

SPECTRA Computer Code Manuals

Volume 2 - User's Guide


Version 24-02

M.M. Stempniewicz

Arnhem, February 2024

K6223/24.277594 MSt-2402

author : M.M. Stempniewicz 

reviewed : E.A.R. de Geus 

744 page(s)

approved : J.J. Meulenbrugge 

Spectra-Vol2.doc

© NRG 2024

Subject to agreement with the client, the information contained in this report may not be disclosed to any third party and NRG is not liable for any damage arising out of the use of such information.

EU DuC = N

Goods labeled with an EU DuC (European Dual-use Codification) not equal to 'N' are subject to European and national export authorization when exported from the EU and may be subject to national export authorization when exported to another EU country as well. Even without an EU DuC, or with EU DuC 'N', authorization may be required due to the final destination and purpose for which the goods are to be used. No rights may be derived from the specified EU DuC or absence of an EU DuC.

SPECTRA Code Manuals - Volume 2: User's Guide

Contents

Abstract	15
Explanation of names and abbreviations	16
1 Introduction	17
2 Description of Input Data	19
2.1 Control Volume Input Data	20
2.1.1 Records: 100000, Control Volume Main Data - Global	20
2.1.2 Records: 100XXX, Control Volume Main Data - Individual	20
2.1.3 Records: 101000, Control Volume Groups - General Data	25
2.1.4 Records: 101XXX, Control Volume Groups- Individual Data	25
2.1.5 Records: 102XXX, Multiplicity of the Control Volume	25
2.1.6 Records: 105XXX, Control Volume Name	26
2.1.7 Records: 11YXXX, Control Volume Segment Data	26
2.1.8 Records: 111XXX, Control Volume Geometry Data	27
2.1.9 Records: 120XXX, Control Volume Initial Conditions	28
2.1.10 Records: 121XXX, Initial Composition of Atmosphere Gas	29
2.1.11 Records: 122XXX, Initial Data for Atmosphere Droplets	29
2.1.12 Records: 123XXX, Initial Data for Pool Bubbles	30
2.1.13 Records: 124XXX, Initial Composition of Bubble Gas	31
2.1.14 Records: 125XXX, Time-Dependent Parameter Definition for Inactive CV	31
2.1.15 Records: 13YXXX, Control Volume Mass Source Data	35
2.1.16 Records: 130XXX, Optional Mass Source Strength Multipliers	38
2.1.17 Records: 14YXXX, Control Volume Energy Source Data	39
2.1.18 Records: 150000, Liquid De-entrainment, Bubble De-entrainment	40
2.1.19 Records: 150XXX, Liquid De-entrainment, Bubble De-entrainment	40
2.1.20 Records: 151XXX, Drop Flow Regime Parameters	43
2.1.21 Records: 152XXX, Bubbly and Annular Flow Parameters	44
2.1.22 Records: 153XXX, Plume Model for Mass Sources	45
2.1.23 Records: 154XXX, Plume Model for Energy Sources	46
2.1.24 Records: 155000, Bubble Collapse Parameters, Droplet and Bubble Activators	47
2.1.25 Records: 155XXX, Bubble Collapse Parameters, Droplet and Bubble Activators	47
2.1.26 Records: 156000, Velocity Limits to Deactivate Plume Model	50
2.1.27 Records: 156XXX, Velocity Limits to Deactivate Plume Model	50
2.1.28 Records: 157000, CV Velocity Change Limits	50
2.1.29 Records: 157XXX, CV Velocity Change Limits	51
2.1.30 Records: 158000, Treatment of Dispersed Components (Bubbles, Droplets)	51
2.1.31 Records: 158XXX, Treatment of Dispersed Components (Bubbles, Droplets)	51
2.1.32 Records: 159000, Stratification Option	53
2.1.33 Records: 160000, Pump/Compressor/Turbine Power Option	54
2.1.34 Records: 161000, Bubble Distribution Parameter and Terminal Velocity	54
2.1.35 Records: 162000, Critical Depth for Bubble Formation	55

SPECTRA Code Manuals - Volume 2: User's Guide

2.1.36	Records: 163000, Non-equilibrium Mass Transfer Parameters	56
2.1.37	Records: 163XXX, Non-equilibrium Mass Transfer Parameters	56
2.1.38	Records: 164000, Interphase Heat and Mass Transfer Parameters -Global	57
2.1.39	Records: 164XXX, Interphase Heat and Mass Transfer Parameters	59
2.1.40	Records: 165XXX, De-entrainment Calculation Options	60
2.1.41	Records: 166000, Freezing / Exceeding Fluid Property Domain Options	61
2.1.42	Records: 167000, Flow Regime Map Parameters	62
2.1.43	Records: 168000, Heterogeneous/Homogeneous CV, Global Activator	64
2.1.44	Records: 168XXX, Heterogeneous/Homogeneous CV, Individual Activators	64
2.1.45	Records: 169000, Accepting Mass or Energy Error	65
2.1.46	Records: 180000, Hydrogen Burn Model Activator	67
2.1.47	Records: 180XXX, Hydrogen Burn Model Data	67
2.1.48	Records: 181XXX, Propagation Distances	68
2.1.49	Records: 182XXX, Combustion Completeness Model	68
2.1.50	Records: 183XXX, Detonation and Fast Deflagration Criteria	69
2.1.51	Records: 184XXX, Flame Speed Calculation	70
2.1.52	Records: 188000, Burn Model Constants	70
2.1.53	Records: 189000, Additional Print and Plot During Burn	71
2.1.54	Example of Control Volume Input Data	72
2.2	Junction Input Data	74
2.2.1	Records: 200XXX, Junction Main Data	74
2.2.2	Records: 201XXX, Initial Velocities	77
2.2.3	Records: 202XXX, Multiplicity of the Junction	77
2.2.4	Records: 205XXX, Junction Name	78
2.2.5	Records: 210XXX, Friction Loss, Form Loss and Moody Coefficient	78
2.2.6	Records: 220XXX, Valve Data	81
2.2.7	Records: 230XXX, Junction Flow Control	84
2.2.8	Records: 231XXX, Pump/Compressor Model Data	85
2.2.9	Records: 232XXX, Simplified Turbine Data	95
2.2.10	Records: 233XXX, Turbine Model Data	98
2.2.11	Records: 235XXX, Pump/Turbine Additional Data	107
2.2.12	Records: 236XXX, Simplified Pump/Turbine Data	108
2.2.13	Records: 237XXX, Request for Pump Curves	109
2.2.14	Records: 238XXX, User-Defined Fluid Properties - Positive Flow Direction	110
2.2.15	Records: 239XXX, User-Defined Fluid Properties - Negative Flow Direction	111
2.2.16	Records: 240XXX, Flow Composition Parameters	112
2.2.17	Records: 250XXX, Entrainment Indicators	113
2.2.18	Records: 251XXX, Drop Flow Regime Model Parameters	114
2.2.19	Records: 252XXX, Bubbly and Annular Flow Parameters	115
2.2.20	Records: 253XXX, Plume Model for Junction Flows	117
2.2.21	Records: 255XXX, Counter-current Flow Model Constants	117
2.2.22	Records: 256000, Diffusion Model - Global Activator	118
2.2.23	Records: 256XXX, Diffusion Model - Individual Activators	118

SPECTRA Code Manuals - Volume 2: User's Guide

2.2.24	Records: 260000, Options for Critical Velocity, Elevation and Area Checking	119
2.2.25	Records: 261000, Minimum Reynolds Number for Friction Calculation	121
2.2.26	Records: 262000, User-Defined Critical Flow Model	121
2.2.27	Records: 263000, Friction Model Global Activators	122
2.2.28	Records: 264000, Momentum Length, Friction Length Options	123
2.2.29	Records: 265000, Hydraulic Diameter - JN Versus CV	124
2.2.30	Records: 270000, Solution of the Junction Flow Matrix	124
2.2.31	Example of the Junction Data	129
2.3	1-D Solid Heat Conductor Input Data	130
2.3.1	Records: 300XXX, 1-D Solid Heat Conductor Main Data	130
2.3.2	Records: 301000, SC Groups - General Data	133
2.3.3	Records: 301XXX, Initial and Transient Temperatures, SC Group Data	133
2.3.4	Records: 302XXX, Multiplicity of the 1-D Solid Heat Conductor	134
2.3.5	Records: 303000, Numerical Integration Method, Global Activator	134
2.3.6	Records: 303XXX, Numerical Integration Method, Individual Activators	135
2.3.7	Records: 304XXX, Optional Size Change During Transient	136
2.3.8	Records: 305XXX, Name of the 1-D Solid Heat Conductor	137
2.3.9	Records: 310XXX, Cell Data	137
2.3.10	Records: 311XXX, Right Surface Temperature	139
2.3.11	Records: 321XXX, Left (Inside) Side Boundary Conditions	139
2.3.12	Records: 322XXX, Right (Outside) Side Boundary Conditions	149
2.3.13	Records: 323XXX, Left Side Extended Surface Data	164
2.3.14	Records: 324XXX, Right Side Extended Surface Data	167
2.3.15	Records: 325XXX, Left Side Heat Exchanger Temperature Averaging	170
2.3.16	Records: 326XXX, Right Side Heat Exchanger Temperature Averaging	172
2.3.17	Records: 327XXX, Left Side Structure-to-Structure Radiation	176
2.3.18	Records: 328XXX, Right Side Structure-to-Structure Radiation	177
2.3.19	Records: 350XXX, Boundary Fluid Temperature Calculation	178
2.3.20	Records: 351XXX, Boundary Fluid Velocity Multiplier	181
2.3.21	Records: 352XXX, Limit for Simultaneous Transfer to Pool and Atmosphere	182
2.3.22	Records: 353XXX, Plume Model for Heat and Mass Transfer	183
2.3.23	Records: 360000, Global Data: Film Boiling, Slip Ratio, TA, Oxidation	184
2.3.24	Records: 365000, Hydraulic Diameter - SC Versus CV	188
2.3.25	Records: 381XXX, Left Side Oxidation Data	189
2.3.26	Records: 382XXX, Right Side Oxidation Data	190
2.3.27	Record: 330XXX, Failure Parameters	191
2.3.28	Records: 33Y000, Material Properties Needed for Failure Calculations	192
2.3.29	Record: 340000, Definition of Fuel Regions for Gap Calculations	194
2.3.30	Record: 340001, Initial Gap Size and Dynamic Expansion Model	195
2.3.31	Record: 340002, User-defined Gap Conductance	198
2.3.32	Record: 3410XX, Gap Data	198
2.3.33	Record: 342XXX, Definition of Common Fuel Regions for Gap Calculations	203
2.3.34	Record: 343XXX, Composition of the Gap Gas	203

SPECTRA Code Manuals - Volume 2: User's Guide

2.3.35	Record: 344XXX, Reference Parameters of the Gap Gas	204
2.3.36	Record: 345000, Number of Integration Points for the Gap Calculations	205
2.3.37	Record: 390XXX, Axial Conduction and Direct Contact Conduction	207
2.3.38	Record: 399000, Interpolation Factor for Boundary Temperature	216
2.3.39	Examples of the 1-D Solid Heat Conductor Input Data	216
2.4	2-D Solid Heat Conductor Input Data	221
2.4.1	Records: 400XXX, 2-D Solid Heat Conductor Main Data	221
2.4.2	Records: 401000, TC Groups - General Data	223
2.4.3	Records: 401XXX, Initial and Transient Temperatures	223
2.4.4	Records: 402XXX, Multiplicity of the 2-D Solid Heat Conductor	224
2.4.5	Records: 405XXX, Name of the 2-D Solid Heat Conductor	224
2.4.6	Records: 410XXX, Number of Cells of the 2-D Solid Heat Conductor	224
2.4.7	Records: 411XXX, Cell Sizes - <i>x</i> -direction	225
2.4.8	Records: 412XXX, Cell Sizes - <i>y</i> -direction	225
2.4.9	Records: 413XXX, Cell Types	226
2.4.10	Records: 414XXX, Material Data	227
2.4.11	Records: 415XXX, Internal Power Distribution	228
2.4.12	Records: 416XXX, Initial Temperatures	228
2.4.13	Records: 420XXX, Boundary Conditions	229
2.4.14	Records: 425XXX, Heat Exchanger Temperature Averaging	238
2.4.15	Records: 450XXX, Boundary Fluid Temperature Calculation	242
2.4.16	Records: 451XXX, Boundary Fluid Velocity Multiplier	245
2.4.17	Records: 452XXX, Limit for Simultaneous Transfer to Pool and Atmosphere	246
2.4.18	Records: 460000, Global Data: Film Boiling, Slip Ratio, TA, Oxidation	246
2.4.19	Records: 465000, Hydraulic Diameter - TC Versus CV	250
2.4.20	Records: 480XXX, Boundary Cell Oxidation Data	251
2.4.21	Records: 430XXX, Failure Parameters	252
2.4.22	Records: 43Y000, Material Properties Needed for Failure Calculations	254
2.4.23	Record: 490XXX, Axial Conduction and Direct Contact Conduction	256
2.4.24	Record: 499000, Interpolation Factor for Boundary Temperature	263
2.4.25	Example of the 2-D Solid Heat Conductor Input Data	264
2.5	MCCI Input Data	266
2.5.1	Records: 440000, MCCI Main Data	266
2.5.2	Records: 44010X, MCCI Material Property Data	268
2.5.3	Records: 4402XX, Concrete Composition	270
2.5.4	Records: 440300, Model Coefficients	271
2.5.5	Records: 441001, Initial Velocities, Horizontal (Radial) Direction	273
2.5.6	Records: 441002, Initial Velocities, Vertical (Axial) Direction	273
2.5.7	Records: 441003, Initial Porosities	274
2.5.8	Records: 441004, Initial Concrete Fractions	274
2.5.9	Records: 441005, Initial Ablated Concrete Fractions	275
2.6	Thermal Radiation Input Data	276
2.6.1	Records: 500Y00, Thermal Radiation Model Selection	276

SPECTRA Code Manuals - Volume 2: User's Guide

2.6.2	Records: 505Y00, Radiating System Name	277
2.6.3	Records: 510YXX, Radiating Surface Data	277
2.6.4	Records: 520YXX, View Factors	279
2.6.5	Records: 530YXX, Beam Lengths	280
2.6.6	Records: 531YXX, Beam Lengths for Multiple CV Paths	281
2.6.7	Records: 5400XX, Radiation Properties of Gases	281
2.6.8	Records: 541000, Radiation Properties of Aerosols	283
2.6.9	Example of Thermal Radiation Input Data	285
2.7	Tabular Function Input Data	289
2.7.1	Records: 605XXX, Tabular Function Name	289
2.7.2	Records: 601XXX, Scaling Factor and Additive Constant	289
2.7.3	Records: 602XXX, Lower and Upper Limits, Rate Change Limits	289
2.7.4	Records: 603XXX, Rate Change Limits for Generating Message	290
2.7.5	Records: 610XXX, Interpolation Type, Interactive Type	290
2.7.6	Records: 611XXX, Automatic Reset Option for Interactive TF	291
2.7.7	Records: 600XXX, Tabular Function Data Records	292
2.7.8	Examples of Tabular Function Input and Use of *.TFD	292
2.8	Control Function Input Data	295
2.8.1	Records: 700XXX, Control Function Main Data	295
2.8.2	Records: 701XXX, Initial Value	295
2.8.3	Records: 702XXX, Lower and Upper Limits, Rate Change Limits	297
2.8.4	Records: 703XXX, Rate Change Limits for Generating Message	297
2.8.5	Records: 705XXX, Control Function Name	298
2.8.6	Records: 708XXX, Y-Coordinate Points for 2-D Tabular Functions	298
2.8.7	Records: 709000, Implicit/Explicit Use of Arguments - Global Activator	301
2.8.8	Records: 709XXX, Implicit/Explicit Use of Arguments	301
2.8.9	Records: 710XXX, Control Function Arguments	302
2.8.10	Records: 715000, Implicit Solution of All Control Functions	324
2.8.11	Examples of Control Function Input Data	325
2.9	Reactor Kinetics Input Data	328
2.9.1	Record: 750000, Reactor Kinetics Main Data	328
2.9.2	Record: 750XXX, Nodal Point Kinetics - Main Data	330
2.9.3	Record: 750990, Nodal Point Kinetics - Additional Data	332
2.9.4	Record: 750999, Nodal and Point Kinetics - Initialization Requests	332
2.9.5	Record: 751000, Volume, Initial Fission Power and Initial Reactivity Data	334
2.9.6	Record: 751XXX, Nodal Point Kinetics - Volume, etc. Data	334
2.9.7	Record: 755000, External Neutron Source Data	335
2.9.8	Record: 755XXX, Nodal Point Kinetics - External Neutron Source Data	336
2.9.9	Record: 760000, Control Rod Reactivity Data	336
2.9.10	Record: 760XXX, Nodal Point Kinetics - Control Rod Reactivity Data	337
2.9.11	Record: 761000, Power Control	337
2.9.12	Record: 770XXX, Delayed Neutron Precursor Data	338
2.9.13	Records: 780000, Reactivity Feedback Data – Selection of Independent Variable	340

SPECTRA Code Manuals - Volume 2: User's Guide

2.9.14	Records: 781XXX, Reactivity Feedback Data - Fuel Temperatures	340
2.9.15	Records: 782XXX, Reactivity Feedback Data - Moderator Temperatures/densities	340
2.9.16	Record: 783XXX, Reactivity Feedback Data - Void Fractions	340
2.9.17	Record: 784XXX, Reactivity Feedback Data - Reactivities	341
2.9.18	Record: 791XXX, Weighting Factors - Fuel Temperatures	346
2.9.19	Record: 792XXX, Weighting Factors - Moderator Temperatures or Densities	347
2.9.20	Record: 793XXX, Weighting Factors - Void Fractions	349
2.9.21	Example of Reactor Kinetics Input Data	351
2.9.22	Record: 740000, Isotope Transformation Data - Initial Core Composition	355
2.9.23	Records: I05XXX, Isotope Transformation Data - Isotope Names	355
2.9.24	Records: 740XXX, Isotope Transformation Data - Initial Isotope Concentrations	356
2.9.25	Records: 741XXX, Isotope Transformation Data - Decay Data	357
2.9.26	Records: 742XXX, Isotope Transformation Data - Absorption Data	358
2.9.27	Records: 743XXX, Isotope Transformation Data - Fission Data	360
2.9.28	Records: 746XXX, Isotope Transformation Data - Fuel Composition	361
2.9.29	Record: 747XXX, Isotope Transformation Data - Fuel Removal/Loading Data	362
2.9.30	Records: 720XXX, Isotope Transformation Data - Multipliers for Fuel Removal	363
2.9.31	Records: 72YXXX, Isotope Transformation Data - Loaded Fuel Data	364
2.9.32	Records: 73YXXX, Isotope Transformation Data - Loaded Non-fuel Data	364
2.9.33	Record: 748000, Point Kinetics Model for Circulating Fuel	365
2.9.34	Record: 749000, Isotope Transformation Data - Normalization Indicators	373
2.9.35	Examples of Isotope Transformation Input Data	375
2.9.36	Built-In Isotope Transformation Data	378
2.10	Material Property Input Data	386
2.10.1	Records: 801XXX, Thermal Conductivity Data	386
2.10.2	Records: 802XXX, Density Data	386
2.10.3	Records: 803XXX, Specific Heat Data	387
2.10.4	Records: 804XXX, Diffusion Coefficients for Fission Product Vapors	387
2.10.5	Records: 805XXX, Material Name	388
2.10.6	Records: 806XXX, Materials Composed of Different Materials	388
2.10.7	Records: 800XXX, Constant Multipliers on the Material Properties	390
2.10.8	Examples of Material Property Input Data	391
2.11	User-Defined Gas Data	393
2.11.1	Record: G05XXX, Name of the User-Defined Gas	393
2.11.2	Record: 830XXX, Molar Weight, Diffusion Volume, Reference Energy	394
2.11.3	Record: 831XXX, Specific Heat	396
2.11.4	Record: 832XXX, Dynamic Viscosity	396
2.11.5	Record: 833XXX, Thermal Conductivity	397
2.11.6	Examples of the User-Defined Gas Data	398
2.12	Alternative Fluid (Liquid Metal, Molten Salt, etc.) Property Data	399
2.12.1	Record: 840000, Alternative Fluid Activator	399
2.12.2	Record: A05000, Name of the Alternative Fluid	400
2.12.3	Records: 841000, Thermodynamic Properties of the Alternative Fluid	400

SPECTRA Code Manuals - Volume 2: User's Guide

2.12.4	Records: 842000, Thermo-Physical Properties of the Alternative Fluid	402
2.12.5	Record: 843000, Heat Transfer Option	403
2.12.6	Record: 843XXX, Heat Transfer Correlations for Alternative Fluid	404
2.12.7	Record: 843YYY, Heat Transfer Correlation Sets for Alternative Fluid	406
2.12.8	Example of the Alternative Fluid Data - Data for Liquid Lead	407
2.13	Heat Transfer Model Coefficients	408
2.13.1	Records: 810010, CHF Model Data	408
2.13.2	Records: 810020, Heat and Mass Transfer Model Data	410
2.13.3	Records: 810030, BDC and CHF/MFB Model Data	412
2.14	Material Oxidation Data	415
2.14.1	Records: 8500XX, Oxidation Reaction Definition	415
2.14.2	Records: O050XX, Oxidation Reaction Name	417
2.14.3	Records: 8510XX, Temperature-Dependent Reaction Rate	418
2.14.4	Records: 8511XX, Corrector for Temperature-Dependent Reaction Rate	421
2.14.5	Records: 8520XX, Velocity-Dependent Reaction Rate	422
2.14.6	Records: 8530XX, Pressure-Dependent Reaction Rate	423
2.14.7	Records: 8540XX, Burn-off Factor	423
2.14.8	Records: 855000, Options for Insufficient Oxidant	425
2.14.9	Built-in Oxidation Models	426
2.14.10	Examples of the User-Defined Oxidation Models	428
2.15	Radioactive Particle Transport Data	433
2.15.1	Record: 860000, RT Package Global Activators, Main Aerosol Data	433
2.15.2	Records: 170XXX, Control Volume Activators	435
2.15.3	Records: 270XXX, Junction Activators	436
2.15.4	Records: 370XXX, 1-D Solid Heat Conductor Activators	436
2.15.5	Records: 470XXX, 2-D Solid Heat Conductor Activators	436
2.15.6	Records: 171000, Control Volume – Pool Related Data	437
2.15.7	Records: 171XXX, Control Volume – Pool Related Data	437
2.15.8	Records: 172000, Option for Pool-Gas Transport of Particles – Global	438
2.15.9	Records: 172XXX, Option for Pool-Gas Transport of Particles – Individual	438
2.15.10	Records: 271000, Aerosol Transport Through Junctions	439
2.15.11	Records: 271XXX, Aerosol Transport Through Junctions	439
2.15.12	Records: 371XXX, 1-D Solid Heat Conductors - Junctions Associations	441
2.15.13	Records: 471XXX, 2-D Solid Heat Conductors – Junctions Associations	443
2.15.14	Records: 372XXX, 1-D Solid Heat Conductors Gravity Factors	445
2.15.15	Records: 472XXX, 2-D Solid Heat Conductors Gravity Factors	447
2.15.16	Records: 361XXX, Electric Field Strength at 1-D Solid Heat Conductors	448
2.15.17	Records: 461XXX, Electric Field Strength at 2-D Solid Heat Conductors	448
2.15.18	Record: 861000, Aerosol Size Sections	449
2.15.19	Record: 861001, Aerosol Surface Areas	449
2.15.20	Records: 173XXX, Initial Airborne Aerosol Masses	450
2.15.21	Records: 174XXX, Initial Masses of Aerosols Deposited in the Pool	451
2.15.22	Records: 373XXX, Initial Deposition on the Left Surface of a SC	451

SPECTRA Code Manuals - Volume 2: User's Guide

2.15.23 Records: 374XXX, Initial Deposition on the Right Surface of a SC	452
2.15.24 Records: 474XXX, Initial Deposition on the Boundary Surfaces of a TC	452
2.15.25 Records: 175XXX, External Sources of Aerosols	453
2.15.26 Records: 375XXX, External Sources of Aerosols Deposited on 1-D Surfaces	453
2.15.27 Records: 475XXX, External Sources of Aerosols Deposited on 2-D Surfaces	454
2.15.28 Records: 275XXX, Aerosol Filter Model	455
2.15.29 Records: 276XXX, Pool Scrubbing Model	456
2.15.30 Record: 376XXX, Inertial Impaction Model for 1-D Solid Heat Conductors	457
2.15.31 Record: 476XXX, Inertial Impaction Model for 2-D Solid Heat Conductors	460
2.15.32 Record: 862000, Agglomeration Shape Factors	461
2.15.33 Record: 863000, Dynamic Shape Factors	461
2.15.34 Record: 864000, Cunningham Slip Correction Factor Model Data	461
2.15.35 Record: 865000, Deposition Model Data	462
2.15.36 Record: 865001, Electrophoretic Deposition - Particle Charge	467
2.15.37 Record: 865002, Global Activators of Deposition Processes	467
2.15.38 Record: 866000, Coagulation Model Data	468
2.15.39 Records: 377XXX, 1-D Solid Heat Conductors Resuspension Model Selection	471
2.15.40 Records: 477XXX, 2-D Solid Heat Conductors Resuspension Model Selection	472
2.15.41 Record: 867000, Parametric Resuspension Model - Main Data	473
2.15.42 Records: 868XXX, Parametric Resuspension Model - V-Coefficients	475
2.15.43 Records: 869XXX, Parametric Resuspension Model - P-Coefficients	477
2.15.44 Records: 8700XX, Mechanistic Resuspension - Main Data	479
2.15.45 Records: 87YYXX, Mechanistic Resuspension - Adhesion Force Distribution	483
2.15.46 Records: 8791XX, Mechanistic Resuspension - Asperity Size Distribution	485
2.15.47 Records: 8792XX, Mechanistic Resuspension - Adhesion Force Calculation	487
2.15.48 Records: 8793XX, Mechanistic Resuspension - Drag Force Calculation	490
2.15.49 Records: 8794XX, Mechanistic Resuspension, C_1 and C_2 , All Sections	491
2.15.50 Records: 8795XX, Mechanistic Resuspension, C_1 Per Size Section	491
2.15.51 Records: 8796XX, Mechanistic Resuspension, C_2 Per Size Section	492
2.15.52 Record: 880000, Fission Product Main Data	493
2.15.53 Records: F05XXY, Fission Product Data - Isotope Names	496
2.15.54 Records: 880XXY, Fission Product Data – Initial Masses, Molar Weights, etc.	497
2.15.55 Records: 881XXY, Fission Product Data - Decay Data	499
2.15.56 Records: 882XXY, Fission Product Data – Neutron Capture Data	500
2.15.57 Record: 883000, Definition of Fuel Regions for FP Release	501
2.15.58 Record: 883101, Definition of Cladding Failure Criteria	503
2.15.59 Record: 883102, Initial Cladding State	503
2.15.60 Record: 8832XX, Definition of Common Fuel Regions for Cladding Failure	504
2.15.61 Record: 884XXY, Initial Fractions of Released (Gap) Fission Products	505
2.15.62 Record: 885000, Release Model Indicator	505
2.15.63 Record: 885XXY, Release Classes	506
2.15.64 Record: 886000, Fission Product Condensation	506
2.15.65 Record: 886XXY, Fission Product Vapor Pressure and Diffusion Volume	507

SPECTRA Code Manuals - Volume 2: User's Guide

2.15.66 Record:	8900XX, Fission Product Release Coefficients – CORSOR-M Model	508
2.15.67 Record:	890000, CORSOR-M Model Constants	510
2.15.68 Record:	8910XX, Fission Product Release Coefficients – ARSAP Model	510
2.15.69 Record:	891000, ARSAP Model Constants	512
2.15.70 Record:	892XXX, Fission Product Release Coefficients – HTR-FPR Model	513
2.15.71 Record:	8930XX, Fission Product Vapor Pressure Coefficients	516
2.15.72 Record:	8931XX, Minimum Half-Life for Vapor Class Isotopes	518
2.15.73 Record:	8932XX, Particle Size and Density of Vapor Class Isotopes	519
2.15.74 Record:	8941XX, Chemical Reactions of Fission Product Vapors – Element A	520
2.15.75 Record:	8942XX, Chemical Reaction of Fission Product Vapors – Element B	521
2.15.76 Record:	8943XX, Chemical Reaction Kinetics	522
2.15.77 Records:	895YXX, Sorption of Fission Product Vapors on Surfaces	524
2.15.78 Records:	395XXX, Selection of Sorption Processes on SC Surfaces	537
2.15.79 Records:	495XXX, Selection of Sorption Processes on TC Surfaces	538
2.15.80 Records:	396XXX, Sorption Related Parameters for SC Surfaces	539
2.15.81 Records:	496XXX, Sorption Related Parameters for TC Surfaces	539
2.15.82 Records:	191XXX, Initial Masses of Isotopes in CV Atmosphere and Pool	540
2.15.83 Records:	391XXX, Initial Masses of Isotopes in SC	540
2.15.84 Records:	491XXX, Initial Masses of Isotopes in TC	541
2.15.85 Records:	192XXX, External Sources of Isotopes	541
2.15.86 Records:	392XXX, Initial Distribution of Vapors on the Surfaces of SC	542
2.15.87 Records:	492XXX, Initial Distribution of Vapors on the Surfaces of TC	543
2.15.88 Records:	393XXX, Initial Distribution of Vapor Classes Inside SC	543
2.15.89 Records:	493XXX, Initial Distribution of Vapor Classes Inside TC	544
2.15.90 Records:	194XXX, Decay Heat Distribution Parameters for CV	545
2.15.91 Records:	394XXX, Decay Heat Distribution Parameters for SC	545
2.15.92 Records:	494XXX, Decay Heat Distribution Parameters for TC	546
2.15.93 Records:	295XXX, Vapor Filter Model	547
2.15.94 Records:	296XXX, Pool Scrubbing Model for Fission Product Vapors	548
2.15.95 Records:	195000, Pool-Gas Transport of FP Vapors - Global	549
2.15.96 Records:	195XXX, Pool-Gas Transport of FP Vapors - Individual	549
2.15.97 Records:	196000, Option for Pool-Gas Transport of FP Vapors – Global	550
2.15.98 Records:	196XXX, Option for Pool-Gas Transport of FP Vapors – Individual	550
2.15.99 Records:	8960XX, Pool-Gas Transport of FP Vapors Sh Correlation	551
2.15.100	Records: 385XXX, Leaching Input Parameters for SC	555
2.15.101	Records: 386000, Leaching Model General Parameters	556
2.15.102	Records: 8970XX, List of RT Isotopes Mapped to CV Gases	557
2.15.103	Records: 898000, Selection of Sorption Processes on Aerosol Particles	557
2.15.104	Records: 197XXX, Initial Masses of Isotopes on Aerosol Particles	559
2.15.105	Records: 397XXX, Initial Masses of Isotopes on Particles Deposited on SC	561
2.15.106	Records: 497XXX, Initial Masses of Isotopes on Particles Deposited on TC	562
2.15.107	Records: 198XXX, Isotopes on External Sources of Aerosols	563
2.15.108	Records: 398XXX, Isotopes on External Sources of SC-Deposited Aerosols	564

SPECTRA Code Manuals - Volume 2: User's Guide

2.15.109	Records: 498XXX, Isotopes on External Sources of TC-Deposited Aerosols	565
2.15.110	Records: 199XXX, Radiation Exposure and Dose Parameters	566
2.15.111	Built-in Fission Product Chains (Decay Chains)	567
2.16	Transient Solution and Output Frequency Parameters	572
2.16.1	Record: 900000, Initial Time	572
2.16.2	Records: 900XXX, Time Step Data	572
2.16.3	Record: 905000, Read Initial Conditions from a File	576
2.16.4	Record: 910000, Advancement Message Frequency, Extended Diagnostics	578
2.16.5	Record: 920000, Iteration Parameters	579
2.16.6	Record: 925000, Reduction of Solid Material Specific Heat for Steady State	584
2.16.7	Record: 930000, Suppressing the Diagnostics File	584
2.16.8	Record: 931000, Adjusting Time Step at the End of Time Domain	585
2.16.9	Record: 940000, Interactive Simulation Activation	585
2.16.10	Record: 950000, Scrambling Input Files	586
2.16.11	Example of Transient Solution and Output Frequency Data	586
2.17	Exporting Input Data to Other Programs	587
2.17.1	Record: 960000, Request for Exporting Data to Other Programs	588
2.18	Requests for External Data Files	590
2.18.1	Record: 9800000, EDF Main Data	591
2.18.2	Record: E0500X, File Name of the Write-EDF	594
2.18.3	Record: D0500X, File Name of the Read-EDF	594
2.18.4	Records: 981000X, Definition of Variables Present in the Write-EDF	594
2.18.5	Records: 982000X, Definition of Variables Present in the Read-EDF	596
2.18.6	Examples of EDF Input and Output	597
2.19	Requests for Plot Variables	601
2.19.1	Record: 9900000, Full Plot File Option	601
2.19.2	Record: 9910000, Requests for Specific Component	601
2.19.3	Record: 9920000, Requests for Specific Variable	602
2.19.4	Record: 9930000, Individual Requests (Specific Component and Variable)	604
2.19.5	Example of Plot Requests Data	606
2.20	Restarting	607
2.20.1	Interactive Input on Restart	607
2.21	Maximum Problem Size – Summary	609
2.22	Applicability Restrictions	610
3	Description of the Output Files	611
3.1	Description of the Printed Output (*.OUT)	611
3.1.1	SPECTRA Main Program Output	612
3.1.2	Control Volume Output	613
3.1.3	Junction Output	627
3.1.4	1-D Solid Heat Conductor Output	632
3.1.5	2-D Solid Heat Conductor Output	640
3.1.6	Thermal Radiation Output	648

SPECTRA Code Manuals - Volume 2: User's Guide

3.1.7	Tabular Function Output	655
3.1.8	Control Function Output	656
3.1.9	Reactor Kinetics Output	658
3.1.10	Material Property Output	666
3.1.11	Transient Solution (SOLVER) Data	667
3.2	Description of the Diagnostics File (*.DIA)	669
3.3	Description of the Plot File (*.PLT)	673
3.3.1	Using S-GRAPH to Make Plots	674
3.3.2	Using VISOR as a Post-Processor	678
3.4	Restart File (*.RST)	681
3.5	The Initial Condition File (*.ICF)	684
3.6	The Tabular Function Data File (*.TFD)	685
3.7	Message File (*.MES)	686
3.8	Stop File (*.STP)	686
4	SPECTRA Installation Guide	689
4.1	Hardware and Software Requirements	689
4.2	Installation of the SPECTRA Code	689
4.3	Execution of the Code	690
4.4	Manual Verification	692
4.5	Automatic Verification	695
4.6	Other Verification Runs	697
	Literature	698
	appendix A Pump/Compressor Maps	703
A.1	Approach	703
A.2	Pump/Compressor Maps	705
A.2.1	Reduced Parameters	705
A.2.2	Pump/Compressor Maps - Ideal Map with no Surge	708
A.2.3	Pump/Compressor Maps - Degradation of Head (Surge Model)	719
	appendix B Turbine Maps	727
	appendix C Pressure Loss Coefficients for Valves	741
C.1	Pressure Loss Coefficient Given by an Analytical Expression	741
C.2	Pressure Loss Coefficient Given by a Table	744

Abstract

SPECTRA (Sophisticated Plant Evaluation Code for Thermal-hydraulic Response Assessment) is a fully integrated system analysis code, that models thermal-hydraulic behavior of Nuclear Power Plants, including reactor cooling system, emergency and control systems, containment, reactor building, etc. of various reactor types, like BWR, PWR, HTR. It can also be used to assess thermal-hydraulic response of non-nuclear plants, for example cooling systems of chemical reactors.

The full documentation of SPECTRA consists of the following four volumes:

- Volume 1: Program Description
- Volume 2: User's Guide
- Volume 3: Verification and Validation
- Volume 4: Code Structure, Development, Hardware and Software Requirements

This report presents Volume 2 of the SPECTRA Code Manuals - User's Guide. A detailed description of input data is provided in this volume. Examples of input files are shown. This volume presents also a description of the output files. The variables printed in the main SPECTRA output data file are shown and shortly described. Examples of output files are presented. Finally, a description of the plot file, and the procedure to make plots using the SPECTRA post-processor is given.

The SPECTRA Manuals are freely available in internet and are also supplied together with the SPECTRA code. The Volume 2 of the Code Manuals is provided in the file **Spectra-Vol2.pdf**.

Explanation of names and abbreviations

CF	Control Function
CV	Control Volume
DIA	Diagnostics file
ICF	Initial Condition File
IT	Isotope Transformation
JN	Junction
MP	Material Properties
OUT	Output file
OX	Material Oxidation
PLT	Plot file
RK	Reactor Kinetics
RT	Radioactive Particle Transport
SC	1-D Solid Heat Conductor
SPECTRA	S ophisticated P lant E valuation C ode for T hermal-hydraulic R esponse A ssessment
TC	2-D Solid Heat Conductor
TF	Tabular Function
TFD	Tabular Function Data file
TR	Thermal Radiation

1 Introduction

SPECTRA (Sophisticated Plant Evaluation Code for Thermal-hydraulic Response Assessment) is a fully integrated system analysis code, that models the thermal-hydraulic behavior of Nuclear Power Plants, including reactor cooling system, emergency and control systems, containment, reactor building, etc. of various reactor types, like BWR, PWR, HTR. It can also be used to assess thermal-hydraulic response of non-nuclear plants, for example cooling systems of chemical reactors. The structure of SPECTRA is shown in Figure 1-1.

The SPECTRA Code Manuals consists of the following four volumes:

- Volume 1: Program Description
- Volume 2: User's Guide
- Volume 3: Verification and Validation
- Volume 4: Code Structure, Development, Hardware and Software Requirements

This report presents Volume 2 of the SPECTRA Code Manuals (SCM) - User's Guide. The full description of the input data needed to run the program as well as the output data is given.

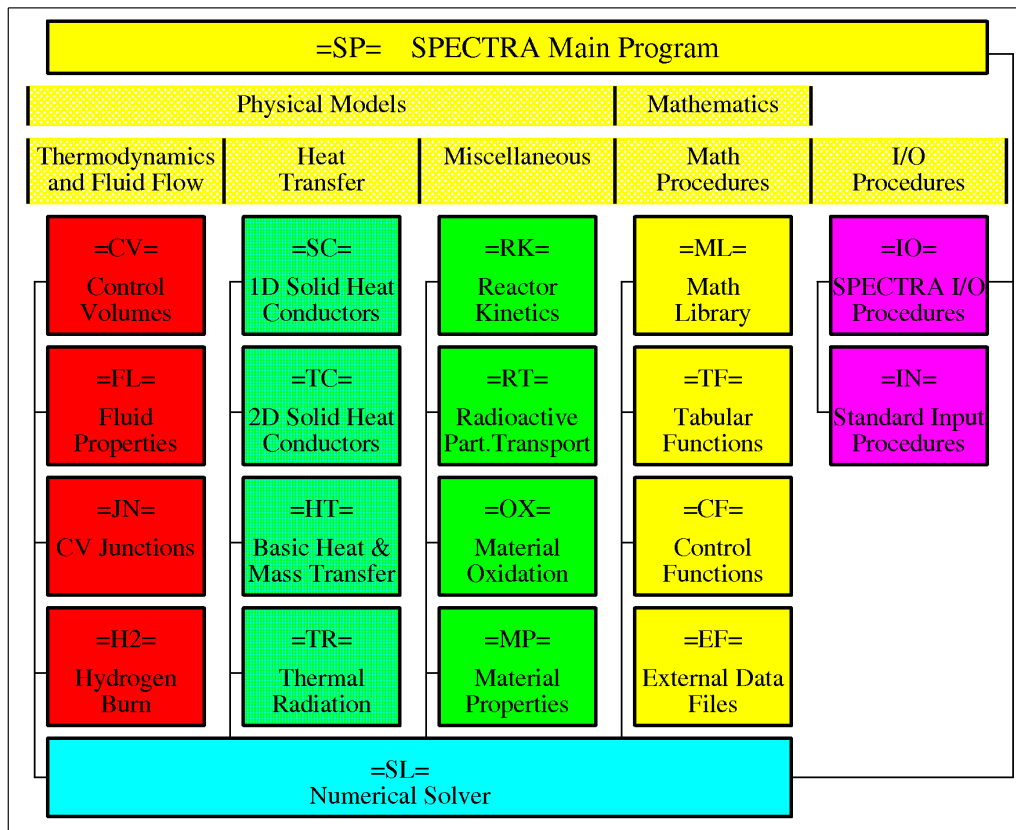


Figure 1-1 SPECTRA code structure.

SPECTRA Code Manuals - Volume 2: User's Guide

Chapter 2 gives a detailed description of input data. Examples of input files are shown.

Chapter 3 presents a description of the output files. The variables printed in the main SPECTRA output data file are shown and shortly described. Examples of output are presented. This chapter provides also the description of the plot file and the procedure to make plots using the SPECTRA post-processor, use of the stop file to terminate calculations, use of the ICF file to provide the initial conditions, use of the TFD file for interactive Tabular Function definitions.

Chapter 4 presents an installation guide. Hardware and software requirements are specified. Installation and execution of the code are described. A verification test case is presented.

Several appendices are included, showing example cases and explaining the effect of using certain input parameters. The appendices show the influence of the user-defined parameters on the maps of pumps/compressors and turbines, as well as the influence of the user-defined parameters on valve loss factors.

2 Description of Input Data

SPECTRA input file must have an extension ".SPE". The name must not be longer than 510 characters or shorter than 5 characters, including extension, i.e. there must be at least one character and no more than 506 characters before the extension. The input file consists of a sequence of input records. Five different record types may be distinguished:

- title record,
- comment records,
- data records,
- requests for file attachments,
- terminator record.

The **title record** is optional and need not to be entered, but it is recommended to enter title for each problem, to have easy way to identify the problem. A title record is identified by an equal sign (=) in the first column. The title is printed in the output and the diagnostics file. If more than one title record is entered, the last one is used.

A **comment record** has an asterisk sign (*) as the leftmost non-blank character. All characters to the right of an asterisk are interpreted as comments. Completely blank lines are interpreted as comments.

A **data record** may contain an arbitrary number of data words that may be integer (I), real (R), or alphanumeric (A), and, optionally, a comment preceded by an asterisk sign. Up to 512 characters are read by the program so the data words cannot be written on fields further to the right. The leftmost word of a data record is interpreted as the record identifier, the remaining words as the data words. Every data record must have a valid identifier.

If less data is entered than is expected in a given record, zeroes are assumed for the remaining words and a warning message is printed to the diagnostics file. If more data is entered than is expected, the remaining values are omitted and a warning message is printed to the diagnostics file.

The User's Guide gives a detailed description of every input entry (Word). Most of the input entries have an acceptable range and a default value. The acceptable ranges and default values are listed in the Chapter 2, describing the input data records. If the value for a given parameter is not entered or it is entered as zero then the default value (if exists) is assumed. In the cases when a non-zero value is the default value and zero is a valid input value, an instruction is given how to set the value to zero. If the input value is outside the acceptable range an error message is printed to the diagnostics file and the run is terminated at the end of the input processing phase.

Files may be attached to the input file using **requests for file attachment**, which has the form:

```
ATTACH FILENAME
```

The word ATTACH has to be written from the first column of a record. The input file can have as many attachments as desired, however no multiple level attachments are allowed. That means, an attached file cannot contain the ATTACH statement. Attaching files is convenient when a (large) model has to be used for calculations of multiple accidents. In such cases the base input deck remains the same, only small accident specific changes need to be made. The base deck can be stored and, when needed, attached at the top of input file, followed by the accident scenario inputs, which will replace the data in the base deck.

The input deck is terminated by the **terminator record**. The terminator record is identified by a period sign (.) in the first column. The terminator record is optional. If there is no terminator record in the data file, all records in the file are read, if the terminator record is present then all the following records are treated as comments.

2.1 Control Volume Input Data

2.1.1 Records: 100000, Control Volume Main Data - Global

Using this record one may specify the parameters described in record 100XXX for all Control Volumes in the model - see description of record 100XXX below.

2.1.2 Records: 100XXX, Control Volume Main Data - Individual

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

W-1 (I) :	ITYPCV	Control volume type, (-).
	ITYPCV = 0:	normal (active) volume, transient conditions are calculated from mass and energy balance, unless the CV solution is switched off by the Solver option IOPSL - see record 900XXX, Word 6.
	ITYPCV > 0:	user-defined conditions. This CV type is typically used to supply boundary conditions. The CV parameters (such as pressure, temperature, etc.) are either constant and equal to their initial values (for example pressure and temperature are entered in record 120XXX, section 2.1.9), or time-dependent, defined by Tabular or Control Functions specified in record 125XXX (section 2.1.14).
	ITYPCV < 0:	user-defined conditions for $t < 0.0$ s. At $t = 0.0$ s it is converted to a normal (active) CV. May be used to specify boundary conditions at the initial (for example steady state) phase of calculations. In that case the start time for the steady state calculations should be defined as negative.
	ITYPCV > 1000:	user-defined conditions if the value of the Tabular Function TF-YYY is greater than 0.0, where $YYY = ITYPCV - 1000$, normal (active) CV otherwise. Similar to $ITYPCV < 0$, but in this case CV may be activated and deactivated many times during calculations.
	<i>Acceptable range:</i>	any integer < 1000, must be a valid reference number of a Tabular Function, if > 1000.
	<i>Default value:</i>	0 if no values are set in the record 125XXX, 1 otherwise

- W-2 (I) : IDSPCV Pointer to a Tabular or Control Function that defines the atmosphere Density Stratification Parameter (DSP) for this volume, (-). If the number is positive, then DSP will be defined by a Tabular Function with the reference number: IDSPCV. If the number is negative, then DSP will be defined by a Control Function with the reference number: $|IDSPCV|$. At any given time of the transient DSP will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 0.0, DSP will be set to 0.0. If it is larger than 1.0, DSP will be set to 1.0. If no value is entered, or the entered value is equal to zero, the DSP will be equal to 0.0 (perfect mixing) throughout the whole transient.
Note that the actual value of DSP may be different from that specified by the Tabular or Control Function. The code internally calculates the minimum and maximum value of DSP based on thermodynamic conditions and thermal stratification. If the value defined by Tabular or Control Function is greater than the maximum limit calculated by the code then the maximum limit is used. If the value defined by Tabular or Control Function is smaller than the minimum limit calculated by the code then the minimum limit is used.
Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.
Default value: 0.
- W-3 (I) : ITSPCV Pointer to a Tabular or Control Function that defines the atmosphere Thermal Stratification Parameter (TSP) for this volume, (-). If the number is positive, then TSP will be defined by a Tabular Function with the reference number: ITSPCV. If the number is negative, then TSP will be defined by a Control Function with the reference number: $|ITSPCV|$. If the current value of the Tabular or Control Function is smaller than 0.0, TSP will be set to 0.0. If it is larger than 1.0, TSP will be set to 1.0. If no value is entered, or the entered value is equal to zero, then TSP will be equal to 0.0 (perfect mixing) throughout the whole transient. Note that the value of TSP is restricted further by the minimum and maximum temperatures, determined by the words 4 and 5 below. Thus the actual value of TSP may differ from the value defined by the Tabular or Control Function.
Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.
Default value: 0.
- W-4 (I) : ITMNCV Pointer to a Tabular or Control Function that defines the minimum atmosphere temperature (at the bottom of atmosphere part of CV) in case when the stratification model is applied (ITSPCV is non-zero). If the number is positive, then the minimum temperature will be defined by a Tabular Function with the reference number: ITMNCV. If the number is negative, then the minimum temperature will be defined by a Control Function with the reference number: $|ITMNCV|$. If the number is zero the minimum temperature is calculated internally by the code (recommended).

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-5 (I) : ITMXCV Pointer to a Tabular or Control Function that defines the maximum temperature (at the top of the atmosphere part of CV). in case when the stratification model is applied (ITSPCV is non-zero). If the number is positive, then the maximum temperature will be defined by a Tabular Function with the reference number: ITMXCV. If the number is negative, then the maximum temperature will be defined by a Control Function with the reference number: |ITMXCV|. If the number is zero the maximum temperature is calculated internally by the code (recommended).

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-6 (I) : IPSPCV Pointer to a Tabular or Control Function that defines the Pool (thermal) Stratification Parameter (PSP) for this volume, (-). If the number is positive, then PSP will be defined by a Tabular Function with the reference number: IPSPCV. If the number is negative, then PSP will be defined by a Control Function with the reference number: |IPSPCV|. If the current value of the Tabular or Control Function is smaller than 0.0, PSP will be set to 0.0. If it is larger than 1.0, PSP will be set to 1.0. If no value is entered, or the entered value is equal to zero, then PSP will be equal to 0.0 (perfect mixing) throughout the whole transient. Note that the value of PSP is restricted further by the minimum and maximum temperatures, determined by the words 7 and 8 below. Thus the actual value of PSP may differ from the value defined by the Tabular or Control Function.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-7 (I) : IPMNCV Pointer to a Tabular or Control Function that defines the minimum pool temperature (at the bottom of pool) in case when the stratification model is applied (IPSPCV is non-zero). If the number is positive, then the minimum temperature will be defined by a Tabular Function with the reference number: IPMNCV. If the number is negative, then the minimum temperature will be defined by a Control Function with the reference number: |IPMNCV|. If the number is zero the minimum temperature is calculated internally by the code (recommended).

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-8 (I) : IPMXCV Pointer to a Tabular or Control Function that defines the maximum pool temperature (at the top of pool) in case when the stratification model is applied (IPSPCV is non-zero). If the number is positive, then the maximum temperature will be defined by a Tabular Function with the reference number: IPMXCV. If the number is negative, then the

SPECTRA Code Manuals - Volume 2: User's Guide

maximum temperature will be defined by a Control Function with the reference number: |IPMXCV|. If the number is zero the maximum temperature is calculated internally by the code (recommended).

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-9 (I) : DTSPCV Maximum value of the ratio DSP/TSP. This parameter may be used to limit the atmosphere density stratification, DSP, based on the atmosphere thermal stratification, TSP. Usually TSP is easier to estimate than DSP, and this limit prevents from obtaining unrealistically large DSP. This word does not affect the TSP. If a negative value is entered then DSP is independent of TSP, but the saturation limit is used. The saturation limit is applied to prevent, as much as possible, the local steam partial pressure to increase above the saturation pressure. The saturation limit is used if DTSPCV > -99. If DTSPCV ≤ -99 then the saturation limit is not used, and DSP is given directly by the Tabular or Control Function. For Best Estimate analysis the default value is recommended. If the user wishes to force the desired density stratification, for example for conservative or sensitivity calculations, then the DTSPCV should be set to ≤ -99.

Acceptable range: DTSPCV ≤ 1000 .

Default value: -1.0 if ITSPCV=0 (Word 3 above),
+3.0 otherwise.

W-10 (R) : DSPCV Initial value of Density Stratification Parameter, DSP, (-). DSP is defined as follows (see Volume 1):

$$\frac{dx_i(z)}{dz} = \tan \left(\frac{\pi}{2} DSP \right)$$

where $x_i(z)$ is the molar concentration of gas i (the lightest gas) at the relative elevation z in the atmosphere. The value of z is equal to zero at the pool surface elevation (at the bottom of the CV if pool is not present), and equal to one at the top of CV.

For example, suppose that the hydrogen concentration at the bottom of the CV is 0.2% (0.002), while the concentration at the top of the CV is 5% (0.05). The value of DSP is obtained from:

$((0.05 - 0.002) / 1.0) = \tan(\pi/2 \cdot DSP)$, or:

$DSP = 2/\pi \cdot \text{atan}((0.05 - 0.002) / 1.0) = 0.0305$

Acceptable range: $0.0 \leq DSPCV \leq 1.0$.

Default value: 0.0 .

W-11 (R) : TSPCV Initial value of Thermal Stratification Parameter, TSP, (-). TSP is defined as follows (see Volume 1):

$$TSP = \frac{T_{top}^{atms} - T_{bot}^{atms}}{T_{ave}^{atms}}$$

SPECTRA Code Manuals - Volume 2: User's Guide

where T^{atms} is the atmosphere temperature, and the subscripts refer to the top, bottom, and average values.

For example, suppose that the initial atmosphere temperature is equal to 300 K at the pool surface elevation (at the bottom of CV if pool is not present), and is equal to 340 K at the top of CV. Average temperature is thus 320 K (this value needs to be entered in record 120XXX - see section 2.1.9 below). The value of TSP is equal to: $TSP = (340 - 300) / 320 = 0.125$.

Acceptable range: $0.0 \leq TSP_{CV} \leq 1.0$.

Default value: 0.0.

W-12 (R) : PSPCV Initial value of Pool Stratification Parameter, PSP, (-). PSP is defined as follows (see Volume 1):

$$PSP = \frac{T_{top}^{pool} - T_{bot}^{pool}}{T_{ave}^{pool}}$$

where T^{pool} is the pool temperature, and the subscripts refer to the top, bottom, and average values.

For example, suppose that the initial pool temperature is equal to 280 K at the pool bottom and 300 K at the pool surface elevation. The average temperature is thus 290 K (this value needs to be entered in record 120XXX - see section 2.1.9 below). The value of PSP is equal to: $PSP = (300 - 280) / 290 = 0.069$.

Acceptable range: $0.0 \leq TSP_{CV} \leq 1.0$.

Default value: 0.0.

W-13 (R) : DDDTCV Maximum value of the rate of change of DSP, $d(DSP)/dt$, (1/s).
Acceptable range: $10^{-5} \leq DTSP_{CV} \leq 1.0$.
Default value: $3.3 \cdot 10^{-3}$ with this value it takes at least 5 min (300 s) to remix a perfectly stratified layer,

W-14 (I) : IRSBCV Indicator determining whether eventual stratification should be removed during hydrogen burns.
 = 1: stratification is removed during slow deflagrations, fast deflagrations and detonations,
 = 2: stratification is removed during fast deflagrations and detonations,
 = 3: stratification is removed during detonations,
 > 3: stratification is not removed during hydrogen burns.
Acceptable range: $IRSBCV > 0$.
Default value: 1.

W-15 (I) : ILEVCV Interpretation of the initial pool level definition (input parameter ZPLSCV, record 120XXX).
 = 0: ZPLSCV is the pool level (m), relative to the bottom of CV
 = 1: ZPLSCV is the relative pool level (-), $0.0 \leq ZPLSCV \leq 1.0$
Acceptable range: $ILEV_{CV} = 0$ or 1
Default value: 0

2.1.3 Records: 101000, Control Volume Groups - General Data

- W-1 (I) : KGRPCV Default CV group number. CV groups are introduced for editing; at the end of input processing an altitude-volume table is printed for each CV group. CV groups may be used to check the fluid volumes for primary system, secondary system, etc. Additionally, RK/RT Packages may use a CV group to define primary system (IDSORK, record 748000).
Acceptable range: $1 \leq \text{KGRPCV} \leq 20$
Default value: 1
- W-2 (I) : NAVTCV Number of data points in the altitude-volume table, printed for each CV group at the end of input processing.
Acceptable range: $10 \leq \text{NAVTCV} \leq 100$
Default value: 50

2.1.4 Records: 101XXX, Control Volume Groups- Individual Data

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

- W-1 (I) : IGRPCV CV group number. CV groups are introduced for editing; at the end of input processing an altitude-volume table is printed for each CV group. CV groups may be used to check the fluid volumes for primary system, secondary system, etc. Additionally, RK/RT Packages may use a CV group to define primary system (IDSORK, record 748000).
Acceptable range: $1 \leq \text{IGRPCV} \leq 20$
Default value: KGRPCV (defined in record 101000)

2.1.5 Records: 102XXX, Multiplicity of the Control Volume

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

- W-1 (R) : XMLTCV Multiplicity of the Control Volume. This is the number of Control Volumes that are identical to the Control Volume XXX. If the number is not equal to 1.0, then the segment flow areas, the average flow areas, the segment volumes, and total volume of this Control Volume, entered in the input deck, are multiplied by this number.
Acceptable range: $0.0 < \text{XMLTCV} < 10^{10}$
Default value: 1.0

Summarizing, there are four optional inputs in this record:

- 110XXX Height (m) Horizontal area (m²)
- 115XXX Height (m) Volume (m³)
- 116XXX Top elevation (m) Horizontal area (m²)
- 117XXX Top elevation (m) Volume (m³)

Note that the last option corresponds to the MELCOR input of altitude/volume (with a negative volume entry, which in MELCOR signifies the segment volume rather than the cumulative volume). The total volume, VOLTCV, and total height, HEIGCV, of CV are calculated from:

$$VOLTCV = \sum_{j=1}^{N_{SEG}} HSEGCV_j \cdot ASEGCV_j$$

$$HEIGCV = \sum_{j=1}^{N_{SEG}} HSEGCV_j$$

2.1.8 Records: 111XXX, Control Volume Geometry Data

XXX is the Control Volume reference number, 001 ≤ XXX ≤ 999. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

- W-1 (R) : ELVBCV Elevation of bottom of Control Volume, (m). ELVBCV gives the difference between the bottom of CV and a reference elevation. The choice of the reference elevation is arbitrary, but all CV must use the same reference elevation.
Acceptable range: any real number.
Default value: 0.0.
- W-2 (R) : AHORCV Representative horizontal flow area of Control Volume, (m²). Used to calculate vertical velocities. **It is recommended to use the flow area for the main flow direction for both AHORCV and AVERCV (below)** - see Volume 3, test runs for pipes with different inclinations.
Acceptable range: >0, >max. area of all connected JN, if ICVAJN=1
Default value: Maximum value of the horizontal cross sections of the segments, ASEGCV
- W-3 (R) : AVERCV Representative vertical flow area of Control Volume, (m²). Used to calculate horizontal velocities. **It is recommended to use the flow area for the main flow direction for both AVERCV and AHORCV (above)** - see Volume 3, test runs for pipes with different inclinations
Acceptable range: >0, >max. area of all connected JN, if ICVAJN=1
Default value: Maximum value of the horizontal cross sections of the segments, ASEGCV
- W-4 (R) : DIPSCV Characteristic dimension for pool surface interphase heat and mass transfer calculations. If a positive value is entered then the characteristic dimension will always be equal to DIPSCV. If a negative value is

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: DDWFCV (defined in record 158XXX, see section 2.1.31) .

- W-4 (R) : ZDRPCV Position of the average droplet in the atmosphere of CV, (m) (related to the top of Control Volume).
Acceptable range: if there are no droplets in the atmosphere (that means: VOLFCV(IDROP)=0.0) then ZDRPCV must be equal to:
 $ZDRPCV = H_{CV,tot} - ZPLSCV$.
if there are droplets in the atmosphere (that means: VOLFCV(IDROP) > 0.0) then:
 $0.0 < ZDRPCV < H_{CV,tot} - ZPLSCV$.
Default value: if there are no droplets in the atmosphere (that means: VOLFCV(IDROP) = 0.0) then the default value of ZDPCV is be equal to:
 $H_{CV,tot} - ZPLSCV$.
if there are droplets in the atmosphere (that means: VOLFCV(IDROP) > 0.0) then the default value of ZDRPCV is:
 $(H_{CV,tot} - ZPLSCV) \cdot ZDWFCV$ (defined in record 158XXX, see section 2.1.31) .

2.1.12 Records: 123XXX, Initial Data for Pool Bubbles

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

- W-1 (R) : VOLFCV Volumetric fraction of bubbles in the pool, (-), (volume of bubbles
 (IBUBB) divided by the volume of water and bubbles in the pool).
Acceptable range: $0.0 \leq VOLFCV(IBUBB) \leq 0.9$.
Default value: 0.0 .
- W-2 (R) : TEMPCV Temperature of bubbles in the pool of Control Volume, (K).
 (IBUBB) *Acceptable range:* $273.2 \leq TEMPCV(IBUBB) \leq 3067.0$ K .
Default value: pool liquid temperature TEMPCV(IPOOL).
- W-3 (R) : DBUBCV Diameter of the average bubble in the pool of Control Volume, (m).
Acceptable range: $0.0 \leq DBUBCV \leq 1.0$.
Default value: DBWFCV (defined in record 158XXX, see section 2.1.31)
- W-4 (R) : ZBUBCV Position of the average bubble in the pool of CV, (m) (related to the bottom of Control Volume).
Acceptable range: if there are no bubbles in the pool (that means: VOLFCV(IBUBB) = 0.0) then ZBUBCV must be equal to:
 $ZBUBCV = ZPLSCV$.

if there are bubbles in the pool (that means: VOLFCV(IBUBB) > 0.0) then:
0.0 < ZBUBCV < ZPLSCV.
Default value: if there are no bubbles in the pool (that means: VOLFCV(IBUBB) = 0.0) then the default value of ZBUBCV is be equal to:
ZPLSCV,
if there are bubbles in the pool (that means: VOLFCV(IBUBB) > 0.0) then the default value of ZBUBCV is:
ZPLSCV·ZDWFCV (defined in record 158XXX, see section 2.1.31) .

2.1.13 Records: 124XXX, Initial Composition of Bubble Gas

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version). Those records define the gas composition of the pool bubbles. Several records with the same number may be entered. Each record may define several components of the gas mixture. The total number of entries in this record must be a multiple of 2.

- W-1 (I) : IGAS Gas number, (-). Must be one of the available gases. The built-in gases are: 1 = H₂, 2 = He, 3 = steam, 4 = N₂, 5 = O₂, 6 = CO₂.
Acceptable range: $1 \leq IGAS \leq NGASCV \leq NGMXFL = 20$
Default value: none.
- W-2 (R) : CVPGCV If IGAS ≠ 3 then this word gives the mole fraction of gas IGAS
(IGAS) related to the total mass of noncondensables. If the sum of CVPGCV for all noncondensables is not equal to one then CVPGCV will be normalized during input processing.
If IGAS = 3 then this word is interpreted as the relative humidity, RHUMCV.
Acceptable range: $0.0 \leq CVPGCV(IGAS) \leq 1.0$.
Default value: 1.0 for IGAS = 3; 0.0 otherwise.

2.1.14 Records: 125XXX, Time-Dependent Parameter Definition for Inactive CV

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

This record defines time dependent parameters (such as pressure, temperature, etc.) for inactive Control Volumes (see records 100XXX, section 2.1.1). If the record 125XXX is not used, then the parameters in the inactive Control Volume will be constant, and equal to their initial values (for example, the initial pressure and temperature are defined in records 120XXX, section 2.1.9). Using Record 125XXX the user may define some, or all of these parameters as functions of time.

SPECTRA Code Manuals - Volume 2: User's Guide

Note that if non-zero values are specified in this record and the type of volume is not set as inactive in the record 100XXX, then the type of volume is automatically set to inactive, ITYPECV = 1 (see record 100XXX, section 2.1.2).

- W-1 (I) : IZPLCV Pointer to a Tabular or Control Function that defines the water level in this volume, (-). If the number is positive, then the water level will be defined by a Tabular Function with the reference number: IZPLCV. If the number is negative, then the water level will be defined by a Control Function with the reference number: |IZPLCV|. At any given time of the transient the water level will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 0.0, it will be set to 0.0. If it is larger than 0.99 times the CV height it will be set to 0.99 times the CV height. If no value is entered, or the entered value is equal to zero, the water level will be constant and equal to the value entered in record 120XXX.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.
- W-2 (I) : IPRSCV Pointer to a Tabular or Control Function that defines the pressure in this volume, (-). If the number is positive, then the pressure will be defined by a Tabular Function with the reference number: IPRSCV. If the number is negative, then the pressure will be defined by a Control Function with the reference number: |IPRSCV|. At any given time of the transient the pressure will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 1.0 Pa, it will be set to 1.0 Pa. If it is larger than 2.09×10^7 Pa it will be set to 2.09×10^7 Pa. If no value is entered, or the entered value is equal to zero, the pressure will be constant and equal to the value entered in record 120XXX.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.
- W-3 (I) : ITATCV Pointer to a Tabular or Control Function that defines the atmosphere temperature in this volume, (-). If the number is 1000, the temperature will be set to the saturation temperature at the CV pressure. If the number is smaller than 1000 and positive, then the atmosphere temperature will be defined by a Tabular Function with the reference number: ITATCV. If the number is negative, then the atmosphere temperature will be defined by a Control Function with the reference number: |ITATCV|. At any given time of the transient the atmosphere temperature will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 273.2 K, it will be set to 273.2 K. If it is larger than 3067.0 K it will be set to 3067.0 K. If no value is entered, or the entered value is equal to zero, the atmosphere temperature will be constant and equal to the value entered in record 120XXX.
Acceptable range: 0, or 1000, or a valid reference number of a Tabular, or a Control Function.
Default value: 0.

- W-4 (I) : ITPLCV Pointer to a Tabular or Control Function that defines the pool temperature in this volume, (-). If the number is 1000, the temperature will be set to the saturation temperature at the CV pressure. If the number is smaller than 1000 and positive, then the pool temperature will be defined by a Tabular Function with the reference number: ITPLCV. If the number is negative, then the pool temperature will be defined by a Control Function with the reference number: |ITPLCV|. At any given time of the transient the pool temperature will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 273.2 K, it will be set to 273.2 K. If it is larger than the saturation temperature at the current pressure, then it will be set to the saturation temperature. If no value is entered, or the entered value is equal to zero, the atmosphere temperature will be constant and equal to the value entered in record 120XXX.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.
- W-5 (I) : IATGCV Pointer to a Tabular or Control Function that defines the volume
(1) fraction of H₂ in this volume, (-). If the number is positive, then the H₂ fraction will be defined by a Tabular Function with the reference number: IATGCV(1). If the number is negative, then the H₂ fraction will be defined by a Control Function with the reference number: |IATGCV(1)|. At any given time of the transient the H₂ fraction will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 0.0, it will be set to 0.0. If it is larger than 1.0 it will be set to 1.0. If no value is entered, or the entered value is equal to zero, the H₂ fraction will be constant and equal to the value entered in record 121XXX. The gas fractions are internally normalized, to make sure that the sum is equal to one at any moment of time.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.
- W-6 (I) : IATGCV Pointer to a Tabular or Control Function that defines the volume
(2) fraction of He in this volume, (-). If the number is positive, then the He fraction will be defined by a Tabular Function with the reference number: IATGCV(2). If the number is negative, then the He fraction will be defined by a Control Function with the reference number: |IATGCV(2)|. At any given time of the transient the He fraction will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 0.0, it will be set to 0.0. If it is larger than 1.0 it will be set to 1.0. If no value is entered, or the entered value is equal to zero, the He fraction will be constant and equal to the value entered in record 121XXX. The gas fractions are internally normalized, to make sure that the sum is equal to one at any moment of time.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 0.

- W-7 (I) : IATGCV (3) Pointer to a Tabular or Control Function that defines the relative humidity, (-). If the number is positive, then the relative humidity will be defined by a Tabular Function with the reference number: IATGCV(3). If the number is negative, then the relative humidity will be defined by a Control Function with the reference number: |IATGCV(3)|. At any given time of the transient the relative humidity will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 0.0, it will be set to 0.0. If it is larger than 1.0 it will be set to 1.0. If no value is entered, or the entered value is equal to zero, the relative humidity will be constant and equal to the value entered in record 121XXX.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.
- W-8 (I) : IATGCV (4) Pointer to a Tabular or Control Function that defines the volume fraction of N₂ in this volume, (-). If the number is positive, then the N₂ fraction will be defined by a Tabular Function with the reference number: IATGCV(4). If the number is negative, then the N₂ fraction will be defined by a Control Function with the reference number: |IATGCV(4)|. At any given time of the transient the N₂ fraction will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 0.0, it will be set to 0.0. If it is larger than 1.0 it will be set to 1.0. If no value is entered, or the entered value is equal to zero, the N₂ fraction will be constant and equal to the value entered in record 121XXX. The gas fractions are internally normalized, to make sure that the sum is equal to one at any moment of time.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.
- W-9 (I) : IATGCV (5) Pointer to a Tabular or Control Function that defines the volume fraction of O₂ in this volume, (-). If the number is positive, then the O₂ fraction will be defined by a Tabular Function with the reference number: IATGCV(5). If the number is negative, then the O₂ fraction will be defined by a Control Function with the reference number: |IATGCV(5)|. At any given time of the transient the O₂ fraction will be equal to the current value of the Tabular or Control Function. If the current value of the Tabular or Control Function is smaller than 0.0, it will be set to 0.0. If it is larger than 1.0 it will be set to 1.0. If no value is entered, or the entered value is equal to zero, the O₂ fraction will be constant and equal to the value entered in record 121XXX. The gas fractions are internally normalized, to make sure that the sum is equal to one at any moment of time.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.

IMMSCV > 0: mass source rate is defined by a Tabular Function with the reference number: IMMSCV.

IMMSCV < 0: mass source rate is defined by a Control Function with the reference number: |IMMSCV|.

IMMSCV = 0: mass source rate is zero (source is inactive).

IMMSCV >1000: mass source rate is linked to the isotope list number YY, where YY=IMMSCV-1000. The isotope list YY is defined in the records 8970XX. Usually isotopes are treated as trace species; the isotope mass is not considered in the CV Package. Using this option, the user may link the RT isotope masses to the CV gas masses for the cases when the effect of gas pressurization is considered non-negligible. An example is shown at the description of the record 8970XX. If this option is used, the following mass source is created:

$$S = (\sum M_{i,0} - M_{gas,0}) / \Delta t$$

Here:

$M_{i,0}$ mass of isotope i in the CV number XXX, start of time step, (kg)

$M_{gas,0}$ mass of gas in the CV number XXX, start of time step, (kg)

Δt time step (s)

Because of the applied formulation, the mass of gas in the CV will be lagging by one time step compared to the mass in the RT Package. This is typically not a problem, since the isotope masses are very small a significant accumulation can only be observed for longer time frames. Since this source is intended as a gas source, it is required that the source elevation must be equal to the CV height, ZMSCV = HEIGCV.

An internal limit is imposed on the value obtained from the Tabular or Control Function. If the absolute value is smaller than 10^{-20} (kg/s), then it is set to 0.0.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, or existing list, if non-zero.

Default value: 0.

W-5 (I) : ITMSCV Pointer to a Tabular or Control Function that defines the temperature of the source (K).

ITMSCV > 0: temperature is defined by a Tabular Function with the reference number: ITMSCV.

ITMSCV < 0: temperature is defined by a Control Function with the reference number: |ITMSCV|.

ITMSCV = 0: temperature is equal to the current CV gas temperature.

SPECTRA Code Manuals - Volume 2: User's Guide

The value obtained from the Tabular or Control Function will be restricted to the range of: 273.2 - 3067 K. When the source is negative (mass sink), then the source temperature and pressure are equal to the current temperature and pressure of the fluid being removed.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0.

W-6 (I) : IPMSCV Pointer to a Tabular or Control Function that defines the pressure of the source (Pa).

IPMSCV > 0: pressure is defined by a Tabular Function with the reference number: IPMSCV.

IPMSCV < 0: pressure is defined by a Control Function with the reference number: |IPMSCV|.

IPMSCV = 0: pressure is equal to the current CV pressure. If this is the steam mass source, i.e.. CGMSCV(3)>0.0, then pressure is equal to 0.99×saturation pressure at the CV gas temperature.

The units obtained from the Tabular or Control Function are assumed to be (Pa). The value obtained from the Tabular or Control Function will be restricted to the range of: 1.0 - 2.09×10⁷ Pa. When the source is negative (mass sink), then the source temperature and pressure are equal to the current temperature and pressure of the fluid being removed.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0.

The following data pairs define the composition (mass fractions) of the source. The mass fractions are assumed constant (time independent).

W-7 (I) : I Id. number of the first component in the mixture (-). Zero means liquid water, positive number indicates one of the available gases. The built-in gases are: 0=liquid, 1=H₂, 2=He, 3=steam, 4=N₂, 5=O₂, 6=CO₂.

Acceptable range: 0 ≤ I ≤ NGASCV ≤ NGMXFL = 20

Default value: none.

W-8 (R) : CGMSCV/ Mass fraction of the first component. If Id. number is 0 (water) /CLMSCV then this is CLMSCV - the mass flow of water divided by the total mass flow of gas and water. If Id. number is greater than zero then this is CGMSCV - the mass flow of gas I divided by the total gas flow (gas fractions).

Acceptable range: 0.0 ≤ CGMSCV/CLMSCV ≤ 1.0 .

Default value: 1.0 for I=3 (steam), 0.0 otherwise.

W-9 (I) : I Id. number of second component in the mixture, (-).

Acceptable range: 0 ≤ I ≤ NGASCV ≤ NGMXFL = 20

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: none.

W-10 (R) : CGMSCV/ Mass fraction of the second component.
/CLMSCV *Acceptable range:* $0.0 \leq \text{CGMSCV}/\text{CLMSCV} \leq 1.0$.
Default value: 1.0 for I=3 (steam), 0.0 otherwise.

... etc.

2.1.16 Records: 130XXX, Optional Mass Source Strength Multipliers

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

W-1 (R) : XMMSCV(1) Source strength multiplier on the tabular mass source 1 (defined in record 131XXX). If a non-zero value is entered, then the mass source strength is multiplied by this number.
Acceptable range: $-10^{10} \leq \text{XMMSCV}(1) \leq +10^{10}$
Default value: 0.0

W-2 (R) : XMMSCV(2) Source strength multiplier on the tabular mass source 2 (defined in record 132XXX). If a non-zero value is entered, then the mass source strength is multiplied by this number.
Acceptable range: $-10^{10} \leq \text{XMMSCV}(2) \leq +10^{10}$
Default value: 0.0

... etc.

The source strength multipliers are introduced to have an easy way of defining chemical reactions, for example hydrogen recombiners. The user must define only one function, e.g. defining the hydrogen recombination rate. Then the mass sink of oxygen is obtained by multiplying this function by a constant factor of -8.0, the mass source of steam is obtained by multiplying this function by +9.0, and the energy source is obtained by multiplying this function by heat of reaction per 1 kg of H₂ reacted.

2.1.17 Records: 14YXXX, Control Volume Energy Source Data

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

Y is the energy source number (consecutive, starting with 1). Up to 9 energy sources are allowed for one Control Volume. The energy source is defined here for a single CV; i.e. the value obtained from TF/CF defined below is multiplied by the CV multiplicity (XMLTCV, record 102XXX).

W-1 (R) : ZTESCV Midpoint elevation for the energy source number Y, relative to the bottom of Control Volume, (m).
Acceptable range: ZTESCV must be greater or equal to zero and smaller or equal to height of CV.
Default value: none.

W-2 (I) : ITESCV Pointer to a Tabular or Control Function that defines the energy rate for the source number Y. If the number is positive, then the mass flux will be defined by a Tabular Function with the reference number: ITESCV. If the number is negative, then the energy rate will be defined by a Control Function with the reference number: $|ITESCV|$. The units obtained from the Tabular or Control Function are assumed to be (W). Positive and negative values are allowed. Negative values will yield energy sink.
If ITESCV points to a Reactor Kinetics Control Function (IGRPCF=3, INUMCF=5) and circulating fuel option is used (IFTORK=2), then:

- The source is placed only in the pool of CV.
- The value obtained from the reactor kinetics Control Function is used if the CV has sufficient amount of liquid, i.e. if the liquid fraction in CV is more than the limit XFULRK (record 748000).
- If the pool occupies less than XFULRK of the CV volume, the source obtained from the reactor kinetics Control Function, is interpolated to obtain zero in case of empty volume, i.e. it is multiplied by $(V_{pool}/V_{CV})/XFULRK$. Here V_{pool} is the pool volume in CV and V_{CV} is the total CV volume. This is done to automatically reduce the power generated in the pool of a CV when the pool is removed from this CV.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0.

W-3 (R) : POWMCV Constant power multiplier. The constant power multiplier is introduced to have an easy way of defining for example axial power profile.
Acceptable range: $-10^{10} \leq POWMCV \leq 10^{10}$
Default value: 1.0

2.1.18 Records: 150000, Liquid De-entrainment, Bubble De-entrainment

Using this record one may specify the parameters described in record 150XXX for all Control Volumes in the model - see description of record 150XXX below.

2.1.19 Records: 150XXX, Liquid De-entrainment, Bubble De-entrainment

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

This record is optional. All entries from this record have their default values, recommended for general application.

W-1 (R) : DENHCV De-entrainment ratio for liquid (droplets) in the atmosphere due to horizontal velocity, D_h , (-). The mass change of discontinuous component (liquid droplets) in the atmosphere of a Control Volume is calculated as (see Volume 1):

$$\frac{dM_{drop}}{dt} |_{h,de-ent} = D_h A_h \alpha_{drop} v_{h,drop} \rho_{drop}$$

- D_h - de-entrainment ratio for horizontal flow, DENHCV,
- A_h - atmosphere area for flow in horizontal direction, (m²),
(atmosphere vertical cross section area),
- α_{drop} - droplet volumetric fraction, (-),
- $v_{h,drop}$ - droplet horizontal velocity, (m/s),
- ρ_{drop} - droplet density, (kg/m³).

The value of DENTCV may be useful for example in case of spray system injecting at some angle to the vertical. Some part of the spray droplets will hit the containment walls. In that case however it is needed to modify the drop flow model parameters (section 2.1.20) to properly model the horizontal velocity component of the spray droplets (see Volume 3, simulation of NUPEC tests).

The general idea of entering the value of DENTCV is illustrated in Figure 2-1. Figure 2-1 shows a Control Volume with the cross section area for atmosphere horizontal flow equal to $A_{h,A}$, and a Junction with a flow area of A_{JN} . Assuming that droplet inertia is large the de-entrainment parameter can be estimated as:

$$D_h = \frac{A_{h,A} - A_{JN}}{A_{h,A}}$$

In practice the droplets will change they flow direction together with the gas stream (finite inertia) or bounce back after hitting the wall. This means that the de-entrainment will be somewhat smaller than defined by

the above formula. Moreover the atmosphere cross-section area depends on the pool level and thus changes in time. Consequently it is not always easy to find the right value for the de-entrainment parameter.

Acceptable range: $0.0 \leq \text{DENHCV} < 1.0$.

Default value: 0.0 .

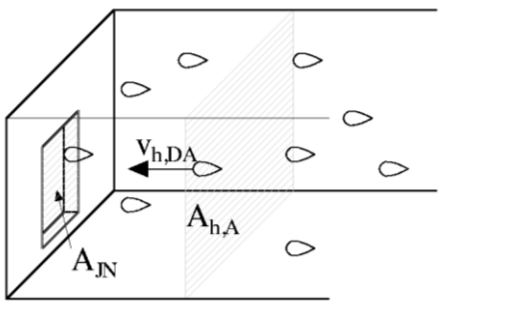


Figure 2-1 Horizontal droplet de-entrainment.

W-2 (R) : DENVCV De-entrainment ratio for liquid (droplets) in the atmosphere due to vertical velocity, D_v , (-). The mass change of discontinuous component (liquid droplets) in the atmosphere of a Control Volume is calculated as (see Volume 1):

$$\frac{dM_{drop}}{dt} /_{v,de-ent} = D_v A_v \alpha_{drop} v_{v,drop} \rho_{drop}$$

- D_v - de-entrainment ratio for vertical flow, DENVCV,
- A_v - either actual pool surface area, or CV segment horizontal cross section area, depending on ISVDCV (Word 3, below), (m^2),
- α_{drop} - droplet volumetric fraction at pool surface elevation,
- $v_{v,drop}$ - droplet vertical velocity, (m/s),
- ρ_{drop} - droplet density, (kg/m^3).

Acceptable range: $0.0 \leq \text{DENVCV} < 1.0$.

Default value: 1.0 (a small number, $< 10^{-50}$, sets the value to 0.0).

W-3 (I) : ISVDCV Indicator for droplet vertical de-entrainment area calculation, A_v .
 ISVDCV = 0 :
 A_v is always equal to the current pool surface area - Figure 2-2 left
 $1 \leq \text{ISVDCV} \leq \text{NSEGCV}$:
 A_v is equal to horizontal area of segment ISVDCV - Figure 2-2 right
Acceptable range: $0 \leq \text{ISVDCV} \leq \text{NSEGCV}$.
Default value: 0 .

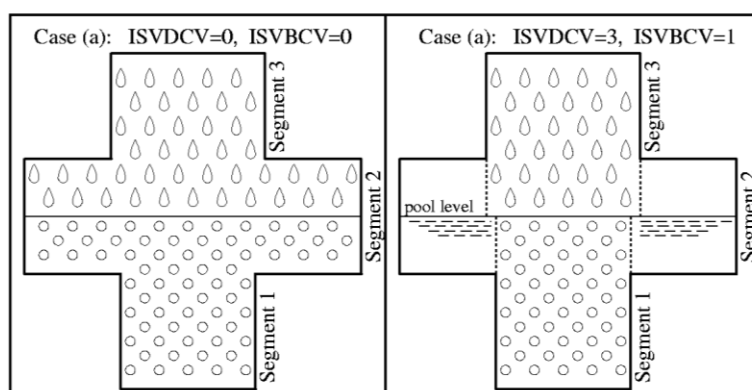


Figure 2-2 Use of ISVDCV, ISVBCV to define droplet and bubble vertical de-entrainment.

W-4 (I) : ISVBCV Indicator for bubble vertical de-entrainment area calculation, A_v .
 ISVBCV = 0 :
 A_v is always equal to the current pool surface area - Figure 2-2 left

$1 \leq \text{ISVBCV} \leq \text{NSEGCV}$:
 A_v is equal to horizontal area of segment ISVBCV - Figure 2-2 right

$\text{ISVBCV} > \text{NSEGCV}$:
 ISVBCV defines a limit, in %, in the relative pool level, above which bubbles are not transported to the pool surface. For example, if $\text{ISVBCV}=90$, then when liquid level is above 90% of the CV height there is no transport of bubbles to the pool surface ($A_v = 0.0$). A transition zone of $0.1 \times \text{ISVBCV}$ is defined, where A_v is interpolated between 0.0 and the full value. In the considered example, the full area will be for liquid levels $\leq 0.9 \times \text{ISVBCV} = 0.81$.

This option may be useful for vertical pipes nodalized with multiple CVs. In such case use of a homogeneous CV is more appropriate - (record 168XXX, Figure 2-5). Use of heterogeneous CV leads to undesired multiple liquid levels in the pipe, with bubbles transported to the pool surface and then as atmosphere in the junction - Figure 2-3 left. Use of the ISVBCV as a cut-off parameter allows the user to define the liquid level in the CV above which there will be no transport of bubbles to the pool surface and thus there will be a flow of pool and bubbles only in all junctions - Figure 2-3 right.

Note 1: this option works also for aerosol particles suspended in the pool. If the particle vertical velocity is positive ($\text{VINPRT} > 0.0$ or drag coefficient is used with particle density < pool density), then flow of particles to the pool surface will be eliminated when liquid level is above ISVBCV %.

Note 2: This option requires that there is a JN connected at the top of the CV. This JN is associated with ISVBCV and is given a name JSVBJN.

Acceptable range: $0 \leq \text{ISVBCV} \leq 100$

Default value: 0

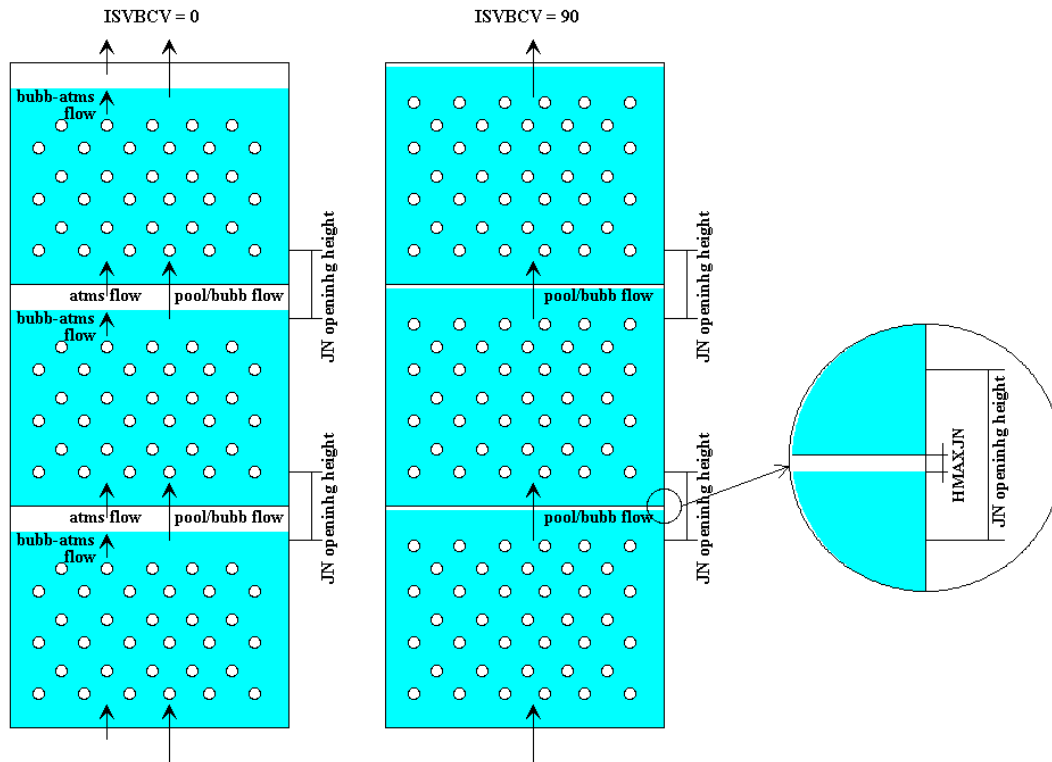


Figure 2-3 Use of ISVBCV to define vertical pool / bubble flow

2.1.20 Records: 151XXX, Drop Flow Regime Parameters

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

This record defines data for the drift flux model, which is used for the droplet transport in atmosphere of CV. This record is optional. All entries from this record have their default values, recommended for general application.

W-1 (R) : C0VACV Constant C_0 for drift flux model for CV atmosphere, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $C_{0,vA}$, (-).
Acceptable range: $0.0 \leq C0VACV \leq 10.0$. If no value or zero is entered, then $C_{0,vA}$ is calculated by the Drop Flow Regime Model, as described in Volume 1.
Default value: 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0

W-2 (R) : VIVACV Terminal velocity, v_∞ , for drift flux model for CV atmosphere, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty,v,A}$, (m/s).
Acceptable range: $-100.0 \leq VIVACV \leq 100.0$. If no value or zero is entered, then $v_{\infty,v,A}$ is calculated by the Drop Flow Regime Model, as described in Volume 1.

SPECTRA Code Manuals - Volume 2: User's Guide

- Default value:* 0.0, a small value ($\leq 10^{-50}$) value will set v_∞ to 0.0
- W-3 (R) : XVACV Exponent x for drift flux model for CV atmosphere, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{v,A}$, (-).
Acceptable range: $0.0 \leq XVACV \leq 10.0$. If no value or zero is entered, then $x_{v,A}$ is calculated by the Drop Flow Regime Model, as described in Volume 1.
Default value: 0.0
- W-4 (R) : COHACV Constant C_0 for drift flux model for CV atmosphere, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $C_{0,hA}$, (-).
Acceptable range: $0.0 \leq COHACV \leq 10.0$. If no value or zero is entered, then $C_{0,hA}$ is calculated by the Drop Flow Regime Model, as described in Volume 1.
Default value: 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0
- W-5 (R) : VIHACV Terminal velocity, v_∞ , for drift flux model for CV atmosphere, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty,h,A}$, (m/s).
Acceptable range: $-100.0 \leq VIHACV \leq 100.0$. If no value or zero is entered, then $v_{\infty,h,A}$ is calculated by the Drop Flow Regime Model, as described in Volume 1.
Default value: 0.0, a small value ($\leq 10^{-50}$) value will set v_∞ to 0.0
- W-6 (R) : XHACV Exponent x for drift flux model for CV atmosphere, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{h,A}$, (-).
Acceptable range: $0.0 \leq XHACV \leq 10.0$. If no value or zero is entered, then $x_{h,A}$ is calculated by the Drop Flow regime Model, as described in Volume 1.
Default value: 0.0

2.1.21 Records: 152XXX, Bubbly and Annular Flow Parameters

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

This record defines data for the drift flux model, which is used for the bubble transport in pool of CV. This record is optional. All entries from this record have their default values, recommended for general application.

- W-1 (R) : COVPCV Constant C_0 for drift flux model for CV pool, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $C_{0,vP}$, (-).
Acceptable range: $0.0 \leq COVPCV \leq 10.0$. If no value or zero is entered, then $C_{0,vP}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1.
Default value: 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0

SPECTRA Code Manuals - Volume 2: User's Guide

W-2 (R) :	VIVPCV	Terminal velocity, v_{∞} , for drift flux model for CV pool, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty,v,P}$, (m/s). <i>Acceptable range:</i> $-100.0 \leq \text{VIVPCV} \leq 100.0$. If no value or zero is entered, then $v_{\infty,v,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set v_{∞} to 0.0
W-3 (R) :	XVPCV	Exponent x for drift flux model for CV pool, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{v,P}$, (-). <i>Acceptable range:</i> $0.0 \leq \text{XVPCV} \leq 10.0$. If no value or zero is entered, then $x_{v,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0
W-4 (R) :	C0HPCV	Constant C_0 for drift flux model for CV pool, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $C_{0,h,P}$, (-). <i>Acceptable range:</i> $0.0 \leq \text{C0HPCV} \leq 10.0$. If no value or zero is entered, then $C_{0,h,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0
W-5 (R) :	VIHPCV	Terminal velocity, v_{∞} , for drift flux model for CV pool, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty,h,P}$, (m/s). <i>Acceptable range:</i> $-100.0 \leq \text{VIHPCV} \leq 100.0$. If no value or zero is entered, then $v_{\infty,h,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set v_{∞} to 0.0
W-6 (R) :	XHPCV	Exponent x for drift flux model for CV pool, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{h,P}$, (-). <i>Acceptable range:</i> $0.0 \leq \text{XHPCV} \leq 10.0$. If no value or zero is entered, then $x_{h,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0
W-7 (R) :	IANNCV	Annular flow model selection. =1: Default model, (see Volume 1). =2: Dartmouth correlation, (see Volume 1). <i>Acceptable range:</i> 1 or 2. <i>Default value:</i> 1 .

2.1.22 Records: 153XXX, Plume Model for Mass Sources

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

SPECTRA Code Manuals - Volume 2: User's Guide

These records activate plume models for one or more mass sources present in the Control Volume. The plume model may be activated only if stratification is calculated for the Control Volume (record 100XXX, section 2.1.2).

Description of the plume model is given in Volume 1. If stratifications are calculated then the plume model may be activated for any of the mass sources present in the Control Volume. To activate the model for a single source and a single component, a set of three integer numbers, described below, must be entered. To activate the model for several mass sources, several sets of three integer numbers should be entered in this record.

- | | | |
|-----------|--------|---|
| W-1 (I) : | I | Number of the mass source for which the plume model is desired. Must be equal to one of the mass sources defined for this Control Volume through records 13YXXX (section 2.1.15).
<i>Acceptable range:</i> $1 \leq I \leq$ No. of sources defined on 13YXXX,
<i>Default value:</i> none. |
| W-2 (I) : | J | Identifier of component, for which the plume model is desired. J=1: atmosphere; J=3: pool.
<i>Acceptable range:</i> 1 or 3.
<i>Default value:</i> none. |
| W-3 (I) : | IPLMCV | Plume model activator. If IPLMCV = 0 then the plume model is not active. If IPLMCV \neq 0 then the plume model is active for the mass source I, in the component J of the Control Volume XXX.
Note that the plume model is used only when stratification models are active. That means, the plumes may be activated in the atmosphere of the Control Volume only if ITSPCV \neq 0 (section 2.1.2), and in the pool of the Control Volume only if IPSPCV \neq 0 (section 2.1.2).
<i>Acceptable range:</i> any integer.
<i>Default value:</i> 0. |

... etc., until all plumes are defined.

2.1.23 Records: 154XXX, Plume Model for Energy Sources

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

These records activate plume models for one or more energy sources, present in the Control Volume. The plume model may be activated only if stratification is calculated for the Control Volume (record 100XXX, section 2.1.2).

Description of the plume model is given in Volume 1. If stratifications are calculated then the plume model may be activated for any of the energy sources present in the Control Volume. To activate the model for a single source and a single component, a set of three integer numbers, described below, must be entered. To activate the model for several energy sources, several sets of three integer numbers must be entered in this record.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-1 (I) : I Number of the energy source for which the plume model is desired. Must be equal to one of the energy sources defined for this Control Volume through records 14YXXX (section 2.1.17).
Acceptable range: $1 \leq I \leq$ No. of sources defined on 14YXXX,
Default value: none.
- W-2 (I) : J Identifier of component, for which the plume model is desired. J=1: atmosphere; J=3: pool.
Acceptable range: J=1, or J=3.
Default value: none.
- W-3 (I) : IPLECV Plume model activator. If IPLECV = 0 then the plume model is not active. If IPLECV \neq 0 then the plume model is active for the energy source I, in the component J of the Control Volume XXX.
Note that the plume model is used only when stratification models are active. That means, the plumes may be activated in the atmosphere of the Control Volume only if ITSPCV \neq 0 (section 2.1.2), and in the pool of the Control Volume only if IPSPCV \neq 0 (section 2.1.2).
Acceptable range: any integer.
Default value: 0.

... etc., until all plumes are defined.

2.1.24 Records: 155000, Bubble Collapse Parameters, Droplet and Bubble Activators

Using this record one may specify the parameters described in record 155XXX for all Control Volumes in the model - see description of record 155XXX below.

2.1.25 Records: 155XXX, Bubble Collapse Parameters, Droplet and Bubble Activators

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. NOTE: if XXX = 000, then the parameters defined in this record are applied to all Control Volumes.

This record is optional. All entries from this record have their default values, recommended for general application. Note! Switching off the bubble collapse models can lead to numerical convergence problems. Specifically for boiling surfaces (XBCMCV(2)) the bubble collapse model ought not to be switched off.

- W-1 (R) : XBCMCV Bubble collapse model at Junctions.
(1) XBCMCV(1) < 0.0: model inactive,
 XBCMCV(1) \geq 0.0: model active.
Acceptable range: all real numbers.
Default value: +1, if an alternative fluid is used (see section 2.12),
 then the default value is -1
- W-2 (R) : XBCMCV Bubble collapse model at Solid Heat Conductor surfaces (boiling).
(2) XBCMCV(2) < 0.0: model inactive,

SPECTRA Code Manuals - Volume 2: User's Guide

- XBCMCV(2) \geq 0.0: model active.
Acceptable range: all real numbers.
Default value: +1, if an alternative fluid is used (see section 2.12), then the default value is -1
- W-3 (R) : XBCMCV Bubble collapse model at Tabular Mass Sources.
(3) XBCMCV(3) $<$ 0.0: model inactive,
XBCMCV(3) \geq 0.0: model active.
Acceptable range: all real numbers.
Default value: +1, if an alternative fluid is used (see section 2.12), then the default value is -1
- W-4 (R) DTBCCV Pool subcooling to switch off the bubble collapse model at Solid Heat Conductors and bubble flow or pure steam atmosphere flow through Junctions, (K). If the value of XBCMCV(2) (Word 2 above) is greater than zero, then the bubble collapse model at the Solid Heat Conductor (boiling) surfaces is used as follows. When the pool subcooling is larger than 2-DTBCCV then the bubble collapse model is used. When the pool subcooling is smaller than DTBCCV then the bubble collapse model is not used. Interpolation is performed for the pool subcooling between DTBCCV and 2-DTBCCV. The same logic applies for the bubbles flowing through Junctions.
Acceptable range: DTBCCV $>$ 0.0. It is not recommended to decrease DTBCCV below its default value.
Default value: 0.5
- W-5 (I) IDRPCV Droplet model activator at Junctions, Solid Heat Conductors, and Tabular Mass Sources. If IDRPCV is equal to 1 then created liquid is always deposited directly in the pool. If IDRPCV is equal to 2 then the liquid is either deposited in the pool (if Junction, SC/TC, or TMS elevation is below the pool surface) or converted to droplets and suspended in CV atmosphere (if elevation is above the pool surface).
Acceptable range: 1 or 2.
Default value: 1 .
- W-6 (I) IBUBCV Bubble model activator at Junctions, Solid Heat Conductors, and Tabular Mass Sources. If IBUBCV is equal to 1 then the created gas is always deposited directly in the atmosphere. If IBUBCV is equal to 2 then the gas is either deposited in the atmosphere (if Junction, SC/TC, or TMS elevation is above the pool surface) or converted to bubbles and suspended in the pool (if elevation is below the pool surface).
Acceptable range: 1 or 2
Default value: 2
NOTE: In the earlier versions (prior to July 2018) the default value for alternative fluids was 1. This may speed up calculations in cases when bubble tracking is not important, which may be the case for example in liquid metal reactors.
- W-7 (R) DMBLCV Maximum depth at which bubbles are created when boiling occurs at the surface of Solid Heat Conductors, (m). If DMBLCV is less than 0.0, then bubbles are created at the true elevation of the Solid Heat Conductor

SPECTRA Code Manuals - Volume 2: User's Guide

surface. In reality, if the boiling surface is deeply submerged, there is very little bubbles in the deep pool. Bubbles are rapidly created near the pool surface, where pressure is close to saturation. To simulate this the parameter *DMBLCV* is used. When *DMBLCV* is set to a positive number then the bubbles will be created not deeper than *DMBLCV* (m) below the pool surface.

Acceptable range: $DMBLCV \leq 0$, or $0.5 \leq DMBLCV \leq 100$.

Default value: 5.0.

- W-8 (R) *DMNBCV* Maximum depth at which bubbles are created during non-equilibrium boiling, (m). If *DMNBCV* is less than or equal to 0.0, then bubbles are created in the middle of the pool. If *DMNBCV* is set to a positive number then the bubbles will be created not deeper than *DMNBCV* (m) below the pool surface. Note that *DMNBCV* is used only when bubbles from non-equilibrium boiling are activated (*MNMTCV* \neq 0, record 163XXX, section 2.1.37).
- Acceptable range:* $DMNBCV \leq 0$, or $0.5 \leq DMNBCV \leq 100$.
- Default value:* 2.0.
- W-9 (I) *IDDCCV* Calculation of the diameter of droplets created due to Junction flows or Tabular Mass Sources.
- IDDCCV* = 1: Use only Taylor instability model.
- IDDCCV* = 2: Maximum of Kutateladze-Styrikovic and Taylor.
- Acceptable range:* 1 or 2.
- Default value:* 1 (Note! Use of the second option may give unrealistic results when only small part of Junction flow area is occupied by liquid).
- W-10 (R) *DDMNCV* Lower limit for diameter of droplets created due to Junction flows or Tabular Mass Sources.
- Acceptable range:* $1.0 \times 10^{-5} \leq DDMNCV \leq 1.0 \times 10^{-2}$.
- Default value:* 1.0×10^{-3} .
- W-11 (R) *DDMXCV* Upper limit for diameter of droplets created due to Junction flows or Tabular Mass Sources.
- Acceptable range:* $DDMNCV \leq DDMXCV \leq 1.0 \times 10^{-1}$.
- Default value:* 2.0×10^{-2} .
- W-12 (R) *DBMNCV* Lower limit for diameter of bubbles created due to Junction flows or Tabular Mass Sources.
- Acceptable range:* $1.0 \cdot 10^{-4} \leq DBMNCV \leq 1.0 \times 10^{-1}$.
- Default value:* 1.0×10^{-3} .
- W-13 (R) *DBMXCV* Upper limit for diameter of bubbles created due to Junction flows or Tabular Mass Sources.
- Acceptable range:* $DBMNCV \leq DBMXCV \leq 1.0 \times 10^{+0}$.
- Default value:* 9.0×10^{-2} .

2.1.26 Records: 156000, Velocity Limits to Deactivate Plume Model

Using this record one may specify the parameters described in record 156XXX for all Control Volumes in the model - see description of record 156XXX below.

2.1.27 Records: 156XXX, Velocity Limits to Deactivate Plume Model

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

This record is optional. All entries from this record have their default values, recommended for general application.

- W-1 (R) : VPLCCV Velocity to deactivate atmosphere plume model in Junctions, (m/s).
 (iatms) Used when Junction flow of atmosphere gas enters the atmosphere of CV, and the atmosphere plume model for this Junction is active (see section 2.2.20). If the atmosphere velocity in the Junction exceeds VPLCCV(iatms), then the atmosphere plume model is deactivated for this Junction.
Acceptable range: $0.1 \leq \text{VPLCCV}(\text{iatms}) \leq 1000.0$
Default value: 1.0 .
- W-2 (R) : VPLCCV Velocity to deactivate pool plume model in Junctions, (m/s).
 (ipool) Used when Junction flow of liquid enters the pool of CV, and the pool plume model for this Junction is active (see section 2.2.20). If the pool velocity in the Junction exceeds VPLCCV(ipool), then the pool plume model is deactivated for this Junction.
Acceptable range: $0.1 \leq \text{VPLCCV}(\text{ipool}) \leq 1000.0$
Default value: 1.0 .
- W-3 (R) : VPLCCV Velocity to deactivate pool plume model in Junctions, (m/s).
 (ibubb) Used when Junction flow of atmosphere gas enters the pool of CV, and the pool plume model for this Junction is active (see section 2.2.20). If the atmosphere velocity multiplied by: $(1 - c_{\text{H}_2\text{O}})$ (where $c_{\text{H}_2\text{O}}$ is the volumetric fraction of steam), in the Junction exceeds VPLCCV(ibubb), then the pool plume model is deactivated for this Junction.
Acceptable range: $0.1 \leq \text{VPLCCV}(\text{ibubb}) \leq 1000.0$
Default value: 1.0 .

2.1.28 Records: 157000, CV Velocity Change Limits

Using this record one may specify the parameters described in record 157XXX for all Control Volumes in the model - see description of record 157XXX below.

2.1.29 Records: 157XXX, CV Velocity Change Limits

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

This record is optional. All entries from this record have their default values, recommended for general application.

- W-1 (R) : DVDTCV Maximum velocity change rate for atmosphere velocities inside CV,
 (iatms) dV_{atms}/dt , (m/s²).
 Acceptable range: $1.0 \times 10^{-2} \leq DVDTCV(iatms) \leq 1.0 \times 10^6$
 Default value: 50.0
- W-2 (R) : DVDTCV Maximum velocity change rate for droplet velocities inside CV,
 (idrop) dV_{drop}/dt , (m/s²).
 Acceptable range: $1.0 \times 10^{-2} \leq DVDTCV(idrop) \leq 1.0 \times 10^6$
 Default value: 50.0
- W-3 (R) : DVDTCV Maximum velocity change rate for pool velocities inside CV,
 (ipool) dV_{pool}/dt , (m/s²).
 Acceptable range: $1.0 \times 10^{-2} \leq DVDTCV(ipool) \leq 1.0 \times 10^6$
 Default value: 5.0
- W-4 (R) : DVDTCV Maximum velocity change rate for bubble velocities inside CV,
 (ibubb) dV_{bubb}/dt , (m/s²).
 Acceptable range: $1.0 \times 10^{-2} \leq DVDTCV(ibubb) \leq 1.0 \times 10^6$
 Default value: 5.0

2.1.30 Records: 158000, Treatment of Dispersed Components (Bubbles, Droplets)

Using this record one may specify the parameters described in record 158XXX for all Control Volumes in the model - see description of record 158XXX below.

2.1.31 Records: 158XXX, Treatment of Dispersed Components (Bubbles, Droplets)

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

Data entered in this record defines how the dispersed components (bubbles and droplets are treated in the Control Volume. Note that by default a simple model is employed, where the number of bubbles/droplets and the average position of the bubble/droplet are not tracked (bubble/droplet count and position equations are disabled). The most accurate results are obtained with the bubble/droplet count and the bubble/droplet position calculated. This option is however more time consuming and should be employed only for selected Control Volumes, where the particle transport is particularly important.

- W-1 (I) : IWATCV Dispersed component treatment indicator:
 IWATCV = -1: Detailed treatment of dispersed components (droplets, bubbles). Both bubble/droplet count and position equation are employed to calculate bubble/droplet average diameter and average position. This option gives most accurate results for bubbles and droplets but is most time consuming.
 IWATCV = 1: Detailed treatment of dispersed components (droplets, bubbles). Simplified heat and mass transfer at the bubble-pool interphase (droplets are not affected). Use this option in case when detailed treatment of bubbles is desired but numerical problems with bubbles are encountered when IWATCV = -1 is used.
 IWATCV=2: Detailed treatment of dispersed components (droplets, bubbles). Additionally mass transfer at the pool surface is deactivated. Bubble vertical de-entrainment (bubble flow to the pool surface) is deactivated if the average bubble volumetric fraction in the pool is below the limit DEWFCV (Word 2 below). This option is intended only for eventual sensitivity calculations and only for Control Volumes that are permanently filled with water (i.e. the pool level is during the whole calculations at or near the top of the Control Volume). It is not recommended to use this option.
 IWATCV=3: Simplified treatment of dispersed components (droplets, bubbles), with user input average particle diameters (Words 3 and 4 below), and average particle positions (Words 5 and 6 below). This is the default option, giving fast but less accurate results for bubbles/droplets.
 IWATCV=4: Simplified treatment of dispersed components (droplets, bubbles), with user input average particle diameters (Words 3 and 4 below), and average particle positions (Words 5 and 6 below). Additionally mass transfer at the pool surface is deactivated. Bubble vertical de-entrainment (bubble flow to the pool surface) is deactivated if the average bubble volumetric fraction in the pool is below the limit DEWFCV (Word 2 below). This option is intended only for eventual sensitivity calculations and only for Control Volumes that are permanently filled with water (i.e. the pool level is during the whole calculations at or near the top of the Control Volume). It is not recommended to use this option.
 Acceptable range: any integer
 Default value: 3
- W-2 (R) : DEWFCV Minimum value of the average bubble volumetric fraction to activate the bubble de-entrainment (flow through pool surface to the atmosphere), (-). Used if IWATCV = 2, or IWATCV = 4.
 Acceptable range: $0.0 < DEWFCV \leq 0.90$
 Default value: 0.90
- W-3 (R) : DDWFCV Average droplet diameter, (m). Used if IWATCV = 3, or 4. If no value is entered, then the droplet diameter is obtained from correlations for breakup of a jet flows and atomization (see Volume 1).
 Acceptable range: $0.0001 \leq DDWFCV \leq 0.02$
 Default value: 0.01

SPECTRA Code Manuals - Volume 2: User's Guide

- W-4 (R) : DBWFCV Average bubble diameter, (m). Used if IWATCV = 3, or 4. If no value is entered, then the bubble diameter is obtained from correlations for bubbly and slug flow, based on flow regime map defined in record 167000 (see section 2.1.42).
Acceptable range: $0.0001 \leq \text{DBWFCV} \leq 0.1$, if non-zero
Default value: 0.0
- W-5 (R) : ZDWFCV Average relative droplet position (distance from the top of CV to the average droplet position, divided by the height of the CV atmosphere), (-). Used if IWATCV = 3, or 4.
Acceptable range: $0.5 \leq \text{ZDWFCV} \leq 0.9$
Default value: 0.5
- W-6 (R) : ZBWFCV Average relative bubble position (distance from the bottom of CV to the average bubble position, divided by the height of the CV pool), (-). Used if IWATCV = 3, or 4.
Acceptable range: $0.5 \leq \text{ZBWFCV} \leq 0.9$.
Default value: 0.5
- W-7 (R) : A1WFCV Lower value of the average bubble volumetric fraction for the bubble - annular transition, (-). When the average bubble volumetric fraction is smaller than A1WFCV, then the bubble average position is equal to ZBWFCV. When the average bubble volumetric fraction is larger than A2WFCV (Word 7 below), then the bubble average position is equal to 0.5. Used if IWATCV = 3, or 4.
Acceptable range: $0.1 \leq \text{A1WFCV} \leq 0.8$
Default value: 0.75
- W-8 (R) : A2WFCV Upper value of the average bubble volumetric fraction for the bubble - annular transition, (-). When the average bubble volumetric fraction is smaller than A1WFCV (Word 6 above), then the bubble average position is equal to ZBWFCV. When the average bubble volumetric fraction is larger than A2WFCV, then the bubble average position is equal to 0.5. Used if IWATCV = 3, or 4.
Acceptable range: $\text{A1WFCV} + 0.05 \leq \text{A2WFCV} \leq 0.85$
Default value: 0.80

2.1.32 Records: 159000, Stratification Option

- W-1 (I) : ISTRCV Stratification option. Used only for these Control Volumes for which IDSPCV is not equal to zero (see section 2.1.2).
ISTRCV=0: the stratification parameter DSPCV is applied for all gases present in a given Control Volume. The stratification gradient is therefore the same for all gases.
ISTRCV>0: the stratification parameter DSPCV is applied for a single gas only. The gas identification number is equal to ISTRCV (see list of available gases in the section 2.1.10). All other gases are assumed to be well mixed.
Acceptable range: $0 \leq \text{ISTRCV} \leq \text{NGASCV} \leq \text{NGMXFL} = 20$

Default value: 0

2.1.33 Records: 160000, Pump/Compressor/Turbine Power Option

W-1 (I) : IPPOCV Pump power option.
 IPPOCV=0: the pump/compressor/turbine power, calculated by the JN Package (calculated always for the Type 2 pumps and the mechanistic turbine models), is added to a downstream Control Volume.
 IPPOCV>1: the pump/compressor/turbine power is ignored in the CV energy balance.
Acceptable range: 0 and 1
Default value: 0

2.1.34 Records: 161000, Bubble Distribution Parameter and Terminal Velocity

The model for bubble distribution parameter calculation may be selected using this record. This record is optional. All entries from this record have their default values, recommended for general application.

The parameters defined in this record affect the bubble rise model in all Control Volumes and all Junctions

W-1 (I) : MODC0 Selection of the model for bubble distribution parameter, C_0 , calculation. The model selected by this record will be used only if C_0 is calculated by the code, and not specified as an input. This means:
 for CV: C0VPCV = 0 (record 152XXX, section 2.1.21)
 for JN: C0VPJN = 0 (record 252XXX, section 2.2.19)
 MODC0=1: Zuber and Findlay correlation: $C_0 = 1.2$
 MODC0=2: Sun et al. correlation: $C_0 = 1 / (0.82 + 0.12 p / p_{crit})$
Acceptable range: 1 or 2
Default value: 1

W-2 (I) : MODVI Selection of the model for bubble (and particle) terminal velocity, v_∞ , calculation. The model selected by this record will be used only if v_∞ is calculated by the code, and not specified as an input. This means:
 for CV: VIVPCV = 0 (record 152XXX, section 2.1.21)
 for JN: VIVPJN = 0 (record 252XXX, section 2.2.19)
 MODVI=1: Default set of correlations is applied for bubbles (Hadamard & Rybczynski, Peebles & Garber, Zuber, Davies & Taylor) and droplets (Hadamard & Rybczynski, Wallis) with drag coefficient C_D defined by CDRGCV, below. Three C_D regimes are described in Volume 1
 MODVI=2: Alternative correlation is applied for bubbles, droplets and particles in the pool (if VINPRT>100, VINFRT>100). The correlation is based on drag coefficient:

$$v_\infty = \left(\frac{4/3 \cdot Dg(\rho_f - \rho_p)}{C_D \cdot \rho_f} \right)^{1/2}$$

SPECTRA Code Manuals - Volume 2: User's Guide

g gravity constant, = 9.81 (m/s²)
 ρ_f fluid density, (kg/m³)
 ρ_p bubble (particle) density, (kg/m³)
 D bubble diameter, (m)
 C_D drag coefficient, (CDRGCV below), five C_D regimes are described in Volume 1
Acceptable range: 1 or 2
Default value: 1

W-3 (R) : CDRGCV Definition of drag coefficient
< 1000: CDRGCV = drag coefficient for large Re, $C_{D,Re \rightarrow \infty}$
> 1000: drag coefficient is defined by a Tabular Function number CDRGCV-1000, as a function of Re: $C_D = f(\text{Re})$. The values obtained from the TF are limited to the minimum of 10^{-2} and a maximum of 10^2 . Use of TF is possible only when the alternative correlation is used, MODVI=2.
Acceptable range: $0.0 < \text{CDRGCV} \leq 100.0$
or reference to a Tabular Function
Default value: 0.44 if MODVI = 1 (applied to droplets only; bubble correlation has no user-defined parameters, see Volume 1, section "Bubble velocities")
0.47 if MODVI = 2 (applied to droplets, bubbles and particles suspended in the liquid pool)

W-4 (R) : CSMLCV Constant C_{small} in the correlation for small particles:

$$v_{\infty} = \frac{1}{18} \cdot \frac{D_p^2 g (\rho_f - \rho_p)}{\eta_f} \cdot C_{small}$$

Used if MODVI=2. If a non-zero value is provided, the correlation is used if the absolute value obtained from this correlation is smaller than the absolute value obtained from the drag of the correlation.
Acceptable range: $0.1 < \text{CSMLCV} \leq 10.0$ or 0.0
Default value: 1.0 (a small value, <0.1, sets the value to zero)

Note that in order to model most accurately bubbly flow in a series of Control Volumes, the option ISVBCV should be used (Figure 2-3). This will allow to avoid bubble flow to the pool surface in CV and let the bubbles flow directly from the pool of one CV to another (see record 150XXX).

2.1.35 Records: 162000, Critical Depth for Bubble Formation

The model for bubble distribution parameter calculation may be selected using this record. This record is optional. All entries from this record have their default values, recommended for general application. The parameters defined in this record affect the bubble rise model in all Control Volumes.

W-1 (R) : TCMCV Critical depth/height of bubble/droplet source for the bubble/droplet formation (m). If the distance of a bubble/droplet source is smaller than TCMCV from the pool surface, then the bubbles/droplets are placed directly in the atmosphere/pool of CV. If the depth/height is larger than

SPECTRA Code Manuals - Volume 2: User's Guide

$2 \times \text{TCMCV}$, the bubbles/droplets are created (if the activators IBUBCV/IDRPCV are on). An interpolation is performed for depths between TCMCV and $2 \times \text{TCMCV}$.

Acceptable range: $0.001 < \text{TCMCV} \leq 0.1$

Default value: 0.01 (0.05 in code versions before Nov 2018)

The following parameters determine how the tabular mass sources for a Control Volume are handled.

- If the elevation of a tabular mass source is higher than the current pool surface + DZUPCV, then the mass source is purely for atmosphere of CV (liquid sources create droplets).
- If the elevation of a tabular mass source is lower than the current pool surface – DZDNCV, then the mass source is purely for pool of CV (gas sources create bubbles).
- If the elevation of a tabular mass source is between pool surface – DZDNCV and pool surface + DZUPCV, then the gas mass sources are placed in the atmosphere and liquid sources are placed in the pool of CV (bubbles or droplets are not created)

W-2 (R) : DZUPCV If a tabular mass source is placed higher than the pool surface + DZUPCV, then the mass source is purely for atmosphere of CV.

Acceptable range: $0.001 < \text{DZUPCV} \leq 0.1$

Default value: 0.01 (0.1 in code versions before Nov 2018)

W-3 (R) : DZDNCV If a tabular mass source is placed lower than the pool surface – DZUPCV, then the mass source is purely for pool of CV.

Acceptable range: $0.001 < \text{DZDNCV} \leq 0.1$

Default value: 0.01 (0.1 in code versions before Nov 2018)

2.1.36 Records: 163000, Non-equilibrium Mass Transfer Parameters

Using this record one may specify the parameters described in record 163XXX for all Control Volumes in the model - see description of record 163XXX below.

2.1.37 Records: 163XXX, Non-equilibrium Mass Transfer Parameters

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

The constants used in the non-equilibrium mass transfer models (bulk boiling and the bulk condensation - see Volume 1) may be redefined in this record. This record is optional. All entries from this record have their default values, recommended for general application.

W-1 (R) : CBBACV Bulk boiling model constant, C_{BB} . The model can be disabled by setting CBBACV to a value ≤ -1.0 .

Acceptable range: $10^{-4} \leq \text{CBBACV} \leq 0.1$, or $\text{CBBACV} \leq -1.0$.

Default value: 0.005.

W-2 (R) : CBCACV Bulk condensation model constant, C_{BC} . The model can be disabled by setting CBCACV to a value ≤ -1.0

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $10^{-4} \leq \text{CBCACV} \leq 0.1$, or $\text{CBCACV} \leq -1.0$.
Default value: 0.005 .

- W-3 (I) : MNPBCV Treatment of steam created due to non-equilibrium boiling.
MNPBCV < 0: steam is placed at the pool-atmosphere interphase. This is not a physically rigorous treatment, but it saves computing effort.
MNPBCV > 0: steam bubbles are suspended in the pool. This is a rigorous physical treatment of the non-equilibrium mass transfer. However it may result in time step cuts and therefore slower calculations. This method is necessary only for rapid depressurization, for example RPV blowdown.
Acceptable range: all integers.
Default value: +1.
- W-4 (I) : MNPCCV Treatment of water created due to non-equilibrium condensation.
MNPCCV < 0: water is placed at the pool-atmosphere interphase. See comment to the Word 3 above.
MNPCCV > 0: water droplets are suspended in the atmosphere (fog creation). See comment to the Word 3 above.
Acceptable range: all integers.
Default value: -1 .
- W-5 (I) : MNMDCV Activator of the non-equilibrium mass transfer model inside droplets.
MNMDCV < 0: the model is inactive,
MNMDCV > 0: the model is active.
Typically there is no need to use the model. The model should be switched on if hot liquid, from a relatively high pressure source, is present in a Control Volume (for example RPV blowdown - see Volume 3), or when droplets are present in a strongly superheated atmosphere.
Acceptable range: all integers.
Default value: -1.
- W-6 (I) : MNMBCV Activator of the non-equilibrium mass transfer model inside bubbles.
MNMBCV < 0: the model is inactive,
MNMBCV > 0: the model is active.
Typically there is no need to use the model. The model should be activated if the bubble relative humidity is observed to exceed 1.0 .
Acceptable range: all integers.
Default value: -1.
- W-7 (R) : DFOGCV Fog/mist diameter, (m). Used if MNPCCV>0 (Word 4) as a diameter of droplets created due to non-equilibrium condensation (fogging), or as a droplet diameter in mist flow for homogeneous volumes (IHOMCV=2)
Acceptable range: $1.0 \times 10^{-5} \leq \text{DFOGCV} \leq 1.0 \times 10^{-2}$
Default value: 1.0×10^{-4} if IHOMCV=1 (heterogeneous CV)
 1.0×10^{-3} if IHOMCV=2 (homogeneous CV)

2.1.38 Records: 164000, Interphase Heat and Mass Transfer Parameters -Global

The interphase heat and mass transfer model can be deactivated using this record. This record is optional. All entries from this record have their default values, recommended for general application.

SPECTRA Code Manuals - Volume 2: User's Guide

- (IPLAT) pool-atmosphere interphase.
Acceptable range: $0.0 < XINGCV(IPLAT) \leq 1.0$
Default value: 1.0
- W-8 (I) : XINGCV Multiplier on the interphase heat and mass transfer calculation for the
(IDPAT) droplet-atmosphere interphase.
Acceptable range: $0.0 < XINGCV(IDPAT) \leq 1.0$
Default value: 1.0
- W-9 (I) : XINGCV Multiplier on the interphase heat and mass transfer calculation for the
(IBBPL) bubble-pool interphase.
Acceptable range: $0.0 < XINGCV(IBBPL) \leq 1.0$
Default value: 0.1 (This default value was chosen to improve the computational speed. Typically, results are not significantly affected.)

2.1.39 Records: 164XXX, Interphase Heat and Mass Transfer Parameters

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version). The interphase heat and mass transfer model can be deactivated using this record. This record is optional. All entries from this record have their default values, recommended for general application.

- W-1 (I) : MINTCV Interphase heat and mass transfer model individual activator.
(IPLAT) Pool-atmosphere interphase.
MINTCV(IPLAT) = -1: inactive
MINTCV(IPLAT) = +1: heat and mass transfer models are active
MINTCV(IPLAT) = +2: only heat transfer is active. Exactly the same effect is obtained with MINTCV(IPLAT) = +1 if the Sherwood number multiplier, XSHPHT - section 2.13.2, is set to 0.0.
Acceptable range: -1, +1, +2, if alternative fluid is used: -1 or +2
Default value: MINGCV(IPLAT) - record 164000
- W-2 (I) : MINTCV Interphase heat and mass transfer model individual activator.
(IDPAT) Droplet-atmosphere interphase.
MINTCV(IDPAT) = -1: inactive
MINTCV(IDPAT) = +1: heat and mass transfer models are active
MINTCV(IDPAT) = +2: only heat transfer is active. Exactly the same effect is obtained with MINTCV(IDPAT) = +1 if the Sherwood number multiplier, XSHDHT - section 2.13.2, is set to 0.0.
Acceptable range: -1, +1, +2, if alternative fluid is used: -1 or +2
Default value: MINGCV(IDPAT) - record 164000
- W-3 (I) : MINTCV Interphase heat and mass transfer model individual activator.
(IBBPL) Bubble-pool interphase.
MINTCV(IBBPL) = -1: inactive
MINTCV(IBBPL) = +1: heat and mass transfer models are active
MINTCV(IBBPL) = +2: only heat transfer is active. Exactly the same effect is obtained with MINTCV(IBBPL) = +1 if the Sherwood number multiplier, XSHBHT - section 2.13.2, is set to 0.0.

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 1.

W-2 (I) : MDEBCV Bubble vertical de-entrainment calculation indicator.
MDEBCV = 1: implicit (recommended),
MDEBCV = 2: explicit.
Acceptable range: 1 or 2.
Default value: 1.

2.1.41 Records: 166000, Freezing / Exceeding Fluid Property Domain Options

W-1 (I) : IFRZCV Freezing option.
IFRZCV=1: freezing not allowed (code stops if freezing encountered).
IFRZCV=2: freezing ignored. Temperature is set to 273 K. In this case the mass and energy balances are violated (mass and energy errors should be checked in the output file; search for :'=CV= DATA SUMMED FOR ALL CONTROL VOLUMES"). This option is convenient in case of sudden depressurization of accumulator volumes or gas cooled reactors (HTR, PBMR).
Acceptable range: 1 or 2
Default value: 1

W-2 (I) : IHTOCV High temperature option.
IHTOCV=1: temperatures above the maximum temperature in the Fluid Property data tables not allowed (the code stops).
IHTOCV=2: temperatures above the maximum temperature in the Fluid Property data tables are ignored. Temperature is set to a maximum value in the Fluid Property data tables and calculations are continued. In this case the mass and energy balances are violated (mass and energy errors should be checked in the output file; search for :'=CV= DATA SUMMED FOR ALL CONTROL VOLUMES").
Acceptable range: 1 or 2
Default value: 1

W-3 (I) : ILPOCV Low pressure option.
ILPOCV=1: pressures below the minimum pressure in the Fluid Property data tables not allowed (the code stops).
ILPOCV=2: pressures below the maximum pressure in the Fluid Property data tables are ignored. Pressure is set to a minimum value in the Fluid Property data tables and calculations are continued. In this case the mass and energy balances are violated (mass and energy errors should be checked in the output file; search for :'=CV= DATA SUMMED FOR ALL CONTROL VOLUMES").
Acceptable range: 1 or 2
Default value: 1

W-4 (I) : IHPOCV High pressure option.
IHPOCV=1: pressures above the maximum pressure in the Fluid Property data tables not allowed (the code stops).
IHPOCV=2: pressures above the maximum pressure in the Fluid Property data tables are ignored. Pressure is set to a maximum value in the Fluid Property data tables and calculations are continued. In this case

the mass and energy balances are violated (mass and energy errors should be checked in the output file; search for :”=CV= DATA SUMMED FOR ALL CONTROL VOLUMES”).

Acceptable range: 1 or 2

Default value: 1

- W-5 (R) : HMAXCV Minimum distance between the top of CV and the initial pool level in CV, (m). The value should be consistent with the parameter HMAXJN. Used when the elevation checking option is set (ICELJN<2). If the distance is lower than this value, then the liquid level is changed in such a way that the distance will be equal to this value and appropriate message is written to the diagnostics file.
- Acceptable range:* $0.0 < \text{HMAXCV} \leq 5.0 \times 10^{-2}$
- Default value:* 1.0×10^{-2}

2.1.42 Records: 167000, Flow Regime Map Parameters

The parameters defined in this record are used to determine bubble size when IWATCV = 3 or 4, and DBWFCV = 0.0 (record 158XXX, section 2.1.31).

- W-1 (R) : A1BSCV Critical void fraction for bubbly-slug transition, low mass flux, $\alpha_{1,BS}$.
- Acceptable range:* $0.1 \leq \alpha_{1,BS} \leq 0.7$
- Default value:* 0.25
- W-2 (R) : A2BSCV Critical void fraction for bubbly-slug transition, high mass flux, $\alpha_{2,BS}$.
- Acceptable range:* $0.1 \leq \alpha_{2,BS} \leq 0.7$
- Default value:* 0.5
- W-3 (R) : G1BSCV Upper limit on mass flux to use $\alpha_{1,BS}$, $G_{1,BS}$, (kg/m²-s). For the mass fluxes G lower than this limit, the critical void fraction fro the bubbly - slug transition, α_{BS} , is equal to $\alpha_{1,BS}$.
- Acceptable range:* $100.0 \leq G_{1,BS} \leq 5000.0$
- Default value:* 2000.0
- W-4 (R) : G2BSCV Lower limit on mass flux to use $\alpha_{2,BS}$, $G_{2,BS}$, (kg/m²-s). For the mass fluxes G higher than this limit, the critical void fraction fro the bubbly - slug transition, α_{BS} , is equal to $\alpha_{2,BS}$.
- Acceptable range:* $G_{1,BS} + 100.0 \leq G_{1,BS} \leq 10,000.0$
- Default value:* 3000.0

For the mass fluxes G within the range $G_{1,BS}$ and $G_{2,BS}$, a linear interpolation is performed:

$$\alpha_{BS} = \alpha_{1,BS} + (\alpha_{2,BS} - \alpha_{1,BS}) \times \frac{G - G_{1,BS}}{G_{2,BS} - G_{1,BS}}$$

- W-5 (R) : DABSCV Bubbly-slug transition zone width, $\Delta\alpha_{BS}$, (-).
- Pure bubbly flow occurs for: $\alpha < \alpha_{BS} - \Delta\alpha_{BS}/2$

SPECTRA Code Manuals - Volume 2: User's Guide

Pure slug flow occurs for: $\alpha > \alpha_{BS} + \Delta\alpha_{BS}/2$

An interpolation zone is defined for void fractions within the range:

$$\alpha_{BS} - \Delta\alpha_{BS}/2 < \alpha < \alpha_{BS} + \Delta\alpha_{BS}/2$$

Acceptable range: $0.01 \leq \Delta\alpha_{BS} \leq 0.1$

Default value: 0.05

W-6 (R) : A1SACV Void fraction for transition from bubbly/slug to annular, α_{SA} , (-). Applied only in Control Volumes with homogeneous thermodynamics (IHOMCV=1).

Acceptable range: $0.80 \leq \alpha_{SA} \leq 0.95$

Default value: 0.90

W-7 (R) : DASACV Slug-annular transition zone width, $\Delta\alpha_{SA}$, (-).

Pure bubbly flow occurs for: $\alpha < \alpha_{SA} - \Delta\alpha_{SA}/2$

Pure slug flow occurs for: $\alpha > \alpha_{SA} + \Delta\alpha_{SA}/2$

An interpolation zone is defined for void fractions within the range:

$$\alpha_{SA} - \Delta\alpha_{SA}/2 < \alpha < \alpha_{SA} + \Delta\alpha_{SA}/2$$

Acceptable range: $0.01 \leq \Delta\alpha_{SA} \leq 0.02$

Default value: 0.02

W-8 (R) : A1AMCV Void fraction for transition from annular to mist, α_{AM} , (-). Applied only in Control Volumes with homogeneous thermodynamics (IHOMCV=1).

Acceptable range: $0.98 \leq \alpha_{AM} \leq 0.999$

Default value: 0.99

W-9 (R) : DAAMCV Annular-mist transition zone width, $\Delta\alpha_{AM}$, (-).

Pure bubbly flow occurs for: $\alpha < \alpha_{AM} - \Delta\alpha_{AM}$

Pure slug flow occurs for: $\alpha > \alpha_{AM}$

An interpolation zone is defined for void fractions within the range:

$$\alpha_{AM} - \Delta\alpha_{AM} < \alpha < \alpha_{AM}$$

Acceptable range: $0.001 \leq \Delta\alpha_{AM} \leq 0.02$

Default value: 0.01

W-10 (R) : GSTRCV Critical mass flux for stratified flow, G_{strat} , (kg/m²-s). Stratified flow occurs when:

$$G < G_{strat}$$

Acceptable range: $1.0 \leq GSTRCV \leq 10,000.0$

Default value: 3000.0

W-11 (R) : VSTRCV Critical velocity for stratified flow, Δv_{strat} , (m/s). Stratified flow occurs when:

$$|v_{gas} - v_{liq}| < \Delta v_{strat}$$

Acceptable range: $0.01 \leq VSTRCV \leq 100.0$

Default value: 1.0

W-12 (R) : CHORCV Constant C_{hor} The stratified flow conditions are checked if the CV flow is defined as horizontal (IHORCV=1, record 168XXX), or if the CV is not defined and the following condition is satisfied:

SPECTRA Code Manuals - Volume 2: User's Guide

$$v_{hor} > v_{ver} \cdot C_{hor}$$

Acceptable range: $0.001 \leq \text{CHORCV} \leq 1000.0$

Default value: 2.0

2.1.43 Records: 168000, Heterogeneous/Homogeneous CV, Global Activator

W-1 (I) : IHMGCV Heterogeneous/homogeneous CV option, global activator. The option selected in this record will be applied to all Control Volumes, unless differently specified for individual Control Volumes in the records 168XXX.

IHMGCV=1: heterogeneous CV, with pool/bubbles at the bottom of a CV and atmosphere/droplets at the top (MELCOR type Control Volumes) - see Figure 2-4.

IHMGCV=2: homogeneous CV. Bubbles and droplets are deactivated; only pool and atmosphere exist in a Control Volume. Atmosphere and pool are assumed to be homogeneously mixed (RELAP-type Control Volumes) - see Figure 2-5. The CV void fraction and gas mass fraction are given as CV-XXX-VolF-atms and CV-XXX-MasF-atms (see Table 2-23). Other volume and mass fractions, as well as the pool level, should not be used as output and plot parameters. The volume-center Control Volume pressure is available as the plot parameter: CV-XXX-Pres-pool. The plot parameter: CV-XXX-Pres-atms gives the pressure at the collapsed liquid level in CV (in a gas-filled CV this is the pressure at the CV bottom; in a liquid-filled CV this is the pressure at the CV top).

Acceptable range: 1 or 2

Default value: 1

2.1.44 Records: 168XXX, Heterogeneous/Homogeneous CV, Individual Activators

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$ or $\text{XXX} = 000$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

W-1 (I) : IHOMCV Heterogeneous/homogeneous CV option, individual activator. The option selected in this record will be applied to Control Volume number XXX.

IHOMCV=1: heterogeneous CV, with pool/bubbles at the bottom of a CV and atmosphere/droplets at the top (MELCOR type Control Volumes) - see Figure 2-4.

IHOMCV=2: homogeneous CV. Bubbles and droplets are deactivated; only pool and atmosphere exist in a Control Volume. Atmosphere and pool are assumed to be homogeneously mixed (RELAP-type Control Volumes) - see Figure 2-5. The CV void fraction and gas mass fraction are given as CV-XXX-VolF-atms and CV-XXX-MasF-atms (see Table 2-23). Other volume and mass fractions, as well as the pool level, should not be used as output and plot parameters. The volume-center Control Volume pressure is available as the plot parameter: CV-XXX-Pres-pool. The plot parameter: CV-XXX-Pres-atms gives the pressure at the

SPECTRA Code Manuals - Volume 2: User's Guide

collapsed liquid level in CV (in a gas-filled CV this is the pressure at the CV bottom; in a liquid-filled CV this is the pressure at the CV top).

Acceptable range: 1 or 2.

Default value: IHMGCV, defined in record 168000

W-2 (I) : IHORCV Indicator for flow direction in a Homogeneous Control Volume.
IHORCV=1: a horizontal flow CV, stratified flow is possible.
IHORCV=2: a vertical flow CV, stratified flow is not possible.
IHORCV=0: undefined CV, the criterion: $v_{hor} > v_{ver} \cdot C_{hor}$ (see record 167000, CHORCV), is used to determine whether the stratified flow is possible.
Acceptable range: 0, 1, 2
Default value: 0

2.1.45 Records: 169000, Accepting Mass or Energy Error

W-1 (I) : IMERCV Option for mass and energy error.
IMERCV=1: no mass or energy error allowed. The code stops if the flow solution results in water level in any Control Volume being higher than the volume height. In such case an error message is printed in the diagnostics file, recommending use of the second option (below).
IMERCV=2: mass or energy error allowed. The code continues if the flow solution results in water level in any Control Volume being higher than the volume height. In such case the excess of water is removed automatically. The amount of removed mass and error is stored, so the user can check what is the total mass and energy error made due to this procedure.
Acceptable range: 1 or 2.
Default value: 1.

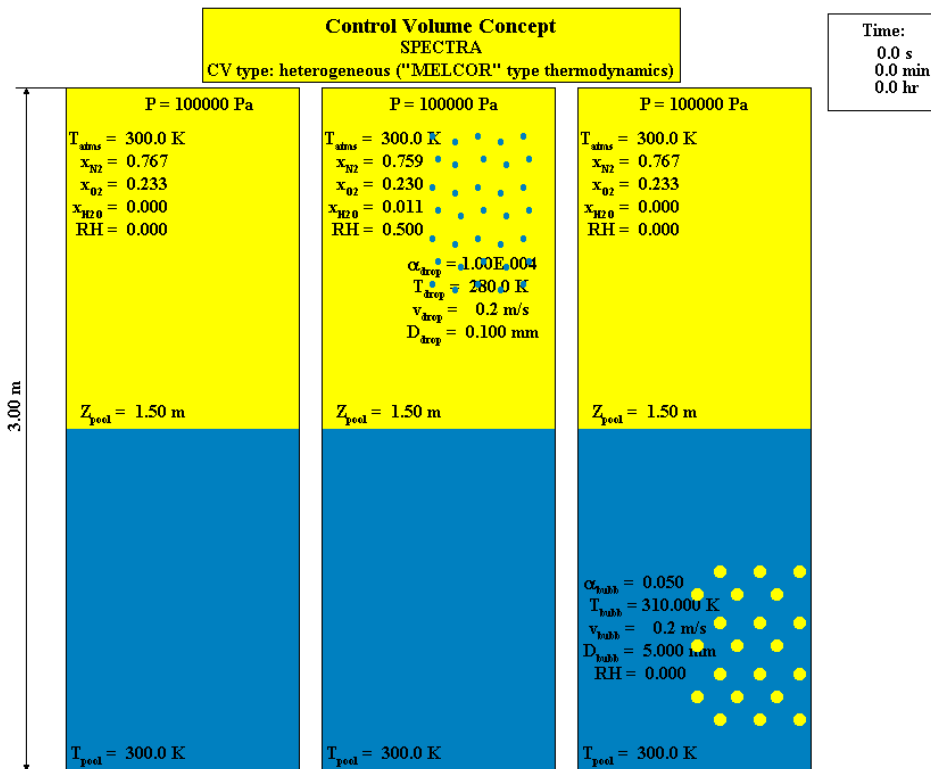


Figure 2-4 SPECTRA Control Volume concept: heterogeneous CV (MELCOR-type)

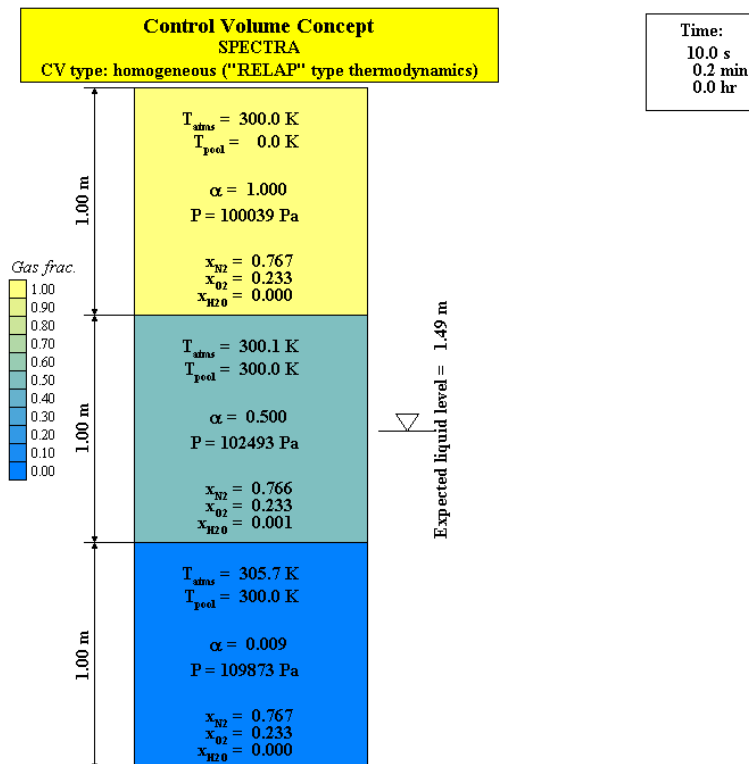


Figure 2-5 SPECTRA Control Volume concept: homogeneous CV (RELAP-type)

2.1.48 Records: 181XXX, Propagation Distances

With this record user can define distances required for burn to propagate to another control volume. XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

- W-1 (I) : IJN Junction number of a junction connected to the control volume XXX.
Acceptable range: Must be one of the junctions connected to the control volume number XXX.
Default value: 0.
- W-2 (R) : PRPDH2 Propagation distance, (m). Minimum distance that the flame must cover in the control volume XXX, before it can propagate to the control volume connected by the junction number IJN.
Acceptable range: $0.01 \leq PRPDH2 \leq 1000.0$.
Default value: 70% of the burn characteristic dimension, DIMH2
- W-3 (I) : IJN Junction number of next junction connected to the control volume number XXX.
- W-4 (R) : PRPDH2 Propagation distance, (m).
- . . . etc. until propagation distances are defined for all junctions connected to the control volume number XXX.

2.1.49 Records: 182XXX, Combustion Completeness Model

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

- W-1 (R) : CCC1H2 Combustion completeness for slow deflagrations.
CCC1H2 < 0.0 : Use correlation from HECTR 1.5.
CCC1H2 > 0.0 : use constant value, equal to CCC1H2.
Acceptable range: CCC1H2 ≤ 1.0 , if positive.
Default value: 0.99 .
- W-2 (R) : CCC2H2 Combustion completeness for detonations and fast turbulent deflagrations.
CCC2H2 < 0.0 : Use correlation from HECTR 1.5.
CCC2H2 > 0.0 : use constant value, equal to CCC2H2.
Acceptable range: CCC2H2 ≤ 1.0 , if positive.
Default value: 0.99 .

2.1.50 Records: 183XXX, Detonation and Fast Deflagration Criteria

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

W-1 (R) : CDCH2 Parameter selecting detonation criteria.
 CDCH2 = 0.0 : use only the default detonation criterion.
 CDCH2 > 0.0 : use only the criterion based on the detonation cell width, λ (called also "the λ criterion"). The criterion is: $D/\lambda > C$, where D is the burn characteristic dimension, equal to DIMH2, and C is a constant, equal to CDCH2.

 CDCH2 < 0.0 : use both the default criterion and the criterion based on detonation cell width: $D/\lambda > C$, where D is the burn characteristic dimension, equal to DIMH2, and C is a constant, equal to $|CDCH2|$. Detonation occurs if any of the two criterions is satisfied.
Acceptable range: $|CDCH2| < 100.0$. The value of 6.0 is recommended, if the λ criterion is used.
Default value: 0.0 .

W-2 (R) : CFCH2 Parameter selecting fast turbulent deflagration criteria.
 CFCH2 = 0.0 : use only the default fast deflagration criterion.
 CFCH2 > 0.0 : use only the criterion based on the expansion ratio, σ (called also "the σ criterion"). The criterion is: $\sigma > \sigma^*(T)$, where σ is the expansion ratio - the ratio of specific volumes (m^3/kg) of burned to unburned gas at constant pressure, and $\sigma^*(T)$ is the critical value of the expansion ratio, calculated as follows:

$$\sigma^*(T) = 1.0 + (\sigma^*(T_0) - 1.0) \cdot \left(\frac{T_0}{T}\right)^{1.5}$$

with:
 T_0 - reference temperature, equal to 300 K,
 $\sigma^*(T_0)$ - value of σ^* at the reference temperature, equal to CFCH2.

CFCH2 < 0.0 : use both the default criterion and the criterion based on the expansion ratio: $\sigma > \sigma^*(T)$, where σ is the expansion ratio - the ratio of specific volumes (m^3/kg) of burned to unburned gas at constant pressure, and $\sigma^*(T)$ is the critical value of the expansion ratio, calculated as shown above, with $\sigma^*(T_0)$ equal to $|CFCH2|$.
Acceptable range: $|CFCH2| < 100.0$. The value of 3.5 is recommended, if the σ criterion is used.
Default value: 0.0 .

SPECTRA Code Manuals - Volume 2: User's Guide

W-3 (R) : CMSWH2 Multiplier on Mach number in shock wave calculation equation, C_M , (see Volume 1).
Acceptable range: $1.0 \leq \text{CMSWH2} \leq 2.0$.
Default value: 1.4 .

2.1.51 Records: 184XXX, Flame Speed Calculation

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. The Control Volume reference numbers, XXX, need not be consecutive. The maximum number of Control Volumes is 550 (999 in LINUX version).

W-1 (R) : RVMAH2 Ratio of maximum to average gas velocity in Control Volume. The value is used to calculate turbulent flame speed. The default value has been set based on results of CFD calculations (see Volume 1).
Acceptable range: $0.1 \leq \text{RVMAH2} \leq 100.0$
Default value: 8.0

W-2 (R) : RVTMH2 Ratio of turbulent to maximum local gas velocity in Control Volume. The value is used to calculate turbulent flame speed. The default value has been set based on results of CFD calculations (see Volume 1).
Acceptable range: $0.01 \leq \text{RVTMH2} \leq 10.0$
Default value: 0.45

W-3 (R) : TLAMH2 Gas temperature used for the laminar flame velocity calculation.
<0.0: use the current gas temperature
>0.0: use a constant temperature, TLAMH2. A value of 1150 K results in laminar flame velocities close to those calculated by the HECTR model (used by the MELCOR code) - see Volume 1. (Note that this was the default value in the earlier SPECTRA versions.)
Acceptable range: $\text{TLAMH2} < 0.0$ or $270.0 \leq \text{TLAMH2} \leq 3000.0$
Default value: -1.0

2.1.52 Records: 188000, Burn Model Constants

W-1 (I) : CKLIH2 Constant C in the Klimov expression for $g(q, v_{lam})$:

$$g(q, v_{lam}) = C \cdot \left(\sqrt{q} / v_{lam} \right)^{0.7}$$

Here v_{lam} is the laminar flame speed, q, v_{lam} is the kinetic energy density, and C is constant, equal to CKLIH2. The best estimate value is 2.4 (see Volume 1). A value of zero will eliminate Klimov correlation. In such case only the Williams correlation is used. If CWILH2 (Word 2 below) is also set to zero, the turbulent flame speed is not taken into account and the flame speed in the slow deflagrations is always calculated from the laminar flame speed, Liu and MacFarlane correlation.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0 \leq \text{CKLIH2} \leq 100.0$
a small value ($\leq 10^{-50}$) value will set it to 0.0
Default value: 2.4

W-2 (I) : CWILH2 Constant C in the Williams expression for $g(q, v_{lam})$:

$$g(q, v_{lam}) = \left[\frac{1}{2} \cdot \left(1 + \sqrt{1 + (8/3) \cdot C \cdot (2q / v_{lam}^2)} \right) \right]^{1/2}$$

Here v_{lam} is the laminar flame speed, q, v_{lam} is the kinetic energy density, and C is constant, equal to CWILH2. The best estimate value is 2.4 (see Volume 1). A value of zero will eliminate the Williams correlation. In such case only the Klimov correlation is used. If CKLIH2 is also set to zero, the turbulent flame speed is not taken into account and the flame speed in the slow deflagrations is always calculated from the laminar flame speed, Liu and MacFarlane correlation.

Acceptable range: $0 \leq \text{CWILH2} \leq 100.0$
a small value ($\leq 10^{-50}$) value will set it to 0.0
Default value: 2.4

2.1.53 Records: 189000, Additional Print and Plot During Burn

Rapid change of parameters that may occur during burn requires that additional printouts (print edits) and plot edits should be made during burn. The additional edits are requested in this record. By default the additional edits are active, they may be deactivated by the user if too large output and plot files are being produced.

W-1 (I) : IPRTH2 Indicator defining if additional printouts are made during burn.
IPRTH2 = 1 : no additional printouts are made during burn.
IPRTH2 = 2 : additional printout is made at the start of each burn.
Acceptable range: IPRTH2 = 1 or 2 .
Default value: 2 .

W-2 (I) : IPLTH2 Indicator defining if additional plot points are made during burn.
IPLTH2 = 1 : no additional plot points are made during burn.
IPLTH2 = 2 : additional plot point is made every time step during burn.
Acceptable range: IPLTH2 = 1 or 2 .
Default value: 2 .

2.1.54 Example of Control Volume Input Data

An example input for a single Control Volume is provided below. The Control Volume name is: "Example volume". There are four segments with different horizontal cross section areas. The bottom segment is 1 m height with an area of 5 m². The bottom elevation of the CV is 5.0 m. The total height is 9 m. One of the CV segments is significantly longer than the others. Therefore the default value of the representative horizontal flow area, which is 5.0 m² (maximum of all segment areas), is overwritten by the input value. The area of the longest segment - 2.2 m², is used as the representative horizontal flow area.

The default value is used for the representative vertical flow area. In this case the code will assume 13.35 m² as the vertical flow area. Since DIPSCV is entered as zero the square root of the current pool surface area will be used as characteristic dimension for pool surface heat and mass transfer. The initial pressure is 1 bar, the gas temperature 300 K. The pool level is 2 m above the floor; the pool temperature is 295 K. The atmosphere consists of 80 % (volume fraction) nitrogen, 20 % oxygen. The relative humidity is 60 %.

There is a mass source of hydrogen. The source is located at the elevation of 7 m, the flow area is 0.0004 m². The mass flow rate of H₂ is defined by the Tabular Function TF-002. The temperature and pressure of the hydrogen source are given by the TF-003 and TF-004 respectively. There is an energy (heat) source. The energy source is located at the elevation of 9 m. The heat power is defined by the Tabular Function 007.

The H₂ burn model is activated in Control Volume CV-150. The characteristic dimension for burn is not specified, thus default value will be used. An igniter is assumed to be present. The igniter temperature is defined as a function of time, by the tabular function TF-011.

The distances required to propagate burn to adjacent Control Volumes are set as 10.0 m and 20.0 respectively, for the junctions number 1 and 2. (These junctions must be connected to the control volume CV-150.)

The alternative detonation criterion, based on the detonation cell size, is requested. The value of constant is set to 6.0. Thus, the selected detonation criterion is:

$$\frac{D}{\lambda} = 6.0$$

The alternative fast deflagration criterion, based on the expansion ratio, is requested. The value of constant is set to 3.5. Thus, the selected fast turbulent deflagration criterion is:

$$\sigma > \sigma^*(T) = 1.0 + (3.5 - 1.0) \cdot \left(\frac{300}{T} \right)^{1.5}$$

SPECTRA Code Manuals - Volume 2: User's Guide

```
*      Definition of Control Volume No. 150
*      =====
*
105150  Example volume
*
*      Height      Area      Segment data
110150  1.00      5.00      * Seg. 1
110150  6.00      2.20      * Seg. 2
110150  1.00      1.50      * Seg. 3
110150  1.00      5.00      * Seg. 4
*
111150  5.0        2.2      0.0      0.0      * Elevation, A-hor, A-ver, D-pool
120150  1.0E+5     300.0    2.0      295.0    * Pressure, Tatms, Zpool, Tpool
*
121150  4           0.80     * atms gas: N2 - mole fraction = 80 %
121150  5           0.20     * atms gas: O2 - mole fraction = 20 %
121150  3           0.60     * atms gas: H2O - relative humidity = 60 %
*
*      Elev. Area   Diam. IMT ITT IPT Gas No. Mass Frac.
131150  7.0 0.0004 0.02 002 003 004 1 1.0 * H2 mass source
*
*      Elev. IQT
141150  9.0 7 * Energy source
*
*      Definition of burn parameters for control volume No. 150
*      =====
*
180000  1           * Global activation of the burn model
180001  0 0.0 011 * CV-001:
*          * - Use global activation
*          * - Use default characteristic dimension
*          * - Igniter present, temperature defined by TF-011
*
*      Propagation distances
*      JN Dist. (m) JN Dist. (m)
181001  1 10.0 2 20.0
*
*      Combustion completeness
*      Deflagration Detonation
182001  0.0 0.0 * Use default values
*
*      Detonation and fast turbulent deflagration criteria
*      D/λ σ*(300 K) * use alternative criteria
183001  6.0 3.5 * for detonation and fast deflagration
*          * The constants in the alternative criteria are:
*          * D/λ = 6.0; σ*(300 K) = 3.5
```

2.2 Junction Input Data

2.2.1 Records: 200XXX, Junction Main Data

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version). No more than 50 Junctions may be connected to a single CV.

- W-1 (I) : ICVFJN "From" Control Volume number, (-).
Acceptable range: must be a valid CV reference number
Default value: none
- W-2 (I) : ICVTJN "To" Control Volume number, (-).
Acceptable range: must be a valid CV reference number
Default value: none
- W-3 (R) : AMAXJN Flow area of fully open Junction, (m²).
Acceptable range: $0.0 < AMAXJN < 10^{10}$.
Default value: $\pi \text{ DIAMJN}^2 / 4$
- W-4 (R) : ELEVJN Elevation of middle point of the Junction, (m). If -999 is entered, then the JN is automatically allocated to match the elevations of CV-s: $\{\text{Min}[Z_{TOP}(CV_1), Z_{TOP}(CV_2)] + \text{Max}[Z_{BOT}(CV_1), Z_{BOT}(CV_2)]\} / 2$. Here Z_{TOP} and Z_{BOT} are top and bottom elevations of the "From" volume CV_1 and the "To" volume CV_2 . The automatic allocation of a Junction is illustrated in Figure 2-6.
Acceptable range: bottom and top elevations of the Junction must lie within the Control Volumes it connects. The bottom and top elevations are calculated based on Junction height (HEIGJN) and vertical orientation (IVERJN) - see Words 7 and 8, and Table 2-1.
Default value: none
- W-5 (R) : XLENJN Momentum length, L , of the Junction, (m). (The value is used at the left hand side of the momentum equation: $L \cdot dv/dt$). The recommended value is:
- $$L_m = L + \frac{V_1}{2A_1} + \frac{V_2}{2A_2}$$
- see Figure 2-7. A more detailed discussion is provided in Volume 1, section "Momentum Length and Friction Length". To use the recommended value, enter IMFLJN=1 (record 264000) and XLENJN=0.0 or IMFLJN=2.
Acceptable range: $10^{-3} \leq XLENJN \leq 10^{10}$
Default value: none

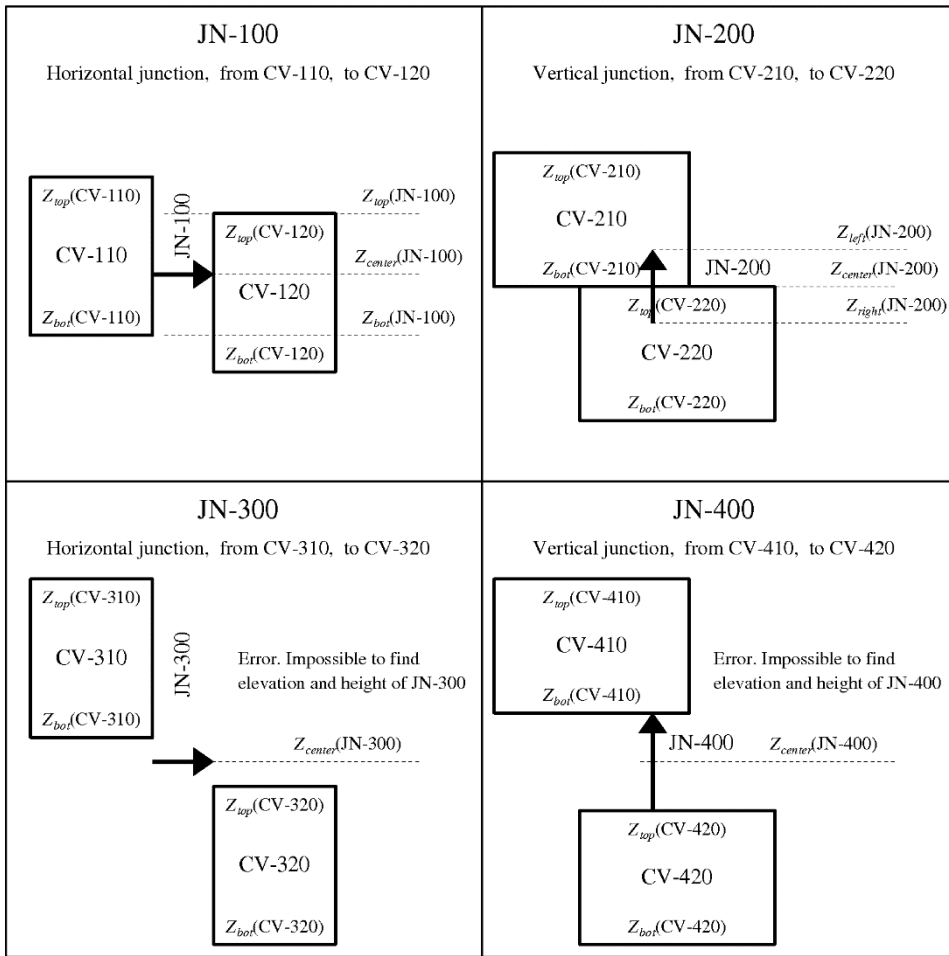


Figure 2-6 Automatic allocation of JN within the boundary Control Volumes

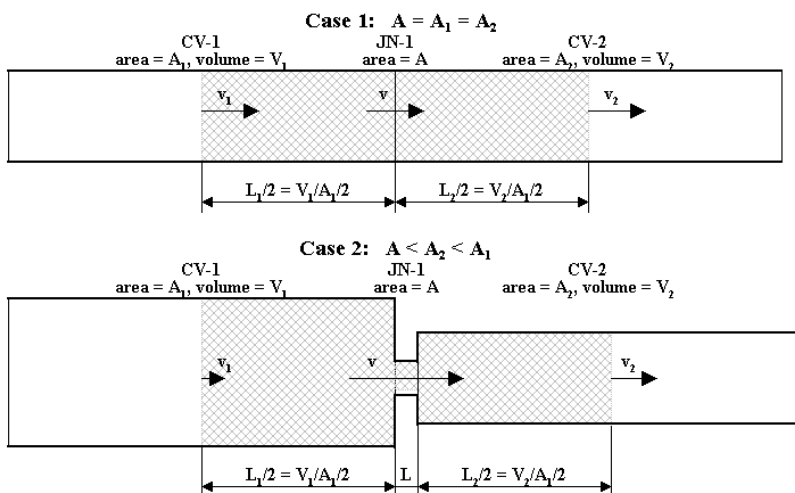


Figure 2-7 Momentum length and friction length of a Junction

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-1 Bottom and top elevations of Junctions.

IVERJN	"From" CV		"To" CV	
	Z _{BOT}	Z _{TOP}	Z _{BOT}	Z _{TOP}
0 (horizontal)	ELEVJN- HEIGJN/2	ELEVJN+HEIGJN/2	ELEVJN- HEIGJN/2	ELEVJN+HEIGJN/2
-1 (vert. down)	ELEVJN	ELEVJN+HEIGJN/2	ELEVJN- HEIGJN/2	ELEVJN
1 (vertical up)	ELEVJN- HEIGJN/2	ELEVJN	ELEVJN	ELEVJN+HEIGJN/2

- W-6 (R) : DIAMJN Diameter of the Junction, (m).
Acceptable range: DIAMJN > 0.0
Default value: $(4 \cdot \text{AMAXJN} / \pi)^{1/2}$
- W-7 (R) : HEIGJN Height of the Junction, (m). Used to determine bottom and top elevations of the Junction opening (Table 2-1). See Volume 1, section 4 for more explanation of the meaning of HEIGJN.
Acceptable range: $0.001 \leq \text{HEIGJN} \leq 10^{10}$ (internal limit ≥ 0.02 m)
Default value: horizontal: = DIAMJN
 vertical: = DIAMJN / 2.0
 The Junction height defined here is used in the code to set the opening heights in both volumes it connects. Additional limits are applied during this process - see: HMINJN, HMAXJN in the record 260000.
- W-8 (I) : IVERJN Flow direction in the Junction, (-).
 -1 : vertical flow, downwards when the flow is positive,
 0 : horizontal flow,
 +1 : vertical flow, upwards when the flow is positive.
 The bottom and top elevations of the Junction, are calculated based on this entry, as well as the middle point elevation, ELEVJN and height, HEIGJN, as shown in Table 2-1.
Acceptable range: $-1 \leq \text{IVERJN} \leq 1$
Default value: 0
- W-9 (R) : EDSMJN Smoothness of Junction edges. EDSMJN equal to 0.0 means the Junction has smooth flanges. EDSMJN equal to 1.0 means that the Junction has sharp edged flanges. The value is used with flooding correlations. Values of the constants in the flooding correlations are obtained as:

$$C = (1 - \text{EDSMJN}) \cdot C_{smooth} + \text{EDSMJN} \cdot C_{sharp}$$

where C_{smooth} (=1.0), C_{sharp} (=0.525) are the values of the constant C appropriate for the sharp and the smooth edges respectively.

Acceptable range: $0.0 \leq \text{EDSMJN} \leq 1.0$

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 0.474 . This value results in $C=0.775$, the same as in the Dartmouth correlation - see Volume 1. A small number ($<10^{-50}$) sets the value to zero.

The following parameter is used only if $IMFLJN = 1$ (record 264000). It is used to calculate the friction length and the momentum length from the recommended formulae (see description of $XLENJN$ and $FRLNJN$).

W-10 (R) : XORFJN The “orifice length” of the Junction, (m). If the junction area is different than the area of the connected volumes, then this is the length with the JN area, denoted by L in Figure 2-7, Case 2.
Acceptable range: $0.0 \leq XORFJN \leq 1.0$
Default value: 0.0

2.2.2 Records: 201XXX, Initial Velocities

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

W-1 (I) : INIVJN Initial velocity calculation indicator.
1: Velocities are calculated from the initial pressure differences.
2: Input values (Words 2 and 3 below) are used. Use this option also when velocities should be read from an Initial Condition File - ICF (section 2.16.3).
Acceptable range: 1, 2
Default value: 2

W-2 (R) : VCMPJN Initial velocity of atmosphere, (m/s).
(IATMS) *Acceptable range:* any real
Default value: 0.0

W-3 (R) : VCMPJN Initial velocity of pool, (m/s).
(IPOOL) *Acceptable range:* any real
Default value: 0.0

2.2.3 Records: 202XXX, Multiplicity of the Junction

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

W-1 (R) : XMLTJN Multiplicity of the Junction. This is the number of Junctions that are identical to the Junction XXX. If the number is not equal to 1.0, then the flow area of this Junction, entered in the input deck, is multiplied by this number.
Acceptable range: $0.0 < XMLTJN < 10^{10}$
Default value: 1.0

2.2.4 Records: 205XXX, Junction Name

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

W-1 (A) : NAMEJN User defined name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.
Acceptable range: any string of up to 50 characters.
Default value: 50 "underline" characters: "_" .

2.2.5 Records: 210XXX, Friction Loss, Form Loss and Moody Coefficient

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

W-1 (R) : FRLNJJ Friction length, L_f , (m). The value is also used to calculate L_f/D ratio (where D is the diameter - Word 3 below), used by the critical flow model. The recommended value is:

$$L_f = L + \frac{V_1}{2A_1} \cdot \left(\frac{D}{D_1}\right) \cdot \left(\frac{A}{A_1}\right)^2 + \frac{V_2}{2A_2} \cdot \left(\frac{D}{D_2}\right) \cdot \left(\frac{A}{A_2}\right)^2$$

see Figure 2-7. A more detailed discussion is provided in Volume 1, section "Momentum Length and Friction Length". To use the recommended value, enter IMFLJN=1 (record 264000) and FRLNJJ=0.0 or IMFLJN=2.

Acceptable range: $0.0 < FRLNJJ < 10^{10}$.
Default value: XLENJJ

W-2 (R) : FRRGJJ Roughness, R , (m). The relative roughness is obtained as: $e = R/D$.
Acceptable range: $0.0 \leq FRRGJJ < FRDHJJ$
Default value: 0.0

W-3 (R) : FRDHJJ Diameter, D , (m). The value is also used to calculate L/D ratio (where L is the friction length - Word 1 above), used by the critical flow model.
Acceptable range: $0.0 < FRDHJJ < 10^{10}$
Default value: DIAMJJ

W-4 (R) : FLCFJJ Form loss coefficient, K_F , forward flow, (-).
 FLCFJJ > 0: $K_F = \text{constant}$, equal to FLCFJJ
 FLCFJJ = -XXX: $K_F = \text{Control Function XXX}$
 FLCFJJ = -1XXX: $K_F = \text{Tabular Function XXX versus Re}$
 Limits of 0.0 and 10^{10} are applied for the value obtained from CF / TF.
 CF/TF cannot be used for a valve (i.e. when 220XXX is present).

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq \text{FLCFJN} \leq 10^{10}$ or reference to CF / TF.
The value must be positive for a valve junction.

Default value: 0.0

- W-5 (R) : FLCRJN Form loss coefficient, K_R , reverse flow, (-).
 FLCRJN > 0: $K_F = \text{constant}$, equal to FLCRJN
 FLCRJN = -XXX: $K_F = \text{Control Function XXX}$
 FLCRJN = -1XXX: $K_F = \text{Tabular Function XXX versus Re}$
 Limits of 0.0 and 10^{10} are applied for the value obtained from CF / TF.
 CF/TF cannot be used for a valve (i.e. when 220XXX is present).
Acceptable range: $0.0 \leq \text{FLCRJN} \leq 10^{10}$ or reference to CF / TF.
 The value must be positive for a valve junction.
Default value: 0.0
- W-6 (R) : RFFJN Empirical coefficient in the Griffith-Rohsenow correlation for the two-phase form loss factor multiplier, r_f , forward flow, (-). Values of r_f are shown in Table 2-2. The multiplier is equal to: $1.0 + r_f \cdot X \cdot v_{fg} / v_f$.
Acceptable range: $0.0 \leq \text{RFFJN} \leq 10^3$
Default value: RFFGJN (see global activators, record 263000, a small number, $<10^{-50}$, sets the value to 0.0)
- W-7 (R) : RFRJN Empirical coefficient in the Griffith-Rohsenow correlation for the two-phase form loss factor multiplier, r_f , reverse flow, (-). Values of r_f are shown in Table 2-2. The multiplier is equal to: $1.0 + r_f \cdot X \cdot v_{fg} / v_f$.
Acceptable range: $0.0 \leq \text{RFRJN} \leq 10^3$
Default value: RFRGJN (see global activators, record 263000, a small number, $<10^{-50}$, sets the value to 0.0)
- W-8 (R) : CMJN Moody coefficient for liquid flow, C_M , (-). The value of CMJN is applied for pure liquid flow ($X=0.0$). For $X>0$ the value is interpolated, to give 1.0 when $X=1.0$. Thus, the effective multiplier on the critical flow is equal to: $\text{CMJN} + X \cdot (1 - \text{CMJN})$, see Volume 1. The best estimate value is 0.7 (Volume 3).
Acceptable range: $0.1 \leq \text{CMJN} \leq 1.0$
Default value: CMGJN (see global activators, record 263000, a small number, $<10^{-50}$, sets the value to 0.0)

Table 2-2 Values of r_f for two phase form loss factor multiplier (reproduced from [7], table 7.4).

Fitting	Pressure range	Quality range (%)	r_f
Bend-short	$p/p_{\text{crit}} < 0.15$	0 - 10	1.5
Bend-short	$p/p_{\text{crit}} > 0.10$	0 - 50	4.0
Bend-long	$p/p_{\text{crit}} > 0.10$	0 - 50	2.2
Tee (serving as L)	$p/p_{\text{crit}} > 0.10$	0 - 50	1.6
Gate valve	$p/p_{\text{crit}} < 0.10$	0 - 50	1.5
Contractions	$0.015 < p/p_{\text{crit}} < 1$	0 - 50	1.0
Expansions	$0.15 < p/p_{\text{crit}} < 1$	0 - 50	1.1

SPECTRA Code Manuals - Volume 2: User's Guide

W-9 (I) : MODFJN Model to calculate friction factor, f , (-), (see Volume 1),

= 1 : non-uniform roughness, Colebrook-White formula

= 2 : uniform roughness, Nikuradse formula

= 3 : simplified method, Blasius and Prandtl-Nikuradse

= 11 : non-uniform roughness, Beluco-Camano formula

= 12 : non-uniform roughness, Churchill formula

>1000 : $f(Re,E)$ is given by Control Function with the number (MODFJN – 1000). It must be a 2-D Tabular Function with the first arguments being the Reynolds number (Re) and the second argument being the the relative roughness (E). The values of Re and E are those for the junction XXX, therefore the same CF may be used for multiple junctions. The actual arguments entered for the CF are not used for friction factor calculation (they will only be used to calculate the value of CF printed in the CF block output).

Example:

```

*          Length  Roughness  Diameter  K-for  K-rev  rf-for  rf-rev  CM  MODFJN
*          (m)      (m)       (m)      (-)    (-)    (-)    (-)  (-)  (-)
210100    0.1      1.0E-5    0.1      0.5    0.5    1.0    1.0  0.7  1100 * Use CF-100

705100 2-D Tabular Function Defining f(Re,E) for JN-100
*      Group Number Fact. Const.
700100 1      5      1.0    0.0    *      Type : General TF
*      E=0.000  E=0.005  E=0.010  E=0.05
708100 0.000    0.005    0.010    0.05 * y-coordinate data points (relative roughness)
* Arguments
* s : (1) (2) (3) (4) Fact. Const.
710100 9 000 1 0 1.0 0.0 * x-argument: dummy argument, for the f(Re,E) calculation it
*                               will be replaced by the Re-number for the given JN
710100 6 101 1 0 1.0 0.0 * uses TF-101 for y = 0.000
710100 6 102 1 0 1.0 0.0 * uses TF-102 for y = 0.005
710100 6 103 1 0 1.0 0.0 * uses TF-103 for y = 0.010
710100 6 104 1 0 1.0 0.0 * uses TF-103 for y = 0.050
710100 9 000 1 0 1.0 0.0 * y-argument: dummy argument, for the f(Re,E) calculation it
*                               will be replaced by the relative roughness for the given JN

605101 f(Re,E=0.000)
*      Re      f
600101 1.0e5    0.001
600101 2.0e5    0.002
*
605102 f(Re,E=0.005)
*      Re      f
600102 1.0e5    0.005
600102 2.0e5    0.006
*
605103 f(Re,E=0.010)
*      Re      f
600103 1.0e5    0.010
600103 2.0e5    0.020
*
605104 f(Re,E=0.050)
*      Re      f
600104 1.0e5    0.050
600104 2.0e5    0.060

```

The following limits are set internally on the value obtained from the Control Function: $10^{-6} \leq f(Re,E) \leq 10^6$.

Acceptable range: MODFJN = 1, 2, 3, 11, 12, or reference to a CF

Default value: MODGJN (see global activators, record 263000)

W-10 (I) : M2PFJN Model to calculate two-phase friction multiplier, Φ_f^2 , (-), (see Vol. 1),

SPECTRA Code Manuals - Volume 2: User's Guide

- = 1 : no two-phase multiplier,
- = 2 : Hancox-Nicoll model,
- = 3 : Levy Model.
- > 1000: Φ_f^2 is given by a Tabular Function with the number: (M2PFJN – 1000). The argument is void fraction. The range of independent argument (void fraction) must cover the range from 0.0 to 1.0, inclusive. The TF value must be =1.0 for the void fraction of 0.0 and >1.0 for void fractions >0.0.

Acceptable range: M2PFJN = 1, 2, 3, or reference to a TF

Default value: M2PGJN (see global activators, record 263000)

- W-11 (R) : CLAMJN Correction factor for non-circular tubes, C_{lam} . It may also be used as a multiplier for wire-wrapped rods. The friction factor in laminar flow is obtained from:

$$f_{wall} = \frac{64 \cdot C_{lam}}{Re}$$

Rectangular channel, dimensions $0.0 < b/a < 1.0$ [10] (Dia. 2-6)

$C_{lam} = 1.50$ $b/a \rightarrow 0.0$

$C_{lam} = 0.89$ $b/a \rightarrow 1.0$ (square)

Tube bundle, pitch-to-diameter ratios $1.0 < (P/D) < 1.5$ [10] (Dia. 2-9):

$C_{lam} = 0.89 \cdot (P/D) + 0.63$ triangular pitch

$C_{lam} = 0.96 \cdot (P/D) + 0.63$ rectangular pitch

For wire-wrapped rods, Engel correlation [50] gives: $f = 110/Re$, so $C_{lam} = 1.50 / 64 = 1.718$

Acceptable range: $0.1 \leq CLAMJN \leq 10.0$

Default value: CLAGJN (see global activators, record 263000)

- W-12 (R) : CTURJN Friction factor multiplier for turbulent flow. Applicable for example for wire-wrapped rod assemblies in fast reactors.

For wire-wrapped rods, Engel correlation [50] gives: $f = 0.55/Re^{0.25}$, so compared to the smooth friction factor (Blasius): $f = 0.316/Re^{0.25}$, $C_{lam} = 0.55 / 0.316 = 1.741$. A good overview of correlations: [51].

Acceptable range: $0.1 \leq CTURJN \leq 10.0$

Default value: CTUGJN (see global activators, record 263000)

2.2.6 Records: 220XXX, Valve Data

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

If the Junction flow area should change in calculations then the valve model can be used for the Junction. This is done using this record. Two types of valves are available: motor valve and check valve. Valves may only be used if the flow in this Junction is not controlled by Tabular or Control Functions (see flow control - records 230XXX, section 2.2.7).

- W-1 (I) : IMVLJN Indicator for "motor valve". If IMVLJN is zero then the Junction flow area is not restricted by the motor valve, and is always equal to the fully open area unless a check valve is present. If the number is positive, then

SPECTRA Code Manuals - Volume 2: User's Guide

a Tabular Function with the reference number: IMVLJN will define the open fraction. If it is negative, then the open fraction will be defined by a Control Function with the reference number: $|IMVLJN|$. If the value obtained from Tabular or Control Function is smaller than zero it will be set to zero. If it is greater than 1.0 it will be set to 1.0. The rate of change of the valve area is restricted by RACVJN (Word 4 below).

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0

W-2 (R) : DPOVJN Opening pressure difference for check valve, Δp_{open} , (Pa) (or pressure difference in the positive flow direction required to open a burst disk, $\Delta p_{open,+}$, see IBDVJN, Word 9). If DPOVJN is zero then the Junction flow area is not restricted by a check valve, and is always equal to the fully open area unless a motor valve is present. If the number is non-zero then check valve is present and DPOVJN is the pressure difference (Pa) required to open the check valve when closed.

Acceptable range: any real. A check valve may be used together with a motor valve (see Word 1, above). In such case the valves are assumed to be serial; the actual flow area is equal to the smaller of the two. A valve cannot be used if the Junction flow is controlled by Tabular or Control Functions (see section 2.2.7). Thus DPOVJN and IMVLJN must be zero if IGFCJN \neq 0.

Default value: 0.0

W-3 (R) : DPCVJN Closing pressure difference for check valve, Δp_{close} , (Pa) (or pressure difference in the negative flow direction required to open a burst disk, $\Delta p_{open,-}$, see IBDVJN, Word 9). If the check valve is present (see Word 2 above) then DPCVJN is the pressure difference (Pa) required to close the check valve when opened.

Acceptable range: DPCVJN < DPOVJN if check valve is present, zero otherwise.

Default value: 0.0

W-4 (R) : RACVJN Rate of area change for a check valve, maximum rate of area change for a motor valve, $(1/A_{TOT}) \cdot (dA/dt)$, (1/s).

Acceptable range: $0.001 \leq RACVJN \leq 1000.0$ if a valve is present, zero otherwise.

Default value: 1.0

W-5 (R) : VIFOJN Initial open fraction, (-). VIFOJN = 0.0 means the valve is initially closed. VIFOJN = 1.0 means the valve is initially fully open.

Acceptable range: $0.0 \leq VIFOJN \leq 1.0$

Default value: 0.0

W-6 (R) : VLFOJN Leakage open fraction for nominally closed valve (-). If positive value is entered then the valve open fraction will never be smaller than VLFOJN.

Acceptable range: $0.0 \leq VLFOJN < 1.0$

Default value: 0.0

SPECTRA Code Manuals - Volume 2: User's Guide

W-7 (R) : VMFOJN Maximum open fraction for nominally open valve, (-). If positive value is entered then the valve open fraction will never be greater than VMFOJN.
Acceptable range: VLFOJN < VMFOJN < 1.0
Default value: 1.0

W-8 (R) : CVVLJN Coefficient used to calculate change of valve resistance with changing open fraction, (-).
 If a positive value is entered then the loss factors (forward and reverse) are calculated from:

$$K_v = K_0 \left[C_v + (1 - C_v) \frac{A_v}{A_0} \right]$$

where: K_v current valve loss coefficient, (-),
 K_0 loss coefficient for fully open valve, (-), (FLCFJN or FLCRJN, specified in records 210XXX - see section 2.2.5).
 C_v valve resistance increase coefficient, CVVLJN, (-),
 A_v current valve open area, (m²),
 A_0 area for fully open valve, (m²).

The limiting values of the loss coefficients are equal to:

$$K_v \rightarrow K_0 \quad \text{when } A_v \rightarrow A_0$$

$$K_v \rightarrow K_0 \cdot C_v \quad \text{when } A_v \rightarrow 0.0$$

Values of C_v may be estimated based on data in [10], chapter 9. Values appropriate for several common valve types are shown in Appendix C.1. (Typical values are: 7.0 for a butterfly valve, 25.0 for a gate valve, 1.0 for a check valve).

If a negative value is entered then the loss factor is multiplied by the value of Tabular Function number -CVVLJN, calculated for the open fraction as an argument. The loss factors (forward and reverse) are calculated from (see example in Appendix C.2):

$$K_v = K_0 \cdot TF(A_v / A_0)$$

where: TF value of Tabular Function evaluated for the current valve open fraction, A_v/A_0 , (-),

Acceptable range: $1.0 \leq CVVLJN < 10^4$ or a valid reference number of a Tabular Function when negative.

Default value: 5.0

W-9 (I) : IBDVJN Burst disc indicator. If IBDVJN=1, then this valve is considered as a burst disc, with opening pressure differences for positive and negative flow directions, $\Delta p_{open,+}$, $\Delta p_{open,-}$, defined by DPOVJN and DPCVJN respectively. Once open the valve will stay open. For a burst disc both DPOVJN and DPCVJN must be positive. If IBDVJN=0 this valve is a check valve with DPOVJN and DPCVJN being the opening and closing setpoints, as described by Words 2 and 3 above.
Acceptable range: 0 or 1
Default value: 0

2.2.7 Records: 230XXX, Junction Flow Control

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

The user can define flow through Junctions using these records. If these records are used then the valves (records 220XXX) cannot be used. Note that if the Pump Model 1 is used (see record 231XXX, section 2.2.8), then the interpretation of the input values is different than described below. Interpretation of IGFCJN and ILFCJN for such case is described in section 2.2.8.

W-1 (I) : IGFCJN Flow control for atmosphere gas. If IGFCJN = 0 then this is a "normal" Junction with flow calculated by the program. If IGFCJN > 0 then IGFCJN is the Tabular Function number which defines gas mass flow rate. If IGFCJN < 0 then the Control Function |IGFCJN| defines the mass flow of gas. Gas flow will occur only if the liquid level in the upstream Control Volume is below the Junction top elevation. The value is applied only for the atmosphere gas flow. Note that the total gas flow may be different than specified by the Tabular or Control Function defined by IGFCJN, if there is a non-zero liquid flow (controlled by ILFCJN - see Word 2 below). If bubbles are present in the pool in the upstream CV then they are carried with the pool flow and the bubble gas flux will be added to the atmosphere gas flux to give the total gas flow for this Junction.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero
if ILFCJN=0 then IGFCJN=0
if ILFCJN≠0 then IGFCJN≠0

Default value: 0

W-2 (I) : ILFCJN Flow control for pool liquid. If ILFCJN = 0 then this is a "normal" Junction with flow calculated by the program. If ILFCJN > 0 then ILFCJN is the Tabular Function number which defines liquid mass flow rate. If ILFCJN < 0 then the Control Function |ILFCJN| defines the mass flow of liquid. Liquid flow will occur only if the liquid level in the upstream Control Volume is above the Junction bottom elevation. The value is applied only for the pool liquid flow. Note that the total liquid flow may be different than specified by the Tabular or Control Function defined by ILFCJN, if there is a non-zero gas flow (controlled by IGFCJN - see Word 1 above). If droplets are present in the atmosphere in the upstream CV then they are carried with the atmosphere flow and the droplet liquid flux will be added to the pool liquid flux to give the total liquid flow for this Junction.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero
if ILFCJN=0 then IGFCJN=0
if ILFCJN≠0 then IGFCJN≠0

Default value: 0

2.2.8 Records: 231XXX, Pump/Compressor Model Data

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

There are two types of pumps in SPECTRA. The Pump Type 1 is treated as a special kind of Junction with Flow Control (see section 2.2.7), for which the volumetric flow, V_{pump} , is calculated from the user specified pump map and the pressure difference, ΔP_{pump} : $V_{pump} = f(\Delta P_{pump})$. The Pump Type 2 is a standard junction for which the pressure head is added on the right hand side of the momentum equation (see Volume 1). The pressure head, ΔP_{pump} , (or pressure ratio) is calculated based on pump map, and the current parameters, such as volumetric flow, V_{pump} , pump speed, ω , and eventually temperature: $\Delta P_{pump} = f(V_{pump}, \omega, T)$. A junction with Pump Type 2 is included in the flow solution matrix, while a junction with Pump Type 1 is calculated separately, outside the flow solution matrix, as all junctions with user prescribed flow (section 2.2.7) and junctions with critical flow. Pump Type 2 offers more modelling options; it allows including temperature in the map definition (useful for compressor modelling), it allows to calculate power entering the fluid (important for compressors, typically negligible for pumps), and it allows to calculate the pump speed using the rotor inertia equation based on user specified motor torque. Therefore Type 2 is generally recommended for modelling pumps or compressors.

The pump model is based on a pump map applicable for a single-phase flow. If a two-phase mixture flows through the pump, then the map is significantly altered (see for example [4], section 8). This fact can be taken into account in calculations by using Control Functions to introduce a two-phase multiplier on the pump speed data. An example of such analysis is shown in Volume 3.

W-1 (R) : DPNPJN Nominal pressure head, ΔP_N , (Pa) (if > 1000.0), or nominal pressure ratio Π_N , (-) (if ≤ 1000.0). If Π_N is specified, then the pressure head is equal to: $\Delta P_N(t) = (\Pi_N - 1) \cdot P_0(t)$, where $P_0(t)$ is the current pressure upstream the pump. For gas compressors this option is more appropriate than using constant pressure head ΔP_N .

If DPNPJN is equal to zero then the pump model is not present and the junction is either a normal junction (with flow calculated from momentum equation), or a junction with flow controlled by Tabular or Control Functions (as described in section 2.2.7). If DPNPJN is greater than zero then the pump model is used.

If Pump Type 1 is used, then parameters IGFCJN, ILFCJN must be specified in record 230XXX (section 2.2.7). These parameters are interpreted as pointers to Tabular or Control Functions, which define pump speed, ω , (1/s), as a function of time.

If Pump Model 2 is used, then parameters IGFCJN, ILFCJN must not be specified in record 230XXX (section 2.2.7). The pump speed, ω , (1/s), is defined by the pointers IOAPJN, IOPPJN (words 4 and 5 below), or by the inertia equation if the rotor moment of inertia is entered (Word 23 below).

Acceptable range:

DPNPJN ≥ 1.01 if Π_N is specified (DPNPJN $\leq 10^3$)

DPNPJN $\geq 1.01 \times 10^3$ if ΔP_N is specified (DPNPJN $> 10^3$)

Default value: 0.0

W-2 (R) : VFNPNJN Nominal pump volumetric flow, V_N , (m^3/s).

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: VFNPJN > 0.0 .

Default value: none .

- W-3 (R) : OMNPJN Nominal pump speed, ω_N , (1/s).
Acceptable range: OMNPJN > 0.0 .
Default value: none .

Words 4 and 5 are interpreted differently for the Pump Type 1 (nonzero values entered for IGFCJN and ILFCJN in record 230XXX - section 2.2.7), and for the Pump Model 2 (no values or zeroes entered in record 230XXX - section 2.2.7).

- Pump Type 1

For this pump model the pump speed, ω , (1/s), is defined by Tabular or Control Functions, indicated by the pointers IGFCJN, ILFCJN (record 230XXX). The meaning of Words 4 and 5 is as follows:

- W-4 (R) : RCAPJN Maximum rate of change of atmosphere flow through the pump, (1/s). The value is used as: $(1/V_N) \cdot dV_{atms}/dt \leq RCAPJN$. This parameter is applied to simulate in a simplified way the flow inertia, which is not taken into account in the Type 1 pump model.
Acceptable range: $0.01 \leq RCAPJN \leq 100.0$.
Default value: 10.0 .

- W-5 (R) : RCPPJN Maximum rate of change of pool flow through the pump, (1/s). The value is used in as: $(1/V_N) \cdot dV_{pool}/dt \leq RCPPJN$. This parameter is applied to simulate in a simplified way the flow inertia, which is not taken into account in the Type 1 pump model.
Acceptable range: $0.01 \leq RCPPJN \leq 100.0$.
Default value: 0.1 .

- Pump Type 2 (general pump model)

If the rotor moment of inertia is not used (see Word 23 below), then the next two words define the pump speed, ω , (1/s). If the rotor moment of inertia is used (see Word 23 below), then the next two words define the power of the pump motor, Q_m , (W).

- W-4 (I) : IOAPJN Pointer to a tabular or a control function, which defines pump speed, ω , (1/s), or power of the pump motor, Q_m , (W) for the atmosphere gas flow through the pump.
If IOAPJN = 0 then the pump speed is equal to zero, or the motor power is equal to zero.
If IOAPJN > 0 then the tabular function with reference number IOAPJN defines the pump speed, ω , (1/s), or the power of the motor, Q_m , (W).
If IOAPJN < 0 then the control function with reference number | IOAPJN | defines the pump speed, ω , (1/s), or the power of the motor, Q_m , (W).
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if nonzero.
Default value: 0 .

SPECTRA Code Manuals - Volume 2: User's Guide

W-5 (I) : IOPPJN Pointer to a tabular or a control function, which defines pump speed, ω , (1/s), or power of the pump motor, Q_m , (W) for the pool flow through the pump.
If IOPPJN = 0 then the pump speed is equal to zero, or the motor power is equal to zero.
If IOPPJN > 0 then the tabular function with reference number IOPPJN defines the pump speed, ω , (1/s), or the power of the motor, Q_m , (W).
If IOPPJN < 0 then the control function with reference number |IOPPJN| defines the pump speed, ω , (1/s), or the power of the motor, Q_m , (W).
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if nonzero.
Default value: 0 .

It is seen from the above description that the pump speed is defined separately for the gas flow and the liquid flow. For the gas flow the pump speed is defined by either Tabular/Control Function |IGFCJN| (Pump Type 1), or by the Tabular/Control Function |IOAPJN| (Pump Type 2). For the liquid flow the pump speed is defined by either Tabular/Control Function |ILFCJN| (Pump Type 1), or by the Tabular/Control Function |IOPPJN| (Pump Type 2). This is done to allow modelling of a two-phase degradation factor. An example case with the definition of such degradation factor is shown in Volume 3.

W-6 (R) : VF0PJN Volumetric flow at zero pump head, V_0 , (m^3/s). In the previous SPECTRA version this input entry was defining the pump constant, C_P , (-), (CPMPJN). This input entry was changed to make the pump/compressor input consistent with the turbine input (see section 2.2.10). The relation between the new and the old parameter is: $(V_0/V_N) = (C_P / (C_P - 1))^{(1/c)}$, where V_N is the nominal flow (Word 2 above), and c is the exponent CEXPJN (Word 20 below). The inverse relation is: $C_P = (V_0/V_N)^c / ((V_0/V_N)^c - 1)$. Note that in the previous SPECTRA version the exponent CEXPJN, was not defined by user, but it had a fixed value of 2.0.
Acceptable range: Type 1: $1.001 \leq (VF0PJN / VFNPJN) \leq 10$
 Type 2: $1.01 \leq (VF0PJN / VFNPJN) \leq 1000$.
Default value: $2.0 \times VFNPJN$ (value corresponding to $C_P=1.33$, for $c=2.0$).

W-7 (R) : CRSPJN Degradation factor for reverse pump speed, C_{RS} , (-). This is the ratio of the pressure head in normal pump speed to the head in reverse speed: $C_{RS} = \Delta P_{reverse} / \Delta P_{max}$, both at zero flow (see Figure 2-8). If the value is positive then at reverse pump speed the fluid is pumped in the same direction as in case of normal speed (centrifugal machines). If the value is negative then at reverse pump speed the fluid is pumped in the opposite direction (axial machines) - see appendix A.
Acceptable range: $-100.0 \leq CRSPJN \leq +100.0$ (a warning message is printed if the value is outside the following range: $-1.0 < CRSPJN < +1.0$).
Default value: 0.1. The default value is appropriate for centrifugal pumps (see discussion of the pump maps below).

Pump/Compressor Model - Test MAP

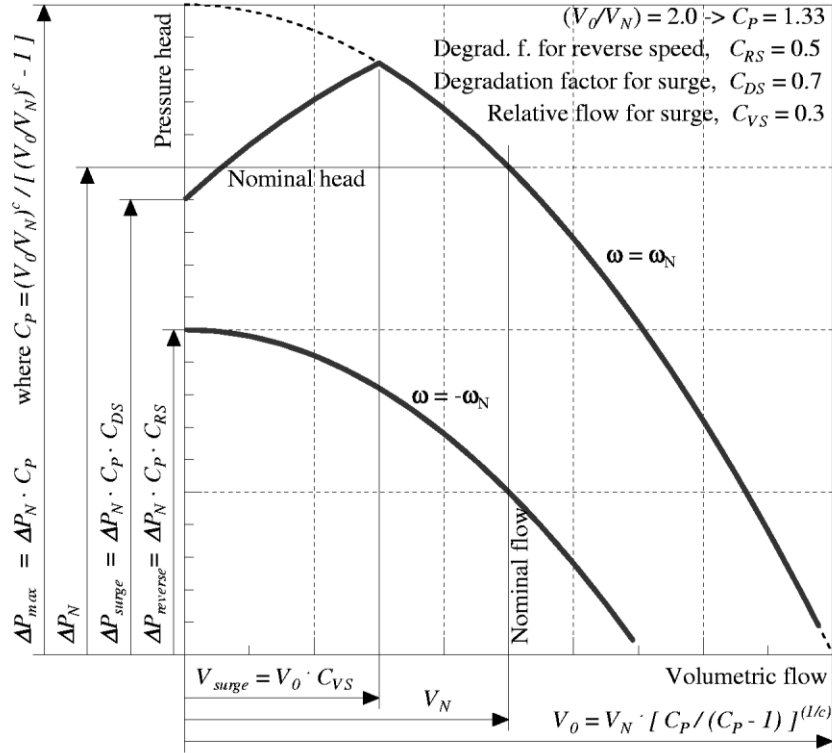


Figure 2-8 Influence of input parameters: V_0 , C_{RS} , C_{DS} , C_{VS} , on the pump map.

- W-8 (R) : CRFPJN Degradation factor for reverse flow, C_{RF} , (-). The flow-dependent term in the pressure head formula is multiplied by this factor, whenever the flow is negative (reverse) - see pump model description in Appendix A.2.2, Figure 4-8.
Acceptable range: $0.0 < CRFPJN \leq +100.0$ (a warning message is printed if the value is outside the range $-CRFPJN \leq +1.0$).
Default value: 1.0.
- W-9 (R) : CDSPJN Low flow degradation factor (surge factor), C_{DS} , (-). This is a ratio between the true pressure head (with surge) at zero flow, and the theoretical pressure head (no surge) at zero flow: $C_{DS} = \Delta P_{surge} / \Delta P_{max}$ (see Figure 2-8, appendix A). In order to obtain a stable map in the entire flow range the value of C_{DS} should be:

$$C_{DS} \geq 1 - C_{VS}^c$$

where C_{VS} is defined by the word 10 below, the exponent c is defined by the word 20 below, and the surge exponent, s , (word 26 below), should be: $s \leq 0.5$ - see appendix A.

Acceptable range: $0.0 \leq CDSPJN \leq 1.0$.

SPECTRA Code Manuals - Volume 2: User's Guide

- Default value:* 0.8. (0.8-1.0 for typical water pumps, ~0.0 for gas compressors - see discussion of the pump maps below).
- W-10 (I) : IVSPJN Pointer to a tabular function defining the limit for the low flow (surge) degradation as a function of the pump speed, $C_{VS}(\omega)$ (-). C_{VS} is defined as a ratio between the volumetric flow for which surge occurs to the volumetric flow at zero head: $C_{VS}(\omega) = V_{surge}(\omega)/V_0(\omega)$ (see Figure 2-8). If the current value of the tabular function is smaller than 0.0, it will be set to 0.0. If it is larger than 1.0 it will be set to 1.0. The argument for the Tabular Function is always the actual pump speed in rev/s. If no value is entered, or the entered value is equal to zero, then the surge model will not be used and the parabolic equation will be used for the whole flow range. If the model is used, then for the volumetric flows smaller than $V_{surge}(\omega) = C_{VS}(\omega) V_0(\omega)$ pressure head will be degraded by a factor that depends on the input parameter C_{DS} (CDSPJN, Word 9 above) - see Figure 2-8.
Acceptable range: must be a valid reference number of a Tabular Function, if nonzero.
Default value: none .
- W-11 (I) : INFPJN Indicator defining back flow through the pump.
INFPJN = 1: Back flow is allowed (no check valve).
INFPJN = 2: Back flow is not allowed (check valve present).
INFPJN = 3: As 2, additionally valve closes when pump is stopped.
Acceptable range: 1, 2, 3.
Default value: 1.
- W-12 (I) : IMPPJN Indicator defining flow solution scheme. IMPPJN=1: implicit. IMPPJN=2: explicit. (See Volume 3, pump model tests).
Acceptable range: 1, 2 . For Pump Type 2 only the implicit option is available (1). When the pressure ratio is small (typical fan), and Type 1 is used, then the explicit option is recommended. The program will automatically set the explicit option for pressure ratios smaller than 1.02.
Default value: 1 .
- W-13 (R) : OMEMJN Minimum relative pump speed to change flow control junction into a normal junction type, ω_{min}/ω_N (-). Used only for the Type 1 pumps. When pump is stopped, then in case of the Type 1 pump the flow will be equal to zero. OMEMJN converts a junction from a flow control junction into normal junction. Therefore it allows flow through the pump when the pump is stopped or pump velocity is small.
Acceptable range: $10^{-3} \leq OMEMJN \leq 0.5$.
Default value: 0.1 .
- W-14 (R) : DOMPJN Maximum relative rate of change of pump speed, $(1/\omega_N)(d\omega/dt)$, (1/s)
Acceptable range: $10^{-5} \leq DOMPJN \leq 10^3$.
Default value: 0.5

W-15 (R) : TPNPJN Nominal temperature for compressors, T_N , (K). This word is used only for the Type 2 pumps. If no value is entered, or the entered value is equal to zero (typical pump), then the reduced volumetric flow (value used on the horizontal axis of pump maps) and the reduced speed are defined as the ratios of the current value to the nominal value (see for example [28]):

$$V_R = \left(\frac{V}{V_N} \right) \quad \omega_R = \left(\frac{\omega}{\omega_N} \right)$$

If a positive value is entered (typical compressor), then the reduced flow (value used on the horizontal axis of pump maps) and the reduced speed are defined as the ratios of the current value to the nominal value, divided by the square root of the temperature ratio:

$$V_R = \frac{\left(\frac{V}{V_N} \right)}{\sqrt{\frac{T}{T_N}}} \quad \omega_R = \frac{\left(\frac{\omega}{\omega_N} \right)}{\sqrt{\frac{T}{T_N}}}$$

If the dynamic terms in p , T can be neglected ($p_{tot} = p$, $T_{tot} = T$), and the gas composition does not change during calculations, the above definition is consistent with the “corrected flow”, commonly used for the compressor maps. The corrected flow, W_{corr} , is defined as:

$$W_{corr} = W \frac{\sqrt{T_{tot}}}{p_{tot}}$$

where W is the mass flow rate, p_{tot} and T_{tot} are the total (static plus dynamic) pressure, and the temperature corresponding to the total (internal plus kinetic) energy - see for example reference [29] (Chapter 5) for the corrected flow definition. Derivation of the reduced flow, as used in SPECTRA, from the dimensional corrected flow is provided in Appendix A.2.

If the user wishes to take into account the dynamic terms, then he should specify the nominal velocity, v_N , (Word 16). If the user wishes to take into account possible gas composition changes, then he should specify the nominal gas constant, R_N , (Word 17).

Acceptable range: TPNPJN > 273.1, or 0.0. (For the Type 1 pumps: TPNPJN = 0.0).

Default value: 0.0 .

W-16 (R) : VPNPJN Nominal velocity, v_N , (m/s). This word is used only for the Type 2 pumps. If the value is not entered, or the entered value is zero, then the reduced flow (value used on the horizontal axis of pump maps) definition depends on the nominal temperature entry, TPNPJN (as described above). A positive value of VPNPJN may only be entered if

TPNPJN is positive. If VPNPJN is positive, then the reduced flow (value used on the horizontal axis of pump maps) is defined as:

$$V_R = \frac{\left(\frac{V}{V_N}\right) \sqrt{\frac{1+v^2/2c_p T}{1+v_N^2/2c_p T_N}}}{\sqrt{\frac{T}{T_N}} \left(\frac{1+v^2/2RT}{1+v_N^2/2RT_N}\right)}$$

If the gas composition does not change during calculations, the above definition is consistent with the corrected flow, W_{corr} , commonly used for the compressor maps. Derivation of the reduced flow, as used in SPECTRA, from the dimensional corrected flow is provided in Appendix A.2.

If the user wishes to take into account possible gas composition changes, then he should specify the nominal gas constant, R_N , (Word 17).

Acceptable range: VPNPJN = 0.0 or VPNPJN ≥ 1.0

Default value: 0.0

W-17 (R) : RPNPJN Nominal gas constant, R_N , (J/kg/K). This word is used only for the Type 2 pumps. (Note that when R_N is needed, it can be taken from the SPECTRA printout - the values of R are printed in the SPECTRA Control Volume output, in the block titled fluid property data). If the value is not entered, or the entered value is zero, then the reduced flow (value used on the horizontal axis of pump maps) definition depends on the nominal temperature, TPNPJN, and velocity, VPNPJN (described above). A positive value of RPNPJN may only be entered if TPNPJN is positive. If RPNPJN is positive, then the reduced flow (value used on the horizontal axis of pump maps) is defined as described below.

- If v_N (VPNPJN, Word 16) is zero:

$$V_R = \frac{\left(\frac{V}{V_N}\right)}{\left(\frac{R}{R_N}\right) \sqrt{\frac{T}{T_N}}}$$

- If positive v_N (VPNPJN, Word 16) is specified:

$$V_R = \frac{\left(\frac{V}{V_N}\right) \sqrt{\frac{1+v^2/2c_p T}{1+v_N^2/2c_p T_N}}}{\left(\frac{R}{R_N}\right) \sqrt{\frac{T}{T_N}} \left(\frac{1+v^2/2RT}{1+v_N^2/2RT_N}\right)}$$

The last definition is always (even when the gas composition changes) consistent with the corrected flow, W_{corr} , commonly used for the

SPECTRA Code Manuals - Volume 2: User's Guide

compressor maps. Derivation of the reduced flow, as used in SPECTRA, from the dimensional corrected flow is provided in Appendix A.2.

Acceptable range: $100.0 \leq \text{RPNPJN} \leq 10000.0$, or $\text{RPNPJN} = 0.0$.

Default value: 0.0.

- W-18 (R) : AEXPJN Exponent a in the pump map (see description of the pump maps, appendix A). This word is used only for the Type 2 pumps.
Acceptable range: $\text{AEXPJN} > 0.0$, and $\text{BEXPJN} \leq \text{AEXPJN} \leq 10.0$.
Default value: 2.0.
- W-19 (R) : BEXPJN Exponent b in the pump map (see description of the pump maps, appendix A). This word is used only for the Type 2 pumps.
Acceptable range: $-10.0 \leq \text{BEXPJN} \leq 10.0$. Negative b , although generally not recommended, was found useful for matching some compressor map data. If $b < 0.0$, then the term with ω_R^b is becoming large when the speed is small, giving unrealistically large pump head or compressor pressure ratio for a slowly turning machine. To prevent this a limit is imposed on ω_R^b : $\omega_R^b < \omega_{lim}^b = \text{BLMPJN}$ (Word 27). For lower speeds the term is linearly interpolated to give zero for zero speed (see appendix A, Figure 4-21).
Default value: 1.0 (a small number, $< 10^{-50}$, sets the value to 0.0).
- W-20 (R) : CEXPJN Exponent c in the pump map (see description of the pump maps, appendix A). This word is used only for the Type 2 pumps.
Acceptable range: $0.0 < \text{CEXPJN} \leq 10.0$.
Default value: 2.0.
- W-21 (I) : IEPPJN Pointer to a Tabular or Control Function defining pump efficiency for positive flow. This word is used only for the Type 2 pumps. If the value is positive then the efficiency will be defined by a tabular function with the number IEPPJN. If the value is negative the efficiency will be defined by a control function with the number $|\text{IEPPJN}|$. If the current value of the Tabular or Control Function is smaller than the minimum acceptable value (see the *Acceptable range*, below), it will be set to the minimum acceptable value. If it is larger than 1.0 it will be set to 1.0. If no value is entered then the efficiency will always be equal to 1.0. The efficiency is defined as follows:
 For gas compressors this is an isentropic efficiency, defined as:

$$\eta = \frac{V \rho c_p T (\Pi^{(\kappa-1)/\kappa} - 1)}{Q_{hydr}}$$

where V is the volumetric flow (m^3/s), ρ is the density (kg/m^3), c_p is the specific heat ($\text{J}/\text{kg}/\text{K}$), T is the inlet temperature (K), Π is the pressure ratio, and Q_{hydr} is the total power source for the fluid (W) (the value is positive during normal pump/compressor operation). If the power, Q_{hydr} , becomes negative, then the efficiency is given by inverse of the above formula.

For water pumps the efficiency is defined as:

$$\eta = \frac{V \Delta P}{Q_{hydr}}$$

where V is the volumetric flow (m^3/s), ΔP is the pressure head (Pa), and Q_{hydr} is the total power source for the fluid (W) (the value is positive during normal pump/compressor operation). If the power, Q_{hydr} , becomes negative, then the efficiency is given by inverse of the above formula.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if nonzero. (For the Type 1 pumps the value must be zero.) The efficiency is restricted by the maximum value of 1.0, and the minimum value, which depends on the power sign. In case of positive power (typical pump/compressor) the efficiency can only be positive, and the minimum limit is set at 0.1. In case of negative power (typical turbine) negative efficiency is possible (see Figure 2-10). The negative efficiency that the fluid is being decompressed and in spite of this the machine is consuming power – point 2c in Figure 2-10. Physically it means a large amount of energy is dissipated as heat due to large friction. This may happen for example in case of a turbine running with reverse speed - see appendix B. In case of negative power the minimum limit of efficiency is set to – 10.0

Default value: 0 .

W-22 (I) : IENPJN Pointer to a Tabular or Control Function defining the pump efficiency for negative flow. This word is used only for the Type 2 pumps. The efficiency definitions are similar as above, with V replaced by $|V|$. If the value is positive then the efficiency will be defined by a tabular function with the number IENPJN. If the value is negative the efficiency will be defined by a control function with the number $|IENPJN|$. If the current value of the Tabular or Control Function is smaller than the minimum acceptable value (see the *Acceptable range*, of IEPPJN, above), it will be set to the minimum acceptable value. If it is larger than 1.0 it will be set to 1.0. If no value is entered then the efficiency will always be equal to 1.0.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if nonzero. (For the Type 1 pumps the value must be zero.)

Default value: 0 .

W-23 (R) : PMIPJN Pump rotor moment of inertia, I , ($kg \cdot m^2$). This word is used only for the Type 2 pumps. If no value is entered, or the entered value is equal to zero, then the inertia equation is not used, and the pump speed is determined by the Tabular or Control Functions indicated by IOAPJN

SPECTRA Code Manuals - Volume 2: User's Guide

and IOPPJN (words 4 and 5 above). If a positive value is entered, then the pump speed is determined by the inertia equation:

$$I \frac{d(2\pi\omega)}{dt} = T_m - T_{hydr} - T_{fric}$$

where ω is the pump speed (rev/s), T is torque, and the subscripts m , $hydr$, $fric$, signify motor, hydraulic and friction respectively. The factor 2π is a consequence of ω being expressed in revolutions per second rather than radians per second. The friction torque is assumed to be proportional to the speed, with the proportionality constant C_f , ($T_{fric} = C_f \cdot 2\pi\omega$) The above equation is re-written using power instead of torque ($Q = 2\pi\omega T$):

$$I \frac{d(2\pi\omega)}{dt} = \frac{Q_m}{2\pi\omega} - \frac{Q_{hydr}}{2\pi\omega} - C_f 2\pi\omega$$

or:

$$\frac{d\omega}{dt} = \frac{1}{I} \left(\frac{Q_m - Q_{hydr}}{4\pi^2\omega} - C_f \omega \right)$$

This equation is used to determine the pump/compressor speed. The motor torque, Q_m , is defined by a tabular or a control function indicated by IOAPJN and IOPPJN. (Thus, if $I > 0.0$ then the interpretation of IOAPJN, IOPPJN is different than when $I = 0.0$). The friction coefficient, C_f , is defined below.

Acceptable range: PMIPJN \geq 0.0, (for the Type 1 pumps: PMIPJN=0.0).

Default value: 0.0 .

W-24 (R) : CF1PJN Friction coefficient, C_f , ($W \cdot s^2$)=($kg \cdot m^2/s$). This word is used for the Type 2 pumps, when the rotor moment of inertia is used to determine the pump speed (PMIPJN $>$ 0). The value is used to calculate the friction power in the pump inertia equation. The friction power is equal to $Q_f = 4\pi^2 C_f \omega |\omega|$ (see the equation shown at PMIPJN description, above).
Acceptable range: CF1PJN \geq 0.0, (for the Type 1 pumps: CF1PJN=0.0).
Default value: 0.0 .

W-25 (R) : ISNPJN Pointer to a Tabular or Control Function, which controls the eventual synchronization of the pump. ISNPJN is used only if a positive moment of inertia, PMIPJN (Word 23) is specified.
If the value of the Tabular or Control Function is smaller than, or equal to zero, then the pump's motor is not synchronized, and the pump speed is calculated using the pump moment of inertia, PMIPJN (Word 23), and the motor power, Q_m , defined by a tabular or a control function indicated by IOAPJN and IOPPJN (Words 4 and 5).
If the value of the tabular or a control function is greater than zero, then the pump's motor is synchronized, and the pump speed is constant and equal to the nominal speed, OMNPJN (Word 3), multiplied by the value obtained from the Tabular or Control Function indicated by ISNPJN. At the moment the pump is synchronized (the value of Tabular or Control

Function |ISNPJN| turns positive), its speed begins to change and it changes until the target speed is reached. The relative rate of this change is equal to DOMPJN (Word 14).

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if nonzero.

Default value: 0.

W-26 (R) : SEXPJN Exponent s , applied in the surge region (see description of the pump maps, appendix A). The value is used to define the pressure head through the "effective speed", ω' , defined as:

$$\omega' = \omega \cdot [C_{DS}^{1/a} + (1 - C_{DS}^{1/a}) \cdot (V / V_{surge})^{1/s}]$$

where ω is the true speed, C_{DS} is the surge degradation factor (CDSPJN), V is the volumetric flow, V_{surge} is the volumetric flow at surge (defined by IVSPJN), and a is the exponent (AEXPJN). In order to obtain stable performance of the pump, SEXPJN should be set to 0.5 (or smaller) - see description of the word CDSPJN above and appendix A.

Acceptable range: $0.1 < \text{SEXPJN} \leq 10.0$.

Default value: 1.0.

W-27 (R) : BLMPJN Limit on ω_R^b in case of negative b (see description of the pump maps, appendix A, Figure 4-21).

Acceptable range: $1.0 < \text{BLMPJN} \leq 10.0$

Default value: 2.0

2.2.9 Records: 232XXX, Simplified Turbine Data

XXX is the Junction reference number, $001 \leq \text{XXX} \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

This record describes a simple turbine model, not recommended for general modelling. This was the first turbine model applied in an early version of SPECTRA, and it is preserved in the code to keep compatibility with earlier input decks. A more sophisticated turbine model, recommended for general application, is based on maps similar to those defining pump/compressors, and is described in the next section.

The simplified "turbine" is treated as a special kind of Junction with flow loss coefficient that may vary in time. An effective "turbine loss coefficient" is calculated based on the turbine data specified below (such as nominal turbine pressure difference, nominal flow, etc.), and is added to the normal loss coefficients, FLCFJN, FLCRJN, which are defined in record 210XXX (section 2.2.5), to determine the overall loss coefficient during the transient. If the nominal turbine data indicate that the overall loss coefficient should be smaller than FLCFJN, then an error message is printed and execution is stopped. In such case user should increase the flow area of turbine Junction, or decrease FLCFJN.

The nominal turbine parameters define the nominal turbine loss factor, C_N , as:

SPECTRA Code Manuals - Volume 2: User's Guide

$$C_N = \Delta P_N \cdot \frac{2 \cdot A_{JN}^2}{\rho_N \cdot V_N^2}$$

- where: ΔP_N - nominal turbine pressure drop, (Pa), (DPNTJN),
 A_{JN} - Junction flow area, (m²), (AMAXJN, section 2.2.1),
 ρ_N - nominal turbine density, (kg/m³), (RHNTJN), this is the density in the volume upstream the turbine Junction,
 V_N - nominal turbine flow, (kg/s), (VFNTJN).

The actual turbine loss coefficient, C_t , is obtained during the transient from:

$$C_t = C_N f_t \left(\frac{\omega}{\omega_N} \right)$$

- where: ω_N - nominal turbine speed, (1/s), (OMNTJN),
 ω - actual turbine speed, (1/s), defined by a Tabular or a Control Function, indicated by the pointer IOMTJN,
 f_t - Tabular Function defining "turbine map", that means relative turbine loss factor C_t/C_N as a function of relative turbine speed ω/ω_N .

W-1 (R) : DPNTJN Nominal pressure ratio Π_N , (-) (if ≤ 1000.0), or nominal pressure head, ΔP_N , (Pa) (if > 1000.0). If Π_N is specified, then turbine pressure head is equal to: $\Delta P_N(t) = \Pi_N \cdot P_0(t)$, where $P_0(t)$ is the current pressure upstream the turbine. For gas turbines this option is more appropriate than using constant pressure head ΔP_N .

If DPNTJN is equal to zero then the turbine model is not used and the flow loss coefficients in this Junction are constant, and equal to the values of FLCFJN, FLCRJN, defined in record 210XXX (section 2.2.5). If DPNTJN is positive, then the turbine model is used, and the turbine loss coefficient, C_t , calculated as shown above, is added to FLCFJN, FLCRJN, to obtain the overall loss coefficient for this JN.

Acceptable range:

DPNPJN ≥ 1.01 if Π_N is specified (DPNPJN $\leq 10^3$)
 DPNPJN $\geq 1.01 \times 10^3$ if ΔP_N is specified (DPNPJN $> 10^3$)

Default value: 0.0

W-2 (R) : VFNTJN Nominal turbine volumetric flow, V_N , (m³/s).

Acceptable range: VFNTJN > 0.0

Default value: none

W-3 (R) : OMNTJN Nominal turbine speed, ω_N , (1/s).

Acceptable range: OMNTJN > 0.0

Default value: none

W-4 (I) : IOMTJN Pointer to a Tabular Function or a Control Function which defines the turbine speed, $\omega(t)$. If the number is positive then the turbine speed will be defined by the Tabular Function IOMTJN. If the number is negative then the turbine speed will be defined by the value of Control Function -IOMTJN.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 0

- W-5 (R) : DOMTJN Maximum relative rate of change of turbine speed, $(1/\omega_N)(d\omega/dt)$, (1/s)
Acceptable range: $10^{-5} \leq \text{DOMTJN} \leq 10^3$
Default value: 0.5
- W-6 (R) : PRNTJN Nominal turbine pressure (in upstream CV), p_N , (kg/m³).
Acceptable range: PRNTJN > 0.0
Default value: initial pressure in the upstream CV
- W-7 (R) : RHNTJN Nominal turbine density (in upstream CV), ρ_N , (kg/m³).
Acceptable range: RHNTJN > 0.0
Default value: initial gas density in the upstream CV
- W-8 (I) : ITCTJN Number of the Tabular Function defining turbine map. If positive, then the TF number ITCTJN defines relative turbine loss factors: C_t/C_N , as a function of relative turbine speed ω/ω_N . If zero then the relative loss factor is always equal to one, which means: $C_t = C_N$. If the value obtained from the TF is smaller than zero then it will be set to zero.
Acceptable range: must be a valid reference number of a Tabular Function, if non-zero
Default value: 0
- W-9 (I) : IEPPJN Pointer to a Tabular or Control Function defining turbine efficiency for positive flow. If the value is positive then the efficiency will be defined by a tabular function with the number IEPPJN. If the value is negative the efficiency will be defined by a control function with the number $|\text{IEPPJN}|$. If the current value of the tabular function is smaller than the minimum acceptable value (see the *Acceptable range*, below), it will be set to the minimum acceptable value. If it is larger than 1.0 it will be set to 1.0. If no value is entered then the efficiency will always be equal to 1.0. The efficiency is defined as follows:
For gas turbine this is an isentropic efficiency, defined as:

$$\eta = \frac{Q_{hydr}}{V \rho c_p T [(1/\Pi)^{(\kappa-1)/\kappa} - 1]}$$

where V is the volumetric flow (m³/s), ρ is the density (kg/m³), c_p is the specific heat (J/kg/K), T is the inlet temperature (K), Π is the turbine pressure ratio, and Q_{hydr} is the total power source for the fluid (W) (the value is negative during normal turbine operation; note that the denominator is also negative during normal operation). If the power, Q_{hydr} , becomes positive, then the efficiency is given by inverse of the above formula.

For water turbines the efficiency is defined as:

$$\eta = \frac{Q_{hydr}}{V \Delta P}$$

where V is the volumetric flow (m^3/s), ΔP is the pressure head (Pa), and Q_{hydr} is the total power source for the fluid (W) (the value is negative during normal turbine operation). If the power, Q_{hydr} , becomes positive, then the efficiency is given by inverse of the above formula.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if nonzero. The efficiency is further restricted as described in section 2.2.10, Word 21.

Default value: 0

- W-10 (I) : IENPJN Pointer to a Tabular or Control Function defining the turbine efficiency for negative flow. The efficiency definitions are similar as above, with V replaced by $|V|$.
- Acceptable range:* must be a valid reference number of a Tabular or a Control Function, if nonzero.
- Default value:* 0 .

2.2.10 Records: 233XXX, Turbine Model Data

XXX is the Junction reference number, $001 \leq \text{XXX} \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

The turbine model is based on the same approach as the pump/compressor Type 2 model (see section 2.2.8). In fact the turbine model uses exactly the same subroutine as the Type 2 pump/compressor. Only the input procedures are slightly different. Most of the input parameters are the same as in case of the Type 2 pump/compressor. The turbine nominal parameters, such as nominal flow and pressure ratio or head, are internally converted by the code into nominal parameters of an “equivalent pump”, as shown in Figure 2-9. The equivalent pump is defined as a pump/compressor that has exactly the same map as the turbine, if the map is plotted in terms of the pump pressure ratio (outlet divided by inlet pressure) rather than the turbine pressure ratio (inlet divided by outlet pressure).

The “equivalent pump” approach allows to perform calculations using the same subroutines that calculate pumps/compressors. The discussion of turbine maps is provided in appendix B.

- W-1 (R) : DPNPJN Nominal pressure ratio Π_N , (-) (if ≤ 1000.0), or nominal pressure head, ΔP_N , (Pa) (if > 1000.0). If Π_N is specified, then turbine pressure head is equal to: $\Delta P_N(t) = \Pi_N \cdot P_o(t)$, where $P_o(t)$ is the current pressure upstream the turbine. For gas turbines this option is more appropriate than using constant pressure head ΔP_N .
- If DPNPJN is equal to zero then the turbine model is not present and the junction is a normal junction (with flow calculated from momentum equation), a junction with flow controlled by Tabular or Control Functions (as described in section 2.2.7), or a simplified turbine (described in section 2.2.9). If DPNPJN is greater than zero then the turbine model is used. The turbine model cannot be used if pump model is used for the same junction (record 231XXX).
- Acceptable range:*
- DPNPJN ≥ 1.01 if Π_N is specified (DPNPJN $\leq 10^3$).
- DPNPJN $\geq 1.01 \times 10^3$ if ΔP_N is specified (DPNPJN $> 10^3$).
- Default value:* 0.0 .

Turbine Model - Test MAP

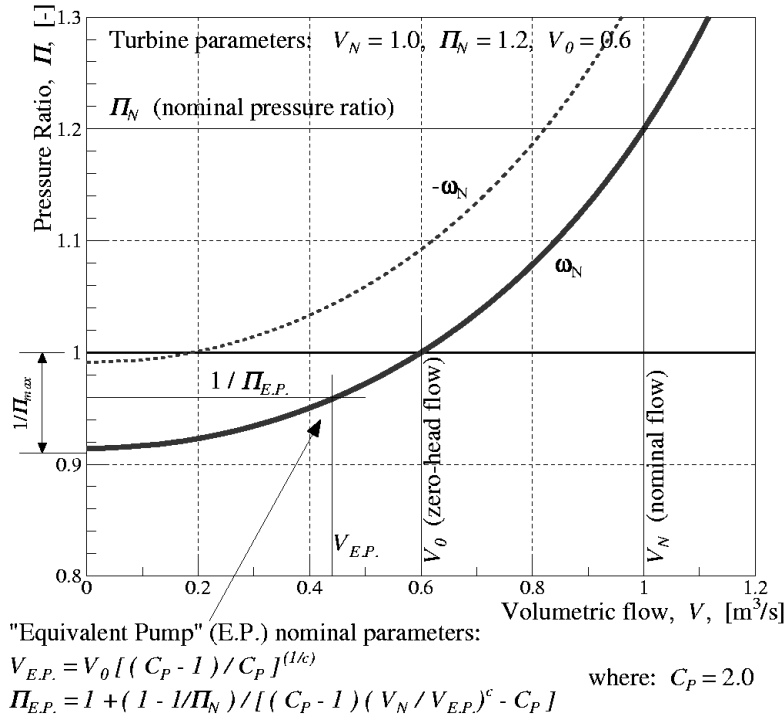


Figure 2-9 Turbine map - conversion of the turbine parameters into the "Equivalent Pump" parameters, performed internally by the code.

- W-2 (R) : VFNPJN Nominal turbine volumetric flow, V_N , (m^3/s).
 Acceptable range: VFNPJN > 0.0 .
 Default value: none .
- W-3 (R) : OMNPJN Nominal turbine speed, ω_N , (1/s).
 Acceptable range: OMNPJN > 0.0 .
 Default value: none .
- W-4 (I) : IOAPJN Pointer to a tabular or a control function, which defines turbine speed, ω , (1/s) (if the rotor moment of inertia is not used), or power of the machine receiving power (generator), Q_m , (W) (if the rotor moment of inertia is specified - Word 20 below) for the atmosphere gas flow through the turbine. Note that if receiving power, Q_m , is specified, then the value is normally negative (power is taken from the turbine).
 If IOAPJN = 0 then the turbine speed is zero, or the motor power is equal to zero.
 If IOAPJN > 0 then the tabular function with reference number IOAPJN defines the turbine speed, ω , (1/s), or the power of the machine receiving power (generator), Q_m , (W).
 If IOAPJN < 0 then the control function with reference number |IOAPJN| defines the turbine speed, ω , (1/s), or the power of the machine receiving power (generator), Q_m , (W).

SPECTRA Code Manuals - Volume 2: User's Guide

- Acceptable range:* must be a valid reference number of a Tabular, or a Control Function, if nonzero.
Default value: 0.
- W-5 (I) : IOPPJN Pointer to a tabular or a control function, which defines turbine speed, ω , (1/s) (if the rotor moment of inertia is not used), or power of the machine receiving power (generator), Q_m , (W) (if the rotor moment of inertia is specified - Word 20 below) for the pool flow through the turbine. Note that if receiving power, Q_m , is specified, then the value is normally negative (power is taken from the turbine).
If IOPPJN = 0 then the turbine speed is zero, or the motor power is equal to zero.
If IOPPJN > 0 then the tabular function with reference number IOPPJN defines the turbine speed, ω , (1/s), or the power of the machine receiving power (generator), Q_m , (W).
If IOPPJN < 0 then the control function with reference number |IOPPJN| defines the turbine speed, ω , (1/s), or the power of the machine receiving power (generator), Q_m , (W).
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if nonzero.
Default value: 0.
- W-6 (R) : VF0PJN Volumetric flow for zero-head $\Delta P = 0.0$ (or $\Pi=1.0$), V_0 , (m³/s).
Acceptable range: $0.01 \leq (VF0PJN / VFNPJN) \leq 0.95$.
Default value: $0.6 \times VFNPJN$.
- W-7 (R) : CRSPJN Degradation factor for reverse speed, C_{RS} (-). Defined as in case of the pump/compressor model, as the ratio of the pressure head (pressure ratio) in normal turbine speed to the head in reverse speed, both at zero flow: $C_{RS} = (1/\Pi_{reverse}) / (1/\Pi_{max})$ (see Figure 2-9). If the value is positive then at reverse turbine speed the pressure head is in the same direction (i.e. the line crosses the $\Pi = 1.0$ line - see Figure 2-9). If the value is negative then at reverse turbine speed the pressure head has opposite direction (i.e. the dashed line shown in Figure 2-9 would be above the $\Pi = 1.0$ line). Note that the pressure head (thus the hydraulic torque) is larger when the turbine turns on reverse than during normal operation.
Acceptable range: $-100.0 \leq CRSPJN \leq +100.0$.
Default value: -1.5. The default value was selected based on turbine data from reference [27] - see appendix B.
- W-8 (R) : CRFPJN Degradation factor for reverse flow, C_{RF} , (-). The flow-dependent term in the pressure head formula is multiplied by this factor, whenever the flow is negative (reverse) - see pump model description in Appendix A.2.2.
Acceptable range: $0.0 < CRFPJN \leq +100.0$ (a warning message is printed if the value is outside the range $-0.0 < CRFPJN < +1.0$).
Default value: 0.05. The default value was selected based on turbine data from reference [27] - see appendix B.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-9 (R) : CDSPJN Low flow degradation factor, C_{DS} , (-). Defined as in case of pump/compressor model, as a ratio between the true pressure head at zero flow, to theoretical pressure head at zero flow. This parameter is typically not used for turbine modelling. Should a value less than 1.0 be entered, the line ω_N in Figure 2-9 would bend at low flow range (say for $V < 0.2 \text{ m}^3/\text{s}$) towards the point ($II = 1.0, V < 0.0$).
Acceptable range: $0.0 \leq \text{CDSPJN} \leq 1.0$.
Default value: 1.0 .
- W-10 (I) : IVSPJN Pointer to a tabular function defining the limit for the low flow (surge) degradation as a function of the turbine speed, $C_{VS}(\omega)$ (-). As the word above, this is a pump/compressor model parameter and typically is not be used for turbines. It is defined as a ratio between the volumetric flow for which surge occurs to the volumetric flow at zero head: $C_{VS}(\omega) = V_{surge}(\omega)/V_0(\omega)$ (compare Figure 2-8). If the current value of the tabular function is smaller than 0.0, it will be set to 0.0. If it is larger than 1.0 it will be set to 1.0. The argument for the Tabular Function will always be the current turbine speed in rev/s. If no value is entered, or the entered value is equal to zero, then surge model will not be used and the parabolic equation will be used for the whole flow range.
Acceptable range: must be a valid reference number of a Tabular Function, if nonzero.
Default value: none .
- W-11 (I) : INFPJN Indicator defining back flow through the turbine.
 INFPJN = 1: Back flow is allowed (no check valve).
 INFPJN = 2: Back flow is not allowed (check valve present).
 INFPJN = 3: As 2, additionally valve closes when pump is stopped.
Acceptable range: 1 and 2 .
Default value: 1 .
- W-12 (I) : IMPPJN Indicator defining flow solution scheme. IMPPJN=1: implicit. IMPPJN=2: explicit.
Acceptable range: 1. For turbines only the implicit method is allowed.
Default value: 1.
- W-13 (R) : OMEMJN Not used for turbine. (pump Type 1 parameter - see section 2.2.8)
- W-14 (R) : DOMPJN Maximum relative rate of change of turbine speed, $(1/\omega_N)(d\omega/dt)$, (1/s)
Acceptable range: $10^{-5} \leq \text{DOMPJN} \leq 10^3$.
Default value: 0.5
- W-15 (R) : TPNPJN Nominal temperature, T_N , (K). If no value is entered, or the entered value is equal to zero, then the reduced flow (value used on the horizontal axis of turbine maps) and the reduced speed are defined as the ratios of the current value to the nominal value:

$$V_R = \frac{V}{V_N} \qquad \omega_R = \frac{\omega}{\omega_N}$$

If positive value is entered, then the reduced flow (value used on the horizontal axis of turbine maps) and the reduced speed are defined as the ratios of the current value to the nominal value, divided by the square root of the inlet temperature ratio:

$$V_R = \frac{\left(\frac{V}{V_N}\right)}{\sqrt{\frac{T}{T_N}}} \quad \omega_R = \frac{\left(\frac{\omega}{\omega_N}\right)}{\sqrt{\frac{T}{T_N}}}$$

If the dynamic terms in p , T can be neglected ($p_{tot} = p$, $T_{tot} = T$), and the gas composition does not change during calculations, the above definition is consistent with the “corrected flow”, commonly used for the gas turbine maps. The corrected flow is defined as:

$$W_{corr} = W \frac{\sqrt{T_{tot}}}{P_{tot}}$$

where p_{tot} and T_{tot} are the total (static plus dynamic) pressure, and the temperature corresponding to the total (internal plus kinetic) energy - see for example reference [29] (Chapter 5) for the corrected flow definition. Derivation of the reduced flow, as used in SPECTRA, from the dimensional corrected flow is provided in Appendix A.2.

If the user wishes to take into account the dynamic terms, then he should specify the nominal velocity, v_N , (Word 15). If the user wishes to take into account possible gas composition changes, then he should specify the nominal gas constant, R_N , (Word 16).

Acceptable range: TPNPJN>273.1, or 0.0.

Default value: 0.0 .

W-16 (R) : VPNPJN Nominal velocity, v_N , (m/s). If the value is not entered, or the entered value is zero, then the reduced flow (value used on the horizontal axis of turbine maps) definition depends on the nominal temperature entry, TPNPJN (as described above). A positive value of VPNPJN may only be entered if TPNPJN is positive. If VPNPJN is positive, then the reduced flow (value used on the horizontal axis of pump maps) is defined as:

$$V_R = \frac{\left(\frac{V}{V_N}\right)}{\sqrt{\frac{T}{T_N}}} \frac{\sqrt{\frac{1 + v^2 / 2c_p T}{1 + v_N^2 / 2c_p T_N}}}{\left(\frac{1 + v^2 / 2RT}{1 + v_N^2 / 2RT_N}\right)}$$

If the gas composition does not change during calculations, the above definition is consistent with the corrected flow, W_{corr} , commonly used for the gas turbine maps. Derivation of the reduced flow, as used in SPECTRA, from the dimensional corrected flow is provided in Appendix A.2.

SPECTRA Code Manuals - Volume 2: User's Guide

If the user wishes to take into account possible gas composition changes, then he should specify the nominal gas constant, R_N , (Word 16).

Acceptable range: VPNPJN = 0.0 or VPNPJN \geq 1.0

Default value: 0.0

W-17 (R) : RPNPJN Nominal gas constant, R_N , (J/kg/K). (Note that when R_N is needed, it can be taken from the SPECTRA printout - the values of R are printed in the SPECTRA Control Volume output, in the block titled fluid property data). If the value is not entered, or the entered value is zero, then the reduced flow (value used on the horizontal axis of turbine maps) definition depends on the nominal temperature, TPNPJN, and velocity, VPNPJN (described above). A positive value of RPNPJN may only be entered if TPNPJN is positive. If RPNPJN is positive, then the reduced flow (value used on the horizontal axis of pump maps) is defined as described below.

- If v_N (VPNPJN, Word 15) is zero:

$$V_R = \frac{\left(\frac{V}{V_N}\right)}{\left(\frac{R}{R_N}\right) \sqrt{\frac{T}{T_N}}}$$

- If positive v_N (VPNPJN, Word 15) is specified:

$$V_R = \frac{\left(\frac{V}{V_N}\right)}{\left(\frac{R}{R_N}\right) \sqrt{\frac{T}{T_N}}} \frac{\sqrt{\frac{1 + v^2 / 2c_p T}{1 + v_N^2 / 2c_p T_N}}}{\left(\frac{1 + v^2 / 2RT}{1 + v_N^2 / 2RT_N}\right)}$$

The last definition is always (even when the gas composition changes) consistent with the corrected flow, W_{corr} , commonly used for the gas turbine maps. Derivation of the reduced flow, as used in SPECTRA, from the dimensional corrected flow is provided in Appendix A.2.

Acceptable range: 100.0 \leq RPNPJN \leq 10000.0, or RPNPJN = 0.0 .

Default value: 0.0 .

W-18 (R) : AEXPJN Exponent a in the turbine map (see description of the turbine maps, appendix B).

Acceptable range: AEXPJN $>$ 0.0, and BEXPJN \leq AEXPJN \leq 10.0

Default value: 2.0 .

W-19 (R) : BEXPJN Exponent b in the turbine map (see description of the turbine maps, appendix B).

Acceptable range: -10.0 \leq BEXPJN \leq 10.0 .

Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0).

SPECTRA Code Manuals - Volume 2: User's Guide

W-20 (R) : CEXPJN Exponent c in the turbine map (see description of the turbine maps, appendix B).
Acceptable range: $0.0 < \text{CEXPJN} \leq 10.0$.
Default value: 2.0 .

W-21 (I) : IEPPJN Pointer to a Tabular or Control Function defining turbine efficiency for positive flow. If the value is positive then the efficiency will be defined by a tabular function with the number IEPPJN. If the value is negative the efficiency will be defined by a control function with the number $|\text{IEPPJN}|$. If the current value of the tabular function is smaller than the minimum acceptable value (see the *Acceptable range*, below), it will be set to the minimum acceptable value. If it is larger than 1.0 it will be set to 1.0. If no value is entered then the efficiency will always be equal to 1.0. The efficiency is defined as follows:

For gas turbine this is an isentropic efficiency, defined as:

$$\eta = \frac{Q_{hydr}}{V \rho c_p T [(1/\Pi)^{(\kappa-1)/\kappa} - 1]}$$

where V is the volumetric flow (m^3/s), ρ is the density (kg/m^3), c_p is the specific heat ($\text{J}/\text{kg}/\text{K}$), T is the inlet temperature (K), Π is the turbine pressure ratio, and Q_{hydr} is the total power source for the fluid (W) (the value is negative during normal turbine operation; note that the denominator is also negative during normal operation). If the power, Q_{hydr} , becomes positive, then the efficiency is given by inverse of the above formula.

For water turbines the efficiency is defined as:

$$\eta = \frac{Q_{hydr}}{V \Delta P}$$

where V is the volumetric flow (m^3/s), ΔP is the pressure head (Pa), and Q_{hydr} is the total power source for the fluid (W) (the value is negative during normal turbine operation). If the power, Q_{hydr} , becomes positive, then the efficiency is given by inverse of the above formula.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if nonzero. The efficiency is further restricted by the maximum value of 1.0, and the minimum value, which depends on the power sign. In case of positive power (typical pump/compressor) the efficiency can only be positive, and the minimum limit is set at 0.1. In case of negative power (typical turbine) negative efficiency is possible (see Figure 2-10). The negative efficiency means that the fluid is being decompressed and in spite of this the machine is consuming power – point 2c in Figure 2-10. Physically it means a large amount of energy is dissipated as heat due to large friction. This may happen for example in case of a turbine running with

reverse speed - see appendix B. In case of negative power the minimum limit of efficiency is set to -10.0.

Default value: 0.

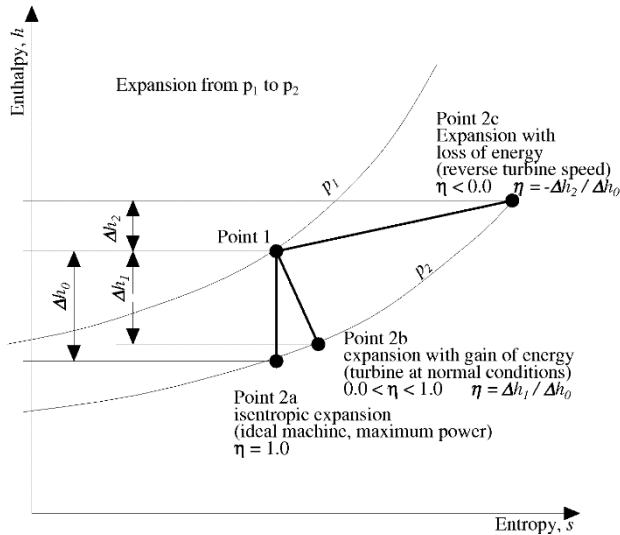


Figure 2-10 Turbine decompression in a h - s diagram.

W-22 (I) : IENPJJ Pointer to a Tabular or Control Function defining the turbine efficiency for negative flow. The efficiency definitions are similar as above, with V replaced by $|V|$.
 If the value is positive then the efficiency will be defined by a tabular function with the number IENPJJ. If the value is negative the efficiency will be defined by a control function with the number $|IENPJJ|$. If the current value of the Tabular or Control Function is smaller than the minimum acceptable value (see the *Acceptable range*, of IEPPJJ, above), it will be set to the minimum acceptable value. If it is larger than 1.0 it will be set to 1.0. If no value is entered then the efficiency will always be equal to 1.0.
Acceptable range: must be a valid reference number of a Tabular or a Control Function, if nonzero.
Default value: 0.

W-23 (R) : PMIPJJ Turbine rotor moment of inertia, I , ($\text{kg} \cdot \text{m}^2$). If no value is entered, or the entered value is equal to zero, then the inertia equation is not used, and the turbine speed is determined by the Tabular or Control Functions indicated by IOAPJJ and IOPPJJ (words 4 and 5 above). If a positive value is entered, then the turbine speed is determined by the inertia equation:

$$I \frac{d(2\pi\omega)}{dt} = T_m - T_{hydr} - T_{fric}$$

where ω is the turbine speed, T is torque, and the subscripts $m, hydr, fric$, signify machine receiving power (generator), hydraulic and friction

respectively. The factor 2π is a consequence of ω being expressed in revolutions per second rather than radians per second. The friction torque is assumed to be proportional to the speed, with the proportionality constant C_f , ($T_{fric} = C_f \cdot 2\pi\omega$). The above equation is re-written using power instead of torque ($Q = 2\pi\omega T$):

$$I \frac{d(2\pi\omega)}{dt} = \frac{Q_m}{2\pi\omega} - \frac{Q_{hydr}}{2\pi\omega} - C_f 2\pi\omega$$

or:

$$\frac{d\omega}{dt} = \frac{1}{I} \left(\frac{Q_m - Q_{hydr}}{4\pi^2\omega} - C_f \omega \right)$$

This equation is used to determine the turbine speed. The motor torque, Q_m , is defined by a tabular or a control function indicated by IOAPJN and IOPPJN. (Thus, if $I > 0.0$ then the interpretation of IOAPJN, IOPPJN is different from their interpretation when $I = 0.0$). The friction coefficient, C_f , is defined below.

Acceptable range: PMIPJN ≥ 0.0 .

Default value: 0.0 .

- | | | |
|------------|--------|--|
| W-24 (R) : | CF1PJN | Friction coefficient, C_f , (W/s ²). The value is used to calculate the friction power in the turbine inertia equation. The friction power is equal to $Q_f = 4\pi^2 C_f \omega \omega $ (see the equation shown at PMIPJN description, above).
<i>Acceptable range:</i> CF1PJN ≥ 0.0 .
<i>Default value:</i> 0.0 . |
| W-25 (R) : | ISNPJN | Pointer to a Tabular or Control Function, which controls the eventual synchronization of the turbine. ISNPJN is used only if a positive moment of inertia, PMIPJN (Word 20) is specified.
If the value of the Tabular or Control Function is smaller than, or equal to zero, then the turbine's motor (generator) is not synchronized, and the turbine speed is calculated using the turbine moment of inertia, PMPIJN (Word 20), and the motor power, Q_m , defined by a tabular or a control function indicated by IOAPJN and IOPPJN (Words 5 and 6).
If the value of the Tabular or Control Function is greater than zero, then the turbine's motor (generator) is synchronized, and the turbine speed is constant and equal to the nominal speed, OMNPJN (Word 4), multiplied by the value obtained from the Tabular or Control Function indicated by ISNPJN. At the moment the turbine is synchronized (the value of a Tabular or Control Function turns positive), its speed begins to change and it changes until the target speed is reached. The relative rate of this change is limited by DOMPJN (Word 14).
<i>Acceptable range:</i> must be a valid reference number of a Tabular or a Control Function, if nonzero.
<i>Default value:</i> 0 . |
| W-26 (R) : | SEXPJN | Exponent s , applied in the surge region. This exponent is analogical to the same exponent in the pump/compressor model. Since the surge |

model is typically not applied for turbines, the value of s is meaningless for the turbine.

Acceptable range: $0.1 < \text{SEXPJN} \leq 10.0$.

Default value: 1.0.

W-27 (R) : BLMPJN Limit on ω^b in case of negative b (see description of the pump maps, appendix A).

Acceptable range: $2.0 < \text{BLMPJN} \leq 20.0$.

Default value: 10.0.

2.2.11 Records: 235XXX, Pump/Turbine Additional Data

XXX is the Junction reference number, $001 \leq \text{XXX} \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version). In this record the user can define:

- The initial speed and speed limits for a pump (if record 231XXX is present for this Junction) or a turbine (if record 233XXX is present for this Junction).
- The minimum reduced flow used for power calculation in nearly zero flow region. Typically the efficiency of pumps/compressors decrease with decreasing flow. In the limit of zero flow, the efficiency is zero; the isentropic power is zero; and the true power is positive. In the code the true power to fluid, Q_{hydr} , is computed from:

$$Q_{hydr} = \frac{Q_{isent}}{\eta}$$

In case of zero flow both Q_{isentr} and η are zero, so the symbol becomes undefined. In order to be able to define a non-zero power at zero flow (pump operating with valve closed), the concept of minimum velocity for power calculation is introduced.

W-1 (R) : OTAPJN Initial speed, ω , of a pump (if record 231XXX is present for this Junction) or a turbine (if record 233XXX is present for this Junction).

Acceptable range: $-10 \cdot \omega_N < \omega < 10 \cdot \omega_N$ (ω_N is the nominal speed).

Default value: 0.0 .

W-2 (R) : VFAPJN Initial volumetric flow of atmosphere (gas), V_a , through a pump (if record 231XXX is present for this Junction) or a turbine (if record 233XXX is present for this Junction).

Acceptable range: $-10 \cdot V_N < V_a < 10 \cdot V_N$ (V_N is the nominal flow).

Default value: 0.0 .

W-3 (R) : VFPPJN Initial volumetric flow of pool (liquid), V_p , through a pump (if record 231XXX is present for this Junction) or a turbine (if record 233XXX is present for this Junction)

Acceptable range: $-10V_N < V_p < 10V_N$. (V_N is the nominal flow).

Default value: 0.0 .

W-4 (R) : OM1PJN Minimum rotational speed, ω_{min} , of a pump (if record 231XXX is present for this Junction) or a turbine (if record 233XXX is present for this Junction)

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $\omega_{min} < \omega_N$. (ω_N is the nominal speed).

Default value: $-100.0 \omega_N$.

W-5 (R) : OM2PJN Maximum rotational speed, ω_{max} , of a pump (if record 231XXX is present for this Junction) or a turbine (if record 233XXX is present for this Junction)

Acceptable range: $\omega_{max} > \omega_N$. (ω_N is the nominal speed).

Default value: $+100.0 \omega_N$.

W-6 (R) : VMNPJN Multiplier defining the minimum reduced flow for power calculation. Used whenever the reduced flow is smaller than V_{min} , defined as:

$$V_{min} = VMNPJN \times V_N \times \left(\frac{\omega_R^a}{\omega_R^b} \right)^{1/c}$$

where V_N is the nominal flow of a pump. In case of a turbine this is a nominal flow of the “equivalent pump” (the “equivalent pump” data is printed in the output file). ω_R is the reduced speed, and a, b, c are the exponents in the pump/compressor/turbine map. The power is calculated by replacing the actual reduced flow by the minimum flow. For example, in case of water pump the power is given by:

$$Q_{hydr} = V_{min} \Delta P$$

The efficiency is then re-defined. The actual efficiency is given by:

$$\eta = \frac{V \Delta P}{Q_{hydr}}$$

Thus when the pump flow is zero, $V=0.0$, then the efficiency (above formula) is zero, and the power, which enters the fluid, is positive ($=V_{min} \cdot \Delta P$)

Acceptable range: $10^{-2} \leq VMNPJN \leq 2.0$.

Default value: 0.5 .

2.2.12 Records: 236XXX, Simplified Pump/Turbine Data

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version). In this record the user can define the pump head through a Tabular or Control Function. The value obtained from the TF / CF may be positive (pump) as well as negative (turbine).

W-1 (I) : IPTAJN Pointer to a Tabular or Control Function that defines the pump/turbine head (Pa) for the atmosphere flow through the Junction XXX. If the number is positive, then the head will be defined by a Tabular Function with the reference number: IPTAJN. If the number is negative, then the head will be defined by a Control Function with the reference number: $|IPTAJN|$.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-2 (I) : ITPPJJ Pointer to a Tabular or Control Function that defines the pump/turbine head (Pa) for the pool flow through the Junction XXX. If the number is positive, then the head will be defined by a Tabular Function with the reference number: ITPPJJ. If the number is negative, then the head will be defined by a Control Function with the reference number: | ITPPJJ |.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

Note: in case of TF, the user defines the pump head as a function of time.

2.2.13 Records: 237XXX, Request for Pump Curves

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

Pump characteristic curves (performance maps) are determined by the input parameters such as VF0PJJ, CRSPJJ, etc., defined in the input records 231XXX. In order to make it easy to compare the curves with source data, SPECTRA prints the pump curves for several selected pump speeds. In this record the user can define the pump speeds for which the curves will be printed in the output file. By default the curves are printed for reduced speeds of 0.2, 0.4, 0.6, 0.8, 1.0, and 1.2. The curves are printed for both positive and negative speeds. An example of such printout is shown below.

REDUCED PRESSURE HEAD FOR FORWARD PUMP SPEED:

i	V-red	N-red = 2.000E-01	N-red = 4.000E-01	N-red = 6.000E-01	N-red = 8.000E-01	N-red = 1.000E+00	N-red = 1.200E+00
0	0.00000E+00	5.33333E-02	2.13333E-01	4.80000E-01	8.53333E-01	1.33333E+00	1.92000E+00
1	2.00000E-01	4.00000E-02	2.00000E-01	4.66667E-01	8.40000E-01	1.32000E+00	1.90667E+00
2	4.00000E-01	2.08167E-17	1.60000E-01	4.26667E-01	8.00000E-01	1.28000E+00	1.86667E+00
3	6.00000E-01	-6.66667E-02	9.33333E-02	3.60000E-01	7.33333E-01	1.21333E+00	1.80000E+00
4	8.00000E-01	-1.60000E-01	8.32667E-17	2.66667E-01	6.40000E-01	1.12000E+00	1.70667E+00
5	1.00000E+00	-2.80000E-01	-1.20000E-01	1.46667E-01	5.20000E-01	1.00000E+00	1.58667E+00
6	1.20000E+00	-4.26667E-01	-2.66667E-01	2.22045E-16	3.73333E-01	8.53333E-01	1.44000E+00
7	1.40000E+00	-6.00000E-01	-4.40000E-01	-1.73333E-01	2.00000E-01	6.80000E-01	1.26667E+00
8	1.60000E+00	-8.00000E-01	-6.40000E-01	-3.73333E-01	3.33067E-16	4.80000E-01	1.06667E+00
9	1.80000E+00	-1.02667E+00	-8.66667E-01	-6.00000E-01	-2.26667E-01	2.53333E-01	8.40000E-01
10	2.00000E+00	-1.28000E+00	-1.12000E+00	-8.53333E-01	-4.80000E-01	2.22045E-16	5.86667E-01

W-1 (R) : OMRPJJ(1) Relative pump speed (ω/ω_N) number 1
Acceptable range: $0.0 < \text{OMRPJJ}(1) < 2.0$
Default value: 0.2

W-2 (R) : OMRPJJ(2) Relative pump speed (ω/ω_N) number 2
Acceptable range: $0.0 < \text{OMRPJJ}(2) < 2.0$
Default value: 0.4

W-3 (R) : OMRPJJ(3) Relative pump speed (ω/ω_N) number 3
Acceptable range: $0.0 < \text{OMRPJJ}(3) < 2.0$
Default value: 0.6

SPECTRA Code Manuals - Volume 2: User's Guide

current value of the Tabular or Control Function with the following limits: $273.2 \leq T_{pool} \leq T_{sat}$.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-3 (I) : IGS1JN(1) Pointer to a Tabular or Control Function that defines the mole fraction of gas 1 flowing through the junction. If the number is positive, the fraction will be defined by a Tabular Function with the reference number: IGS1JN. If the number is negative, the fraction will be defined by a Control Function with the reference number: $|IGS1JN|$. At any given time of the transient the mole fractions will be equal to the current value of the Tabular or Control Function with the following limits: $0.0 \leq X(1) \leq 1.0$.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-4 (I) : IGS1JN(2) The same for gas number 2. Note that the user-defined gas mole fractions must either be specified for all gases or none.

(...) until all gases are defined. Normalization is performed to ensure that sum of all fractions is equal to 1.0.

2.2.15 Records: 239XXX, User-Defined Fluid Properties - Negative Flow Direction

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

This record defines the same parameters as record 238XXX but these to be applied **only when the flow direction is negative**. Changing the definition of JN flow direction in the input file and replacing 238XXX by 239XXX will yield the identical results. Simultaneous use of 238XXX and 239XXX indicate erroneous input model definition and in such case a warning is given in the diagnostics file.

W-1 (I) : IAT2JN Pointer to a Tabular or Control Function that defines the temperature of atmosphere gas flowing through the junction. If the number is positive, the temperature will be defined by a Tabular Function with the reference number: IAT2JN. If the number is negative, the temperature will be defined by a Control Function with the reference number: $|IAT2JN|$. At any given time of the transient the temperature will be equal to the current value of the Tabular or Control Function with the following limits: $T_{sat} \leq T_{ams} \leq 3070$.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-2 (I) : IPL2JN Pointer to a Tabular or Control Function that defines the temperature of pool flowing through the junction. If the number is positive, the temperature will be defined by a Tabular Function with the reference number: IPL2JN. If the number is negative, the temperature will be

defined by a Control Function with the reference number: $|IPL2JN|$.
 At any given time of the transient the temperature will be equal to the current value of the Tabular or Control Function with the following limits: $273.2 \leq T_{pool} \leq T_{sat}$.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-3 (I) : IGS2JN(1) Pointer to a Tabular or Control Function that defines the mole fraction of gas 1 flowing through the junction. If the number is positive, the fraction will be defined by a Tabular Function with the reference number: IGS2JN. If the number is negative, the fraction will be defined by a Control Function with the reference number: $|IGS2JN|$. At any given time of the transient the mole fractions will be equal to the current value of the Tabular or Control Function with the following limits: $0.0 \leq X(1) \leq 1.0$.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-4 (I) : IGS2JN(2) The same for gas number 2. Note that the user-defined gas mole fraction must either be specified for all gases or none.

(...) until all gases are defined. Normalization is performed to ensure that sum of all fractions is equal to 1.0.

2.2.16 Records: 240XXX, Flow Composition Parameters

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

The user can influence the composition of gas flowing through Junctions using these records. The Flow Composition Parameters (FCP) may be defined for each gas by those records. If those records are not present then the gas composition will always be equal to the gas composition in the upstream Control Volume, at the elevation of the Junction. If the FCP are entered then the volume fractions for each gas are multiplied by the FCP for this gas and divided by the sum of FCP for all gases. Using the FCP the user can introduce additional conservatism into the analysis. For example in BWR containments the steam flow through vacuum breakers can be restricted, which will typically result in higher containment pressures. Several records with the same number may be entered. Each record defines FCP for one gas. Flow Composition Parameters are applied only for the atmosphere gases and not for the bubble gases.

W-1 (I) : IGAS Gas number, (-). Must be one of the available gases. The built-in gases are: 1 = H₂, 2 = He, 3 = steam, 4 = N₂, 5 = O₂, 6 = CO₂.

Acceptable range: $1 \leq IGAS \leq NGASCV \leq NGMXFL = 20$

Default value: none.

W-2 (I) : IFCPJN Indicator for Flow Composition Parameter (FCP) for gas IGAS. If IFCPJN is zero then the FCP for this gas is equal to 1.0. If the number is

positive then the Tabular Function IFCPJN will define the FCP for this gas. If it is negative the FCP will be defined by the Control Function – IFCPJN. The following limits are imposed on the values of FCP: $1.0 \times 10^{-3} < FCP < 1.0 \times 10^3$. If the value obtained from the Tabular or Control Function is outside this range it will be set to the nearest value within the range. If FCP are used then the gas composition in Junction is determined as:

$$v_{i,JN} = \frac{v_{i,CV} \cdot FCP_i}{\sum_{k=1}^{N_{GAS}} v_{k,CV} \cdot FCP_k}$$

where: $v_{i,JN}$ is the volume fraction of gas i in the Junction, $v_{k,CV}$ is the volume fraction of gas k in the upstream CV, at the Junction elevation, FCP_k is the Flow Composition Parameter for the gas k.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

2.2.17 Records: 250XXX, Entrainment Indicators

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version). The use of the entrainment indicators is explained in Volume 1, in the section describing the equation of mass conservation.

W-1 (R) : ENTRJN(1) Entrainment indicator for atmosphere flow, E_{atms} . If $E_{atms}=0.0$ then the JN atmosphere flow is deposited in atmosphere of the receiving CV, as long as the liquid level in the receiving CV is below the top of the Junction. When the liquid level is above the top of the Junction then the atmosphere flow is a source of bubbles in the receiving CV. If $E_{atms}=1.0$ then part of the JN atmosphere flow is entrained into pool as bubbles, whenever the pool level in the receiving CV is above the pool level in the Junction. Note that bubbles are created in the receiving CV only when the bubble model is activated for that volume (IBUBCV=2 - see record 155XXX).

Acceptable range: $0.0 \leq ENTRJN(1) \leq 1.0$

Default value: 0.0.

W-2 (R) : ENTRJN(2) Entrainment indicator for droplet flow, E_{drop} . If $E_{drop}=0.0$ then the JN droplet flow is deposited in the pool of the receiving CV, as long as the liquid level in the receiving CV is above the bottom of the Junction. When the liquid level is below the bottom of the Junction then the droplet flow is a source of droplets in the receiving CV. If $E_{drop}=1.0$ then part of the JN droplet flow is entrained into atmosphere, already when the pool level in the receiving CV is below the top of the Junction. Note that droplets are created in the receiving CV only when the droplet model is activated for that volume (IDRPCV=2 - see record 155XXX).

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq \text{ENTRJN}(2) \leq 1.0$

Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0).

W-3 (R) : ENTRJN(3) Entrainment indicator for pool flow, E_{pool} . If $E_{pool}=0.0$ then the JN pool flow is deposited in the pool of the receiving CV, as long as the liquid level in the receiving CV is above the bottom of the Junction. When the liquid level is below the bottom of the Junction then the pool flow is a source of droplets in the receiving CV. If $E_{pool}=1.0$ then part of the JN pool flow is entrained into atmosphere as droplets, whenever the pool level in the receiving CV is below the pool level in the Junction. Note that droplets are created in the receiving CV only when the droplet model is activated for that volume (IDRPCV =2 - see record 155XXX).
Acceptable range: $0.0 \leq \text{ENTRJN}3 \leq 1.0$
Default value: 0.0 .

W-4 (R) : ENTRJN(4) Entrainment indicator for bubble flow, E_{bubb} . If $E_{bubb}=0.0$ then the JN bubble flow is deposited in the atmosphere of the receiving CV, as long as the liquid level in the receiving CV is below the top of the Junction. When the liquid level is above the top of the Junction then the bubble flow is a source of bubbles in the receiving CV. If $E_{bubb}=1.0$ then part of the JN bubble flow is entrained into pool, already when the pool level in the receiving CV is above the bottom of the Junction. Note that bubbles are created in the receiving CV only when the bubble model is activated for that volume (IBUBCV=2 - see record 155XXX).
Acceptable range: $0.0 \leq \text{ENTRJN}4 \leq 1.0$
Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0).

2.2.18 Records: 251XXX, Drop Flow Regime Model Parameters

XXX is the Junction reference number, $001 \leq \text{XXX} \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

W-1 (R) : COVAJN Constant C_0 for drift flux model for Junction atmosphere, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: C_0 , v_A , (-).
Acceptable range: $0.0 \leq \text{COVAJN} \leq 10.0$. If no value or zero is entered, then C_0 , v_A is calculated by the Drop Flow Regime Model, as described in Volume 1.
Default value: 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0

W-2 (R) : VIVAJN Terminal velocity, v_∞ , for drift flux model for Junction atmosphere, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty, A}$, (m/s).
Acceptable range: $-100.0 \leq \text{VIVAJN} \leq 100.0$. If no value or zero is entered, then $v_{\infty, A}$ is calculated by the Drop Flow Regime Model, as described in Volume 1.
Default value: 0.0, a small value ($\leq 10^{-50}$) value will set v_∞ to 0.0

SPECTRA Code Manuals - Volume 2: User's Guide

W-3 (R) :	XVAJN	Exponent x for drift flux model for Junction atmosphere, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{v,A}$, (-). <i>Acceptable range:</i> $0.0 \leq XVAJN \leq 10.0$. If no value or zero is entered, then $x_{v,A}$ is calculated by the Drop Flow Regime Model. <i>Default value:</i> 0.0
W-4 (R) :	C0HAJN	Constant C_0 for drift flux model for Junction atmosphere, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $C_{0,hA}$, (-). <i>Acceptable range:</i> $0.0 \leq C0HAJN \leq 10.0$. If no value or zero is entered, then $C_{0,hA}$ is calculated by the Drop Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0
W-5 (R) :	VIHAJN	Terminal velocity, v_∞ , for drift flux model for Junction atmosphere, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty,hA}$, (m/s). <i>Acceptable range:</i> $-100.0 \leq VIHAJN \leq 100.0$. If no value or zero is entered, then $v_{\infty,hA}$ is calculated by the Drop Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set v_∞ to 0.0
W-6 (R) :	XHAJN	Exponent x for drift flux model for Junction atmosphere, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{h,A}$, (-). <i>Acceptable range:</i> $0.0 \leq XHAJN \leq 10.0$. If no value or zero is entered, then $x_{h,A}$ is calculated by the Drop Flow Regime Model. <i>Default value:</i> 0.0
W-7 (I) :	IDFAJN	Droplet flow activator: = 0: droplet flow through junctions is possible $\neq 0$: droplet flow through junctions is not possible <i>Acceptable range:</i> any integer <i>Default value:</i> 0

2.2.19 Records: 252XXX, Bubbly and Annular Flow Parameters

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

W-1 (R) :	C0VPJN	Constant C_0 for drift flux model for Junction pool, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $C_{0,vP}$, (-). <i>Acceptable range:</i> $0.0 \leq C0VPJN \leq 10.0$. If no value or zero is entered, then $C_{0,vP}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1. <i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0
-----------	--------	---

SPECTRA Code Manuals - Volume 2: User's Guide

W-2 (R) :	VIVPJN	<p>Terminal velocity, v_{∞}, for drift flux model for Junction pool, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty,v,P}$, (m/s).</p> <p><i>Acceptable range:</i> $-100.0 \leq \text{VIVPJN} \leq 100.0$. If no value or zero is entered, then $v_{\infty,v,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1.</p> <p><i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set v_{∞} to 0.0</p>
W-3 (R) :	XVPJN	<p>Exponent x for drift flux model for Junction pool, vertical velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{v,P}$, (-).</p> <p><i>Acceptable range:</i> $0.0 \leq \text{XVPJN} \leq 10.0$. If no value or zero is entered, then $x_{v,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1.</p> <p><i>Default value:</i> 0.0 .</p>
W-4 (R) :	C0HPJN	<p>Constant C_0 for drift flux model for Junction pool, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $C_{0,hP}$, (-).</p> <p><i>Acceptable range:</i> $0.0 \leq \text{C0HPJN} \leq 10.0$. If no value or zero is entered, then $C_{0,hP}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1.</p> <p><i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set C_0 to 0.0</p>
W-5 (R) :	VIHPJN	<p>Terminal velocity, v_{∞}, for drift flux model for Junction pool, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $v_{\infty,h,P}$, (m/s).</p> <p><i>Acceptable range:</i> $-100.0 \leq \text{VIHPJN} \leq 100.0$. If no value or zero is entered, then $v_{\infty,h,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1.</p> <p><i>Default value:</i> 0.0, a small value ($\leq 10^{-50}$) value will set v_{∞} to 0.0</p>
W-6 (R) :	XHPJN	<p>Exponent x for drift flux model for Junction pool, horizontal velocity (see Volume 1). This is the value denoted in Volume 1 as: $x_{h,P}$, (-).</p> <p><i>Acceptable range:</i> $0.0 \leq \text{XHPJN} \leq 10.0$. If no value or zero is entered, then $x_{h,P}$ is calculated by the Bubbly Flow Regime Model, as described in Volume 1.</p> <p><i>Default value:</i> 0.0 .</p>
W-7 (I) :	IANNJN	<p>Annular flow model selection.</p> <p>=1: Default model, see Volume 1.</p> <p>=2: Dartmouth correlation, see Volume 1.</p> <p><i>Acceptable range:</i> 1 or 2.</p> <p><i>Default value:</i> 1 .</p>
W-8 (I) :	IBFAJN	<p>Bubble flow activator:</p> <p>= 0: bubble flow through junctions is possible</p> <p>$\neq 0$: bubble flow through junctions is not possible</p> <p><i>Acceptable range:</i> any integer</p> <p><i>Default value:</i> 0</p>

2.2.20 Records: 253XXX, Plume Model for Junction Flows

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

These records activate plume models for the material flowing through the Junction. The plume model is used in Control Volumes in which stratification is calculated. Thus, it will be used only if there is stratification model active in one (or both) Control Volumes connected by this Junction. A description of the plume model is given in Volume 1. To activate the model for a single component, a set of two integer numbers, described below, must be entered. To activate the model for two components, two sets of pairs should be entered in this record.

W-1 (I) : J Identifier of component, for which the plume model is desired. J=1: atmosphere; J=3: pool.
Acceptable range: J=1, or J=3.
Default value: none.

W-2 (I) : IPLMJN Plume model activator. If IPLMJN = 0 then the plume model is not active. If IPLMJN \neq 0 then the plume model is active for the component J and Junction XXX.
 Note that the plume model is used only when stratification models are active in Control Volumes. The plume model will be deactivated if Junction velocities exceed certain limits (see section 2.1.27).
Acceptable range: any integer.
Default value: 0 .

... etc., until all plumes are defined.

2.2.21 Records: 255XXX, Counter-current Flow Model Constants

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

W-1 (R) : CCFVJN Counter-current flow constant for vertical flow, $C_{cf, v}$. The counter-current flow limit is defined by the equation:

$$\alpha = \frac{|v_g|}{|v_g| + |v_l| \cdot C_{cf, v}}$$

where α is a void fraction, v_g , v_l are the gas and liquid velocities respectively. Generally, a larger value of CCFVJN causes smaller flow resistance in counter-current flow. A large value ($\geq 10^9$) eliminates the counter current flow.

Acceptable range: $10^{-10} \leq CCFVJN \leq 10^{10}$
Default value: 0.1

W-2 (R) : CCFHJN Counter-current flow constant for horizontal flow, $C_{cf, h}$. The counter-current flow limit is defined by the equation:

$$\alpha = \frac{|v_g|}{|v_g| + |v_l| \cdot C_{cf,h}}$$

where α is a void fraction, v_g , v_l are the gas and liquid velocities respectively. Generally, a larger value of CCFHJN causes smaller flow resistance in counter-current flow. A large value ($\geq 10^9$) eliminates the counter current flow.

Acceptable range: $10^{-10} \leq \text{CCFHJN} \leq 10^{10}$

Default value: 10.0

2.2.22 Records: 256000, Diffusion Model - Global Activator

- W-1 (I) : JDIFJN Global indicator for diffusion calculation in junction.
 = 1: diffusion is not calculated
 = 2: diffusion is calculated.
 If activated, diffusion is calculated for a gas flow through a junction. Diffusion does not result in a net flow but only in change of gas concentrations. A description of the diffusion model is provided in Volume 1. Diffusion is only important in case of a very small velocity in a junction. The diffusion calculation is automatically turned off in those junctions where the gas velocity is higher than a certain limit (set by the input parameter VMDFJN).
Acceptable range: 1 or 2
Default value: 1
- W-2 (I) : LDIFJN Request for diffusion plot parameters
 = 1: diffusion plot parameters not requested
 = 2: diffusion plot parameters requested
 If diffusion parameters are requested, then the volume change due to diffusion is available in the plot file as JN-xxx-VDif-yyyy, where xxx is the junction number and yyyy is the gas name. In such case the plot parameters replace the default parameters JN-xxx-Cgas-yyyy (Table 2-24). The diffusion volume change is always available in the output file *.OUT.
Acceptable range: 1 or 2
Default value: JDIFJN

2.2.23 Records: 256XXX, Diffusion Model - Individual Activators

XXX is the Junction reference number, $001 \leq \text{XXX} \leq 999$. The Junction reference numbers, XXX, need not be consecutive. The maximum number of Junctions is 600 (999 in LINUX version).

- W-1 (I) : IDIFJN Indicator for diffusion calculation in junction.
 = 1: diffusion is not calculated
 = 2: diffusion is calculated.

If activated, diffusion is calculated for a gas flow through a junction. Diffusion does not result in a net flow but only in change of gas concentrations. A description of the diffusion model is provided in Volume 1. Diffusion is only important in case of a very small velocity in a junction. The diffusion calculation is automatically turned off in those junctions where the gas velocity is higher than a certain limit (set by the input parameter VMDFJN).

The model is applied to CV gases, defined in the FL Package. It may also be applied for the fission product vapours, defined in the RT Package. To do so; the user must supply the diffusion volumes (SGFPRT, record 886XXY), needed to calculate diffusion coefficients.

Acceptable range: 1 or 2

Default value: JDIFJN

- W-2 (R) : X1DFJN Diffusion length in the 'from-CV', $L_{from-CV}$, (m).
Acceptable range: $10^{-4} \leq X1DFJN \leq 10^{10}$
Default value: FRLNJV/2.0 (half of the friction length)
- W-3 (R) : X2DFJN Diffusion length in the 'to-CV', L_{to-CV} , (m).
Acceptable range: $10^{-4} \leq X2DFJN \leq 10^{10}$
Default value: FRLNJV/2.0 (half of the friction length)

2.2.24 Records: 260000, Options for Critical Velocity, Elevation and Area Checking

The options below are applied to all Junctions.

- W-1 (R) : VMCFJN Velocity below which the critical flow calculation is bypassed, (m/s).
Acceptable range: $0.0 < VMCFJN \leq 1.0 \times 10^6$
Default value: 10.0
- W-2 (I) : ICELVN Elevation checking option.
=-1: Check elevations close to CV bottom or top. Adjust JN elevations and CV heights if needed. This option, or option +1, should be used for two-phase systems.
=+1: Check elevations close to CV bottom or top. Adjust JN elevations if needed. This option, or option -1, should be used for two-phase systems.
=+2: Do not check nor adjust elevations close to CV bottom or top. This option can be used for single-phase (pure gas) systems.
Acceptable range: -1, 1, 2
Default value: 1
- W-3 (I) : ICVAJN CV horizontal and vertical area (AHORCV, AVERCV, record 111XXX) checking option. In general any of these flow areas should not be smaller than the largest flow area of the Junctions connected to a given CV. If the user wishes to apply smaller flow areas, he must allow the code to accept such input by setting the value to 2.
=1: CV horizontal or vertical area smaller than the largest flow area of the junctions connected to the given CV is flagged as an error and is not accepted for calculations.

SPECTRA Code Manuals - Volume 2: User's Guide

- =2: CV horizontal or vertical area smaller than the largest flow area of the junctions connected to the given CV is accepted.
- =3: CV areas are modified automatically by the code.
 - (A) If CV vertical area (AVERCV) is smaller than the maximum flow area of all horizontal junctions connected to this CV, then it is set to the maximum JN area.
 - (B) If CV horizontal area (AHORCV) is smaller than the maximum flow area of all vertical junctions connected to this CV, then it is set to the maximum JN area.
- =4: Junction flow areas are modified automatically by the code.
 - A) If the flow area of a vertical junction is larger than the minimum horizontal flow area of the two connected CV-s, the junction area is set to the smaller CV horizontal area.
 - B) If the flow area of a horizontal junction is larger than the smaller of the minimum vertical flow area of the two connected CV-s, the Junction area is automatically set to the smaller CV horizontal area.

Acceptable range: 1, 2, 3, 4

Default value: 1

W-4 (R) : HMINJN Minimum distance between bottom of CV and JN bottom, (m). Used when the elevation checking option is set (ICELJN<2). If the JN bottom elevation, calculated from the JN level and JN height specified in the input deck, is lower than the limit imposed by this value, it is automatically reset by the code.

Acceptable range: $0.0 < \text{HMINJN} \leq 1.0 \times 10^{-2}$

Default value: 1.0×10^{-4}

W-5 (R) : HMAXJN Minimum distance between top of JN and CV top, (m). The value should be consistent with the parameter HMAXCV. Used when the elevation checking option is set (ICELJN<2). If the JN top elevation, calculated from the JN level and JN height specified in the input deck, is higher than the limit imposed by this value, it is automatically reset by the code.

Acceptable range: $0.0 < \text{HMAXJN} \leq 5.0 \times 10^{-2}$

Default value: 1.0×10^{-2}

W-6 (R) : VMDFJN Velocity above which the diffusion mass transfer calculation is bypassed, (m/s). See the input parameter IDIFJN.

Acceptable range: $1.0 \times 10^{-3} < \text{VMDFJN} \leq 1.0 \times 10^{-1}$

Default value: 1.0×10^{-2}

W-7 (R) : XMDFJN Interpolation range for the diffusion mass transfer calculation. The velocity-dependent multiplier is defined as:

= 1.0 for the gas velocity $v_{gas} < \text{VMDFJN} \times \text{XMDFJN}$

= 0.0 for the gas velocity $v_{gas} > \text{VMDFJN}$

= $(\text{VMDFJN} - v_{gas}) / (\text{VMDFJN} - \text{VMDFJN} \times \text{XMDFJN})$

Acceptable range: $0.1 < \text{XMDFJN} \leq 0.9$

Default value: 0.5

2.2.25 Records: 261000, Minimum Reynolds Number for Friction Calculation

The value below is applied to all Junctions.

W-1 (R) : REMNJJ Minimum Reynolds number for friction calculation, Re_{min} (-). In the laminar range the friction factor is calculated from:

$$f = \frac{64}{Re}$$

A limit is imposed on the Reynolds number: $Re < Re_{min}$. With the default value, the friction factor is not larger than 10.0. The limit must be decreased to analyze low velocity flows, for which $Re < 6.4$.

Acceptable range: $6.4 \times 10^{-2} < VMCFJN \leq 6.4 \times 10^2$

Default value: 6.4

2.2.26 Records: 262000, User-Defined Critical Flow Model

This record activates the user-defined critical flow model. The model is intended to be applied for alternative liquids or sensitivity calculations. If defined, the values below are applied to all Junctions.

W-1 (I) : ITFGJJ Tabular Function, f_{gas} , defining the critical velocity for the gas phase. The TF value gives critical velocity, c_{gas} (m/s), as a function of gas temperature, T_{gas} (K):

$$c_{gas} = f_{gas}(T_{gas})$$

The following limits are imposed on the value obtained from the Tabular Function: $10.0 \leq c_{gas} \leq 10^6$ m/s.

Acceptable range: 0 or reference to a Tabular Function. A positive value must be used in case of alternative fluid (IFLDFL>1)

Default value: 0

W-2 (I) : ITFLJJ Tabular Function, f_{liq} , defining the critical velocity for the liquid phase. The TF value gives the the critical velocity, c_{liq} (m/s), as a function of liquid temperature, T_{liq} (K):

$$c_{liq} = f_{liq}(T_{liq})$$

The following limits are imposed on the value obtained from the Tabular Function: $100.0 \leq c_{liq} \leq 10^6$ m/s.

Acceptable range: 0 or reference to a Tabular Function. A positive value must be used in case of alternative fluid (IFLDFL>1)

Default value: 0

2.2.27 Records: 263000, Friction Model Global Activators

This records specifies default values of the friction model parameters. The default values can be redefined for each individual junction in the records 210XXX.

- W-1 (R) : RFFGJN Empirical coefficient in the Griffith-Rohsenow correlation for the two-phase form loss factor multiplier, r_f , forward flow, (-). Values of r_f are shown in Table 2-2. The multiplier is equal to: $1.0 + r_f \cdot X \cdot v_{fg} / v_f$.
Acceptable range: $0.0 \leq \text{RFFGJN} \leq 10^3$
Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0)
- W-2 (R) : RFRGJN Empirical coefficient in the Griffith-Rohsenow correlation for the two-phase form loss factor multiplier, r_f , reverse flow, (-). Values of r_f are shown in Table 2-2. The multiplier is equal to: $1.0 + r_f \cdot X \cdot v_{fg} / v_f$.
Acceptable range: $0.0 \leq \text{RFRGJN} \leq 10^3$
Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0)
- W-3 (R) : CMGJN Moody coefficient for liquid flow, C_M , (-). The value of CMJN is applied for pure liquid flow ($X=0.0$). For $X>0$ the value is interpolated, to give 1.0 when $X=1.0$. Thus, the effective multiplier on the critical flow is equal to: $C_M + X \cdot (1 - C_M)$, see Volume 1. The best estimate value is 0.7 (Volume 3).
Acceptable range: $0.1 \leq \text{CMGJN} \leq 1.0$
Default value: 0.7
- W-4 (I) : MODGJN Model to calculate friction factor, f , (-), (see Volume 1),
 = 1 : non-uniform roughness, Colebrook-White formula,
 = 2 : uniform roughness, Nikuradse formula,
 = 3 : simplified method, Blasius and Prandtl-Nikuradse,
 = 11 : non-uniform roughness, Beluco-Camano formula
 = 12 : non-uniform roughness, Churchill formula
Acceptable range: MODGJN = 1, 2, 3, 11, 12
Default value: 11
- W-5 (I) : M2PGJN Model to calculate two-phase friction multiplier, Φ_f^2 , (-), (see Vol. 1),
 = 1 : no two-phase multiplier,
 = 2 : Hancox-Nicoll model,
 = 3 : Levy Model.
 > 1000: Φ_f^2 is given by a Tabular Function with the number: (M2PFJN - 1000). The argument is void fraction. The range of independent argument (void fraction) must cover the range from 0.0 to 1.0, inclusive. The TF value must be =1.0 for the void fraction of 0.0 and >1.0 for void fractions >0.0.
Acceptable range: M2PGJN = 1, 2, or 3.
Default value: 2
- W-61 (R) : CLAGJN Correction factor for non-circular tubes, C_{lam} . It may also be used as a multiplier for wire-wrapped rods. The friction factor in laminar flow is obtained from:

$$f_{wall} = \frac{64 \cdot C_{lam}}{Re}$$

Rectangular channel, dimensions $0.0 < b/a < 1.0$ [10] (Dia. 2-6)

$C_{lam} = 1.50$ $b/a \rightarrow 0.0$

$C_{lam} = 0.89$ $b/a \rightarrow 1.0$ (square)

Tube bundle, pitch-to-diameter ratios $1.0 < (P/D) < 1.5$ [10] (Dia. 2-9):

$C_{lam} = 0.89 \cdot (P/D) + 0.63$ triangular pitch

$C_{lam} = 0.96 \cdot (P/D) + 0.63$ rectangular pitch

For wire-wrapped rods, Engel correlation [50] gives: $f = 110/Re$, so $C_{lam} = 1.50 / 64 = 1.718$

Acceptable range: $0.1 \leq CLAGJN \leq 10.0$

Default value: 1.0

- W-7 (R) : CTUGJN Friction factor multiplier for turbulent flow. Applicable for example for wire-wrapped rod assemblies in fast reactors.
 For wire-wrapped rods, Engel correlation [50] gives: $f = 0.55/Re^{0.25}$, so compared to the smooth friction factor (Blasius): $f = 0.316/Re^{0.25}$, $C_{lam} = 0.55 / 0.316 = 1.741$. A good overview of correlations: [51].
 Acceptable range: $0.1 \leq CTUGJN \leq 10.0$
 Default value: 1.0

2.2.28 Records: 264000, Momentum Length, Friction Length Options

The momentum length, XLENJN is defined in the record 200XXX. In case of liquid-full volumes the momentum length is automatically reduced by the program is to the minimum value, defined in this record.

- W-1 (R) : XLMNJN Minimum momentum length for junctions connecting Control Volumes that are filled with liquid.
 Acceptable range: $0.01 \leq XLMNJN \leq 100.0$
 Default value: 0.05
- W-2 (I) : IMFLJN Option to calculate the momentum length (XLENJN) and the friction length (FRLNJN) automatically by the code:
 = 0 : momentum and friction length are defined by the user,
 = 1 : momentum and friction length are calculated by the code from the recommended formulae (see description of XLENJN and FRLNJN) if XLENJN and FRLNJN are entered as 0.0. If a positive value of XLENJN or FRLNJN is entered, it is compared to the recommended value. If the relative difference is larger than 0.1, a warning message is printed.
 = 2 : momentum and friction length are always calculated by the code from the recommended formulae (see description of XLENJN and FRLNJN), independently of the values entered.
 Acceptable range: 0, 1, 2
 Default value: 0

2.2.29 Records: 265000, Hydraulic Diameter - JN Versus CV

W-1 (I) : IDHDJN Option to calculate the CV hydraulic diameter (DHYDCV) based on JN hydraulic diameter (DIAMJN).
= 1 : option not used. DHYDCV is defined by the user. If no value is defined, then the default value is used.
= 2 : option used. With this option DHYDCV is compared to the junction diameter, DIAMJN. If $DIAMJN < DHYDCV$, then DHYDCV is set to DIAMJN. This option is consistent with SPECTRA version of April 2023 or earlier.
Acceptable range: 1, 2
Default value: 1

2.2.30 Records: 270000, Solution of the Junction Flow Matrix

The "Junction Flow Matrix" (see Volume 1, Chapter 2) is used to calculate flows through all Junctions. The dimension of the matrix is equal to the number of active Junctions (all Junctions except for closed valves, Junctions with tabular flow control and critical Junctions). If the dimension is small then a typical method of matrix solution (L-U decomposition - see Volume 1) is preferable. For matrices of large dimension the bi-conjugate gradient method is available.

W-1 (I) : MSFMJN Method of solving the flow matrix dimension.
1 = only the Full Flow Matrix (FFM) is solved.
2 = the Full Flow Matrix is solved in the first iteration, subsequently the Limited Flow Matrix (LFM) is solved.
Acceptable range: 1, 2
Default value: 1

W-2 (I) : IMSFJN Indicator of the Junction Flow Matrix solution frequency.
1 = Junction Flow Matrix is solved at the beginning of a time step.
2 = Junction Flow Matrix is re-solved during iterations.
Acceptable range: 1, 2; any other entry is set to the default value
Default value: 2

W-3 (I) : MXFSJN Maximum number of Junction flow matrix solutions per time step. Used if IMSFJN (Word 2 above) is equal to 2.
Acceptable range: $2 \leq MXFSJN \leq 10$
Default value: 2

W-4 (R) : XCFMJN Minimum velocity for C_f and C_i calculation, (m/s), (see Volume 1).
Acceptable range: $10^{-6} \leq XCFMJN \leq 0.1$.
Default value: 10^{-3} .

W-5 (R) : CLCMJN Multiplier in the time step limit for gas composition change. The time step is limited if the gas composition in any Junction at the end of the time step is very different than at the beginning of the time step. This limit is specifically important in case of explicit definition of the

SPECTRA Code Manuals - Volume 2: User's Guide

Junction donor quantities (IMPLJN = 2, Word 11 below). The time step is limited to:

$$\Delta t = CLCMJN \times \text{Min} \left(\frac{c_i}{|c_i - c_i^0|} \right) \Delta t'$$

where: c_i - mass fraction of gas i, end of time step,
 c_i^0 - mass fraction of gas i, start of time step,
 $\Delta t'$ - previous value of time step, (s).

Acceptable range: $0.0 < CLCMJN \leq 1.0$

Default value: 0.1

W-6 (R) : CLMAJN Multiplier in the mass change limit for the atmosphere gas transport (Courant Limit for gas flow - see also word 12 below). The time step is limited if the gas mass flows through Junctions are large, compared to the gas mass in a Control Volume. The time step is limited to:

$$\Delta t = CLMAJN \times \text{Min} \left(\frac{M_{atms}}{\text{Max}(|W_{atms}|)} \right)$$

where: M_{atms} - mass of gas in a Control Volume (kg),
 W_{atms} - gas flow through a Junction connected to the Control Volume, (kg/s). Maximum is taken over all Junctions connected to the given Control Volume.

Acceptable range: $0.0 < CLMAJN \leq 1.0$

Default value: 0.50

W-7 (R) : CLCEJN Multiplier in the energy transfer time step limit. The time step is limited if the energy transfer in or from a Control Volume is large, compared to the gas heat capacity in a Control Volume. The time step is limited to:

$$\Delta t = CLCEJN \times \text{Min} \left(\frac{M_{cv} c_p \Delta T_{max}}{|Q_{atms}|} \right)$$

where: M_{cv} - mass of gas in Control Volume (kg),
 c_p - specific heat of the atmosphere gas, (J/kg/K).
 ΔT_{max} - maximum temperature change (=100 K).
 Q_{atms} - total heat in or out the atmosphere of the Control Volume, (W).

Acceptable range: $0.0 < CLMMJN \leq 10.0$

Default value: 1.0

W-8 (R) : CLCPJN Multiplier in the volume flow change limit for compressors and pumps. The criterion applied for all Type 1 Pump/Compressor (see section 2.2.8) Junctions is:

$$\Delta t = CLCPJN \times \text{Min} \left(\frac{1}{\text{Max}(R_{atms,JN}, R_{pool,JN})} \right)$$

where: $R_{atms,JN}$ maximum rate of change of atmosphere flow through the compressor (1/s), = RCAPJN (see 2.2.8),
 $R_{pool,JN}$ maximum rate of change of pool flow through the pump (1/s), = RCPPJN (see section 2.2.8).

The criterion applied for those Type 2 Pump/Compressor (see section 2.2.8) for which moment of inertia is used to calculate the speed, is:

$$\Delta t = CLCPJN \times \frac{I \omega_N \Delta \omega}{Q}$$

where: I - moment of inertia, (kg·m²).
 ω_N - nominal speed, (s⁻¹).
 $\Delta \omega$ - speed change, (s⁻¹), taken equal to 10% of ω_N .
 Q - current power, (W).

Acceptable range: $0.0 < CLCPJN \leq 10.0$

Default value: 1.0

W-9 (R) : CVCLJN Multiplier in the velocity change limit. The velocity change limit may be activated if the change of velocities in the last two time advancements are in the opposite directions (oscillating velocities). The time step is limited to:

$$\Delta t = CVCLJN \times \text{Min} \left(\frac{\Delta v_2}{\Delta v_1} \right) \cdot \Delta t'$$

where: $\Delta v_1 = v_k - v_{k-1}$,
 $\Delta v_2 = v_{k-1} - v_{k-2}$,
 v_k - velocity at k -th (last) advancement, (m/s),
 v_{k-1} - velocity at $k-1$ advancement, (m/s),
 v_{k-2} - velocity at $k-2$ advancement, (m/s),
 $\Delta t'$ - previous value of the time step, (s).

The limit is activated only if $\Delta v_1 > CVCLJN \times \Delta v_2$, and if the absolute value of either v_{k-1} or v_{k-2} is larger than the minimum velocity, defined by the Word 10 below.

Acceptable range: $0.0 < CVCLJN \leq 1.0$

Default value: 0.5 .

W-10 (R) : VVCLJN Minimum velocity to apply velocity change limit (m/s) (see Word 9 above).

Acceptable range: $0.0 < VVCLJN \leq 1000.0$.

Default value: 10.0. If density stratification is active in any Control Volume (IDSPCV≠0) and the link with thermal stratification is not used (DTSPCV<0.0 - see section

2.1.2), or if compressors with surge factor $CDS_{PJN} < 0.1$ (section 2.2.8) are used, then the default value is 1000.0. This means in practice that no velocity change limit is applied. This setting was motivated by observation that strong stratification may sometimes lead to oscillations in flow solution, which have little effect on the overall results. To avoid time step cuts in such cases, the velocity change limit is suppressed.

W-11 (I) : IMPLJN Method of calculating donor quantities in the Junction flow solution matrix. If the value is 1 then the donor quantities (gas compositions, temperatures) are implicit (end of time step value). This may require a very large number of iterations if the number of Junctions is significant. If $IMPLJN = 2$ then the explicit formulation is used and the donor quantities are defined by the beginning of time step values.
Acceptable range: 1, 2 .
Default value: 2 .

W-12 (R) : CLMPJN Multiplier in the mass change limit for the pool transport (Courant Limit for liquid flow - see also Word 6 above). The time step is limited if the liquid mass flows through Junctions are large, compared to the liquid mass in a Control Volume. The time step is limited to:

$$\Delta t = CLMPJN \times \text{Min} \left(\frac{M_{pool}}{\text{Max}(|W_{pool}|)} \right)$$

where: M_{pool} - mass of liquid in a Control Volume (kg),
 W_{pool} - liquid flow through a Junction connected to the Control Volume, (kg/s). Maximum is taken over all Junctions connected to the given Control Volume.

Acceptable range: $0.0 < CLMPJN \leq 1.0$
Default value: CLMAJN (Word 6 above) .

W-13 (I) : IACCJN Acceleration pressure drop calculation. The acceleration pressure drop is calculated from:

$$\Delta p_{acc} = \frac{\rho(v_D^2 - v_U^2)}{2}$$

where v_U , v_D are the average velocities in the upstream and the downstream Control Volumes respectively.

1 : acceleration pressure drop not included (compatible with SPECTRA Version 2.00 and earlier).

2 : acceleration pressure drop included for atmosphere flow only.

3 : acceleration pressure drop included for pool flow only.

4 : acceleration pressure drop included for atmosphere and pool flows.

Acceptable range: 1, 2, 3, 4

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 4

- W-14 (I) : INTFJN Interface friction calculation.
 1 : interface friction not calculated
 2 : interface friction calculated
 Acceptable range: 1, 2
 Default value: 2
- W-15 (I) : INRTJN Inertial “pressure drop” calculation in the Limited Flow Matrix.
 1 : inertial “pressure drop” reduced by with user-defined reduction
 factors, defined by the next two words.
 2 : inertial “pressure drop” calculated without the reduction factors.
 Acceptable range: 1, 2
 Default value: 1
- W-16 (R) : ALFMJN Reduction factor for atmosphere flow. Used if INRTJN =1.
 Acceptable range: $1.0 \times 10^{-4} \leq \text{ALFMJN} \leq 1.0$
 Default value: 1.0
- W-17 (R) : PLFMJN Reduction factor for pool flow. Used if INRTJN =1.
 Acceptable range: $1.0 \times 10^{-4} \leq \text{PLFMJN} \leq 1.0$
 Default value: 1.0×10^{-2}
- W-18 (I) : ILFMJN Immediate time step request activator in case the discrepancy between
 the velocities calculated by the Full Flow Matrix and the Limited Flow
 Matrix are larger than 50% or values have different signs
 1 : a request for an immediate time step cut is send to the numerical
 Solver Package,
 2 : a request for an immediate time step cut is NOT send.
 Acceptable range: 1, 2
 Default value: 2
- W-19 (R) : CLCDJN Multiplier in droplet flow time limit (Courant Limit for droplet flow).
 The time step is limited if the droplet vertical velocity and vertical height
 of Control Volume. The time step is limited to:

$$\Delta t = \text{CLCDJN} \times \left(\frac{H_{CV}}{v_{drop}} \right)$$

where: H_{CV} - height of a Control Volume (m),
 v_{drop} - droplet vertical velocity (m/s)

Acceptable range: $0.00 < \text{CLCDJN} \leq 100.0$

Default value: 1.00

2.2.31 Example of the Junction Data

The example input of Junction data given below defines a check valve Junction, JN-150, named "Example Junction", allowing flow from CV-200 to CV-100, when the pressure in CV-200 is higher by 0.1 bar than the pressure in CV-100, and closes when the CV-200 pressure exceeds the CV-100 pressure by less than 0.01 bar. The steam flow is restricted by the Flow Composition Parameter (FCP) of 10^{-3} . The FCP is defined by Tabular Function TF-100.

```

*      Definition of Junction No. 001
*      =====
*
205150 Example Junction
*
*      Area Elevation Length Diameter Height Flow
*      From To (m2) (m) (m) (m) (m) Direction Edges
200150 200 100 0.05 5.0 0.1 0.1 0.1 0 0.0
*
*      Length Roughness Diameter K-for K-rev rf-for rf-rev CM MOD
*      (m) (m) (m) (-) (-) (-) (-) (-) (-)
210150 0.1 1.0E-5 0.1 0.5 0.5 1.0 1.0 0.7 1
*
*      Valve
*      Motor dP-open dP-close
220150 0 0.10E+5 0.01E+5
*
*      Gas TF number
240150 3 100
*
605100 TF defining CFP for check valve, for conservative BWR analysis.
600100 0.0 1.0E-03
    
```

2.3 1-D Solid Heat Conductor Input Data

2.3.1 Records: 300XXX, 1-D Solid Heat Conductor Main Data

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

W-1 (I) :	IGEOSC	Geometry type, (-). IGEOSC = 1 : rectangular geometry, IGEOSC = 2 : cylindrical geometry, IGEOSC = 3 : spherical geometry. <i>Acceptable range:</i> 1, 2, 3. <i>Default value:</i> none.
W-2 (R) :	SIZESC	Size of solid conductor. The interpretation depends on the geometry: IGEOSC = 1 : area of the conductor surface, (m ²), IGEOSC = 2 : length of the cylinder, (m), IGEOSC = 3 : not used. <i>Acceptable range:</i> $0.0 < SIZESC \leq 10^{10}$. <i>Default value:</i> none.
W-3 (R) :	X0SC	Left (inner) side coordinate. The interpretation depends on the geometry type. IGEOSC = 1 : not used, IGEOSC = 2 : inner radius of the cylinder, (m), IGEOSC = 3 : inner radius of the sphere, (m). <i>Acceptable range:</i> $0.0 \leq X0SC \leq 10^{10}$. <i>Default value:</i> 0.0 .
W-4 (R) :	ELEVSC	Elevation of middle point of the conductor, (m). If -999 is entered, then the SC is automatically allocated to match the elevations of CV-s: $\{\text{Min}[Z_{TOP}(CV_1), Z_{TOP}(CV_2)] + \text{Max}[Z_{BOT}(CV_1), Z_{BOT}(CV_2)]\} / 2$. Here Z_{TOP} and Z_{BOT} are top and bottom elevations of the left boundary volume CV_1 and the right boundary volume CV_2 . The automatic allocation of a 1-D Solid Heat Conductor is illustrated in Figure 2-12 (see also Volume 1, description of the SC boundary conditions). <i>Acceptable range:</i> elevations of the boundary surfaces that transfer heat to Control Volumes must lie within the elevations of the corresponding Control Volumes <i>Default value:</i> 0.0

SPECTRA Code Manuals - Volume 2: User's Guide

- W-5 (I) : IVERSC Vertical orientation of conductor, (-), see Figure 2-11.
 Rectangular: IVERSC = 0 : vertical wall
 IVERSC = +1 : horizontal wall, left surface up
 IVERSC = -1 : horizontal wall, left surface down
 Cylindrical: IVERSC = 0 : vertical cylinder
 IVERSC = +1 : horizontal cylinder
 Acceptable range: -1, 0, +1
 Default value: 0
- W-6 (R) : POWRSC Internal power source, (W). In order to obtain the current internal source, the value of POWRSC is multiplied by the time dependent multiplier defined by IPOWSC (word 7) and by the constant multiplier POWMSC (word 9), if present.
 Acceptable range: $-10^{10} \leq \text{POWRSC} \leq 10^{10}$.
 Default value: 0.0 .

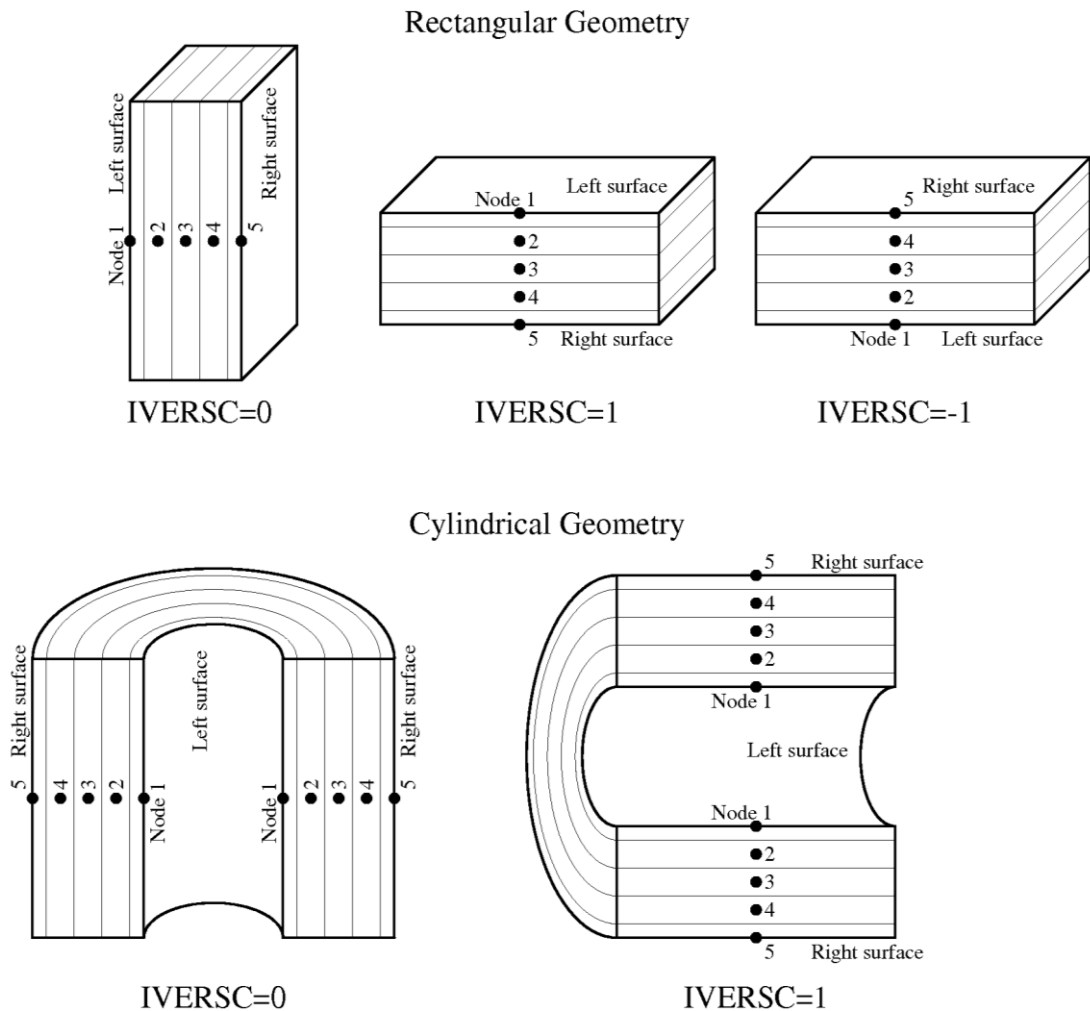


Figure 2-11 Vertical orientations of 1-D Solid Heat Conductors

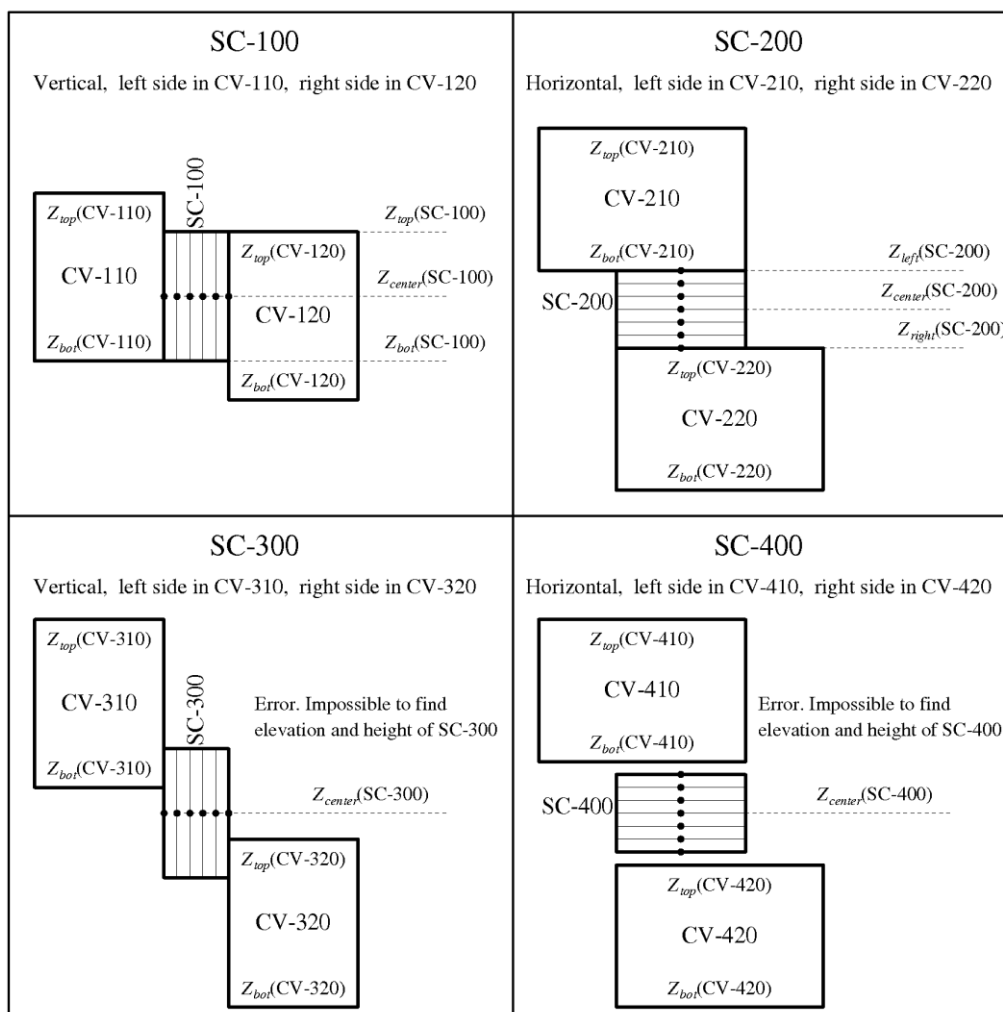


Figure 2-12 Automatic allocation of SC within the boundary Control Volumes

W-7 (I) : IPOWSC Pointer to a Tabular or Control Function which defines the internal power multiplier. If the number is equal to zero, then internal power source is constant, and equal to POWRSC (Word 6). If the number is positive, then the internal power multiplier will be defined by the Tabular Function IPOWSC. If it is negative the multiplier will be defined by the Control Function |IPOWSC|. No lower or upper limit is imposed on the value obtained from a Tabular or Control Function (thus a negative power source is allowed). If there is no internal power source (POWRSC=0.0) then IPOWSC must also be equal to zero.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-8 (R) : HINCSC Inclination of nearly horizontal tubes, (degree). Tubes that have small inclination should be modelled as horizontal (IVERSC= ± 1 , see Word 5 above) with HINCSC $> 0.0^\circ$. The value is used by the condensation model.
Acceptable range: $0.0^\circ \leq \text{HINCSC} \leq 20.0^\circ$.
Default value: 0.0° .
- W-9 (R) : POWMSC Constant power multiplier. The constant power multiplier is introduced to have an easy way of defining for example axial power profile.
Acceptable range: $-10^{10} \leq \text{POWMSC} \leq 10^{10}$
Default value: 1.0

2.3.2 Records: 301000, SC Groups - General Data

- W-1 (I) : KGRPSC Default SC group number. SC groups are introduced for editing; at the end of input processing volumes and masses of all materials is printed for each SC group. SC groups may be used to check the volumes and masses of materials in primary system, secondary system, etc.
Acceptable range: $1 \leq \text{KGRPSC} \leq 20$
Default value: 1

2.3.3 Records: 301XXX, Initial and Transient Temperatures, SC Group Data

XXX is the Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

This record is optional. All entries from this record have their default values, recommended for general application.

- W-1 (I) : INTSC Initial temperature calculation indicator.
1: Initial temperature distribution is calculated. If this option is selected, the program calculates temperature distribution performing conduction calculation with a large ($\Delta t=10^{99}$ s) time step. In rare cases convergence failure may be encountered when performing the initial step. Usually it is good to ignore the convergence failure, since the calculated initial temperatures are typically better than could be obtained by manual initialization. The convergence failure can be ignored, by setting IACSFL (Word 8 in record 920000 - see section 2.16.5).
2: Input values (Words 4 in records 310XXX) are used. Use this option also if temperatures should be read from an Initial Condition File - ICF (section 2.16.3).
Acceptable range: 1, 2.
Default value: 2 .
- W-2 (R) : ITYPSC Transient temperature calculation indicator.

SPECTRA Code Manuals - Volume 2: User's Guide

- 1: Temperatures are time independent; that means the initial temperatures are kept through the transient.
- 2: Transient temperatures are calculated from conduction equation (normal SC type).

Acceptable range: 1, 2.

Default value: 2.

W-3 (I) : IGRPSC SC group number. SC groups are introduced for editing; at the end of input processing volumes and masses of all materials is printed for each SC group. SC groups may be used to check the volumes and masses of materials in primary system, secondary system, etc.
Acceptable range: $1 \leq \text{IGRPSC} \leq 20$
Default value: KGRPSC (defined in record 301000)

2.3.4 Records: 302XXX, Multiplicity of the 1-D Solid Heat Conductor

XXX is the Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

W-1 (R) : XMLTSC Multiplicity of the 1-D solid conductor. This is the number of solid conductors that are identical to the conductor XXX. If XMLTSC<0 then multiplicity will be time-dependent and defined by a Control Function with reference number $|\text{-XMLTSC}|$.
Acceptable range: $0.0 < \text{XMLTSC} < 10^{10}$ or CF reference number
Default value: 1.0 .

2.3.5 Records: 303000, Numerical Integration Method, Global Activator

W-1 (I) : NIMGSC Numerical integration method - Figure 2-13.
=1: Nodes at cell-centers.
 This was the only method available in earlier SPECTRA versions
=2: Nodes at cell-edges (used in MELCOR, RELAP, etc.).
 An advantage is an more accurate stationary state temperature distribution in case of a coarse nodalization and nonuniform power profile - see Volume 3, section: "Integration methods 1 and 2 -Non-uniform Power, Comparison with MELCOR").
Acceptable range: 1 and 2
Default value: 1

W-2 (I) : NDGSC For numerical integration method 2, this is the node number for axial conduction or direct contact conduction.
=1: left boundary node,
=2: right boundary node,
=3: average of the left and right boundary nodes.
Acceptable range: 1, 2, 3
Default value: 1

2.3.6 Records: 303XXX, Numerical Integration Method, Individual Activators

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

- W-1 (R) : NIMISC Numerical integration method - Figure 2-13.
 =1: Nodes at cell-centers.
 This was the only method available in earlier SPECTRA versions
 =2: Nodes at cell-edges (used in MELCOR, RELAP, etc.).
 An advantage is an more accurate stationary state temperature
 distribution in case of a coarse nodalization and nonuniform
 power profile - see Volume 3, section: "Integration methods 1
 and 2 -Non-uniform Power, Comparison with MELCOR").
 Note! Method 2 is used only for temperature distribution calculation.
 The fission product diffusion is always calculated using the Method 1.
 The diffusion results are practically independent of the method used for
 temperature calculation. The only difference is introduced by the
 temperature-dependent diffusion coefficient. If Method 1 is used, then
 there is a direct correspondence between the temperature nodes and the
 diffusion nodes. In such case the diffusion coefficient in cell i is obtained
 using the temperature in the same cell: $D_i = f_i(T_i)$. If Method 2 is used,
 the diffusion coefficient in a given cell is obtained using the average
 temperature of the two temperature nodes bounding the computational
 cell: temperature in the same cell: $D_i = f_i((T_i + T_{i+1})/2)$.
 Acceptable range: 1 and 2.
 Default value: NIMGSC
- W-2 (I) : NDISC For NIMISC=2, this is the node number for axial conduction or direct
 contact conduction.
 =1: left boundary node,
 =2: right boundary node,
 =3: average of the left and right boundary nodes.
 Note: implicit solution of direct contact is available only for NDISC = 1
 or 2. For these values the minimum resistance is 10^{-5} (m-K/W). For
 NDISC=3, the minimum resistance is equal to 10^{-3} (m-K/W) - see
 description of IHAXSC, record 390XXX).
 Acceptable range: 1, 2, 3
 Default value: NDGSC

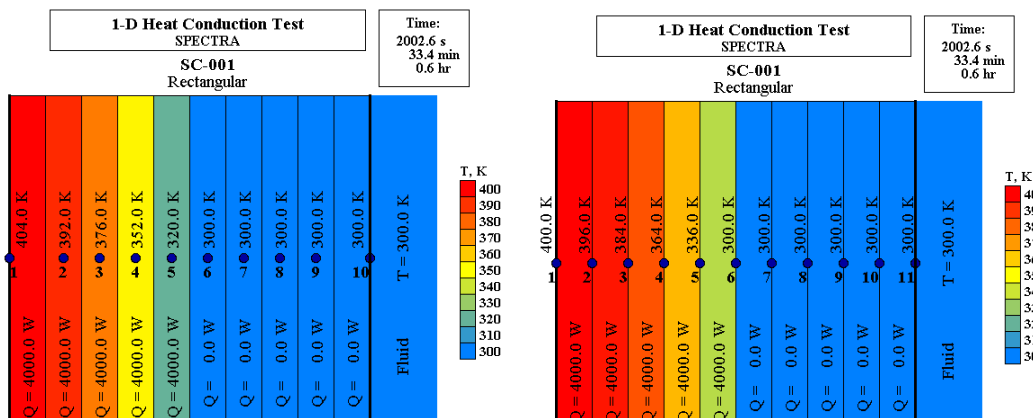


Figure 2-13 Numerical integration methods:
 left: SPECTRA original method, nodes at cell centers
 right: MELCOR/RELAP method, nodes at cell edges

2.3.7 Records: 304XXX, Optional Size Change During Transient

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

W-1 (I) : IAHTSC Pointer to a Tabular or Control Function that defines a multiplier on the SC size (left and right surface area) during the transient. If the number is positive, then the multiplier will be defined by a Tabular Function with the reference number: IAHTSC. If the number is negative, then the multiplier will be defined by a Control Function with the reference number: $|IAHTSC|$. The value obtained from the Tabular or Control Function will be internally limited to the range between 10^{-6} and 1.0. The thickness and node sizes are not affected. If the size change is applied and the SC has an internal heat source, the source strength will follow the size change (i.e. the power density, W/m^3 , will remain the same). The plot parameter SC-xxx-Qcel-xxxx, giving the power generation in each cell, is however not reflecting this fact (it gives power of the “full size” SC, independently of the value of the multiplier). The model can be used for SCs with direct contact (records 390XXX) but in such case the SC size multiplier should be made the same for the SCs that are in contact.

The size change can be applied for the cases when:

1. SC surfaces are convecting heat,
2. simple radiation-model between the SC surface and gas is used,
3. structure-to-structure radiation model is used.

Examples of all three cases are shown in Volume 3. The model cannot be used if SC is a member of the detailed radiation model network (section 2.6), because the radiation view factors do not change in time.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 1

2.3.8 Records: 305XXX, Name of the 1-D Solid Heat Conductor

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

W-1 (A) : NAMESC User defined name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.
Acceptable range: any string of up to 50 characters.
Default value: 50 "underline" characters: "_" .

2.3.9 Records: 310XXX, Cell Data

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

Several records with the same number may be entered. Each record with this number contains data for NC cells. Cell data are read sequentially - the first record in the input is interpreted as containing the data for the first (leftmost) NC cells. The total number of cells of a 1-D Solid Heat Conductor may not exceed 100 and may not be smaller than 2.

W-1 (R) : CELLSC Cell width, (m). For the boundary cells the cell width is compared to the thermal penetration depth (see Volume 1):

$$d_{pen}(t) = C \cdot \sqrt{at} = 7.09 \cdot \sqrt{k / (\rho \cdot c_p) \cdot t}$$

A warning message is printed if:

$$\text{CELLSC} > d_{pen}(10^2) = 70.9 \cdot (k / (\rho \cdot c_p))^{1/2}.$$

An error message is issued if:

$$\text{CELLSC} > d_{pen}(10^4) = 709 \cdot (k / (\rho \cdot c_p))^{1/2}.$$

Acceptable range: $0.0 < \text{CELLSC} < 10^{10}$.

Default value: none.

W-2 (I) : MATCSC Pointer to a material number, (-). Each cell is assumed to be composed of a single material defined by this word.

Acceptable range: must be a valid reference number of a solid material, defined in records 801XXX, 802XXX, 803XXX - see section 2.10).

Default value: none.

W-3 (R) : QFRCSC Relative power density in this cell, (-). The values are relative and may be scaled by any factor. The values will be normalized during the input

SPECTRA Code Manuals - Volume 2: User's Guide

processing so that the total internal power source of the conductor is always equal to POWRSC multiplied by the value of the Tabular or Control Function |IPOWSC| (if used). If the internal power source, POWRSC, is greater than zero, then QFRCSC must be greater than zero for at least one cell. If the internal power source, POWRSC, is equal to zero, then QFRCSC must be equal to zero for all cells.

Acceptable range: $0.0 \leq \text{QFRCSC} \leq 10^{10}$.

Default value: 0.0 .

- W-4 (R) : TINCSC Initial cell temperature, (K). Used only if INTSC=2 (section 2.3.3).
 If NIMISC=1 (nodes at cell-centers) this is the center temperature of the cell.
 If NIMISC=2 (nodes at cell-edges) this is the left temperature of the cell.
 The right temperature of the last cell is in such case specified in record 311XXX.
Acceptable range: $273.0 \leq \text{TINCSC} \leq 10,000.0$.
Default value: none.
- W-5 (I) : NC Number of cells. Data words 1 - 4 are applied for NC cells, starting from the cell number NF, if a nonzero value is specified for Word 6, otherwise from the cell number N+1, where N is the sum of NC for all previous records with this number.
Acceptable range: ≥ 1 . The total number of cells, equal to the sum of NC entered in all records, NCELSC = $\sum(\text{NC})$, must be within the range of: $2 \leq \text{NCELSC} \leq 100$.
Default value: 1
- W-6 (I) : NF Starting cell number. If this number is missing, the starting cell is the first yet unspecified cell, i.e. cell N+1, where N is the sum of NC for all previous records with this number. If NF=N+1, this record defines data for a new cell or cells. If NF<N+1, this is a replacement data.
Acceptable range: $1 \leq \text{NF} \leq \text{N}+1$, where N is the sum of NC for all previous records with this number
Default value: N+1

Example 1: five cells with material 101, two cells with material 102:

*	x-cell	Mat	Power	T (K)	NC	NF	
310101	0.001	101	0.0	300.0	5		* data for cells 1-5, Mat. 101
310101	0.001	102	0.0	300.0	2		* data for cells 6-7, Mat. 102

Example 2: three cells with material 101, two cells with material 105, two cells with material 102:

*	x-cell	Mat	Power	T (K)	NC	NF	
310101	0.001	101	0.0	300.0	5		* data for cells 1-5, Mat. 101
310101	0.001	102	0.0	300.0	2		* data for cells 6-7, Mat. 102
310101	0.001	105	0.0	300.0	2	4	* data for cells 4-5 redefined to Mat. 105

2.3.10 Records: 311XXX, Right Surface Temperature

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

This record is needed if the second numerical integration method is used, NIMISC=2 (nodes at cell-edges).

W-1 (R) : TINRSC Initial temperature at the right surface of SC. This is the right surface temperature of the last cell. The left surface temperatures for all cells are defined in the records 310XXX.
Acceptable range: $273.0 \leq \text{TINRSC} \leq 10,000.0$.
Default value: temperature of the previous node.

2.3.11 Records: 321XXX, Left (Inside) Side Boundary Conditions

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

W-1 (I) : IVLLSC Control Volume number for convective heat transfer. The value specifies the Control Volume, which is associated with the left (inside) boundary surface. If zero is entered, then the left surface is either insulated, or the convective heat transfer coefficient and the fluid temperature are specified by Tabular or Control Functions (defined by words 3 and 4 below). If $\text{IVLLSC} > 0$, then heat is transferred to/from the CV using the standard heat and mass transfer package (Volume 1). It is also possible to overrule the use of the standard heat and mass transfer package, and use a Tabular or Control Function (defined by word 3 below) to determine the heat transfer coefficient. Also the fluid temperature can be altered by a Tabular or Control Function, by using the Word 4 below. In such case the value obtained from the Tabular or Control Function will be taken with weighting factor of 0.5, and the true (Control Volume) fluid temperature will be taken with the weighting factor of 0.5. If the heat transfer coefficient or the fluid temperature are defined by Tabular or Control Functions, then only heat transfer will occur on the surface, mass transfer (boiling/condensation) will not be calculated.
Acceptable range: must be a valid reference number of a Control Volume, if non-zero.
Default value: 0 .

W-2 (R) : HGTLSC Height of the left surface of the SC (elevation difference between the uppermost and the lowermost point of the surface). Used only if $\text{IVLLSC} > 0$. Used to determine pool and atmosphere fractions in case the surface is partly covered by pool.
Acceptable range: $0 \leq \text{HGTLSC} < 10^{10}$.
Default value: RECTANGULAR geometry (IGEOSC=1):

- HORIZONTAL (IVERSC≠0):
zero .
- VERTICAL (IVERSC=0):
square root of the surface area, given by
SIZE SC (section 2.3.1). It is appropriate for
square surfaces, thus for a rectangular
geometry the default value should not
generally be used. The appropriate value,
wall height, should be entered.
- CYLINDRICAL geometry (IGEOSC=2):
- HORIZONTAL (IVERSC≠0):
inner diameter, calculated from XOSC.
- VERTICAL (IVERSC=0):
cylinder length, given by SIZE SC.
- SPHERICAL geometry (IGEOSC=3):
inner diameter, calculated from XOSC.

W-3 (I) : IHTLSC Pointer to a Tabular or Control Function defining the convective heat transfer coefficient (HTC) at the left surface. If zero then the HTC is calculated by the code for the thermal-hydraulic conditions taken from the volume IVLLSC (Word 1). If the value is positive, HTC will be defined by the Tabular Function IHTLSC. If it is negative, it will be defined by the Control Function $|IHTLSC|$. The units of the quantities obtained from the Tabular or Control Function are assumed to be (W/m²/K). If the obtained value is negative, it will be set to zero. Note that if IHTLSC≠0 then the fluid temperature, needed to calculate the boundary heat flux, is taken as:

- if IVLLSC>0 then the fluid temperature in Control Volume IVLLSC is used.
- if ITPLSC≠0 then the fluid temperature is given by a Tabular or Control Function, defined by ITPLSC (word 4 below).
- if IVLLSC=0 and ITPLSC=0 then the fluid temperature is set to 300 K.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0 .

W-4 (I) : ITPLSC Pointer to a Tabular or Control Function defining the fluid temperature at the left surface for convective heat transfer. If the value is positive, the fluid temperature will be defined by the Tabular Function ITPLSC. If it is negative, it will be defined by the Control Function $|ITPLSC|$. The units of quantity obtained from the Tabular or Control Function are assumed to be (K). If the obtained value is negative, it will be set to zero. If ITPLSC≠0 and IVLLSC>0 (heat transfer to a Control Volume), then the value obtained from Tabular or Control Function will be used with the weighting factor of FINTSC. The true fluid temperature (from Control Volume) will be used with the weighting factor of 1.0–FINTSC. Boiling and condensation models will be disabled by setting CSFLSC to –1.0 and ICNLSC to –4. In the past the input combination of IPTLSC≠0 and IVLLSC>0 was used to perform temperature averaging for heat exchangers. Currently it is not recommended to use this method. A more

elaborate temperature averaging model has been developed, and is available through input records 325XXX, 326XXX (see sections 2.3.15 and 2.3.16).

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0.

W-5 (I) : IQLSC Indicator for non-convective heat flux at the left boundary. The heat flux defined by this pointer is used only on the uncovered part of the SC (above water level). With this pointer a user can model in a simple way radiative heat transfer. If the net enclosure thermal radiation model is used, and this surface is associated with one of the radiating surfaces (section 2.6.3), then this parameter must not be used. The meaning is as follows:

IQLSC>1000:

Simple radiation model between the left SC surface and atmosphere gas is used to determine the non-convective heat transfer. The grey gas model is used, atmosphere is assumed to be opaque (the reason for assuming opaque atmosphere is discussed in Volume 3). The heat flux is equal to:

$$q = \varepsilon(T_w)\sigma(T_w^4 - T_g^4)$$

where $\varepsilon(T_w)$ is the wall emissivity, σ is the Stefan-Boltzmann constant, T_w , T_g are the wall and gas temperatures respectively. The emissivity is obtained from the Tabular Function number: (IQLSC – 1000). The argument for the Tabular Function is the wall surface temperature, (K).

0<IQLSC<1000:

The heat flux is obtained from the Tabular Function number IQLSC. The units of the quantities obtained from the Tabular Function are assumed to be: (W/m²). Positive heat flux means that the heat is emitted from the surface.

IQLSC<0:

The heat flux is obtained from the Control Function number |IQLSC|. The units of the quantities obtained from the Control Function are assumed to be: (W/m²). Positive heat flux means that the heat is emitted from the surface.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0.

W-6 (I) : INCLSC Configuration indicator for natural convection. The value is used only when IVLLSC is positive. The meaning of this variable is as follows:

Rectangular geometry: 0 vertical wall,
 -1 horizontal wall facing down,
 +1 horizontal wall facing up.

Cylindrical geometry: 0 vertical cylinder,
 -1 horizontal cylinder, inside,

SPECTRA Code Manuals - Volume 2: User's Guide

Spherical geometry: +1 horizontal cylinder, outside.
 -1 sphere, inside,
 +1 sphere, outside.

Default values are provided for each geometrical configuration, based on IGEO SC and IVER SC parameters (section 2.3.1) - see Table 2-6 and Table 2-7.

Acceptable range: -1, 0, +1.

Default value: RECTANGULAR geometry (IGEO SC=1):
 - VERTICAL (IVER SC=0): 0,
 - HORIZONTAL down (IVER SC=-1): -1,
 - HORIZONTAL up (IVER SC=+1): +1,
 CYLINDRICAL geometry (IGEO SC=2):
 - VERTICAL (IVER SC=0): 0,
 - HORIZONTAL (IVER SC=±1): -1,
 SPHERICAL geometry (IGEO SC=1): -1.

W-7 (R) : DNCLSC Characteristic dimension for natural convection at the left boundary surface, (m). The value is used only when IVLLSC is positive. A best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DNCLSC should be equal to (see Table 2-6 and Table 2-7): for vertical plates - height; for horizontal plates - width; for vertical cylinders - cylinder length; for horizontal cylinders - maximum of length and 2 times the inner diameter; for spheres - inner diameter. Note that the default value for plates (rectangular geometry) is only appropriate for the square surfaces.

Acceptable range: $0.0 < DNCLSC < 10^{10}$.

Default value: height, given by HGTLSC (Word 2 above). If HGTLSC is equal to zero (horizontal rectangular surfaces) then the square root of the surface area, given by SIZE SC (section 2.3.1). The value is appropriate for square surfaces. Thus for horizontal rectangular surfaces the default value should not generally be used. The appropriate value, width, should be entered.

CYLINDRICAL geometry (IGEO SC=2):
 inner diameter, calculated from XOSC (section 2.3.1).

SPHERICAL geometry (IGEO SC=3):
 inner diameter, calculated from XOSC (section 2.3.1).

W-8 (I) : IFCLSC Configuration indicator for forced convection, as well as the nucleate boiling model and the model for critical heat flux calculation. The value is used only when IVLLSC is positive and no alternative liquid is used. For the alternative liquid the forced convection correlation is selected by Word 21 (IHCLSC). The meaning of this variable is as follows:

-1 internal flow, Chen correlation for nucleate boiling, Zuber and USSR Academy of Science models for critical heat flux calculations (Zuber for non-flow, USSR A. S. for flow conditions).

SPECTRA Code Manuals - Volume 2: User's Guide

+1 external flow, Rohsenow correlation for nucleate boiling, Zuber model for critical heat flux calculation.

Default values are provided for each geometrical configuration, based on IGEO SC (section 2.3.1) - see Table 2-8 and Table 2-9.

Acceptable range: -1, +1.

Default value: -1.

W-9 (R) : DFCLSC Characteristic dimension for forced convection at the left boundary surface, (m). The value is used only when IVLLSC is positive. A best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DFCLSC should be equal to (see Table 2-8 and Table 2-9): for internal flow - hydraulic diameter; for external flow - width (rectangular wall). Note that for cylinders and spheres the external flow type, defined by IFCLSC (see above) is not available. For the internal flow type the default value is the same as for the external flow type. Therefore for the internal flow type the default value should not be used. The appropriate value (hydraulic diameter) should be entered.

Acceptable range: $0.0 < DFCLSC < 10^{10}$.

Default value: RECTANGULAR geometry (IGEO SC=1):
 HGTLSC (if entered) or square root of the surface area, given by SIZE SC (section 2.3.1). The value is appropriate for square surfaces. Thus for rectangular geometry the default value should not generally be used. The appropriate value should be entered: for internal flow - hydraulic diameter, for external flow - width.

CYLINDRICAL geometry (IGEO SC=2):
 inner diameter, calculated from XOSC (section 2.3.1).

SPHERICAL geometry (IGEO SC=3):
 inner diameter, calculated from XOSC (section 2.3.1).

W-10 (I) : IFBLSC Configuration indicator for film boiling. The value is used only when IVLLSC is positive. The meaning of this variable is as follows:

- 0 vertical surface,
- ±1 horizontal cylinder,
- 1 horizontal plate, facing down,
- +1 horizontal plate, facing up.

Default values are provided for each geometrical configuration, based on IGEO SC and IVERSC (section 2.3.1) - see Table 2-10 and Table 2-11.

Acceptable range: -1,0, +1.

Default value: RECTANGULAR geometry (IGEO SC=1):
 - VERTICAL (IVERSC=0): 0.
 - HORIZONTAL down (IVERSC=-1): -1,
 - HORIZONTAL up (IVERSC=+1): +1,
 CYLINDRICAL geometry (IGEO SC=2):
 - VERTICAL (IVERSC=0): 0,
 - HORIZONTAL (IVERSC=±1): +1,
 SPHERICAL geometry (IGEO SC=1): +1.

- W-11 (R) : DFBLSC Characteristic dimension for film boiling at the left boundary surface, (m). The value is used only when IVLLSC is positive. A best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DFBLSC should be equal to (see Table 2-10 and Table 2-11): for vertical walls - height; for horizontal plates - width; for cylinders and spheres - inner diameter.
Acceptable range: $0.0 < DFBLSC < 10^{10}$.
Default value: RECTANGULAR geometry (IGEOSC=1):
 square root of the surface area, given by SIZESC (section 2.3.1). The value is appropriate for square surfaces. Thus for rectangular geometry the default value should not generally be used. The appropriate value should be entered: for internal flow - hydraulic diameter, for external flow - width.
 CYLINDRICAL geometry (IGEOSC=2):
 - VERTICAL (IVERSC = 0):
 length, given by SIZESC (section 2.3.1);
 - HORIZONTAL (IVERSC = ±1):
 inner diameter, calculated from XOSC.
 SPHERICAL geometry (IGEOSC=3):
 inner diameter, calculated from XOSC.
- W-12 (I) : ICNLSC Configuration indicator for condensation. The value is used only when IVLLSC is positive. The meaning of this variable is as follows:
 ≤ -4 model disabled
 $= -3$ condensation on horizontal wall facing up,
 $= -2$ condensation on horizontal wall facing down,
 $= -1$ condensation inside horizontal tubes,
 $= 0$ condensation on vertical walls,
 $= +1$ condensation on outside surface of horizontal tube.
 $\geq +2$ condensation on outside surface of horizontal tube bank. ICNLSC is equal to the number of vertical rows of tubes.
 Default values are provided for each geometrical configuration based on IGEOSC and IVERSC (section 2.3.1) - see Table 2-12 and Table 2-13.
Acceptable range: all integers.
Default value: RECTANGULAR geometry (IGEOSC=1):
 - VERTICAL (IVERSC=0): 0;
 - HORIZONTAL down (IVERSC=-1): -2;
 HORIZONTAL up (IVERSC=+1): -3;
 however, if fins are present
 (ITFLSC>0) then: 0;
 CYLINDRICAL geometry (IGEOSC=2):
 - VERTICAL (IVERSC=0): 0;
 - HORIZONTAL (IVERSC=±1): -1;
 SPHERICAL geometry (IGEOSC=3): -1.
- W-13 (R) : DCNLSC Characteristic dimension for condensation at the left boundary surface, (m). The value is used only when IVLLSC is positive. Best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DCNLSC

should be equal to (see Table 2-12 and Table 2-13): for vertical walls (or cylinders) - wall height; inside horizontal tubes - inner diameter; outside surface of horizontal tubes or tube banks - outer diameter; horizontal walls facing up - maximum film thickness (equilibrium thickness of water layer with free fall of liquid at the edges of the wall). The condensation type is defined by ICNLSC (word 12).

In case of vertical walls the user may wish divide the total wall into a certain number of segments, modelled by separate conductors. Thus the conductors are stacked one over the other. To take into account the behavior of the condensate film in this case the characteristic dimension of the conductor number k in the stack (counting from the top) should be defined as follows:

$$DCNLSC(k) = \left(\frac{z_{BOT}(k)^{5/4} - z_{TOP}(k)^{5/4}}{z_{BOT}(k) - z_{TOP}(k)} \right)^4$$

where: $z_{BOT}(k)$ distance from the bottom of the conductor k to the top of the stack, (m),
 $z_{TOP}(k)$ distance from the top of the conductor k to the top of the stack, (m).

If the height of each conductor in the stack is identical then the above formula reduces to:

$$DCNLSC(k) = \left(k^{5/4} - (k-1)^{5/4} \right)^4 \frac{H}{N}$$

where: H - total height of the wall, (m),
 N - number of conductors in the stack.

The ratio: (H/N) is the height of a single conductor in the stack. Note that only for $k=1$ DCNLSC is equal to the physical height of the conductor, (H/N) . For $k>1$ DCNLSC is greater than (H/N) . For $k=N$ DCNLSC is always greater than the total wall height, H .

Acceptable range: $0.0 < DCNLSC < 10^{10}$.

Default value: height, given by HGTLSC (Word 2 above). For horizontal walls facing up the default value is 10^{-2} .

W-14 (R) : CSFLSC The constant C_{sf} in the Rohsenow equation for nucleate boiling (see Volume 1). The values of C_{sf} for different surfaces are given in the Table 2-3. Entering a negative value will disable the full boiling model.
Acceptable range: all reals.
Default value: 0.013 .

Table 2-3 Values of C_{sf} for Rohsenow correlation.

Surface type	C_{sf}	Surface type	C_{sf}
Nickel	0.0060	Platinum	0.0130
Ground and polished stainless steel	0.0080	Brass	0.0060
Teflon pitted stainless steel	0.0058	Polished copper	0.0128
Chemically etched stainless steel	0.0133	Lapped copper	0.0147
Mechanically polished stainless steel	0.0132	Scored copper	0.0068

- W-15 (I) : MCFLSC Critical heat flux model selection. The value is used only when IVLLSC > 0.
- 1 Zuber pool boiling correlation with Ivey-Morris correction for subcooling.
 - 2 Combination of model based on USSR Academy of Sciences CHF look-up tables for high flow, with Zuber and Ivey-Morris for low flow.
 - 3 Combination of Biasi correlation for high flow, with Zuber and Ivey-Morris for low flow.
 - 4 Groeneveld (1986) look-up tables.
- <0 CHF is calculated by a user-defined Control Function with the number |MCFLSC|.
- Acceptable range:* 1, 2, 3 or reference to a Control Function
Default value: 2.
- W-16 (I) : MNCLSC Selection of model for the influence of non-condensable gases for condensation. The value is used only when IVLLSC is positive and ICNLSC is greater than -4. The meaning of this variable is as follows:
- 1 Kuhn-Shrock-Petersen (KSP) correlations - recommended for condensation on the inside surface of tubes,
 - 2 Ogg correlations,
 - 3 Modified Ogg correlations - recommended for condensation on the outside surface of tubes, plates, etc.
- Default values are provided - see Table 2-14 and Table 2-15.
Acceptable range: 1, 2, 3.
Default value: 3.
- W-17 (R) : CFDLSC Indicator of condensate film drainage behaviour.
- If the value is positive then CFDLSC is the height of the left SC surface. The elevation of the lowermost point of this surface is equal to the elevation of its center point, minus CFDLSC/2.0. The drainage from this surface is either deposited in the pool of a CV (if the lowest point of the surface is immersed in pool), or converted to droplets and suspended in the atmosphere of a CV as "rain" drops (if the lowest point of the surface is not immersed in the pool).
- If the value is negative then the drainage is assumed to be deposited on a surface of other (lower) Solid Conductor. The absolute value of CFDLSC must then be equal to the number of SC at the bottom of the stack.
- The use of the drainage parameter, CFDLSC, and the condensation characteristic dimension, DCNLSC, in case of individual and stacked

conductors is illustrated in Figure 2-14 (see also Volume 3). The length of all conductors is assumed to be 0.5 m. Appropriate values of DCNLSC and CFDLSC are shown in Table 2-4.

Acceptable range: if $CFDLSC < 0.0$ then the left surface of SC No. $|CFDLSC|$ must be connected to a Control Volume (not necessarily equal to IVLLSC), if $CFDLSC > 0.0$ then the bottom elevation of the left surface (center point elevation minus $CFDLSC/2.0$) must be within the boundary Control Volume.

Default value: the default value is set to twice the distance between the center point of the left surface and the bottom of the boundary Control Volume. That value will result in deposition of condensate always in the pool. This is done to avoid numerical problems, and time step reduction, when condensate is converted into droplets.

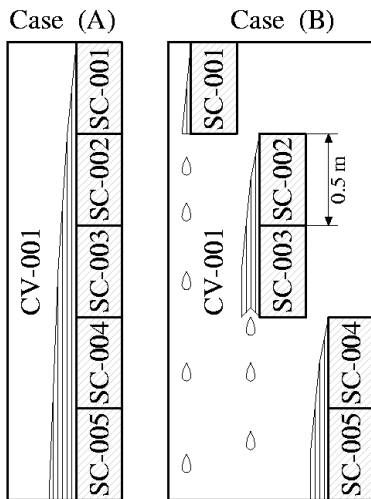


Figure 2-14 Condensation example cases (A) and (B).

Table 2-4 Values of DCNLSC and CFDLSC for the example cases (A) and (B).

SC	Case (A)		Case (B)	
	DCNLSC	CFDLSC	DCNLSC	CFDLSC
1	$0.5 \cdot (1^{5/4} - 0^{5/4})^4 = 0.50$	-5.0	0.50	0.5
2	$0.5 \cdot (2^{5/4} - 1^{5/4})^4 = 1.81$	-5.0	$0.5 \cdot (1^{5/4} - 0^{5/4})^4 = 0.50$	-3.0
3	$0.5 \cdot (3^{5/4} - 2^{5/4})^4 = 3.04$	-5.0	$0.5 \cdot (2^{5/4} - 1^{5/4})^4 = 1.81$	0.5
4	$0.5 \cdot (4^{5/4} - 3^{5/4})^4 = 4.26$	-5.0	$0.5 \cdot (1^{5/4} - 0^{5/4})^4 = 0.50$	-5.0
5	$0.5 \cdot (5^{5/4} - 4^{5/4})^4 = 5.48$	0.5	$0.5 \cdot (2^{5/4} - 1^{5/4})^4 = 1.81$	0.5

SPECTRA Code Manuals - Volume 2: User's Guide

- W-18 (I) : IHDLSC Indicator of CV flow direction relative to the left SC surface. Used only for rectangular (IGEOSC=1) SC's. The meaning is:
 For vertical SC's (IVERSC=0):
 0: CV horizontal flow is parallel, $v_{SC} = (v_{CV,ver}^2 + v_{CV,hor}^2)^{1/2}$,
 1: CV horizontal flow is perpendicular, $v_{SC} = v_{CV,ver}$.
 For horizontal SC's (IVERSC<>0):
 0: CV vertical flow is parallel, $v_{SC} = (v_{CV,ver}^2 + v_{CV,hor}^2)^{1/2}$,
 1: CV vertical flow is perpendicular, $v_{SC} = v_{CV,ver}$.
Acceptable range: $0 \leq \text{IHDLSC} \leq 1$.
Default value: 0 .
- W-19 (I) : THTLSC Contact angle, θ , (degree). Used to determine the diameter of bubbles created during nucleate boiling: $D = 0.0208 \cdot \theta \cdot (\sigma/g/(\rho_{liq} - \rho_{gas}))^{(1/2)}$.
Acceptable range: $10^\circ \leq \text{THTLSC} \leq 180^\circ$.
Default value: 96° .
- W-20 (R) : XRBLSC Multiplier for convective heat transfer, X_{RB} .
 XRBLSC<0.0: HTC is multiplied by |XRBLSC| in both natural and force convection. It may be used to obtain a conservative estimation of heat transfer.
 XRBLSC>0.0: HTC is multiplied by XRBLSC only in case of turbulent forced convection (FC-TUR), internal flow (IFCLSC = -1). It is intended to allow the user to define a rod bundle multiplier in forced convection:

$$Nu_{tur} = X_{RB} 0.023 Re^{0.8} Pr^{0.4}$$

 Appropriate values for parallel flow and cross-flow may be found in literature. The ratio of pitch over diameter is a good approximation (see Volume 1, description of forced convection correlations):

$$X_{RB} = P / D$$

 For tube arrangements other than equilateral triangle pitch, the multiplier is given by:

$$X_{RB} = \left(\frac{P_1 \cdot P_2}{D^2} \right)$$

 Note that the rod bundle multiplier may be different for different fluids. For example, for the liquid metals the value may even show different tendency (see Volume 1, description of liquid metals correlations):

$$X_{RB} = 1 - \exp[-3.8 \cdot (P/D - 1)]$$

Acceptable range: $0.0 \leq |\text{XRBLSC}| \leq 10^6$
Default value: XRBLHT
 (global activator, defined in the record 810020)
- W-21 (I) : IHCLSC Selection of heat transfer correlation for alternative fluid.
Acceptable range: one of the correlations defined in records 843XXX or 843YYY
Default value: rectangular: 1, cylindrical: 2, spherical: 3.

2.3.12 Records: 322XXX, Right (Outside) Side Boundary Conditions

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 1-D Solid Heat Conductors is 550 (999 in LINUX version).

W-1 (I) : IVLRSC Control Volume number for convective heat transfer. The value specifies the Control Volume, which is associated with the right (outside) boundary surface. If zero is entered then the right surface is either insulated, or the convective heat transfer coefficient and fluid temperature are specified by Tabular or Control Functions (defined by words 3 and 4 below). If $IVLRSC > 0$ then heat is transferred to/from the CV using the standard heat and mass transfer package (Volume 1). It is also possible to overrule the use of the standard heat and mass transfer package, and use a Tabular or Control Function (defined by word 3 below) to determine the heat transfer coefficient. Also the fluid temperature can be altered by a Tabular or a Control Function, by using the Word 4 below. In such case the value obtained from the Tabular or Control Function will be taken with weighting factor of 0.5, and the true (Control Volume) fluid temperature will be taken with the weighting factor of 0.5. If the heat transfer coefficient or the fluid temperature are defined by Tabular or Control Functions, then only heat transfer will occur on the surface, mass transfer (boiling/condensation) will not be calculated.

Acceptable range: must be a valid reference number of a Control Volume, if non-zero.

Default value: 0 .

W-2 (R) : HGTRSC Height of the right surface of the SC (elevation difference between the uppermost and the lowermost point of the surface). Used only if $IVLRSC > 0$. Used to determine pool and atmosphere fractions in case the surface is partly covered by pool.

Acceptable range: $0 \leq HGTRSC < 10^{10}$.

Default value: RECTANGULAR geometry (IGEOSC=1):

- HORIZONTAL (IVERSC≠0): zero.
- VERTICAL (IVERSC=0):
square root of the surface area, given by SIZE SC (sec. 1.3.1). It is appropriate for square surfaces, thus for a rectangular geometry the default value should not generally be used. The appropriate value, wall height, should be entered.

CYLINDRICAL geometry (IGEOSC=2):

- HORIZONTAL (IVERSC≠0):
outer diameter, calculated from X0SC and CELLSC.
- VERTICAL (IVERSC=0):
cylinder length, given by SIZE SC.

SPHERICAL geometry (IGEOSC=3):

outer diameter, calculated from X0SC and CELLSC.

- W-3 (I) : IHTRSC Pointer to a Tabular or Control Function defining the convective heat transfer coefficient (HTC) at the right surface. If zero then the HTC is calculated by the code for the thermal-hydraulic conditions taken from the volume IVLRSC (Word 1). If the value is positive, HTC will be defined by the Tabular Function IHTRSC. If it is negative, it will be defined by the Control Function $|IHTRSC|$. The units of the quantities obtained from the Tabular or Control Function are assumed to be (W/m²/K). If the obtained value is negative, it will be set to zero. Note that if IHTRSC≠0 then the fluid temperature, needed to calculate the boundary heat flux, is taken as:
- if IVLRSC>0 then the fluid temperature in Control Volume IVLRSC is used.
 - if ITPRSC≠0 then the fluid temperature is given by a Tabular or Control Function, defined by ITPRSC (word 4 below).
 - if IVLRSC=0 and ITPRSC=0 then the fluid temperature is set to 300 K.
- Acceptable range:* must be a valid reference number of a Tabular, or a Control Function, if non-zero.
- Default value:* 0 .
- W-4 (I) : ITPRSC Pointer to a Tabular or Control Function defining the fluid temperature at the right surface for convective heat transfer. If the value is positive, the fluid temperature will be defined by the Tabular Function ITPRSC. If it is negative, it will be defined by the Control Function $|ITPRSC|$. The units of quantity obtained from the Tabular or Control Function are assumed to be (K). If the obtained value is negative, it will be set to zero. If ITPRSC≠0 and IVLRSC>0 (heat transfer to a Control Volume), then the value obtained from Tabular or Control Function will be used with the weighting factor of FINTSC. The true fluid temperature (from Control Volume) will be used with the weighting factor of 1.0–FINTSC. Boiling and condensation models will be disabled by setting CSFRSC to –1.0 and ICNRSC to –4. In the past the input combination of IPTLSC≠0 and IVLLSC>0 was used to perform temperature averaging for heat exchangers. Currently it is not recommended to use this method. A more elaborate temperature averaging model has been developed, and is available through input records 325XXX, 326XXX (see sections 2.3.15 and 2.3.16).
- Acceptable range:* must be a valid reference number of a Tabular, or a Control Function, if non-zero.
- Default value:* 0 .
- W-5 (I) : IQRRSC Indicator for non-convective heat flux at the right boundary. The heat flux defined by this pointer is used only on the uncovered part of the SC (above water level). With this pointer a user can model in a simple way radiative heat transfer. If the net enclosure thermal radiation model is used, and this surface is associated with one of the radiating surfaces (section 2.6.3), then this parameter must not be used. The meaning is as follows:

IQRRSC>1000:

Simple radiation model between the right SC surface and atmosphere gas is used to determine the non-convective heat transfer. The grey gas model is used, atmosphere is assumed to be opaque (the reason for assuming opaque atmosphere is discussed in Volume 3). The heat flux is equal to:

$$q = \varepsilon(T_w)\sigma(T_w^4 - T_g^4)$$

where $\varepsilon(T_w)$ is the wall emissivity, σ is the Stefan-Boltzmann constant, T_w , T_g are the wall and gas temperatures respectively. The emissivity is obtained from the Tabular Function number: (IQRRSC-1000). The argument for the Tabular Function is the wall surface temperature, (K).

0<IQRRSC<1000:

The heat flux is obtained from the Tabular Function number IQRRSC. The units of the quantities obtained from the Tabular Function are assumed to be: (W/m²). Positive heat flux means that the heat is emitted from the surface.

IQRRSC<0:

The heat flux is obtained from the Control Function number $|IQRRSC|$. The units of the quantities obtained from the Control Function are assumed to be: (W/m²). Positive heat flux means that the heat is emitted from the surface.

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0.

W-6 (I) : INCRSC Configuration indicator for natural convection. The value is used only when IVLRSC is positive. The meaning of this variable is as follows:

Rectangular geometry: 0 vertical wall,
-1 horizontal wall facing down,
+1 horizontal wall facing up.

Cylindrical geometry: 0 vertical cylinder,
-1 horizontal cylinder, inside,
+1 horizontal cylinder, outside.

Spherical geometry: -1 sphere, inside,
+1 sphere, outside.

Default values are provided for each geometrical configuration, based on IGEOSC and IVERSC parameters (section 2.3.1) - see Table 2-6 and Table 2-7.

Acceptable range: -1, 0, +1.

Default value: RECTANGULAR geometry (IGEOSC=1):
- VERTICAL (IVERSC=0): 0,
- HORIZONTAL down (IVERSC=-1): +1,
- HORIZONTAL up (IVERSC=+1): -1,
CYLINDRICAL geometry (IGEOSC=2):
- VERTICAL (IVERSC=0): 0,
- HORIZONTAL (IVERSC=±1): 1,

SPECTRA Code Manuals - Volume 2: User's Guide

however, if fins are present
(ITFRSC=1) then: 0;
SPHERICAL geometry (IGEOSC=1): 1.

- W-7 (R) : DNCRSC Characteristic dimension for natural convection at the right boundary surface, (m). The value is used only when IVLRSC is positive. A best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DNCRSC should be equal to (see Table 2-6 and Table 2-7): for vertical plates - height; for horizontal plates - width; for vertical cylinders - cylinder length; for horizontal cylinders - outer diameter; for spheres - outer diameter. Note that the default value for plates (rectangular geometry) is only appropriate for the square walls.
Acceptable range: $0.0 < DNCRSC < 10^{10}$.
Default value: height, given by HGTRSC (Word 2 above). If HGTRSC is equal to zero (horizontal rectangular surfaces) then the square root of the surface area, given by SIZEESC (section 2.3.1). The value is appropriate for square surfaces. Thus for horizontal rectangular surfaces the default value should not generally be used. The appropriate value, width, should be entered.
CYLINDRICAL geometry (IGEOSC=2):
outer diameter, calculated from X0SC and CELLSC (sections 2.3.1 and 2.3.9).
SPHERICAL geometry (IGEOSC=3):
outer diameter, calculated from X0SC and CELLSC (sections 2.3.1 and 2.3.9).
- W-8 (I) : IFCRSC Configuration indicator for forced convection, as well as the nucleate boiling model and the model for critical heat flux calculation. The value is used only when IVLRSC is positive and no alternative liquid is used. For the alternative liquid the forced convection correlation is selected by Word 21 (IHDRSC). The meaning of this variable is as follows:
-1 internal flow, Chen correlation for nucleate boiling, Zuber and USSR Academy of Science models for critical heat flux calculations (Zuber for non-flow, USSR A. S. for flow conditions).
+1 external flow, Rohsenow correlation for nucleate boiling, Zuber model for critical heat flux calculation.
Default values are provided for each geometrical configuration, based on IGEOSC (section 2.3.1) - see Table 2-8 and Table 2-9.
Acceptable range: $-1 \leq IFCRSC \leq +1$.
Default value: -1.
- W-9 (R) : DFCRSC Characteristic dimension for forced convection at the right boundary surface, (m). The value is used only when IVLRSC is positive. A best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DFCRSC should be equal to (see Table 2-8 and Table 2-9): for internal flow - hydraulic diameter; for external flow - width (rectangular wall) or outer diameter (cylinders, spheres). The internal/external flow type is

defined by IFCRSC (see above). For the internal flow type the default value is the same as for the external flow type. Therefore for the internal flow type the default value should not be used, but the appropriate value for DFCRSC should be entered.

Acceptable range: $0.0 < \text{DFCRSC} < 10^{10}$.

Default value: RECTANGULAR geometry (IGEOSC=1):
HGTRSC (if entered) or square root of the surface area, given by SIZESC (section 2.3.1).
CYLINDRICAL geometry (IGEOSC=2):
outer diameter, calculated from X0SC and CELLSC (sections 2.3.1 and 2.3.9).
SPHERICAL geometry (IGEOSC=3):
outer diameter, calculated from X0SC and CELLSC (sections 2.3.1 and 2.3.9).

W-10 (I) : IFBRSC Configuration indicator for film boiling. The value is used only when IVLRSC is positive. The meaning of this variable is as follows:

- 0 vertical surface,
- ±1 horizontal cylinder,
- 1 horizontal plate, facing down,
- +1 horizontal plate, facing up.

Default values are provided for each geometrical configuration, based on IGEOSC and IVERSC (section 2.3.1) - see Table 2-10 and Table 2-11.

Acceptable range: -1, 0, +1.

Default value: RECTANGULAR geometry (IGEOSC=1):
- VERTICAL (IVERSC=0):
0; not changeable by user,
- HORIZONTAL down (IVERSC=-1):
-1; not changeable by user,
- HORIZONTAL up (IVERSC=+1):
+1; not changeable by user.
CYLINDRICAL geometry (IGEOSC=2):
- VERTICAL (IVERSC=0):
0; not changeable by user,
- HORIZONTAL (IVERSC=±1):
1; not changeable by user,
SPHERICAL geometry (IGEOSC=1):
1; not changeable by user.

W-11 (R) : DFBRSC Characteristic dimension for film boiling at the right boundary surface, (m). The value is used only when IVLRSC is positive. A best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DFBRSC should be equal to (see Table 2-10 and Table 2-11): for vertical walls - height; for horizontal plates - width; for cylinders and spheres - outer diameter.

Acceptable range: $0.0 < \text{DFCRSC} < 10^{10}$.

Default value: RECTANGULAR geometry (IGEOSC=1):
HGTRSC (if entered) or square root of the surface area, given by SIZESC (section 2.3.1).
CYLINDRICAL geometry (IGEOSC=2):

SPECTRA Code Manuals - Volume 2: User's Guide

outer diameter, calculated from XOSC and CELLSC.

SPHERICAL geometry (IGEOSC=3):

outer diameter, calculated from XOSC and CELLSC.

- W-12 (I) : ICNRSC Configuration indicator for condensation. The value is used only when IVLRSC is positive. The meaning of this variable is as follows:
- ≤ -4 model disabled
 - = -3 condensation on horizontal wall facing up,
 - = -2 condensation on horizontal wall facing down,
 - = -1 condensation inside horizontal tubes,
 - = 0 condensation on vertical walls,
 - = +1 condensation on outside surface of horizontal tube.
 - ≥ +2 condensation on outside surface of horizontal tube bank. The value of ICNRSC is equal to the number of rows of tubes in vertical direction.
- Default values are provided for each geometrical configuration based on IGEOSC and IVERSC (section 2.3.1) - see Table 2-12 and Table 2-13.
- Acceptable range:* all integers.
- Default value:*
- RECTANGULAR geometry (IGEOSC=1):
 - VERTICAL (IVERSC=0): 0;
 - HORIZONTAL down (IVERSC=+1): -2;
 - HORIZONTAL up (IVERSC=-1): -3;
 - however, if fins are present (ITFRSC=1) then: 0;
 - CYLINDRICAL geometry (IGEOSC=2):
 - VERTICAL (IVERSC=0): 0;
 - HORIZONTAL (IVERSC=±1): +1;
 - however, if fins are present (ITFRSC=1) then: 0;
 - SPHERICAL geometry (IGEOSC=3): +1.

- W-13 (R) : DCNRSC Characteristic dimension for condensation at the right boundary surface, (m). The value is used only when IVLRSC is positive. Best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DCNRSC should be equal to (see Table 2-12 and Table 2-13): for vertical walls (or cylinders) - wall height; inside horizontal tubes - inner diameter; outside surface of horizontal tubes or tube banks - outer diameter; horizontal walls facing up - maximum film thickness (equilibrium thickness of water layer with free fall of liquid at the edges of the wall). The condensation type is defined by ICNRSC (word 12).
- In case of vertical walls the user may wish divide the total wall into a certain number of segments, modelled by separate conductors. Thus the conductors are stacked one over the other. To take into account the behavior of the condensate film in this case the characteristic dimension of the conductor number k in the stack (counting from the top) should be defined as follows:

$$DCNLSC(k) = \left(\frac{z_{BOT}(k)^{5/4} - z_{TOP}(k)^{5/4}}{z_{BOT}(k) - z_{TOP}(k)} \right)^4$$

where: $z_{BOT}(k)$ distance from the bottom of the conductor k to the top of the stack, (m),
 $z_{TOP}(k)$ distance from the top of the conductor k to the top of the stack, (m).

If the height of each conductor in the stack is identical then the above formula reduces to:

$$DCNLSC(k) = \left(k^{5/4} - (k-1)^{5/4} \right)^4 \frac{H}{N}$$

where: H - total height of the wall, (m),
 N - number of conductors in the stack..

The ratio: (H/N) is the height of a single conductor in the stack.
 Note that only for $k=1$ DCNRSC is equal to the physical height of the conductor, (H/N) . For $k>1$ DCNRSC is greater than (H/N) . For $k=N$ DCNRSC is always greater than the total wall height, H .

Acceptable range: $0.0 < DCNRSC < 10^{10}$.

Default value: height, given by HGTRSC (Word 2 above). For horizontal walls facing up the default value is equal to 10^{-3} .

W-14 (R) : CSFRSC The constant C_{sf} in the Rohsenow equation for nucleate boiling (see Volume 1). The values of C_{sf} for different surfaces are given in Table 2-5. Entering a negative value will disable the full boiling model.
Acceptable range: all reals.
Default value: 0.013 .

Table 2-5 Values of C_{sf} for Rohsenow correlation.

Surface type	C_{sf}	Surface type	C_{sf}
Nickel	0.0060	Platinum	0.0130
Ground and polished stainless steel	0.0080	Brass	0.0060
Teflon pitted stainless steel	0.0058	Polished copper	0.0128
Chemically etched stainless steel	0.0133	Lapped copper	0.0147
Mechanically polished stainless steel	0.0132	Scored copper	0.0068

W-15 (I) : MCFRSC Critical heat flux model selection. The value is used only when IVLRSC > 0 .
 1 Zuber pool boiling correlation with Ivey-Morris correction for subcooling.
 2 Combination of model based on USSR Academy of Sciences CHF look-up tables for high flow, with Zuber and Ivey-Morris for low flow.

- 3 Combination of Biasi correlation for high flow, with Zuber and Ivey-Morris for low flow.
- 4 Groeneveld (1986) look-up tables.
- <0 CHF is calculated by a user-defined Control Function with the number |MCFRSC|.
- Acceptable range:* 1, 2, 3 or reference to a Control Function
- Default value:* 2.
- W-16 (I) : MNCRSC Selection of model for the influence of noncondensable gases for condensation. The value is used only when IVLRSC is positive and ICNRSC is greater than -4. The meaning of this variable is as follows:
- 1 Kuhn-Shrock-Petersen (KSP) correlations - recommended for condensation on the inside surface of tubes,
- 2 Ogg correlations,
- 3 Modified Ogg correlations - recommended for condensation on the outside surface of tubes, plates, etc.
- Default values are provided - see Table 2-14 and Table 2-15).
- Acceptable range:* 1, 2, 3 .
- Default value:* 3.
- W-17 (R) : CFDRSC Indicator of condensate film drainage behavior.
- If the value is positive then CFDRSC is the height of the right SC surface. The elevation of the lowermost point of this surface is equal to the elevation of its center point, minus CFDRSC/2.0.
- The drainage from this surface is either deposited in the pool of a CV (if the lowest point of the surface is immersed in pool), or converted to droplets and suspended in the atmosphere of a CV as "rain" drops (if the lowest point of the surface is not immersed in the pool).
- If the value is negative then the drainage is assumed to be deposited on a surface of other (lower) Solid Conductor. The absolute value of CFDRSC must then be equal to the number of SC at the bottom of the stack.
- The use of the drainage parameter, CFDRSC, and the condensation characteristic dimension, DCNRSC, on the right surface of SC is the same as for the left surface of SC. The use of DCNRSC and CFDRSC in case of individual and stacked conductors is illustrated in Figure 2-14 and Table 2-4, section 2.3.11.
- Acceptable range:* if CFDRSC<0.0 then the right surface of SC No. |CFDRSC| must be connected to a Control Volume (not necessarily equal to IVLRSC),
if CFDRSC>0.0 then the bottom elevation of the right surface (centre point elevation, minus CFDRSC/2.0) must be within the boundary Control Volume.
- Default value:* the default value is set to twice the distance between the centre point of the right surface and the bottom of the boundary Control Volume. That value will result in deposition of condensate always in the pool. This is done to avoid numerical problems, and time step reduction, when condensate is converted into droplets. The most realistic treatment (although typically more time consuming) is obtained by

setting CFDRSC equal to the physical height of the right surface. The influence of the value of CFDRSC on the results is, in practical cases, negligible.

- W-18 (I) : IHDRSC Indicator of CV flow direction relative to the right SC surface. Used only for rectangular (IGEOSC=1) SC's. The meaning is:
 For vertical SC's (IVERSC=0):
 0: CV horizontal flow is parallel, $v_{SC} = (v_{CV,ver}^2 + v_{CV,hor}^2)^{1/2}$,
 1: CV horizontal flow is perpendicular, $v_{SC} = v_{CV,ver}$.
 For horizontal SC's (IVERSC<>0):
 0: CV vertical flow is parallel, $v_{SC} = (v_{CV,ver}^2 + v_{CV,hor}^2)^{1/2}$,
 1: CV vertical flow is perpendicular, $v_{SC} = v_{CV,ver}$.
 Acceptable range: $0 \leq \text{IHDRSC} \leq 1$.
 Default value: 0.
- W-19 (I) : THTRSC Contact angle, θ , (degree). Used to determine diameter of bubbles created during nucleate boiling: $D = 0.0208 \cdot \theta \cdot (\sigma/g/(\rho_{liq} - \rho_{gas}))^{(1/2)}$.
 Acceptable range: $10^\circ \leq \text{THTRSC} \leq 180^\circ$.
 Default value: 96° .
- W-20 (R) : XRBRSC Multiplier for convective heat transfer, X_{RB} .
 XRBRSC<0.0: HTC is multiplied by |XRBRSC| in both natural and force convection. It may be used to obtain a conservative estimation of heat transfer.
 XRBRSC>0.0: HTC is multiplied by XRBRSC only in case of turbulent forced convection (FC-TUR), internal flow (IFCRSC = -1). It is intended to allow the user to define a rod bundle multiplier in forced convection:

$$Nu_{tur} = X_{RB} 0.023 Re^{0.8} Pr^{0.4}$$

Appropriate values for parallel flow and cross-flow may be found in literature. The ratio of pitch over diameter is a good approximation (see Volume 1, description of forced convection correlations):

$$X_{RB} = P / D$$

For tube arrangements other than equilateral triangle pitch, the multiplier is given by:

$$X_{RB} = \left(\frac{P_1 \cdot P_2}{D^2} \right)$$

Note that the rod bundle multiplier may be different for different fluids. For example, for the liquid metals the value may even show different tendency (see Volume 1, description of liquid metals correlations):

$$X_{RB} = 1 - \exp[-3.8 \cdot (P/D - 1)]$$

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq |XRBRSC| \leq 10^6$

Default value: XRBRHT
(global activator, defined in the record 810020)

W-21 (I) : IHCRC Selection of heat transfer correlation for alternative fluid.
Acceptable range: one of the correlations defined in records 843XXX
or 843YYY
Default value: rectangular: 1, cylindrical: 2, spherical: 3.

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-6 Natural convection - input options, characteristic dimensions, equations.

IVE-RSC	Rectangular		Cylindrical		Spherical	
	Left	Right	Left	Right	Left	Right
0	INCLSC: 0 DNCLSC: H Eq. Set: (1) alternative: INCLSC: $\neq 0$	INCRSC: 0 DNCRSC: H Eq. Set: (1) alternative: INCLSC: $\neq 0$	INCLSC: 0 DNCLSC: L Eq. Set: (1) alternative: INCLSC: $\neq 0$	INCRSC: 0 DNCRSC: L Eq. Set: (1) alternative: INCLSC: $\neq 0$	INCLSC: -1 DNCLSC: D Eq. Set: (6) no alternative:	INCRSC: +1 DNCRSC: D Eq. Set: (6) no alternative:
-1	INCLSC: -1 DNCLSC: W Eq. Set: - if $T_w > T_f$ (3) - if $T_w < T_f$ (2)	INCRSC: +1 DNCRSC: W Eq. Set: - if $T_w > T_f$ (2) - if $T_w < T_f$ (3)	INCLSC: -1 DNCLSC: L < 2D Eq. Set: (4) alternative: INCLSC: $\neq -1$	INCRSC: +1 DNCRSC: D Eq. Set: (5) alternative: INCLSC: $\neq +1$		
+1	INCLSC: +1 DNCLSC: W Eq. Set: - if $T_w > T_f$ (2) - if $T_w < T_f$ (3)	INCRSC: -1 DNCRSC: W Eq. Set: - if $T_w > T_f$ (3) - if $T_w < T_f$ (2)				

H - height, W - width, L - length, D - diameter.

Table 2-7 Natural convection correlations (for $(Gr Pr) < 10^4$ the "recommended curves" - see Volume 1 - are used).

Geometry	Open for natural circulation ^(*)	Closed for natural circulation ^(*) (enclosures)
Vertical plate	Source: McAdams, Holman Ch. Dim.: height, H Correl.: $Nu = 0.59 \cdot (Gr \cdot Pr)^{1/4}$ $Nu = 0.10 \cdot (Gr \cdot Pr)^{1/3}$ Set No.: (1)	N/A
Horizontal plate	Source: McAdams Ch. Dim.: width, W Correl.: $Nu = 0.54 \cdot (Gr \cdot Pr)^{1/4}$ $Nu = 0.14 \cdot (Gr \cdot Pr)^{1/3}$ Set No.: (2)	Source: McAdams Ch. Dim.: width, W Correl.: $Nu = 0.27 \cdot (Gr \cdot Pr)^{1/4}$ Set No.: (3)
Vertical cylinder	Source: McAdams, Holman Ch. Dim.: length, L Correl.: $Nu = 0.59 \cdot (Gr \cdot Pr)^{1/4}$ $Nu = 0.10 \cdot (Gr \cdot Pr)^{1/3}$ Set No.: (1)	Source: Holman Ch. Dim.: length, $L < 2D$ Correl.: $Nu = 0.55 \cdot (Gr \cdot Pr)^{1/4}$ Set No.: (4)
Horizontal cylinder	Source: McAdams, Holman Ch. Dim.: diameter, D Correl.: $Nu = 0.53 \cdot (Gr \cdot Pr)^{1/4}$ $Nu = 0.13 \cdot (Gr \cdot Pr)^{1/3}$ Set No.: (5)	Source: Holman Ch. Dim.: diameter, D Correl.: $Nu = 0.55 \cdot (Gr \cdot Pr)^{1/4}$ Set No.: (4)
Sphere	Source: Holman Ch. Dim.: diameter, D Correl.: $Nu = 2 + 0.43 \cdot (Gr \cdot Pr)^{1/4}$ Set No.: (6)	Source: Holman Ch. Dim.: diameter, D Correl.: $Nu = 2 + 0.43 \cdot (Gr \cdot Pr)^{1/4}$ Set No.: (6)

References are: Holman [9], McAdams [18].

^(*) The meaning of "Open" and "Closed" is as follows:

- *Horizontal plates* Open: hot surface facing upwards or cold surface facing downwards.
Closed: cold surface facing upwards or hot surface facing downwards.
- *Cylinders* Open: large vertical cylinders, outer surface of horizontal cylinders that are not enclosed by other surfaces
Closed: inner surface of small cylinders, horizontal cylinders enclosed by other surfaces
- *Spheres* Open: large spheres, outer surface of spheres that are not enclosed by other surfaces
Closed: inner surface of small spheres, sphere surfaces enclosed by other surfaces

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-8 Forced convection - input options, characteristic dimensions, equations.

Rectangular		Cylindrical		Spherical	
Left	Right	Left	Right	Left	Right
IFCLSC: -1	IFCRSC: -1	IFCLSC: -1	IFCRSC: -1	IFCLSC: -1	IFCRSC: -1
DFCLSC: D_{hyd}	DFCRSC: D_{hyd}	DFCLSC: D_{hyd}	DFCRSC: D_{hyd}	DFCLSC: D_{hyd}	DFCRSC: D_{hyd}
Eq. Set: (1)	Eq. Set: (1)	Eq. Set: (1)	Eq. Set: (1)	Eq. Set: (1)	Eq. Set: (1)
alternative: IFCLSC: +1	alternative: IFCLSC: +1	alternative: IFCLSC: +1	alternative: IFCRSC: +1	alternative: IFCLSC: +1	alternative: IFCRSC: +1
DFCLSC: W	DFCLSC: W	DFCLSC: D	DFCRSC: D	DFCLSC: D	DFCRSC: D
Eq. Set: (2)	Eq. Set: (2)	Eq. Set: (2)	Eq. Set: (2)	Eq. Set: (3)	Eq. Set: (3)

W - width, D_{hyd} - hydraulic diameter.

Table 2-9 Forced convection correlations.

Geometry	Internal flow	External flow
Rectangular	Source : Rohsenow Ch.Dim.: hydraulic diameter, D_{hyd} Correl.: $Nu = 3.656$ $Nu = 0.023 Re^{0.8} Pr^{0.4}$ Set No.: (1)	Source : Holman Ch.Dim.: width, W Correl.: $Nu = (0.35+0.56 Re^{0.52}) Pr^{0.3}$ $Nu = 0.037 Re^{0.8} Pr^{1/3}$ Set No.: (2)
Cylindrical	Source : Rohsenow Ch.Dim.: hydraulic diameter, D_{hyd} Correl.: $Nu = 3.656$ $Nu = 0.023 Re^{0.8} Pr^{0.4}$ Set No.: (1)	Source : Holman Ch.Dim.: diameter, D Correl.: $Nu = (0.35+0.56 Re^{0.52}) Pr^{0.3}$ $Nu = 0.037 Re^{0.8} Pr^{1/3}$ Set No.: (2)
Spherical	Source : Rohsenow Ch.Dim.: hydraulic diameter, D_{hyd} Correl.: $Nu = 3.656$ $Nu = 0.023 Re^{0.8} Pr^{0.4}$ Set No.: (1)	Source : Holman Ch.Dim.: diameter, D Correl.: $Nu = 2 + (0.4 Re^{0.5} + Pr^{0.3} + 0.06 Re^{2/3}) Pr^{1/3}$ Set No.: (3)

References: Holman [9], Rohsenow [14].

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-10 Film boiling - input options, characteristic dimensions, equations.

IVE-RSC	Rectangular		Cylindrical		Spherical	
	Left	Right	Left	Right	Left	Right
0	IFBLSC: 0 DFBLSC: H Eq. Set: (1) alternative: IFBLSC ≠ 0	IFBRSC: 0 DFBRSC: H Eq. Set: (1) alternative: IFBLSC ≠ 0	IFBLSC: 0 DFBLSC: L Eq. Set: (1) alternative: IFBLSC ≠ 0	IFBRSC: 0 DFBRSC: L Eq. Set: (1) alternative: IFBLSC ≠ 0	IFBLSC: 0, ±1 DFBLSC: D Eq. Set: (4) no alternative	IFBRSC: 0, ±1 DFBRSC: D Eq. Set: (4) no alternative
-1	IFBLSC: -1 DFBLSC: W Eq. Set: (3) alternative: IFBLSC ≠ -1	IFBRSC: +1 DFBRSC: cw Eq. Set: (2) alternative: IFBLSC ≠ +1	IFBLSC: ±1 DFBLSC: D Eq. Set: (4) alternative: IFBLSC = 0	IFBRSC: ±1 DFBRSC: D Eq. Set: (4) alternative: IFBLSC = 0		
+1	IFBLSC: +1 DFBLSC: cw Eq. Set: (2) alternative: IFBLSC ≠ +1	IFBRSC: -1 DFBRSC: W Eq. Set: (3) alternative: IFBLSC ≠ -1				

H - height, W - width, L - length, D - diameter, cw - critical wavelength, $cw = (\sigma/g(\rho_l - \rho_g))^{1/2}$ (calculated internally by the code).

Except for the spherical geometry, the user can select the film boiling correlation by changing the default value of IFBLSC / IFBRSC. For example, in case of rectangular geometry, IGEO SC = 1, horizontal, left side down structure, IVERSC = -1, the default value on the film boiling indicator on the left surface is IFBLSC = -1 (downwards surface). The user can change it to 0 (vertical) or even +1 (upwards surface), thus activating the appropriate correlations. There should be however a clear reason to change the default settings for the film boiling model.

Table 2-11 Film boiling correlations.

Geometry	Correlation	Geometry	Correlation
Vertical walls	Correl.: Bromley Const. : C = 0.625 Ch.dim.: $D_0 = \text{height, H}$ Eq.No. : (1)	Vertical cylinders	Correl.: Bromley Const. : C = 0.625 Ch.dim.: $D_0 = \text{height, H}$ Eq.No. : (1)
Horizontal walls, facing up	Correl.: Berenson Const. : C = 0.425 Ch.dim.: $D_0 = (\sigma/g(\rho_{liq} - \rho_{vap}))^{1/2}$ Eq.No. : (2)	Horizontal cylinders	Correl.: Bromley Const. : C = 0.620 Ch.dim.: $D_0 = \text{diameter}$ Eq.No. : (4)
Horizontal walls, facing down	Correl.: Berenson Const. : C = 0.425 Ch.dim.: $D_0 = \text{width, W}$ Eq.No. : (3)	Spheres	Correl.: Bromley Const. : C = 0.620 Ch.dim.: $D_0 = \text{diameter}$ Eq.No. : (4)

References: Bromley [19], Berenson [20].

The table above gives the value of the constant C, and the characteristic dimension D_0 , in the general film boiling correlation:

$$h = C \left(\frac{k_{vap}^3 \rho_{vap} g (\rho_{liq} - \rho_{vap}) (h_{l-v} + 0.4c_{p,vap} \Delta T_{sat})}{\eta_{vap} D_0 \Delta T_{sat}} \right)^{0.25}$$

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-12 Pure steam condensation - input options, characteristic dimensions, equations.

IVERSC	Rectangular		Cylindrical		Spherical	
	Left	Right	Left	Right	Left	Right
0	ICNLSC: 0 DCNLSC: H Eq. No. (1) alternative: ICNLSC ≠ 0	ICNRSC: 0 DCNRSC: H Eq. No. (1) alternative: ICNRSC ≠ 0	ICNLSC: 0 DCNLSC: L Eq. No. (1) alternative: ICNLSC ≠ 0	ICNRSC: 0 DCNRSC: L Eq. No. (1) alternative: ICNRSC ≠ 0	ICNLSC: -1 DCNLSC: D Eq. No. (2) alternative: ICNLSC ≠ -1	ICNRSC: -1 DCNRSC: D Eq. No. (2) alternative: ICNRSC ≠ -1
-1	ICNLSC: -2 DCNLSC: cw Eq. No. (4) alternative: ICNLSC ≠ -2	ICNRSC: -3 DCNRSC: δ Eq. No. (5) alternative: ICNRSC ≠ -3	ICNLSC: -1 DCNLSC: D Eq. No. (2) alternative: ICNLSC ≠ -1	ICNRSC: -1 DCNRSC: D Eq. No. (2) alternative: ICNRSC ≠ -1		
+1	ICNLSC: -3 DCNLSC: δ Eq. No. (5) alternative: ICNLSC ≠ -2	ICNRSC: -2 DCNRSC: cw Eq. No. (4) alternative: ICNRSC ≠ -2				

H - height, W - width, L - length, D - diameter, cw - critical wavelength, $cw = (\sigma/g(\rho_l - \rho_g))^{1/2}$ (calculated internally by the code).

Table 2-13 Pure steam condensation correlations.

Configuration	Correlation
Vertical walls and cylinders	Source : Nusselt, Ch.Dim.: wall height, H Correl.: $0.943 (g \rho_{liq} (\rho_{liq} - \rho_{gas})) k_{liq}^3 h_{l-v} / H \eta_{liq} \Delta T_{sat.})^{0.25}$ Eq. No.: (1)
Inside tubes	Source : Nusselt, Chato, Ch.Dim.: inner diameter, D Correl.: $0.555 (g \rho_{liq} (\rho_{liq} - \rho_{gas})) k_{liq}^3 h_{l-v} / D \eta_{liq} \Delta T_{sat.})^{0.25} (1 + \theta^9/100)$ Eq. No.: (2)
Outside tubes and tube banks	Source : Nusselt, Ch.Dim.: outer diameter, D Correl.: $0.728 (g \rho_{liq} (\rho_{liq} - \rho_{gas})) k_{liq}^3 h_{l-v} / N_{row} D \eta_{liq} \Delta T_{sat.})^{0.25}$ Eq. No.: (3)
Horizontal walls, facing down	Source : Gerstmann and Griffith, Ch.Dim.: not used Correl.: $k_{liq} / D_x 0.9 \tau^{-1/6} / (1 + 1.1 \tau^{1/6})$ where D_x is the critical wavelength Eq. No.: (4)
Horizontal walls, facing up	Source : Maximum film thickness concept Ch.Dim.: Maximum film thickness, δ Correl.: k_{liq} / δ Eq. No.: (5)

References: Nusselt [23], Chato [21], Gerstmann and Griffith [22].

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-14 Non-condensable degradation factor - input options, equations.

Rectangular		Cylindrical		Vertical	
Left	Right	Left	Right	Left	Right
MCNLSC: 3 Corr.: M.Ogg Eq. No. (3)	MCNRSC: 3 Corr.: M.Ogg Eq. No. (3)	MCNLSC: 3 Corr.: M.Ogg Eq. No. (3)	MCNRSC: 3 Corr.: M.Ogg Eq. No. (3)	MCNLSC: 3 Corr.: M.Ogg Eq. No. (3)	MCNRSC: 3 Corr.: M.Ogg Eq. No. (3)
alternative: MCNLSC: 1 Corr.: KSP Eq. No.: (1)	alternative: MCNRSC: 1 Corr.: KSP Eq. No.: (1)	alternative: MCNLSC: 1 Corr.: KSP Eq. No.: (1)	alternative: MCNRSC: 1 Corr.: KSP Eq. No.: (1)	alternative: MCNLSC: 1 Corr.: KSP Eq. No.: (1)	alternative: MCNRSC: 1 Corr.: KSP Eq. No.: (1)
MNCLSC: 2 Corr.: Ogg Eq. No.: (2)	MNCRSC: 2 Corr.: Ogg Eq. No.: (2)	MNCLSC: 2 Corr.: Ogg Eq. No.: (2)	MNCRSC: 2 Corr.: Ogg Eq. No.: (2)	MNCLSC: 2 Corr.: Ogg Eq. No.: (2)	MNCRSC: 2 Corr.: Ogg Eq. No.: (2)

Table 2-15 Non-condensable degradation factor correlations.

Model	
Kuhn-Shrock-Petersen	Source : KSP (inside tube condensation) Correl.: steam-air: $f_{NC}=1 - 2.601 X_a^{0.701}$ for $X_a < 0.10$ $1 - X_a^{0.292}$ for $X_a > 0.10$ steam-He: $f_{NC}=1 - 35.81 X_{He}^{1.074}$ for $X_{He} < 0.01$ $1 - 2.09 X_{He}^{0.457}$ for $X_{He} < 0.10$ $1 - X_{He}^{0.137}$ for $X_{He} > 0.10$ Set No.: (1)
Ogg	Source : Ogg (outside wall condensation) Correl.: steam-air: $f_{NC}=1 - 1.165 X_a^{0.26}$ for $X_a < 0.30$ $1 - 0.905 X_a^{0.05}$ for $X_a < 0.90$ $1 - X_a$ for $X_a > 0.90$ steam-He: $f_{NC}=1 - 1.590 X_{He}^{0.29}$ for $X_{He} < 0.11$ $1 - 1.865 X_{He}^{0.014}$ for $X_{He} < 0.86$ $1 - X_{He}$ for $X_{He} > 0.86$ Set No.: (2)
Modified Ogg	Source : Modified Ogg (outside wall condensation) Correl.: steam-air: $f_{NC}=1 - 1.165 X_a^{0.26}$ for $X_a < 0.30$ $0.21 - 0.21 X_a$ for $X_a < 0.30$ steam-He: $f_{NC}=1 - 1.590 X_{He}^{0.29}$ for $X_{He} < 0.12$ $0.16 - 0.16 X_{He}$ for $X_{He} > 0.12$ Set No.: (3)

References: KSP [24], Ogg [25], Modified Ogg [25], [26].

2.3.13 Records: 323XXX, Left Side Extended Surface Data

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. It should be noted that if a Solid Conductor is used to represent a wall with fins or spines then the cell data (records 310XXX) should represent only the wall, and not the fins/spines. Fins/spines are accounted for in calculations using a simplified method, based on theoretical temperature profiles inside fins/spines. Those profiles are appropriate for steady-state conditions (see Volume 1).

W-1 (I) : ITFLSC Type of extended surface:
 1: fins (Figure 2-15 a, b),
 2: spines (Figure 2-15 c).
Acceptable range: 0, 1, 2. Fins are allowed only if IGEOSC = 1 or 2 (rectangular or cylindrical). If fins are used on the left surface of a cylindrical SC, then the rectangular fin model (Figure 2-15 a) is used. This means the inner radius of the cylinder is assumed to be large compared to the fin size. Spines can be used with all geometries. For cylindrical and spherical geometries it is assumed that the surface radius of curvature is large compared to the spine length. Fins and spines can be used only if IVLLSC > 0.
Default value: 0 (no extended surface model).

W-2 (R) : THFLSC Half thickness of fin/spine, (m). THFLSC is denoted in Figure 2-15 as: *t*.
Acceptable range: 0.0 < THFLSC ≤ 1.0 .
Default value: none.

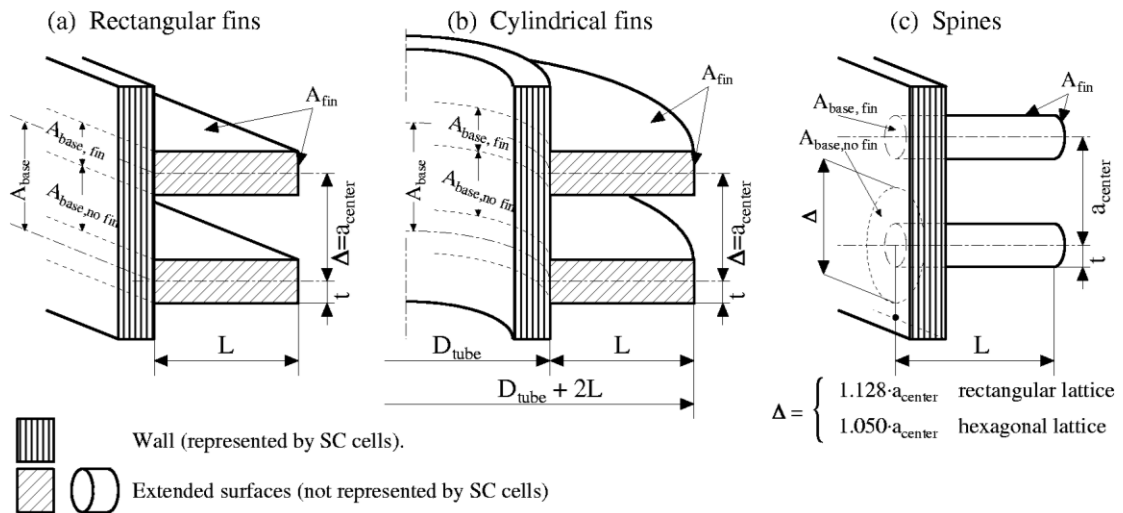


Figure 2-15 Fins and spines.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-3 (R) : XLFLSC Length of fin/spine, (m). XLFLSC is denoted in Figure 2-15 as: L.
Acceptable range: $10^{-10} < \text{XLFLSC} \leq 10.0$. In case of fins on cylinders and spines on cylinders and spheres, the length cannot be greater than 90% of the inner radius $\text{XLFLSC} \leq \text{XOSC} \times 0.90$.
Default value: none.
- W-4 (R) : DDFLSC Effective distance between fin/spines, (m). DDFLSC is denoted in Figure 2-15 as: Δ . In case of fins Δ is equal to the distance between the fin centers - Figure 2-15 (a). In case of spines Δ is equal to the diameter of a circle which has the same area as the area associated with a single spine - Figure 2-15 (c). If the spines are arranged in a square lattice, then the surface area associated with a single spine is equal to: a_{centre}^2 , where a_{centre} is the distance between the centers of two neighboring spines. The effective distance, Δ , is obtained from: $\pi \cdot \Delta^2 / 4 = a_{\text{centre}}^2$. Thus:

$$\Delta = a_{\text{centre}} \cdot 2 / \pi^{1/2} = 1.128 \cdot a_{\text{centre}}.$$
 In case of hexagonal spines arrangement the effective distance is equal to:

$$\Delta = a_{\text{centre}} \cdot (2/\pi)^{1/2} \cdot 3^{1/4} = 1.050 \cdot a_{\text{centre}}.$$
Acceptable range: $2 \cdot t < \text{DDFLSC} \leq 1.0$.
Default value: none.
- W-5 (R) : TCFLSC Thermal conductivity of the fin/spine material, (W/m²K). If a positive number is entered, the fin conductivity is constant and equal to this value while the fin heat capacity is neglected. If a negative number is entered, the absolute value is the reference number of the fin material.
Acceptable range: $\text{TCFLSC} \leq 10^{10}$. Must be a valid reference to an existing material, if less than zero.
Default value: reference number of the boundary cell material. If the fin material is different from the boundary cell material then those materials must have the same or similar heat capacities.
- W-6 (R) : DNFLSC Characteristic dimension for natural convection, (m). When the extended surface model is activated, then the characteristic dimension for the left surface natural convection (DNCLSC, entered in the record 321XXX - section 2.3.11), is overwritten by this value.
Acceptable range: the same as for DNCLSC:
 $0.0 < \text{DNFLSC} < 10^{10}$
 Note! This input entry is only used to overwrite the value of DNCLSC for this surface. Further diagnostics is performed for DNCLSC. Thus if an unacceptable value is entered for DNFLSC then the diagnostics output will point out that DNCLSC is out of the permitted range.
Default value: length of the fin/spine: L.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-7 (R) : DFFLSC Characteristic dimension for forced convection, (m). When the extended surface model is activated, then the characteristic dimension for the left surface forced convection (DFCLSC, entered in the record 321XXX - section 2.3.11), is overwritten by this value.
Acceptable range: the same as for DFCLSC:
 $0.0 < DFFLSC < 10^{10}$.
Note! This input entry is only used to overwrite the value of DFCLSC for this surface. Further diagnostics is performed for DFCLSC. Thus if an unacceptable value is entered for DFFLSC then the diagnostics output will point out that DFCLSC is out of the permitted range.
Default value: effective distance between fins/spines: Δ .
- W-8 (R) : DBFLSC Characteristic dimension for film boiling, (m). When the extended surface model is activated, then the characteristic dimension for the left surface film boiling (DFBLSC, entered in the record 321XXX - section 2.3.11), is overwritten by this value.
Acceptable range: the same as for DFBLSC:
 $0.0 < DBFLSC < 10^{10}$.
Note! This input entry is only used to overwrite the value of DFBLSC for this surface. Further diagnostics is performed for DFBLSC. Thus if an unacceptable value is entered for DBFLSC then the diagnostics output will point out that DFBLSC is out of the permitted range.
Default value: length of the fins/spines: L.
- W-9 (R) : DMFLSC Characteristic dimension for condensation, (m). When the extended surface model is activated, then the characteristic dimension for the left surface condensation (DCNLSC, entered in the record 321XXX - section 2.3.11), is overwritten by this value.
Acceptable range: the same as for DCNLSC:
 $0.0 < DMFLSC < 10^{10}$.
Note! This input entry is only used to overwrite the value of DCNLSC for this surface. Further diagnostics is performed for DCNLSC. Thus if an unacceptable value is entered for DMFLSC then the diagnostics output will point out that DCNLSC is out of the permitted range.
Default value: length of the fins/spines: L.

2.3.14 Records: 324XXX, Right Side Extended Surface Data

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. It should be noted that if a Solid Conductor is used to represent a wall with fins or spines then the cell data (records 310XXX) should represent only the wall, and not the fins/spines. Fins/spines are accounted for in calculations using a simplified method, based on theoretical temperature profiles inside fins/spines. Those profiles are appropriate for steady-state conditions (see Volume 1).

- W-1 (I) : ITFRSC Type of extended surface:
 1: fins (Figure 2-15 a, b),
 2: spines (Figure 2-15 c).
 Acceptable range: 0, 1, 2. Fins are allowed only if IGEOSC = 1 or 2 (rectangular or cylindrical). If fins are used on the right surface of a cylindrical SC, then the cylindrical fin model (Figure 2-15 b) is used. Spines can be used with all geometries. For cylindrical and spherical geometries it is assumed that the surface radius of curvature is large compared to the spine length. Fins and spines can be used only if IVLRSC > 0.
 Default value: 0 (no extended surface model).
- W-2 (R) : THFRSC Half thickness of fin/spine, (m). THFRSC is denoted in Figure 2-15 as: t.
 Acceptable range: $0.0 < \text{THFRSC} \leq 1.0$.
 Default value: none.
- W-3 (R) : XLFRSC Length of fin/spine, (m). XLFRSC is denoted in Figure 2-15 as: L.
 Acceptable range: $10^{-10} < \text{XLFRSC} \leq 10.0$.
 Default value: none.
- W-4 (R) : DDFRSC Effective distance between fin/spines, (m). DDFRSC is denoted in Figure 2-15 as: Δ . In case of fins Δ is equal to the distance between the fin centers - Figure 2-15 (a) and (b). In case of spines Δ is equal to the diameter of a circle that has the same area as the area associated with a single spine - Figure 2-15 (c). If the spines are arranged in a square lattice, then the surface area associated with a single spine is equal to: a_{centre}^2 , where a_{centre} is the distance between the centers of two neighboring spines. The effective distance, Δ , is obtained from:

$$\pi \cdot \Delta^2 / 4 = a_{\text{centre}}^2$$
 Thus:

$$\Delta = a_{\text{centre}} \cdot 2 / \pi^{1/2} = 1.128 \cdot a_{\text{centre}}$$
 In case of hexagonal spines arrangement the effective distance is equal to:

$$\Delta = \Delta_{\text{centre}} \cdot (2/\pi)^{1/2} \cdot 3^{1/4} = 1.050 \cdot a_{\text{centre}}$$
 Acceptable range: $2 \cdot t < \text{DDFRSC} \leq 1.0$.
 Default value: none.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-5 (R) : TCFRSC Thermal conductivity of the fin/spine material, (W/m²/K). If a positive number is entered, the fin conductivity is constant and equal to this value while the fin heat capacity is neglected. If a negative number is entered, the absolute value is the reference number of the fin material.
Acceptable range: $TCFRSC \leq 10^{10}$. Must be a valid reference to an existing material, if less than zero.
Default value: reference number of the boundary cell material. If the fin material is different from the boundary cell material then those materials must have the same or similar heat capacities.
- W-6 (R) : DNFRSC Characteristic dimension for natural convection, (m). When the extended surface model is activated, then the characteristic dimension for the right surface natural convection (DNCRSC, entered in the record 322XXX - section 2.3.12), is overwritten by this value.
Acceptable range: the same as for DNCRSC:
 $0.0 < DNFRSC < 10^{10}$.
Note! This input entry is only used to overwrite the value of DNCRSC for this surface. Further diagnostics is performed for DNCRSC. Thus if an unacceptable value is entered for DNFRSC then the diagnostics output will point out that DNCRSC is out of the permitted range.
Default value: spines and fins for rectangular geometry:
length of the fin/spine: L;
fins for cylindrical geometry:
 $(\pi/4) \cdot (D_{fin}^2 - D_{tube}^2) / D_{fin}$, where D_{tube} is the outer diameter of the tube, and D_{fin} is the outer diameter of the fin, equal to: $(D_{tube} + 2 \cdot L)$ - see Figure 2-15.
The formula applied here is the same as that used typically to determine the characteristic dimension for condensation [3].
- W-7 (R) : DFFRSC Characteristic dimension for forced convection, (m). When the extended surface model is activated, then the characteristic dimension for the right surface forced convection (DFCRSC, entered in the record 322XXX - section 2.3.12), is overwritten by this value.
Acceptable range: the same as for DFCRSC:
 $0.0 < DFFRSC < 10^{10}$.
Note! This input entry is only used to overwrite the value of DFCRSC for this surface. Further diagnostics is performed for DFCRSC. Thus if an unacceptable value is entered for DFFRSC then the diagnostics output will point out that DFCRSC is out of the permitted range.
Default value: effective distance between fins/spines: Δ .

SPECTRA Code Manuals - Volume 2: User's Guide

- W-8 (R) : DBFRSC Characteristic dimension for film boiling, (m). When the extended surface model is activated, then the characteristic dimension for the right surface film boiling (DFBRSC, entered in the record 322XXX - section 2.3.12), is overwritten by this value.
- Acceptable range:* the same as for DFBRSC:
 $0.0 < \text{DBFRSC} < 10^{10}$
- Note! This input entry is only used to overwrite the value of DFBRSC for this surface. Further diagnostics is performed for DFBRSC. Thus if an unacceptable value is entered for DBFRSC then the diagnostics output will point out that DFBRSC is out of the permitted range.
- Default value:* spines and fins for rectangular geometry:
length of the fin/spine: L;
fins for cylindrical geometry:
 $(\pi/4) \cdot (D_{\text{fin}}^2 - D_{\text{tube}}^2) / D_{\text{fin}}$, where D_{tube} is the outer diameter of the tube, and D_{fin} is the outer diameter of the fin, equal to: $(D_{\text{tube}} + 2 \cdot L)$ - see Figure 2-15. The formula applied here is the same as that used typically to determine the characteristic dimension for condensation [3].
- W-9 (R) : DMFRSC Characteristic dimension for condensation, (m). When the extended surface model is activated, then the characteristic dimension for the right surface condensation (DCNRSC, entered in the record 322XXX - section 2.3.12), is overwritten by this value.
- Acceptable range:* the same as for DCNRSC:
 $0.0 < \text{DMFRSC} < 10^{10}$
- Note! This input entry is only used to overwrite the value of DCNRSC for this surface. Further diagnostics is performed for DCNRSC. Thus if an unacceptable value is entered for DMFRSC then the diagnostics output will point out that DCNRSC is out of the permitted range.
- Default value:* spines and fins for rectangular geometry:
length of the fin/spine: L;
fins for cylindrical geometry [3]:
 $(\pi/4) \cdot (D_{\text{fin}}^2 - D_{\text{tube}}^2) / D_{\text{fin}}$, where D_{tube} is the outer diameter of the tube, and D_{fin} is the outer diameter of the fin, equal to: $(D_{\text{tube}} + 2 \cdot L)$ - see Figure 2-15.

2.3.15 Records: 325XXX, Left Side Heat Exchanger Temperature Averaging

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. These records may be used to model a heat exchanger. If these records are used, then an averaging procedure will be applied to calculate the representative fluid temperature at the SC surface. The representative fluid temperature will be equal to the weighted average of the inlet and outlet fluid temperatures. Note that if the temperature averaging is not used, then the representative fluid temperature is always equal to the fluid temperature in the boundary volume, which means it is equal to the outlet temperature. As shown in Volume 3, when the temperature-averaging concept is not used, a large number of nodes (~100) may be required to obtain accurate results. With the temperature averaging the same accuracy may be obtained using only a few nodes. An example of the temperature averaging is shown below - see Figure 2-16 and the corresponding discussion.

Inlet Junction Data:

- | | | |
|-----------|---------------|---|
| W-1 (I) : | JTALSC
(1) | Junction reference number of the inlet Junction on the current (left) side.
<i>Acceptable range:</i> must be a Junction connected to the left boundary Control Volume (IVLLSC), if non-zero.
<i>Default value:</i> none. |
| W-2 (R) : | WTALSC
(1) | Limiting mass flow in the inlet Junction JTALSC(1) for full temperature averaging (W_{TAL} in Figure 2-16 (a)). Applied when there is a flow through JTALSC(1) into IVLLSC and there is no flow through KTALSC(1) into IVLRSC - <u>normal flow direction on both left (primary) and right (secondary) side</u> . The temperature of the fluid entering through the Junction JTALSC(1) will be used with maximum weighting factor if the mass flow at the Junction is larger than WTALSC(1) ($W_{JN} > WTALSC(1)$). Generally speaking, WTALSC(1) is a flow for which the temperature distribution in the left boundary Control Volume is approximately linear, provided that there is flow in through JTALSC(1) and there is no flow in through KTALSC(1). Roughly, this number can be viewed as a nominal flow through the heat exchanger.
<i>Acceptable range:</i> $10^{-10} < WTALSC(1) < 10^{10}$.
<i>Default value:</i> none. |
| W-3 (I) : | KTALSC
(1) | Junction reference number of the outlet Junction on the other (right) side.
<i>Acceptable range:</i> must be a Junction connected to the right boundary Control Volume (IVLRSC), if non-zero.
<i>Default value:</i> none. |
| W-4 (R) : | XTALSC
(1) | Limiting mass flow in the Junction JTALSC(1) for full temperature averaging (X_{TAL} in Figure 2-16 (c)). Applied when there is flow through JTALSC(1) into IVLLSC and simultaneously there is flow through KTALSC(1) into IVLRSC - <u>normal flow direction on the left (primary) side, reversed right (secondary) side flow</u> . The temperature of the fluid entering through the Junction JTALSC(1) will be used with maximum weighting factor if the mass flow at the Junction is larger than XTALSC(1) ($W_{JN} > XTALSC(1)$). The input entries KTALSC(1) and XTALSC(1) allow the user to change the averaging weighting factors |

when flow conditions in the heat exchangers change, for example when a counter-current flow becomes co-current. Typically the temperature averaging is needed in counter-flow conditions, while it is not needed in co-flow conditions. This can be achieved by setting XTALSC(1) to a large number (for example XTALSC(1)=10⁶). Generally speaking, XTALSC(1) is a flow for which the temperature distribution in the left boundary Control Volume is approximately linear, provided that there is flow in through JTALSC(1) and KTALSC(1).

Acceptable range: $10^{-10} < \text{XTALSC}(1) < 10^{10}$.

Default value: none.

Outlet Junction Data:

- W-5 (I) : JTALSC(2) Junction reference number of the outlet Junction on the current (left) side.
Acceptable range: must be a Junction connected to the left boundary Control Volume (IVLLSC), if non-zero.
Default value: none.
- W-6 (R) : WTALSC(2) Limiting mass flow in the outlet Junction JTALSC(2) for full temperature averaging (W_{TAL} in Figure 2-16 (b)). Applied when there is flow through JTALSC(2) into IVLLSC and there is no flow through KTALSC(2) into IVLRSC - reversed flow on the left (primary) side, normal flow direction on the right (secondary) side. The temperature of the fluid entering through the Junction JTALSC(2) will be used with maximum weighting factor if the mass flow at the Junction is larger than WTALSC(2) ($W_{JN} > \text{WTALSC}(2)$). Generally speaking, WTALSC(2) is a flow for which the temperature distribution in the left boundary Control Volume is approximately linear, provided that there is flow in through JTALSC(2) and there is no flow in through KTALSC(2).
Acceptable range: $10^{-10} < \text{WTALSC}(2) < 10^{10}$.
Default value: none.
- W-7 (I) : KTALSC(2) Junction reference number of the outlet Junction on the other (right) side.
Acceptable range: must be a Junction connected to the right boundary Control Volume (IVLRSC), if non-zero.
Default value: none.
- W-8 (R) : XTALSC(2) Limiting mass flow in the outlet Junction JTALSC(2) for full temperature averaging (X_{TAL} in Figure 2-16 (d)). Applied when there is flow through JTALSC(2) into IVLLSC and simultaneously there is flow through KTALSC(2) into IVLRSC - reversed flow on both left (primary) and right (secondary) side. The temperature of the fluid entering through the Junction JTALSC(2) will be used with maximum weighting factor if the mass flow at the Junction is larger than XTALSC(2) ($W_{JN} > \text{XTALSC}(2)$). The input entries KTALSC(2) and XTALSC(2) allow the user to change the averaging weighting factors when flow conditions in the heat exchangers change, for example when a counter-current flow becomes co-current. Typically the temperature averaging is needed in counter-flow conditions, while it is not needed in co-flow conditions. This can be achieved by setting XTALSC(2) to a

large number (for example XTALSC(2)=10⁶). Generally speaking, XTALSC(2) is a flow for which the temperature distribution in the left boundary Control Volume is approximately linear, provided that there is flow in through JTALSC(2) and KTALSC(2).
 Acceptable range: 10⁻¹⁰ < XTALSC(2) < 10¹⁰.
 Default value: none.

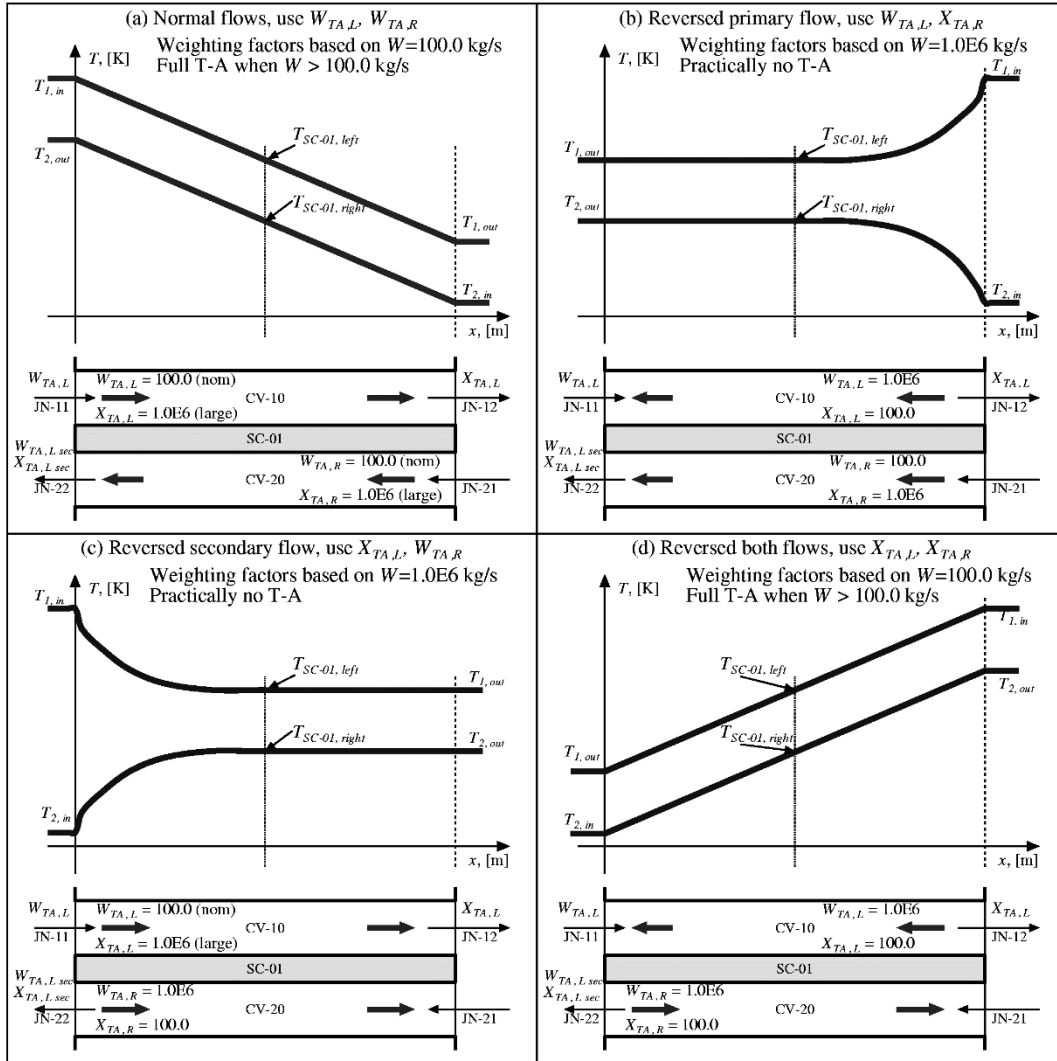


Figure 2-16 Example of temperature averaging for a counter-flow heat exchanger.

2.3.16 Records: 326XXX, Right Side Heat Exchanger Temperature Averaging

XXX is the Solid Heat Conductor reference number, 001 ≤ XXX ≤ 999. These records define the temperature averaging for the right surface of a Solid Heat Conductor (see section 2.3.15).

Inlet Junction Data

SPECTRA Code Manuals - Volume 2: User's Guide

- W-1 (I) : JTARSC (1) Junction reference number of the inlet Junction on the current (right) side.
Acceptable range: must be a Junction connected to the right boundary Control Volume (IVLRSC), if non-zero.
Default value: none.
- W-2 (R) : WTARSC (1) Limiting mass flow in the inlet Junction JTARSC(1) for full temperature averaging ($W_{TA,R}$ in Figure 2-16 (a)). Applied when there is flow through JTARSC(1) into IVLRSC and there is no flow through KTARSC into IVLLSC - normal flow direction on both right (secondary) and left (primary) side. The temperature of the fluid entering through the Junction JTARSC(1) will be used with maximum weighting factor if the mass flow at the Junction is larger than WTARSC(1) ($W_{JN} > WTARSC(1)$). Generally speaking, WTARSC(1) is a flow for which the temperature distribution in the right boundary Control Volume is approximately linear, provided that there is flow in through JTARSC(1) and there is no flow in through KTARSC(1). Roughly, this number can be viewed as a nominal flow through the heat exchanger.
Acceptable range: $10^{-10} < WTARSC(1) < 10^{10}$.
Default value: none.
- W-3 (I) : KTARSC (1) Junction reference number of the outlet Junction on the other (left) side.
Acceptable range: must be a Junction connected to the left boundary Control Volume (IVLLSC), if non-zero.
Default value: none.
- W-4 (R) : XTARSC (1) Limiting mass flow in the Junction JTARSC(1) for full temperature averaging ($X_{TA,R}$ in Figure 2-16 (b)). Applied when there is flow through JTARSC(1) into IVLRSC and simultaneously there is flow through KTARSC(1) into IVLLSC - normal flow direction on the right (secondary) side, reversed left (primary) side flow. The temperature of the fluid entering through the Junction JTARSC(1) will be used with maximum weighting factor if the mass flow at the Junction is larger than XTARSC(1) ($W_{JN} > XTARSC(1)$). The input entries KTARSC(1) and XTARSC(1) allow the user to change the averaging weighting factors when flow conditions in the heat exchangers change, for example when a counter-current flow becomes co-current. Typically the temperature averaging is needed in counter-flow conditions, while it is not needed in co-flow conditions. This can be achieved by setting XTARSC(1) to a large number (for example $XTARSC(1)=10^6$). Generally speaking, XTARSC(1) is a flow for which the temperature distribution in the right boundary Control Volume is approximately linear, provided that there is flow in through JTARSC(1) and KTARSC(1).
Acceptable range: $10^{-10} < XTARSC(1) < 10^{10}$.
Default value: none.

Outlet Junction Data

- W-5 (I) : JTARSC (2) Junction reference number of the outlet Junction on the current (right) side.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: must be a Junction connected to the right boundary Control Volume (IVLRSC), if non-zero.

Default value: none.

- W-6 (R) : WTARSC Limiting mass flow in the outlet Junction JTARSC(2) for full temperature averaging ($W_{TA,R}$ in Figure 2-16 (c)). Applied when there is a through JTARSC(2) into IVLRSC and there is no flow through KTARSC(2) into IVLLSC - reversed flow on the right (secondary) side and normal flow direction on the left (primary) side. The temperature of the fluid entering through the Junction JTARSC(2) will be used with maximum weighting factor if the mass flow at the Junction is larger than WTARSC(2) ($W_{JN} > WTARSC(2)$). Generally speaking, WTARSC(2) is a flow for which the temperature distribution in the right boundary Control Volume is approximately linear, provided that there is flow in through JTARSC(2) and there is no flow in through KTARSC(2).
Acceptable range: $10^{-10} < WTARSC(2) < 10^{10}$.
Default value: none.
- W-7 (I) : KTARSC Junction reference number of the outlet Junction on the other (left) side.
(2) *Acceptable range:* must be a Junction connected to the left boundary Control Volume (IVLLSC), if non-zero.
Default value: none.
- W-8 (R) : XTARSC Limiting mass flow in the outlet Junction JTARSC(2) for full temperature averaging ($X_{TA,R}$ in Figure 2-16 (d)). Applied when there is a through JTARSC(2) into IVLRSC and simultaneously there is flow through KTARSC(2) into IVLLSC - reversed flow on both right (secondary) side and left (primary) side. The temperature of the fluid entering through the Junction JTARSC(2) will be used with maximum weighting factor if the mass flow at the Junction is larger than XTARSC(2) ($W_{JN} > XTARSC(2)$). The input entries KTARSC(2) and XTARSC(2) allow the user to change the averaging weighting factors when flow conditions in the heat exchangers change, for example when a counter-current flow becomes co-current. Typically the temperature averaging is needed in counter-flow conditions, while it is not needed in co-flow conditions. This can be achieved by setting XTARSC(2) to a large number (for example $XTARSC(2)=10^6$). Generally speaking, XTARSC(2) is a flow for which the temperature distribution in the right boundary Control Volume is approximately linear, provided that there is flow in through JTARSC(2) and KTARSC(2).
Acceptable range: $10^{-10} < XTARSC(2) < 10^{10}$.
Default value: none.

An example of temperature averaging for a counter-flow heat exchanger is shown in Figure 2-16. For the case shown in this figure appropriate input entries are:

SC-01 left surface, inlet Junction:

- JTALSC=11 JN-11 is the inlet Junction on the left surface.
- WTALSC= W_{NL} nominal flow for the normal counter-flow conditions - Figure 2-16 (a).

SPECTRA Code Manuals - Volume 2: User's Guide

- KTALSC=22 if there is flow in through JN-11, and simultaneously through JN-22, the flow is co-current and WTALSC needs to be replaced by XTALSC, below.
- XTALSC=10⁶ a large value, appropriate for co-flow conditions - Figure 2-16 (c).

SC-01 left surface, outlet Junction:

- JTALSC=12 JN-12 is the outlet Junction on the left surface; when there is flow in through this Junction, the flow is co-current and WTALSC should be large.
- WTALSC=10⁶ a large value, appropriate for co-flow conditions -Figure 2-16 (b).
- KTALSC=22 if there is flow in through JN-12, and simultaneously through JN-22, the flow is counter-current and WTALSC needs to be replaced by XTALSC, below.
- XTALSC=W_{NL} nominal flow for the reversed counter-flow conditions - Figure 2-16 (d).

SC-01 right surface, inlet Junction:

- JTARSC=21 JN-21 is the inlet Junction on the right surface.
- WTARSC=W_{NR} nominal flow for the normal counter-flow conditions - Figure 2-16 (a).
- KTARSC=12 if there is flow in through JN-21, and simultaneously through JN-12, the flow is co-current and WTARSC needs to be replaced by XTARSC, below.
- XTARSC=10⁶ a large value, appropriate for co-flow conditions - Figure 2-16 (b).

SC-01 right surface, outlet Junction:

- JTARSC=22 JN-22 is the outlet Junction on the left surface; when there is flow in through this Junction, the flow is co-current and WTARSC should be large.
- WTARSC=10⁶ a large value, appropriate for co-flow conditions - Figure 2-16 (c).
- KTARSC=12 if there is flow in through JN-22, and simultaneously through JN-12, the flow is counter-current and WTARSC needs to be replaced by XTARSC, below.
- XTARSC=W_{NLR} nominal flow for the reversed counter-flow conditions - Figure 2-16 (a).

Suppose the nominal flow is 100.0 kg/s on both left and right side. The input deck for the SC-01 Temperature Averaging (Figure 2-16) looks like this:

	INLET JUNCTION				OUTLET JUNCTION				
*	JTALSC	WTALSC	KTALSC	XTALSC	JTALSC	WTALSC	KTALSC	XTALSC	
325001	011	100.0	022	1.0E+6	012	1.0E+6	022	100.0	* Left side
326001	021	100.0	012	1.0E+6	022	1.0E+6	012	100.0	* Right side

Note that the limiting flow for T-A is affected by the multipliers CMN1SC, CMN2SC, defined in the record 360000 (section 2.3.23). Generally one should make sure that the limiting flows, W_{TA}, approximately fulfil the relation:

$$(W_{TA}c_p)_{primary} \approx (W_{TA}c_p)_{secondary}$$

The multipliers will then assure proper temperature averaging in case when the flow on the primary side is becoming very different from the flow on the secondary side.

2.3.17 Records: 327XXX, Left Side Structure-to-Structure Radiation

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : JQRLSC Reference number of the 1-D Solid Heat Conductor member of the structure-to-structure radiation pair. A left side surface of JQRLSC is identified by the use of a negative Solid Conductor number while a right side surface of JQRLSC is identified by a positive Solid Conductor number. A single SC may be a member of a single radiating pair only. The model need to be defined on one of the radiating surfaces. If it is defined on both radiating surfaces, the input must be consistent. Emissivity must be defined for both surfaces:
 IQRLSC > 1000: for the Solid Conductor XXX
 IQRLSC < 1000: for the Solid Conductor -JQRLSC, if JQRLSC < 0
 IQRRSC > 1000: for the Solid Conductor JQRLSC, if JQRLSC > 0
Acceptable range: must be a valid reference number of a 1-D Solid Heat Conductor, if non-zero
Default value: 0
- W-2 (R) : FQRLSC View factor from the smaller surface to the larger surface, F_{1-2} . Note that this always the view factor from the smaller surface of the pair.
Acceptable range: $0.0 < FQRLSC \leq 1.0$.
Default value: 1.0

The effective emissivity of a pair of 1-D Solid Heat Conductor surfaces and the radiation heat fluxes are obtained from:

$$\varepsilon_{1-2} = \left(\frac{1}{\varepsilon_1} + \frac{A_1}{A_2} \cdot \left(\frac{1}{\varepsilon_2} - 1 \right) + \frac{1}{F_{1-2}} - 1 \right)^{-1}$$

$$q_{1-2} = \varepsilon_{1-2} \cdot \sigma \cdot (T_1^4 - T_2^4)$$

$$q_{2-1} = \varepsilon_{1-2} \cdot \sigma \cdot (T_2^4 - T_1^4) \cdot \frac{A_1}{A_2}$$

- q_{1-2} heat flux from surface 1 to 2, W/m²,
 σ Stefan-Boltzmann constant, $=5.67 \times 10^{-8}$ W/(m²·K⁴),
 T_1 temperature of surface 1, K,
 T_2 temperature of surface 2, K,
 ε_{1-2} effective emissivity between surfaces 1 and 2.
 A_1 area of surface 1, m², (the smaller surface)
 A_2 area of surface 2, m², (the larger surface)
 ε_1 emissivity (temperature-dependent) of surface 1,

SPECTRA Code Manuals - Volume 2: User's Guide

ϵ_2 emissivity (temperature-dependent) of surface 2,
 F_{1-2} view factor from surface 1 (the smaller surface) to surface 2 (the larger surface).

2.3.18 Records: 328XXX, Right Side Structure-to-Structure Radiation

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : JQRRSC Reference number of the 1-D Solid Heat Conductor member of the structure-to-structure radiation pair. A left side surface of JQRRSC is identified by the use of a negative Solid Conductor number while a right side surface of JQRRSC is identified by a positive Solid Conductor number. A single SC may be a member of a single radiating pair only. The model need to be defined on one of the radiating surfaces. If it is defined on both radiating surfaces, the input must be consistent. Emissivity must be defined for both surface:
 IQRSC > 1000: for the Solid Conductor XXX
 IQLSC > 1000: for the Solid Conductor -JQRRSC, if JQRRSC<0
 IQRSC > 1000: for the Solid Conductor JQRRSC, if JQRRSC>0
Acceptable range: must be a valid reference number of a 1-D Solid Heat Conductor, if non-zero
Default value: 0

W-2 (R) : FQRRSC View factor from the smaller surface to the larger surface, F_{1-2} . Note that this always the view factor from the smaller surface of the pair.
Acceptable range: $0.0 < FQRRSC \leq 1.0$.
Default value: 1.0

Example 1

The example below defines a radiating pair consisting of the right surface of SC-100 and the left surface of SC-200. Default value of the view factor from the smaller surface, $F_{1-2} = 1.0$, is used. The view factor from the larger surface (computed internally by the code) is equal to $F_{2-1} = A_1/A_2$.

```
328100    -200   *   SC-100 right to SC-200 left
```

Example 2

The example below defines a radiating pair consisting of the right surface of SC-100 and the left surface of SC-200. The view factor from the smaller surface is equal to $F_{1-2} = 0.5$. The view factor from the larger surface (computed internally by the code) is equal to $F_{2-1} = F_{1-2} \times A_1/A_2$.

```
328100    -200   0.5   *   SC-100 right to SC-200 left , view fac=0.5
```

It is sufficient to define the pair for one of the two radiating surfaces. The definition below will give exactly the same results as the definition above:

```
327200    100  0.5  *  SC-200 left  to SC-100 right, view fac=0.5
```

The radiating pair of surfaces may also be defined twice. In this case both definitions must be consistent, otherwise an input error is generated. The following definition:

```
328100   -200  0.5  *  SC-100 right to SC-200 left , view fac=0.5
327200    100  0.5  *  SC-200 left  to SC-100 right, view fac=0.5
```

will give exactly the same results as the definitions shown earlier: Note that the view factor FQRRSC is always interpreted as the view factor from the smaller of the two surfaces. Therefore the value is the same, independently of which record, 328100 or 327200, is used. The view factor from the larger surface is always calculated obtained internally in the code.

2.3.19 Records: 350XXX, Boundary Fluid Temperature Calculation

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record describes boundary fluid temperature calculation in case of intensive boiling. This record is optional. All entries from this record have their default values, recommended for general application.

W-1 (I) : IBPTSC Indicator for boundary fluid temperature calculation for pool-bubble flow. Typically the pool temperature is used as boundary fluid temperature for Solid Heat Conductors. In case of intensive boiling the program assumes that bubbles rise up in a plume of relatively warm water (see Volume 1). The water temperature in this plume is equal to the local saturation temperature, and is therefore higher than the pool average temperature, which is no higher than the saturation temperature at the pool surface pressure. The indicator IBPTSC defines how the program should determine whether the SC surface will be exposed to the warm plume or to the relatively cold pool outside the plume. Three factors may be used by the program: the void fraction factor, f_α , the temperature factor, f_T , and the submergence factor, f_z . Those factors are defined as follows:

a) The void fraction factor, f_α :

$$f_\alpha = \begin{cases} 0.0 & \text{if } \alpha \leq \alpha_1 \\ (3 - 2X)X^2 & \text{if } \alpha_1 < \alpha < \alpha_2 \\ 1.0 & \text{if } \alpha \geq \alpha_2 \end{cases}$$

where α is the average void fraction in the pool, X is the interpolation factor, equal to: $X = (\alpha - \alpha_1) / (\alpha_2 - \alpha_1)$, and the boundary values of void fractions, α_1 , α_2 , are defined below (words 2 and 3). Note that the cubic interpolation is used, which ensures continuity of the function as well as its first derivative.

b) The surface temperature factor, f_T :

$$f_T = \begin{cases} 0.0 & \text{if } T_{SC} \leq T_{int} + \Delta T_1 \\ (3 - 2X)X^2 & \text{if } T_{int} + \Delta T_1 < T_{SC} < T_{int} + \Delta T_2 \\ 1.0 & \text{if } T_{SC} \geq T_{int} + \Delta T_2 \end{cases}$$

where T_{SC} is the surface temperature of the Solid Heat Conductor, T_{int} is the liquid temperature at the pool-bubble interphase, X is the interpolation factor, equal to:

$$X = (T_{SC} - (T_{int} + \Delta T_1)) / ((T_{int} + \Delta T_2) - (T_{int} + \Delta T_1)),$$

and the boundary values of ΔT are defined below (words 4 and 5).

c) The surface submergence factor, f_Z :

$$f_Z = \begin{cases} (3 - 2X_1)X_1^2 & \text{if } 0 \leq Z < Z_{bubb} \\ 1.0 & \text{if } Z_{bubb} \leq Z \leq Z_{bubb}Z_{m1} \\ (3 - 2X_2)X_2^2 & \text{if } Z_{bubb}Z_{m1} < Z < Z_{bubb}Z_{m2} \\ 0.0 & \text{if } Z_{bubb}Z_{m2} \leq Z \end{cases}$$

where Z is the SC submergence (equal to the distance between the pool surface and the elevation of the middle point of this part of the SC which is covered by water), Z_{bub} is the submergence of average bubble, X_1 and X_2 are the interpolation factors, equal to:

$$X_1 = Z/Z_{bub},$$

$$X_2 = (Z - Z_{bub} \cdot Z_{m2}) / (Z_{bub} \cdot Z_{m1} - Z_{bub} \cdot Z_{m2}).$$

Values of the multipliers, Z_{m1} and Z_{m2} , are defined below (words 6, 7).

The parameter IBPTSC defines which of the factors described above should be used. The interpretation is as follows:

IBPTSC = -1 : No factors are used. When the surface is exposed to a boiling pool, the boundary fluid temperature is always equal to the pool temperature, T_{pool} (approximately equal to the saturation temperature for the pressure at the pool surface).

$$T_{fluid} = T_{pool}$$

IBPTSC = 1 : Only the void fraction factor is taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot f_\alpha$$

where T_{pool} is the pool average temperature, and T_{int} is the liquid temperature at the pool-bubble interphase (thus the warm plume temperature, approximately equal to the saturation temperature for the pressure at the elevation of average bubble).

SPECTRA Code Manuals - Volume 2: User's Guide

IBPTSC = 2 : The void fraction factor and the temperature factor are taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot (f_{\alpha} f_T)$$

IBPTSC = 3 : The void fraction factor and the submergence factor are taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot (f_{\alpha} f_Z)$$

IBPTSC = 4 : All factors are taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot (f_{\alpha} f_T f_Z)$$

Acceptable range: $-1 \leq \text{IBPTSC} \leq +4$.

Default value: +4. If IWATCV>0 (see section 2.1.31) then the default value is -1.

- | | | |
|-----------|--------|--|
| W-2 (R) : | ALP1SC | Upper limit of void fraction to use only the pool temperature as boundary fluid temperature for the SC surface, α_1 , (-). Used if IBPTSC (word 1 above) is positive. If the average void fraction in the pool is below α_1 then the Solid Heat Conductor surface is not exposed to the warm plume.
<i>Acceptable range:</i> $10^{-5} \leq \text{ALP1SC} \leq 0.1$.
<i>Default value:</i> 10^{-3} . |
| W-3 (R) : | ALP2SC | Lower limit of void fraction to use the warm plume temperature as boundary fluid temperature for the SC surface, α_2 , (-). Used if IBPTSC (word 1 above) is positive. If the average void fraction in the pool is above α_2 then the Solid Heat Conductor surface can be exposed to the warm plume (depending on other conditions if they are applied).
<i>Acceptable range:</i> $2.0 \cdot \text{ALP1SC} \leq \text{ALP2SC} \leq 0.5$.
<i>Default value:</i> 0.05 . |
| W-4 (R) : | TSC1SC | Upper limit of SC surface superheat to use only the pool temperature as boundary fluid temperature for the SC surface, ΔT_1 , (K). Used if IBPTSC (word 1 above) is equal to 2 or 4. If the SC surface temperature is lower than the liquid temperature at the pool-bubble interphase (warm plume temperature) plus TSC1SC then the Solid Heat Conductor surface is not exposed to the warm plume.
<i>Acceptable range:</i> $0.1 \leq \text{TSC1SC} \leq 10.0$.
<i>Default value:</i> 1.0 . |
| W-5 (R) : | TSC2SC | Lower limit of SC surface superheat to use the warm plume temperature as boundary fluid temperature for the SC surface, ΔT_2 , (K). Used if IBPTSC (word 1 above) is equal to 2 or 4. If the SC surface temperature is lower than the liquid temperature at the pool-bubble interphase (warm plume temperature) plus TSC2SC then the Solid Heat Conductor surface can be exposed to the warm plume (depending on other conditions if they are applied). |

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $2.0 \cdot TSC1SC \leq TSC2SC \leq 30.0$.
Default value: 3.0 .

W-6 (R) : ZSC1SC Lower multiplier on bubble submergence to use the warm plume temperature as boundary fluid temperature for the SC surface, Z_{m1} , (-). Used if IBPTSC (word 1 above) is equal to 3 or 4. If the SC surface submergence is smaller than the average bubble submergence multiplied by ZSC1SC then the Solid Heat Conductor surface can be exposed to the warm plume (depending on other conditions if they are applied).
Acceptable range: $1.0 \leq ZSC1SC \leq 10.0$.
Default value: 2.0 .

W-7 (R) : ZSC2SC Upper multiplier on bubble submergence to use only the pool temperature as boundary fluid temperature for the SC surface, Z_{m2} , (-). Used if IBPTSC (word 1 above) is equal to 3 or 4. If the SC surface submergence is larger than the average bubble submergence multiplied by ZSC2SC then the Solid Heat Conductor surface is not exposed to the warm plume.
Acceptable range: $1.2 \cdot ZSC1SC \leq ZSC2SC \leq 15.0$.
Default value: 4.0 .

2.3.20 Records: 351XXX, Boundary Fluid Velocity Multiplier

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record is optional. The velocity multiplier may be used for to account for own movement of structures, such as for example rotor blades. In such case the relative velocity surface-to-gas velocity is different than the gas velocity in a Control Volume. The user may take into account that difference using a Control Function that depends on the rotational speed, etc.

W-1 (I) : VLMLSC Velocity multiplier, C_v , for the boundary surface velocity calculation. If a positive value is entered, the velocity multiplier is constant, and equal to this value. If a negative value is entered, the velocity multiplier is obtained from the Control Function equal to $|VLMLSC|$. An absolute value of the number obtained from the Control Function is used. Furthermore the value is limited to a maximum of 10^{10} .

The fluid velocity at the SC boundary surface is obtained from:

If IHDLSC=0 (Word 18, record 321XXX):

$$v_{SC} = C_v \cdot \sqrt{v_{CV,hor}^2 + v_{CV,ver}^2}$$

If IHDLSC=1, IVERSC=0 (vertical SC, Word 5, record 300XXX):

$$v_{SC} = C_v \cdot v_{CV,ver}$$

If IHDLSC=1, IVERSC≠0 (horizontal SC, Word 5, record 300XXX):

$$v_{SC} = C_v \cdot v_{CV,hor}$$

Acceptable range: $0.0 \leq VLMLSC \leq 10^{10}$
or reference to a Control Function.
Default value: 1.0

2.3.21 Records: 352XXX, Limit for Simultaneous Transfer to Pool and Atmosphere

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (R) : PMXLSC Critical (maximum) fraction of left surface area covered by pool to allow simultaneous heat transfer to pool and atmosphere. If no value is given, simultaneous heat transfer to pool and atmosphere is always possible. This may lead to too large condensation in some cases. To eliminate it, the user may restrict the simultaneous heat transfer to a situation when the pool-covered fraction is smaller than PMXLSC. This input parameter is similar to CPFPL in the MELCOR code. An interpolation zone is defined. The full transfer to gas occurs when the pool fraction is below 0.9 of the critical value, a linear interpolation is performed in the range between 0.9 and 1.0 times the critical value.

Acceptable range: $0.0 \leq PMXLSC \leq 1.0$
Default value: 0.0 .

W-1 (R) : PMXRSC Maximum fraction of right surface area covered by pool to allow simultaneous heat transfer to pool and atmosphere. The same as PMXLSC but applied for the right surface).

Acceptable range: $0.0 \leq PMXRSC \leq 1.0$
Default value: 0.0 .

As example of such situation is discussed in Volume 1. As a reference case, a fine nodalization is used (Figure 2-17, left). Coarse nodalization and consequent too slow heat up due to artificial heat transfer from atmosphere to pool through the solid structure is shown in Figure 2-17, middle. This is prevented by using the parameter PMXRSC. A value of PMXRSC=0.01 was used (Figure 2-17, right). The heat transfer from atmosphere to pool is practically eliminated. However, a direct heat transfer still exists at the pool-atmosphere interphase. Therefore it is advisable to eliminate the pool-atmosphere heat transfer at the same time (input record 164XXX). This was done in the considered example.

Test for simultaneous pool and atmosphere heat transfer, SPECTRA,

t = 1600 s

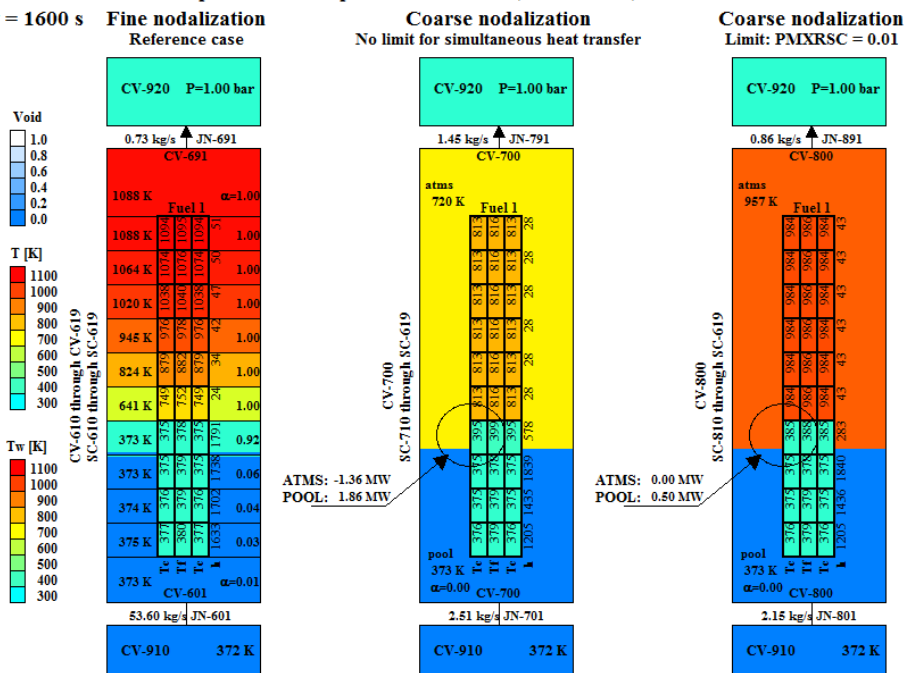


Figure 2-17 Simultaneous heat transfer to fuel pool and atmosphere

2.3.22 Records: 353XXX, Plume Model for Heat and Mass Transfer

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. These records activate plume models for the heat and mass transferred at the surface of the Solid Heat Conductor. The plume model is used in Control Volumes, in which stratification is calculated. Thus, it will be used only if the stratification model is active for the boundary (left or right) volume for this Solid Heat Conductor. A description of the plume model is given in Volume 1. To activate the model for a single component, a set of two integer numbers, described below, must be entered. To activate the model for both atmosphere and pool, two pairs of data should be entered in this record.

W-1 (I) : J Identifier of component, for which the plume model is desired. J=1: atmosphere; J=3: pool.
 Acceptable range: J=1, or J=3.
 Default value: none.

W-2 (I) : IPLMSC Plume model activator. If IPLMSC = 0 then the plume model is not active. If IPLMSC \neq 0 then the plume model is active for the component J and Solid Heat Conductor XXX.
 Note that the plume model is used only when stratification models are active in Control Volumes associated with left or right boundary surface of the Solid Heat Conductor.
 Acceptable range: any integer.
 Default value: 0.

... etc., until all plumes are defined.

2.3.23 Records: 360000, Global Data: Film Boiling, Slip Ratio, TA, Oxidation

Parameters defined in this record are applied for all 1-D Solid Heat Conductors.

- W-1 (R) : AMFBSC First coefficient in the Simon Minimum Film Boiling correlation, A_{MFB} , (-). SPECTRA selects correlation that gives maximum value of the T_{MFB} , therefore the Simon correlation may be deactivated by setting AMFBSC and BMFBSC to small values.
Acceptable range: $0.0 < AMFBSC \leq 1.0$
Default value: 0.13.
- W-2 (R) : BMFBSC Second coefficient in the Simon Minimum Film Boiling correlation, B_{MFB} , (-). SPECTRA selects correlation that gives maximum value of the T_{MFB} , therefore the Simon correlation may be deactivated by setting AMFBSC and BMFBSC to small values.
Acceptable range: $0.0 < BMFBSC \leq 2.0$
Default value: 0.86.
- W-3 (R) : CMFBSC Coefficient in the Berenson Minimum Film Boiling correlation, C_{MFB} , (-). SPECTRA selects correlation that gives maximum value of the T_{MFB} , therefore the Berenson correlation may be deactivated by setting CMFBSC to a small value.
Acceptable range: $0.0 < CMFBSC \leq 1.0$
Default value: 0.127
- W-4 (R) : TFMNSC Minimum value of the Minimum Film Boiling (MFB) temperature minus the Critical Heat Flux (CHF) temperature: $(T_{MFB} - T_{CHF})$, (K). The MFB temperature, calculated from the Simon correlation is limited by this word so that it will never be lower than $T_{CHF} + TFMNSC$.
Acceptable range: $5.0 \leq TFMNSC \leq 1000.0$
Default value: 5.0.
- W-5 (R) : TFMXSC Maximum value of the Minimum Film Boiling (MFB) temperature minus the Critical Heat Flux (CHF) temperature: $(T_{MFB} - T_{CHF})$, (K). The minimum film boiling temperature, calculated from the Simon correlation is limited by this word so that it will never be higher than $T_{CHF} + TFMXSC$.
Acceptable range: $TFMNSC \leq TFMXSC \leq 1000.0$
Default value: 1000.0.
- W-6 (R) : XTRBSC Coefficient in the Kalinin Transition Boiling correlation, X_{TB} , (-).
Acceptable range: $0.5 < XTRBSC \leq 20.0$
Default value: 7.0.
- W-7 (R) : ASFBSC Correction for subcooling in the film boiling correlation, A_{SFB} , (-). In case of a subcooled film boiling, the total heat flux is calculated from:

$$q = q_{FB} + A_{SFB} \cdot h_{conv} \cdot (T_{sat} - T_{fluid})$$

SPECTRA Code Manuals - Volume 2: User's Guide

where q_{FB} is the saturated film boiling heat flux while h_{conv} is a convective heat transfer coefficient, equal to: $\text{Max}(h_{FC}, h_{NC})$ with h_{FC} , h_{NC} being the forced and the natural convective heat transfer coefficients

Acceptable range: $0.0 \leq \text{ASFBSC} \leq 2.0$

Default value: 0.0

W-8 (R) : SMAXSC Maximum value of the slip ratio, (v_{bubb} / v_{pool}), (-). Used for CHF calculations. The slip ratio which is used in the CHF correlation is equal to the minimum of v_{bubb} / v_{pool} and SMAXSC.

Acceptable range: $1.0 \leq \text{SMAXSC} \leq 1000.0$

Default value: 100.0.

W-9 (R) : CMN1SC Multiplier for the first (counter-current) Temperature Averaging (T-A) mode. The nominal flows for the T-A on both primary and secondary side of a heat exchanger are entered in the records 325XXX 326XXX. If the flows exceed the nominal flows, full T-A is performed. If flows are decreased then also the T-A is decreased - see section 2.3.15 and 2.3.16. This treatment is approximately correct if flow changes only on one side of the heat exchanger. If the flow changes simultaneously on both sides of the heat exchanger, then T-A should be used for flows much smaller than nominal. This multiplier defines how much the limiting flow (typically taken as a nominal flow) can be decreased when the flow on the other side of a heat exchanger decreases.

The default value of 0.01 means that in nominal counter-flow conditions full T-A will be performed if the flows decrease down to 1% of the nominal flow, provided that they will decrease simultaneously on both sides of the heat exchanger.

Generally the limiting flow on a given side of a heat exchanger is:

$$W_{TA} = \text{Min} \left[\frac{W_{TA}}{C_{MN1}}, \text{Max} \left(W_{TA} C_{MN1}, W_{TA} \frac{W_{other\ side}}{W_{TA, other\ side}} \right) \right]$$

where W_{TA} is the limiting flow for full T-A, C_{MN1} is the factor CMN1SC, $W_{TA, other\ side}$ is the limiting flow for full T-A on the other side, and $W_{other\ side}$ is the current flow on the other side. Note that with this definition, the limiting flow for T-A can be either decreased or increased, and the actual value will always be within the range:

$$W_{TA} C_{MN1} \leq W_{TA} \leq \frac{W_{TA}}{C_{MN1}}$$

The limiting flow will be small when the other side flow is small, and large when the other side flow is large. This is the most appropriate treatment of a heat exchanger, provided that the limiting flows, defined in records 325XXX, 326XXX for both primary and secondary side, fulfil approximately the relation:

$$(W_{TA} c_p)_{primary} \approx (W_{TA} c_p)_{secondary}$$

Acceptable range: $0.001 \leq \text{CMN1SC} \leq 1.0$

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 0.01.

W-10 (R) : CMN2SC Multiplier for the second (co-current) Temperature Averaging (T-A) mode. Works the same as CMN1SC, but in case when the flow is co-current. Default value means that CMN2SC is not used in co-flow conditions. It is recommended to disable T-A in co-flow by setting the limiting flow to a large value - see section 2.3.15 and 2.3.16. In such case the value of CMN2SC is not very important. For consistency it should be equal to 1.0 when T-A is disabled.

Acceptable range: $0.001 \leq \text{CMN2SC} \leq 1.0$

Default value: 1.0.

W-11 (R) : VGLMSC Gas velocity limit, $v_{g,lm}$ (m/s), to switch off the Temperature Averaging (T-A). Numerical problems may be encountered when T-A is used in case of low velocities and changes of flow direction. To avoid this problems the T-A is turned off when the velocity is smaller than the limit defined by this word. An interpolation zone is defined for gas velocities between VGLMSC and $2 \times \text{VGLMSC}$.

$$X_{TA,eff} = \begin{cases} X_{TA} & \text{if } v_g > 2v_{g,lm} \\ X_{TA} \cdot (v_g - v_{g,lm}) / v_{g,lm} & \text{if } v_{g,lm} < v_g < 2v_{g,lm} \\ 0.0 & \text{if } v_g < v_{g,lm} \end{cases}$$

where X_{TA} is the Temperature Averaging factor for full T-A, $X_{TA,eff}$ is the effective T-A factor, v_g is the gas velocity and $v_{g,lm}$ is the limiting gas velocity, VGLMSC.

Acceptable range: $0.001 \leq \text{VGLMSC} \leq 100.0$

Default value: 1.0

W-12 (R) : VLLMSC Liquid velocity limit, $v_{l,lm}$ (m/s), to switch off the Temperature Averaging (T-A). Numerical problems may be encountered when T-A is used in case of low velocities and changes of flow direction. To avoid this problems the T-A is turned off when the velocity is smaller than the limit defined by this word. An interpolation zone is defined for liquid velocities between VLLMSC and $2 \times \text{VLLMSC}$.

$$X_{TA,eff} = \begin{cases} X_{TA} & \text{if } v_l > 2v_{l,lm} \\ X_{TA} \cdot (v_l - v_{l,lm}) / v_{l,lm} & \text{if } v_{l,lm} < v_l < 2v_{l,lm} \\ 0.0 & \text{if } v_l < v_{l,lm} \end{cases}$$

where X_{TA} is the Temperature Averaging factor for full T-A, $X_{TA,eff}$ is the effective T-A factor, v_l is the liquid velocity and $v_{l,lm}$ is the limiting liquid velocity, VLLMSC.

Acceptable range: $0.001 \leq \text{VLLMSC} \leq 100.0$

Default value: 0.1

W-13 (I) : IOXNSC Option for oxidation on surfaces not connected to Control Volumes.

SPECTRA Code Manuals - Volume 2: User's Guide

=1: oxidation is calculated on SC surfaces not connected to a CV. It will be assumed that all oxidizing gases are always available at the surface.

=2: oxidation is disabled on SC surfaces not connected to a CV.

Acceptable range: 1, 2

Default value: none

- W-14 (I) : ISEQSC Indicator for multiple oxidation reactions.
 =1: all oxidation reactions proceed simultaneously.
 =2: dominant reactions: oxidation reactions proceed in sequence, defined in records 381XXX, 382XXX. If there is enough oxidant (gas fraction > XLIMSC) for the first reaction, only this reaction occurs. If not, second reaction starts, then third, etc. This option is available because, according to [52], reaction with oxygen dominates over reactions with steam and nitrogen.
Acceptable range: 1, 2
Default value: 1
- W-15 (R) : XLIMSC Limit for dominant reactions. The default oxidation starvation limits are:
 C1OX = 1.0×10^{-4} : full strength oxidation
 C0OX = C1OX / 10.0 = 1.0×10^{-5} : no oxidation
 The default value of XLIMSC was selected approximately in the middle of the interpolation zone, when the dominant reaction strength is reduced roughly by half.
Acceptable range: $1.0 \times 10^{-7} \leq \text{XLIMSC} \leq 1.0 \times 10^{-2}$
Default value: XLIMSC = C1OX / 2.0
- W-16 (I) : IMPGSC Implicit/explicit use of gas concentration for oxidation calculations.
 = 1: implicit (end of time step value is used).
 = 2: explicit (beginning of time step value is used).
Acceptable range: 1 or 2
Default value: 1
- W17 - (I) IAVESC Method used to calculate average SC temperature. In SPECTRA output and plot files, the average temperatures are given next to the cell temperatures. This entry defines how the average temperature is obtained.
 = 1: volume average: $\bar{T} = \frac{\sum_i V_i \cdot T_i}{\sum_i V_i}$
 = 2: mass-average: $\bar{T} = \frac{\sum_i M_i \cdot T_i}{\sum_i M_i}$
 Here M_i , V_i , T_i are the mass, volume and temperature of the cell i .
Acceptable range: 1 or 2
Default value: 2
- W-18 (I) : ITAISC A value of ITAISC > 0 activates the averaging scheme (T-A) also for isotopes in circulating fuel. The averaging weighting factor is divided by ITAISC. ITAISC = 1 means full averaging (both current CV value and the value at the inlet to CV are taken with weights of 0.5. A value > 1 means that the current CV value gets higher weight. For example, ITAISC = 3 means that the current CV is taken with the weight of 0.75 and the inlet value with the weight of 0.25 (see Volume 1).

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: ITAISC ≥ 0

Default value: 0

W-19 (I) : IQPLSC Power versus power density as plot parameters - Table 2-25.
= 1: Power (W) is used as plot parameters: SC-XXX-Qcel-YYYY
= 2: Power density (W/m³) is used: SC-XXX-qcel-YYYY
Acceptable range: 1 or 2
Default value: 1

2.3.24 Records: 365000, Hydraulic Diameter - SC Versus CV

W-1 (I) : IDHDSC Option to check consistency between the CV hydraulic diameter (DHYDCV) and the SC hydraulic diameter (DFCLSC/DFCRSC).
= 1 : consistency is not required. If DFCLSC \neq DHYDCV or DFCRSC \neq DHYDCV, then a warning message is issued.
= 2 : consistency is required. If DFCLSC \neq DHYDCV or DFCRSC \neq DHYDCV, then an error message is issued.
Acceptable range: 1, 2
Default value: 1

Second, steel oxidation by O₂ and H₂O for the 1-D Heat Conductor SC-100, right surface. The initial thickness of material which can be oxidized is 0.001 m. The initial oxide thickness is 0.0 m. For steel-steam reaction the built-in model is used (model indicator = -3, see section 2.14.1). For steel-oxygen reaction a user-defined model number 4 is used. The records 850004, 8510004, ..., must be specified in the input deck. Example input for steel-oxygen reaction is shown in section 2.14.1.

```

*
*      Un-oxidized Oxide  Reactions
381100  0.001      0.0  -4 -1 *  Zr oxidation by O2 and H2O
382100  0.001      0.0   4 -3 *  Steel oxidation by O2 and H2O
    
```

2.3.27 Record: 330XXX, Failure Parameters

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record activates the failure model for this 1-D Solid Heat Conductor. The failure model considers the following three failure mechanisms:

- Ultimate strength failure (failure mode = 1)
- Creep rupture (failure mode = 2)
- Meltdown (failure mode = 3)

W-1 (I) : IFFASC Failure model activator.
 =0: failure model not requested for this SC
 >0: failure model requested for this SC. The properties required by the failure model are defined with the material number IFFASC in the records 39Y000
Acceptable range: IFFASC ≥ 0
Default value: 0

W-2 (I) : ITFASC Indicator defining how the representative temperature is obtained for the failure calculations.
 =1: use maximum temperature of all SC nodes
 =2: use volume-weighted average temperature
Acceptable range: 1 or 2
Default value: 1

W-3 (I) : ISFASC Indicator defining which pressures are used for to determine the stress, needed for the failure calculations
 <0: use Control Function number |ISFASC |
 =0: pressure is not used (value is set to 1.0). Stress is constant, and given directly by XSFASC (next word).
 =1: use CV pressure from the left boundary CV
 =2: use CV pressure from the right boundary CV
 =3: use absolute value of the difference between the left and the right volume pressures
Acceptable range: 1 ≤ ISFASC ≤ 3 or reference to a Control Function
Default value: 1 if a CV is present only on the left side of the SC
 2 if a CV is present only on the right side of the SC

3 if CV-s present on both sides of the SC
0 if there is no CV on neither left nor right side

W-4 (R) : XSFASC Ratio of stress and pressure (defined by the word above), (σ/p) . For example in case of a tube with the inner diameter D and the thickness t , the relation between the overpressure inside the tube, p , and the stress, σ , (see Figure 2-18):

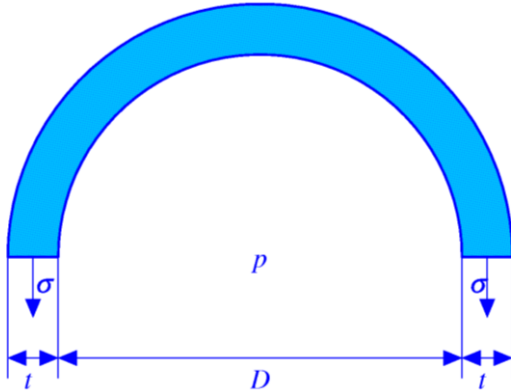


Figure 2-18 Relation between stress and pressure for a tube.

$$p \cdot D = \sigma \cdot 2t$$

Therefore:

$$\sigma = p \cdot (D/2t)$$

This for this case the ratio is equal to XSFASC = $(D/2t)$.

Acceptable range: XSFASC > 0.0

Default value: rectangular geometry: none
cylindrical geometry: $(D/2t)$
spherical geometry: $(D/4t)$

2.3.28 Records: 33Y000, Material Properties Needed for Failure Calculations

Y is the material number, $1 \leq Y \leq 9$. The failure model considers the following three failure mechanisms:

- Ultimate strength failure (failure mode = 1)
- Creep rupture (failure mode = 2)
- Meltdown (failure mode = 3)

Creep rupture is calculated using the method proposed by Larson and Miller [40]. The time to rupture is obtained from the following relation (see Volume 1):

$$\log_{10}(t_r) = \frac{LMP}{T} - C$$

2.3.29 Record: 340000, Definition of Fuel Regions for Gap Calculations

This record is needed if the user wishes to apply the gap conductance model. The record defines core fuel regions, which are to be viewed as structures - 1-D or 2-D Solid Heat Conductors - that represent fuel rods in a nuclear reactor. The gap properties and the location of the gap within the 1-D or the 2-D Solid Heat Conductor, are specified in this record.

If the RT (Radioactive Particle Transport) Package is used, and the RT fuel regions are used (record 883000), the fuel regions in the RT Package must be consistent with the fuel regions for the SC Package, defined in this record. The maximum number of fuel regions is NFRMSC = 200.

- W-1 (I) : L1FRSC Core fuel region indicator 1.
 =1: this fuel region is represented by a 1-D Solid Heat Conductor,
 =2: this fuel region is represented by a 2-D Solid Heat Conductor.
Acceptable range: 1 or 2 .
Default value: if the reactor kinetics model is used, the default values are equal to the regions indicators ITF1RK, specified for the fuel temperature weighting factor in record 791XXX. In this case the region indicator ITF1RK must refer to a 1-D or 2-D Heat Conductor (=1 or 2).
- W-2 (I) : L2FRSC Core fuel region indicator 2. Equal to:
 Reference number of a 1-D Solid Heat Conductor, if L1FRSC = 1,
 Reference number of a 2-D Solid Heat Conductor, if L1FRSC = 2.
Acceptable range: Must be a valid reference number of a 1-D or a 2-D Solid Heat Conductor. The geometry of the Solid Heat Conductor must be cylindrical.
Default value: If the reactor kinetics model is used, the default values are equal to the regions indicators ITF2RK, specified for the fuel temperature weighting factor in record 791XXX.
- W-3 (I) : NGFRSC Cell indicator for the gap model (see record 3410XX). The gap will be present in the cell NGFRSC of the SC with a reference number L2FRSC (if L1FRSC=1), or in the radial ring number NGFRSC of the TC with a reference number L2FRSC (if L1FRSC=2).
Acceptable range: Must not be a boundary cell of a 1-D or a 2-D Solid Heat Conductor. This means:
 =1 < NGFRSC < NCELSC, in case of SC
 =1 < NGFRSC < NCLXTC, in case of TC
Default value: =NCELSC-1, in case of SC (L2FRSC=1),
 =NCLXTC-1, in case of TC (L2FRSC=2).
- W-4 (I) : MGFRSC Gap model indicator (see record 3410XX). The gap model MGFRSC will be applied in the gap present in the cell NGFRSC.
Acceptable range: 1 ≤ MGFRSC ≤ NGPMSC = 10
Default value: none

The set of four words defined above is repeated until all fuel regions are described. The total number of entries in this record must be a multiple of 4. Multiple records with the same record identified (340000) may be entered. Data is read in the order in which these records appear in the input. If the Reactor Kinetics Package is used, the total number of fuel regions must be the same as the number of the weighting factors in the Reactor Kinetics Package.

2.3.30 Record: 340001, Initial Gap Size and Dynamic Expansion Model

- W-1 (R) : DGPISC Gap size, (m), for the core fuel region number 1. If the following six inputs are zero, the gap size will be constant and equal to DGPISC. If non-zero values are entered for the following six inputs, the dynamic expansion model will be used. In such case DGPISC is not used.
Acceptable range: $0.0 \leq \text{DGPISC} \leq 10^{-2}$ m
Default value: thickness of the gap node (node number NGFRSC)
- W-2 (R) : RDFSSC Radial displacement due to fission gas-induced fuel swelling, (m), for the core fuel region number 1.
Acceptable range: $0.0 \leq \text{RDFSSC} \leq 1.0 \times 10^{-2}$ m
Default value: 0.0
- W-3 (R) : RDCCSC Radial displacement due to cladding creepdown, (m), for the core fuel region number 1.
Acceptable range: $-1.0 \times 10^{-2} \leq \text{RDCCSC} \leq 0.0$ m
Default value: 0.0
- W-4 (R) : FCCSSC Fuel-cladding centerline shift ratio, for the core fuel region number 1.
Acceptable range: $0.0 \leq \text{FCCSSC} \leq 1.0$
Default value: 0.0
- W-5 (R) : IFTESSC Tabular Function defining the strain function, $\varepsilon_{FT}(T)$ (-), versus temperature T , for the fuel thermal expansion. The radial displacement of fuel due to thermal expansion is calculated from:

$$x_{FT} = \sum_{i=1}^{N_G-1} d_i \cdot \varepsilon_{FT}(T_i)$$

Here i is the node number, N_G is gap node number (NGFRSC), d_i is the thickness of the node i , T_i is the temperature of the node i (cell-center), ε_{FT} is the strain function calculated from Tabular Function IFTESSC. For UO_2 and PuO_2 fuels, the strain function is given by:

$$\text{UO}_2 : \quad \varepsilon_{FT}(T) = 1.0 \times 10^{-5} T - 3.0 \times 10^{-3} + 4.0 \times 10^{-2} \exp\left(\frac{-6.9 \times 10^{-20}}{k_B T}\right)$$

$$\text{PuO}_2 : \quad \varepsilon_{FT}(T) = 9.0 \times 10^{-6} T - 2.7 \times 10^{-3} + 7.0 \times 10^{-2} \exp\left(\frac{-7.0 \times 10^{-20}}{k_B T}\right)$$

Here T is the temperature (K), $k_B = 1.38 \times 10^{-23}$ J/K is the Boltzmann constant. Values tabulated for relevant temperature range are shown in Figure 2-19.

Acceptable range: a reference to a valid Tabular Function if non-zero, all tabulated values must be within the range $0.0 \leq \varepsilon_{CT}(T) \leq 0.1$

Default value: 0

W-6 (R) : ICTESC Tabular Function defining the strain function, $\varepsilon_{CT}(T)$ (-), versus temperature T , for the cladding thermal expansion. The radial displacement of cladding due to thermal expansion is calculated from:

$$x_{CT} = r_{cm} \cdot \varepsilon_{CT}(T_c)$$

Here r_{cm} is the cladding mid-point radius, T_c is the average cladding temperature (K), ε_{CT} is the strain function calculated from Tabular Function ICTESC. For Zircaloy cladding, the strain function is given by:

$$\varepsilon_{CT}(T) = -2.373 \times 10^{-4} + 6.721 \times 10^{-6}(T - 273) \quad \text{for } T < 1073$$

$$\varepsilon_{CT}(T) = -6.800 \times 10^{-3} + 9.700 \times 10^{-6}(T - 273) \quad \text{for } T > 1273$$

Here T is the temperature (K). Values tabulated for relevant temperature range are shown in Figure 2-19.

Acceptable range: a reference to a valid Tabular Function if non-zero, all tabulated values must be within the range $0.0 \leq \varepsilon_{CT}(T) \leq 0.1$

Default value: 0

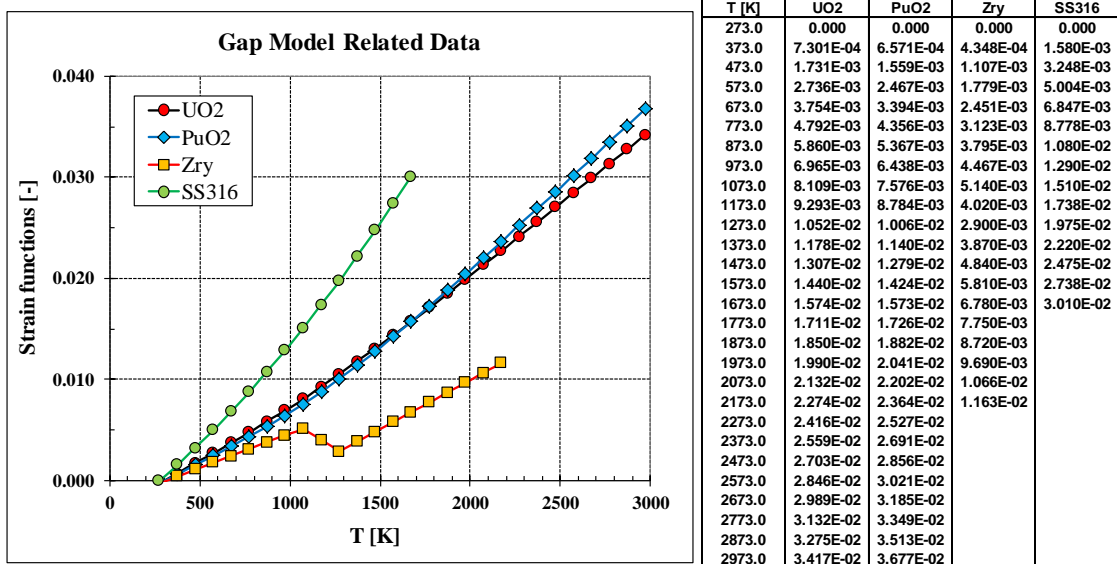


Figure 2-19 Gap model data for frequently used materials - strain function

W-7 (R) : IYMCSC Tabular Function defining the Young modulus $E(T)$ (Pa), versus temperature T , for the cladding. The cladding elastic deformation is calculated from:

$$x_{CE} = r_{cm} \left(\frac{\sigma_h - \nu \sigma_z}{E} \right)$$

Here r_{cm} is the cladding mid-point radius, σ_h is the cladding hoop stress (Pa), σ_z is the cladding axial stress (Pa), ν is the Poisons ratio. The hoop and axial stresses are given by:

$$\sigma_h = \frac{P_I \cdot r_I - P_O \cdot r_O}{r_O - r_I} \quad \sigma_z = \frac{P_I \cdot r_I^2 - P_O \cdot r_O^2}{r_O^2 - r_I^2}$$

P = pressure (Pa), r = cladding radius (m), subscripts: I = inner surface of cladding (gap), O = outer surface of cladding (fluid). E is the Young modulus calculated from Tabular Function IYMCSC. NOTE: cladding elastic deformation is calculated only when there is a boundary volume defined (in 1-D IVLRSC>0, in 2-D IVLBTC>0), because only then the cladding outer pressure, P_O , is available as the pressure in the boundary volume.

For the Zircaloy cladding, the Young modulus is given by:

$$E(T) = 1.088 \times 10^{11} - 5.475 \times 10^7 T \quad \text{for } T < 1090$$

$$E(T) = 9.210 \times 10^{10} - 4.050 \times 10^7 T \quad \text{for } T > 1240$$

Here T is the temperature (K). Values of the Young modulus tabulated for relevant temperature range are shown in Figure 2-20.

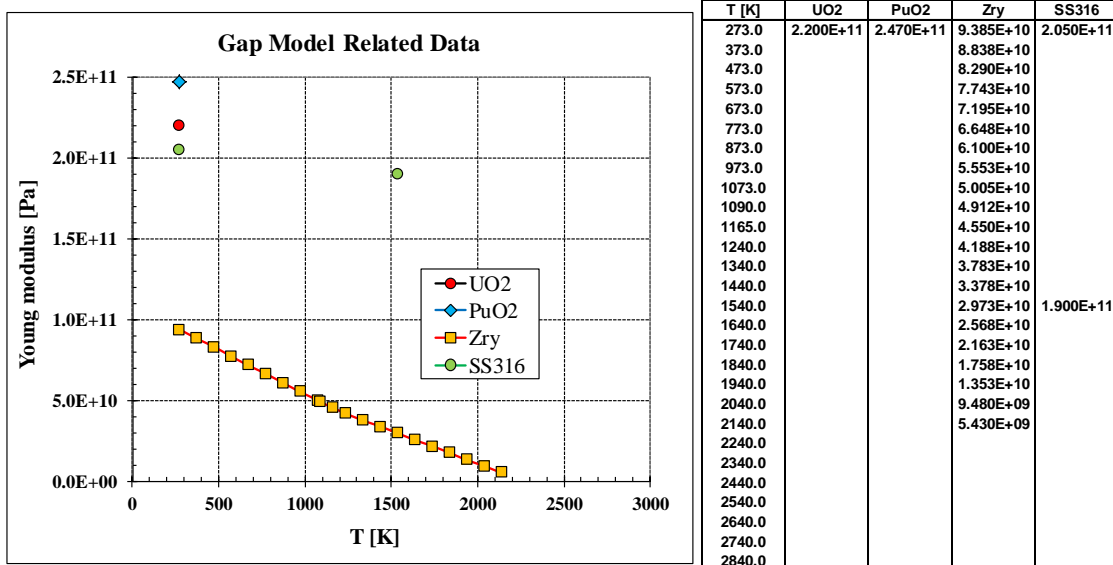


Figure 2-20 Gap model data for frequently used materials - Young modulus

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: a reference to a valid Tabular Function if non-zero, all tabulated values must be within the range $10^7 \leq E(T) \leq 10^{12}$ Pa
Default value: 0

The set of 7 words defined above is repeated until all fuel regions are described. The total number of entries in this record must be a multiple of 7. The number of sets per single input record must not be larger than 5. Multiple records with the same record identified (340001) may be entered. Data is read in the order in which these records appear in the input. The number of fuel regions must be the same as in the records 340000.

2.3.31 Record: 340002, User-defined Gap Conductance

A user-defined gap conductance may be specified in this record. The gap conductance may be either constant or time-dependent, calculated by a Control Function.

W-1 (R) : HGPCSC Gap conductance for the core fuel region number 1, defined as follows:
HGPCSC>0: Constant gap conductance, h_{gap} (W/m²-K)
HGPCSC<0: Gap conductance will be calculated by the Control Function with the number |HGPCSC|. The value obtained from the CF will be interpreted as gap conductance h_{gap} (W/m²-K), with the following limits: $1.0 \leq h_{gap} \leq 1.0 \times 10^{10}$
HGPCSC=0: Gap conductance will be calculated based on the data entered in the following input records.
Acceptable range: $0.0 \leq \text{HGPCSC} \leq 1.0 \times 10^{10}$
Default value: 0.0

... until constant gap conductance is defined for all fuel regions. Multiple records with the same record identified (340002) may be entered. Data is read in the order in which these records appear in the input. If the record is entered, the number of fuel regions must be the same as in the records 340000 and 340001.

2.3.32 Record: 3410XX, Gap Data

XX is the gap model number, $1 \leq \text{XX} \leq 10$. The maximum number of the gap models is 10. The overall heat transfer coefficient in gap is computed as a sum of thee terms:

$$h_{gap} = h_r + h_c + h_s$$

h_r radiation, (W/m²-K)
 h_c conduction through gas, (W/m²-K)
 h_s conduction through solid, due to contact of fuel and cladding, (W/m²-K)

- *Radiation.* The radiation term is obtained as:

$$h_r = \sigma \cdot \left(\frac{1}{\varepsilon_f} + \frac{1}{\varepsilon_c} - 1 \right)^{-1} \cdot (T_f^2 + T_c^2) \cdot (T_f + T_c)$$

Here ε_f , ε_c , are the emissivities of fuel and cladding, T_f , T_c , are the surface temperatures of fuel and cladding, σ is the Stefan-Boltzmann constant, equal to 5.67×10^{-8} (W/m²-K⁴).

- *Gas conduction.* The conduction term is obtained as:

$$h_c = \frac{k_g}{d_{gap} + d_{min} + (g_f + g_c)}$$

Here k_g is the conductivity of the gas mixture, d_{gap} is the gap thickness, d_{min} is related to the roughness of the two surfaces, g_f , g_c , are the temperature jump distances. The d_{min} is obtained from:

$$d_{min} = C_d \cdot (r_f + r_c)$$

Here r_f , r_c , are the surface roughness of fuel and cladding respectively, and C_d is constant. The temperature jump distances are obtained from:

$$(g_f + g_c) = C_j \cdot \frac{k_g \cdot \sqrt{T_g}}{p_g \cdot \sum_{i=1}^{N_{gas}} X_i a_i M_i^{-1/2}}$$

Here C_j is constant, a_i is the accommodation coefficient (-), T_g is the gap gas temperature (K), M_i is the gas molar weight (kg/kmol), X_i is the gas molar fraction (-), and p_g is the gas pressure in the gap (Pa). The thermal accommodation coefficient is based on Ullman data [44]:

$$a_i = a_{He} + \frac{M_i - M_{He}}{M_{Xe} - M_{He}} \cdot (a_{Xe} - a_{He})$$

$$a_{He} = 0.425 - 2.3 \times 10^{-4} \cdot T_g$$

$$a_{Xe} = 0.740 - 2.5 \times 10^{-4} \cdot T_g$$

The gas pressure in the gap is computed from:

$$p_g = \frac{p_0}{T_0} \cdot T_g$$

Here p_0 , T_0 are the gas pressure and temperature in reference state and T_g is the current gas temperature in the gas plenum. The gas plenum is defined by the user for each common region. A CV fluid temperature or SC/TC node temperature may be selected. This should be selected as the volume or structure most closely associated with the non-fuel region in a fuel pin at the top of a stack of fuel pellets.

W-10 (R) : XNGCMP Power n , (-), in the formula for h_s .
 Acceptable range: $0.0 \leq XNGCSC \leq 5.0$
 Default value: 1.0 (Ross and Stoute model [45])

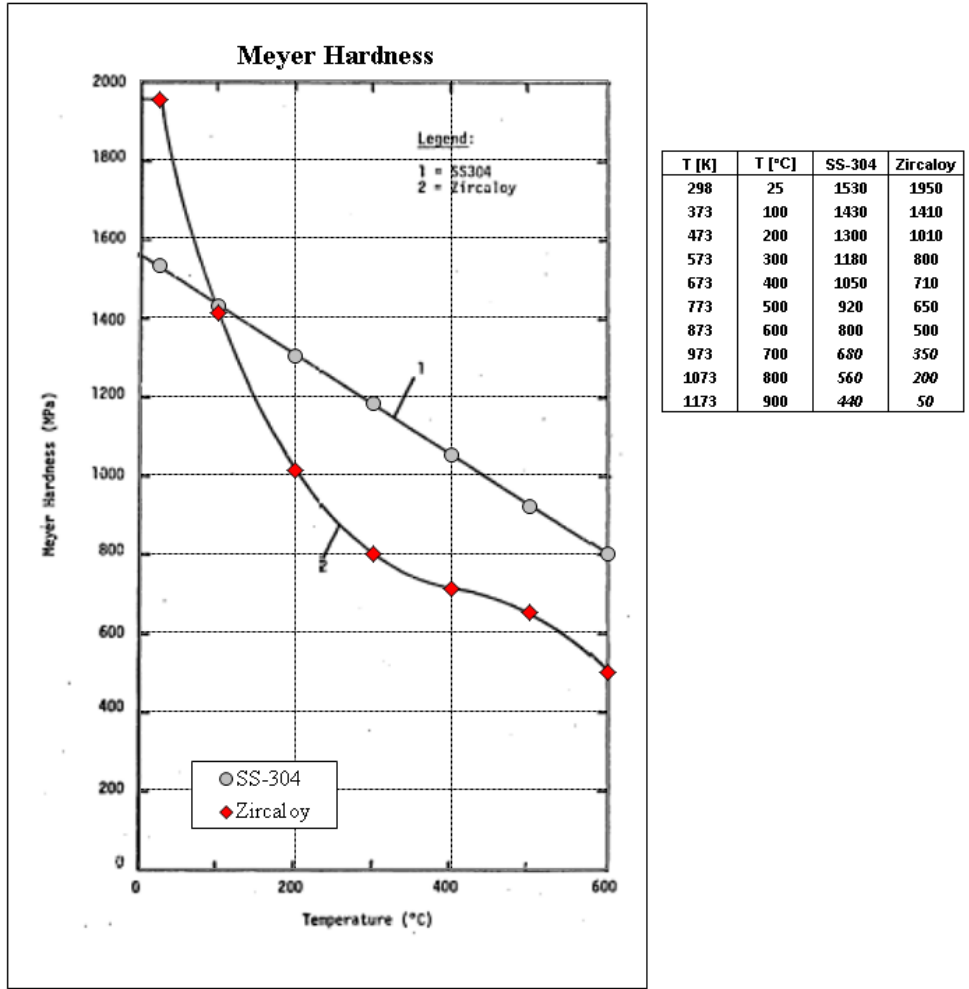


Figure 2-21 Meyer hardness of SS-304 and Zircaloy

W-11 (R) : XPGCMP User-defined multiplier X_p , (-), in the formula for p_a .
 Acceptable range: $0.0 \leq XPGCSC \leq 1.0$
 Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0)

2.3.33 Record: 342XXX, Definition of Common Fuel Regions for Gap Calculations

XXX is the common fuel region for gap calculations (single fuel rod). The region numbers must be consecutive. The common fuel rod regions are introduced for the following reason. If a fuel rod is represented by several Solid Heat Conductors (there is an axial division of the fuel rods), then the gap parameters, such as gas pressure and gas composition in the gap, are common for each such region. Therefore the common fuel regions must reflect the axial nodalization of the fuel rods.

If the Radioactive Particle Transport Package is used, and the RT core regions are used (record 883000), the common fuel regions for cladding failure in the RT Package (records 8832XX) must be consistent with the common fuel regions for gap calculations in the SC Package, defined in this record. The maximum number of common fuel regions is $NCRMSC = 200$.

- W-1 (I) : IICRSC(1) Fuel region number IICRSC(1) (defined in the record 340000) belongs to the common fuel region XX. Gap pressure and gas composition will be the same in the common fuel regions.
Acceptable range: must be one of the core regions defined in records 340000.
Default value: XX.
- W-2 (I) : IICRSC(2) Fuel region number IICRSC(2) (defined in the record 340000) belongs to the common fuel region XX. Gap pressure and gas composition will be the same in the common fuel regions.
Acceptable range: must be one of the core regions defined in records 340000.
Default value: none
- W-3 (I) : IICRSC(3) Fuel region number IICRSC(3) (defined in the record 340000) belongs to the common fuel region XX. Gap pressure and gas composition will be the same in the common fuel regions.
Acceptable range: must be one of the core regions defined in records 340000.
Default value: none

. . . until all members of the common fuel regions are defined. The maximum number of fuel regions in a single common fuel region is 200. Several records with the same number may be entered. Data is read in the order in which these records appear in the input.

2.3.34 Record: 343XXX, Composition of the Gap Gas

XXX is the common fuel region number, $1 \leq XXX \leq 200$. The common fuel regions for fuel rods are defined in the records 342XXX. The maximum number of the common fuel regions is $NCRMSC = 200$. The gas composition in the gap is defined in those records. The total number of entries in this record must be a multiple of 2.

- W-1 (I) : IGAS Gas number, (-). Must be one of the available gases. The built-in gases are: 1 = H₂, 2 = He, 3 = steam, 4 = N₂, 5 = O₂, 6 = CO₂.
Acceptable range: $1 \leq IGAS \leq NGASCV \leq NGMXFL = 20$
Default value: 2 (Helium)

SPECTRA Code Manuals - Volume 2: User's Guide

W-2 (R) : CVCRCSC Mole fraction of gas IGAS. If the sum of CVCRCSC for all noncondensables is not equal to one, then CVCRCSC will be normalized during input processing.
Acceptable range: $0.0 \leq \text{CVCRCSC}(\text{IGAS}) \leq 1.0$
Default value: 0.0 (if no data is specified, assume 100% Helium)

2.3.35 Record: 344XXX, Reference Parameters of the Gap Gas

XXX is the common fuel region number, $1 \leq \text{XXX} \leq 200$. The common fuel regions for fuel rods are defined in the records 342XXX. The maximum number of the common fuel regions is NCRMSC = 200. The gas pressure in the gap is computed from:

$$p_g = \frac{P_0}{T_0} \cdot T_g$$

W-1 (R) : T0CRSC Reference temperature of the gap gas, T_0 (K).
Acceptable range: $270.0 \leq \text{T0CRSC} \leq 10,000.0$
Default value: 300.0

W-2 (R) : P0CRSC Reference pressure of the gap gas, p_0 (Pa) at the reference temperature, T_0 .
Acceptable range: $1.0 \leq \text{P0CRSC} \leq 1.0 \times 10^{10}$
Default value: 1.0×10^5

T_g is the current gas temperature in the gas plenum. The gas plenum is defined below. A CV fluid temperature or SC/TC node temperature may be selected. If nothing is selected by default the temperature of the gap node of the SC or TC listed as first on the common fuel region will be used.

W-3 (I) : IGP1SC Indicator 1 of the gas gap plenum
= 1: CV atmosphere or pool temperature defines the gap gas plenum temperature.
= 2: SC node number defines the gap gas plenum temperature.
= 3: TC node number defines the gap gas plenum temperature.
Acceptable range: 1, 2, and 3
Default value: 2 or 3.

W-4 (I) : IGP2SC Region indicator 2. Defines CV, SC, or TC number.
if IGP1SC=1: CV reference number
if IGP1SC=2: SC reference number
if IGP1SC=3: TC reference number
Acceptable range: must be a valid reference number of a Control Volume, 1-D, or 2-D Solid Heat Conductor.
Default value: SC or TC number which is first on the list for this common region

W-5 (I) : IGP3SC Region indicator 3
if IGP1SC=1: 1 = CV atmosphere, 2 = CV pool temperature
if IGP1SC=2: SC cell number

if IGP1SC=3: TC cell number
 Acceptable range:
 if IGP1SC=1: 1 or 2
 if IGP1SC=2: $1 \leq \text{IGP3SC} \leq \text{No. of cells in SC IGP2SC}$
 if IGP1SC=3: $1 \leq \text{IGP3SC} \leq \text{No. of cells in TC IGP2SC}$
 Default value: gap cell of SC or TC

2.3.36 Record: 345000, Number of Integration Points for the Gap Calculations

In case of fuel-cladding centerline shift (FCCSSC>0.0) the overall gap conductance, h_g , is computed based on the local gap conductances, $h_g'(d_g')$, obtained for the local gap size, d_g' , from the following formula:

$$h_g = \frac{1}{\pi} \int_0^\pi h_g'[d_g'(\theta)] \cdot d\theta = \frac{1}{N} \sum_{i=1}^N h_g'[d_g'(\theta_i)]$$

$$\theta_i = \frac{i-1}{N-1} \cdot \pi$$

The local gap size is obtained from (Figure 2-22):

$$d_g'(\theta_i) \approx R_{c,i} - R_{f,o} - \Delta \cdot \cos(\theta_i)$$

Approximation is good for gaps small compared to the cladding and fuel radii, $d_g \ll R_{c,i} \approx R_{r,o}$.

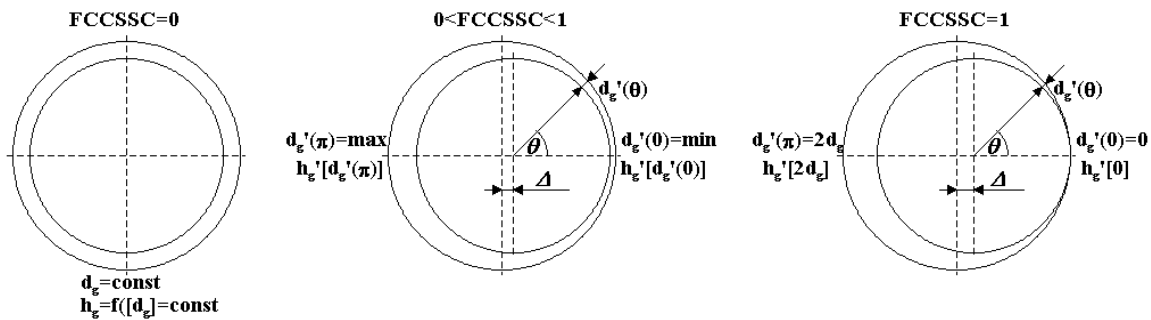


Figure 2-22 Local gap size calculation for fuel-cladding centerline shift

W-1 (I) : NIGCMP Number of integration points. The minimum number of points is 2. In such case the local gap conductance is calculated in two points only, the smallest gap ($\theta = 0$) and the largest gap ($\theta = \pi$). Influence of the number of integration points is shown in Figure 2-23. It is seen that in practice 50 points are sufficient to obtain an accurate (N -independent value of h_{gap}). Figure 2-24 shows the effect of centerline shift on h_{gap} for several different gap thickness. Note that the value of gap conductance for the fuel-cladding centerline shift of 1.0 is between a factor of 2 and a factor of 4 larger than the value for no shift.

Acceptable range: $2 \leq \text{NIGCMP} \leq 1000$
 Default value: 100

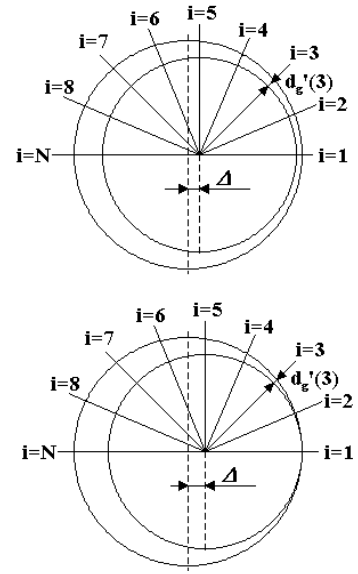
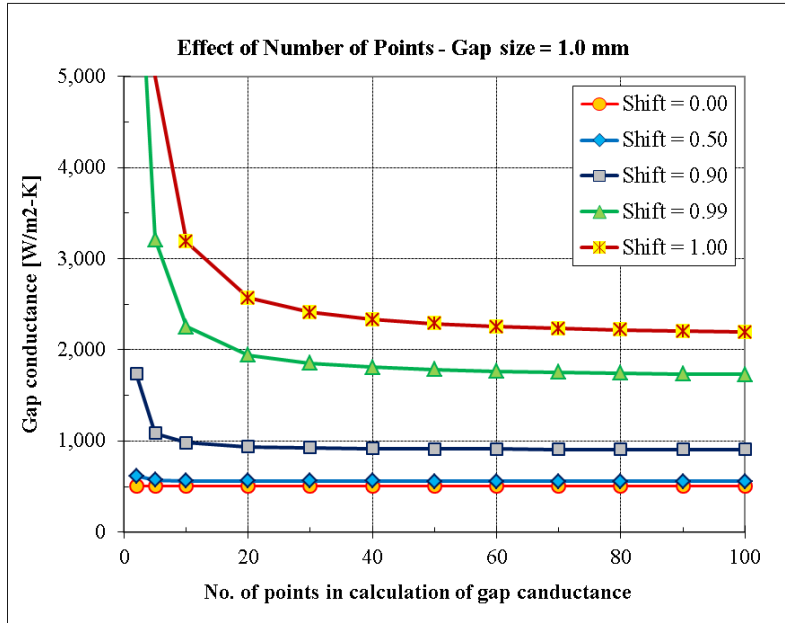


Figure 2-23 Influence of number of points, N , on gap conductance h_{gap}

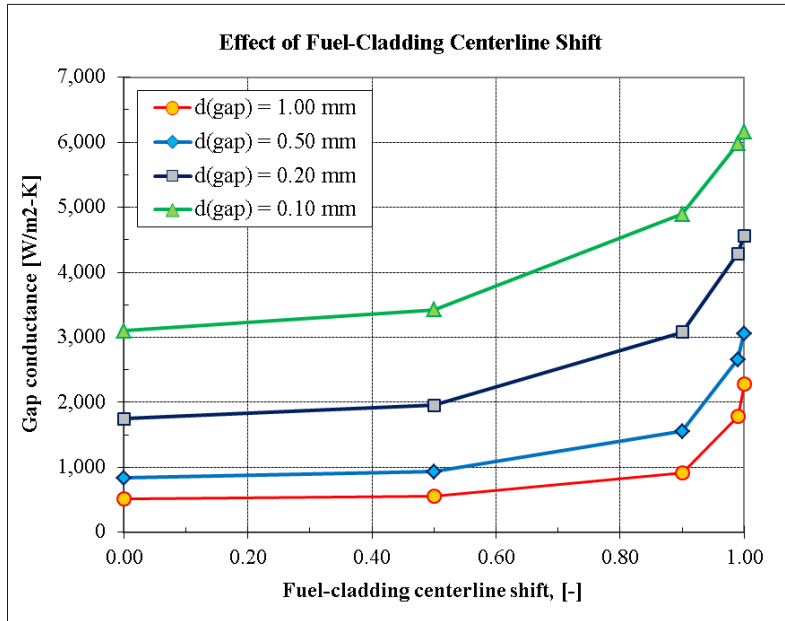


Figure 2-24 Influence of centerline shift on gap conductance

2.3.37 Record: 390XXX, Axial Conduction and Direct Contact Conduction

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record activates the axial heat transfer process for this 1-D Solid Heat Conductor. The maximum number of axial heat transfer processes is 10 for a single 1-D Solid Heat Conductor and 100 for a single 2-D Conductor.

The axial heat conduction or direct contact heat transfer between two structures, i (the “current solid heat conductor”, XXX) and j (the “other solid heat conductor”), is considered - Figure 2-25. The heat transfer between the two solid heat conductors is calculated from:

$$Q_{i-j} = A_{i-j} \frac{T_i - T_j}{R_{i-j}}$$

- Q_{i-j} heat transferred between the solid heat conductors i and j , (W)
- A_{i-j} area of contact between the solid heat conductors i and j , (m²)
- T_i temperature of the solid heat conductor i (local or averaged - see Word 2 below), (K)
- T_j temperature of the solid heat conductor j (local or averaged - see Word 2 below), (K)
- R_{i-j} thermal resistance for the axial heat flow between the solid conductors i and j , (m²-K/W)

The thermal resistance for the heat flow is obtained from:

$$R_{i-j} = \frac{L_i}{k_i} + \frac{1}{h_{i-j}} + \frac{L_j}{k_j}$$

- L_i length for axial conduction in the solid heat conductor i (input parameter X1AXSC)
- k_i thermal conductivity in the solid heat conductor i
- L_j length for axial conduction in the solid heat conductor j (input parameter X2AXSC)
- k_j thermal conductivity in the solid heat conductor j
- h_{i-j} heat transfer coefficient at the point of contact of solid heat conductors i and j

- W-1 (I) : J1AXSC First indicator of the other solid heat conductor (j).
 =1: 1-D Solid Heat Conductor (SC)
 =2: 2-D Solid Heat Conductor (TC) - *not used, transfer between 1-D and 2-D can be defined in the records 490XXX*
 Acceptable range: 1
 Default value: none

- W-2 (I) : J2AXSC Second indicator of the other solid heat conductor (j).
 if J1AXSC=1: SC reference number
 if J1AXSC=2: TC reference number - *not used, transfer between 1-D and 2-D can be defined in the records 490XXX*
 Acceptable range: must be a valid reference number of SC
 Default value: none

- W-3 (I) : I1AXSC Cell number for axial or direct contact heat conduction through the current solid heat conductor, i .
 >0: cell number for direct contact heat transfer (Figure 2-25-b), see Volume 3, discussion on direct contact heat transfer modeling.

SPECTRA Code Manuals - Volume 2: User's Guide

		<p>=0: axial heat transfer with all cells transferring heat to corresponding cell or cells in the other solid heat conductor (Figure 2-25-a). If also I2AXSC = 0, then both solid heat conductors must have identical nodalization.</p> <p><i>Acceptable range:</i> cell number or 0</p> <p><i>Default value:</i> none</p>
W-4 (I) :	I2AXSC	<p>Cell number for axial or direct contact heat conduction through the other solid heat conductor, j.</p> <p>>0: cell number for direct contact heat transfer (Figure 2-25-b), see Volume 3, discussion on direct contact heat transfer modeling.</p> <p>=0: axial heat transfer with all cells transferring heat to corresponding cell or cells in the other solid heat conductor (Figure 2-25-a). If also I1AXSC = 0, then both solid heat conductors must have identical nodalization.</p> <p><i>Acceptable range:</i> cell number or 0</p> <p><i>Default value:</i> none</p>
W-5 (R) :	X1AXSC	<p>Length of the axial heat conduction (Figure 2-25) in the current solid heat conductor, L_i (m).</p> <p><i>Acceptable range:</i> $0.0 \leq X1AXSC \leq 10,000.0$</p> <p><i>Default values:</i> half of the current SC length, if I1AXSC=0 0.0 if I1AXSC>0</p>
W-6 (R) :	X2AXSC	<p>Length of the axial heat conduction (Figure 2-25) in the other solid heat conductor, L_j (m).</p> <p><i>Acceptable range:</i> $0.0 \leq X2AXSC \leq 10,000.0$</p> <p><i>Default values:</i> half of the other SC length, if I2AXSC=0 0.0 if I2AXSC>0</p>
W-7 (I) :	IHAXSC	<p>Pointer to a Tabular or Control Function that defines the direct contact heat transfer coefficient, h_{i-j} (W/m²-K), or resistance, $1/h_{i-j}$ (m²-K/W), depending on MHAXSC (Word 10 below). If the number is positive, then h_{i-j} or $1/h_{i-j}$ will be defined by a Tabular Function with the reference number: IHAXSC. If the number is negative, then h_{i-j} or $1/h_{i-j}$ will be defined by a Control Function with the reference number: IHAXSC . If the current value of the Tabular or Control Function is smaller or equal to 0.0, there will be no resistance at the contact point ($h_{i-j} = \infty$, $1/h_{i-j} = 0.0$). The value obtained from the Tabular or Control Function will be internally limited to the range 10^{-10} - 10^{10}. If direct contact heat transfer is implied (I1AXSC > 0 and I2AXSC > 0) then a very small contact resistance may cause numerical instabilities. A minimum resistance of $1/h_{i-j} = 10^{-3}$ m²-K/W is applied in case of SC-to-TC and TC-to-TC direct contact. However, in case of SC-to-SC a special numerical procedure allows smaller contact resistance. In such case the minimum resistance is $1/h_{i-j} = 10^{-5}$ m²-K/W (see also description of NDISC, record 303XXX).</p> <p><i>Acceptable range:</i> must be a valid reference number of a Tabular or a Control Function, if non-zero.</p> <p><i>Default value:</i> 0.</p>

SPECTRA Code Manuals - Volume 2: User's Guide

- W-8 (R) : A1AXSC Multiplier on the heat transfer area, (-). The area of heat transfer, A_{ij} , is automatically calculated by the code as the smaller of the areas of the connected conductor cells multiplied by the corresponding multiplier. A1AXSC is applied for the cell in the “current” SC (while A2AXSC is applied to the “other” SC). Note that in case of axial heat transfer (heat transfer perpendicular to the normal heat transfer in this conductor), the cross-sectional area of the cell is used. In case of direct contact heat transfer (heat transfer along the normal heat transfer in this conductor), the area of boundary surface. The value obtained in this way is multiplied by A1AXSC. NOTE: The user may also define the area directly, by using the AXAXSC (W-15 below). In this case the multipliers A1AXSC, A2AXSC will be ignored.
Acceptable range: $0.0 < A1AXSC \leq 10^{10}$
Default value: 1.0
- W-9 (R) : A2AXSC Multiplier on the heat transfer area, (-). The area of heat transfer, A_{ij} , is automatically calculated by the code as the smaller of the areas of the connected conductor cells multiplied by the corresponding multiplier. A2AXSC is applied to the “other” SC (while A1AXSC is applied for the cell in the “current” SC). Note that in case of axial heat transfer (heat transfer perpendicular to the normal heat transfer in this conductor), the cross-sectional area of the cell is used. In case of direct contact heat transfer (heat transfer along the normal heat transfer in this conductor), the area of boundary surface. The value obtained in this way is multiplied by A2AXSC. NOTE: The user may also define the area directly, by using the AXAXSC (W-15 below). In this case the multipliers A1AXSC, A2AXSC will be ignored.
Acceptable range: $0.0 < A2AXSC \leq 10^{10}$
Default value: 1.0
- W-10 (I) : MHAXSC Parameter affecting direct contact conduction:
=1: IHAXSC defines the heat transfer coefficient, h_{i-j} (W/m²-K)
=2: IHAXSC defines the resistance, $1/h_{i-j}$ (m²-K/W)
Acceptable range: 1 or 2
Default value: 1
- W-11 (I) : M1AXSC Pointer to a material number which defines thermal conductivity in the current solid heat conductor. If zero or no value is specified the conductivity of the actual material, defined in the records 310XXX, is used. If a positive value is defined then the thermal conductivity of the material M1AXSC is used. For example, in case of a pebble bed model, the actual material should represent the true material of a pebble, to get a correct surface-to-center temperature difference. M1AXSC should be an artificial material, which is used to define the effective conductivity of the pebble bed, for example from Zehner-Schlunder or Robold correlation (see Volume 3, test PBR-k-eff).
Acceptable range: must be a valid reference number of a solid material, defined in records 801XXX, 802XXX, 803XXX - see section 2.10).
Default value: 0

SPECTRA Code Manuals - Volume 2: User's Guide

- W-12 (I) : M2AXSC Pointer to a material number which defines thermal conductivity in the other solid heat conductor. If zero or no value is specified the conductivity of the actual material, defined in the records 310XXX, is used. If a positive value is defined then the thermal conductivity of the material M2AXSC is used. For example, in case of a pebble bed model, the actual material should represent the true material of a pebble, to get a correct surface-to-center temperature difference. M2AXSC should be an artificial material, which is used to define the effective conductivity of the pebble bed, for example from Zehner-Schlunder or Robold correlation (see Volume 3, test PBR-k-eff).
Acceptable range: must be a valid reference number of a solid material, defined in records 801XXX, 802XXX, 803XXX - see section 2.10).
Default value: 0
- W-13 (I) : L1AXSC Option for the direct contact transfer (I1AXSC > 0 and I2AXSC > 0) in the current solid heat conductor.
=0: Cell-to-cell direct contact. The temperature T_i is taken from the cell I1AXSC. The calculated heat is removed/added to the cell I1AXSC.
=1: Global radial transfer. The temperature T_i is equal to the average temperature of the current solid heat conductor (mass-averaged or volume-averaged, depending of IAVESC). The calculated heat is distributed over all cells, proportionally to the cell volume or cell mass. The input parameter I1AXSC is used only to determine the area for the heat transfer. This option is intended to model the effective conductivity of the pebble bed or prismatic blocks (see Volume 3, tests PBR-k-eff, PMR-k-eff).
Acceptable range: 0 or 1
Default value: 0
- W-14 (I) : L2AXSC Option for the direct contact transfer (I1AXSC > 0 and I2AXSC > 0) y in the other solid heat conductor.
=0: Cell-to-cell direct contact. The temperature T_j is taken from the cell I2AXSC. The calculated heat is removed/added to the cell I2AXSC.
=1: Global radial transfer. The temperature T_j is equal to the average temperature of the other solid heat conductor (mass-averaged or volume-averaged, depending of IAVESC). The calculated heat is distributed over all cells, proportionally to the cell volume or cell mass. The input parameter I2AXSC is used only to determine the area for the heat transfer. This option is intended to model the effective conductivity of the pebble bed or prismatic blocks (see Volume 3, tests PBR-k-eff, PMR-k-eff).
Acceptable range: 0 or 1
Default value: 0
- W-15 (R) : AXAXSC Area of heat transfer, (m²). If zero or no value is entered, then the area is calculated as the smaller value of the cell areas (multiplicity included):

$$A_{HT} = \text{MIN} (A_{cell,SC-1} \times A1AXSC , A_{cell,SC-2} \times A2AXSC)$$

If a positive value is entered, then the heat transfer area is equal to the entered value:

SPECTRA Code Manuals - Volume 2: User's Guide

$$A_{HT} = AXAXSC$$

Acceptable range: $0.0 \leq AXAXSC \leq 10^{10}$

Default value: 0.0

W-16 (I) : KAXSC Sequential number of the axial heat transfer process. If no value or zero is entered, then the data are read sequentially - the first record 390XXX in the input file is interpreted as containing the first axial transfer process, the second record with this number the second heat transfer process, etc.
Acceptable range: I = 1, 2, ..., 6
Default value: none

Examples are shown in Figure 2-25. Further examples and discussion is included in Volume 3.

Cases (a) and (c) - cell-to-cell axial heat conduction

```
* SC-100 heat transfer to SC-200
* - cell-to-cell transfer for all cells
* - "axial" heat transfer - perpendicular to the normal conduction heat flow
* - conduction length: L = 0.5 m for SC-100, L=0.6 m for SC-200
* - contact h = TF-900
*
*            SC   Cell-i   Cell-j   L-i   L-j   h
390100 1 200       0       0       0.5   0.6   900 * Input for SC-100
```

alternatively the following input may be defined for SC-200:

```
*            SC   Cell-i   Cell-j   L-i   L-j   h
390200 1 100       0       0       0.6   0.5   900 * Input for SC-200
*
```

If both records are present, then an error "double specification of axial transfer" - will be encountered.

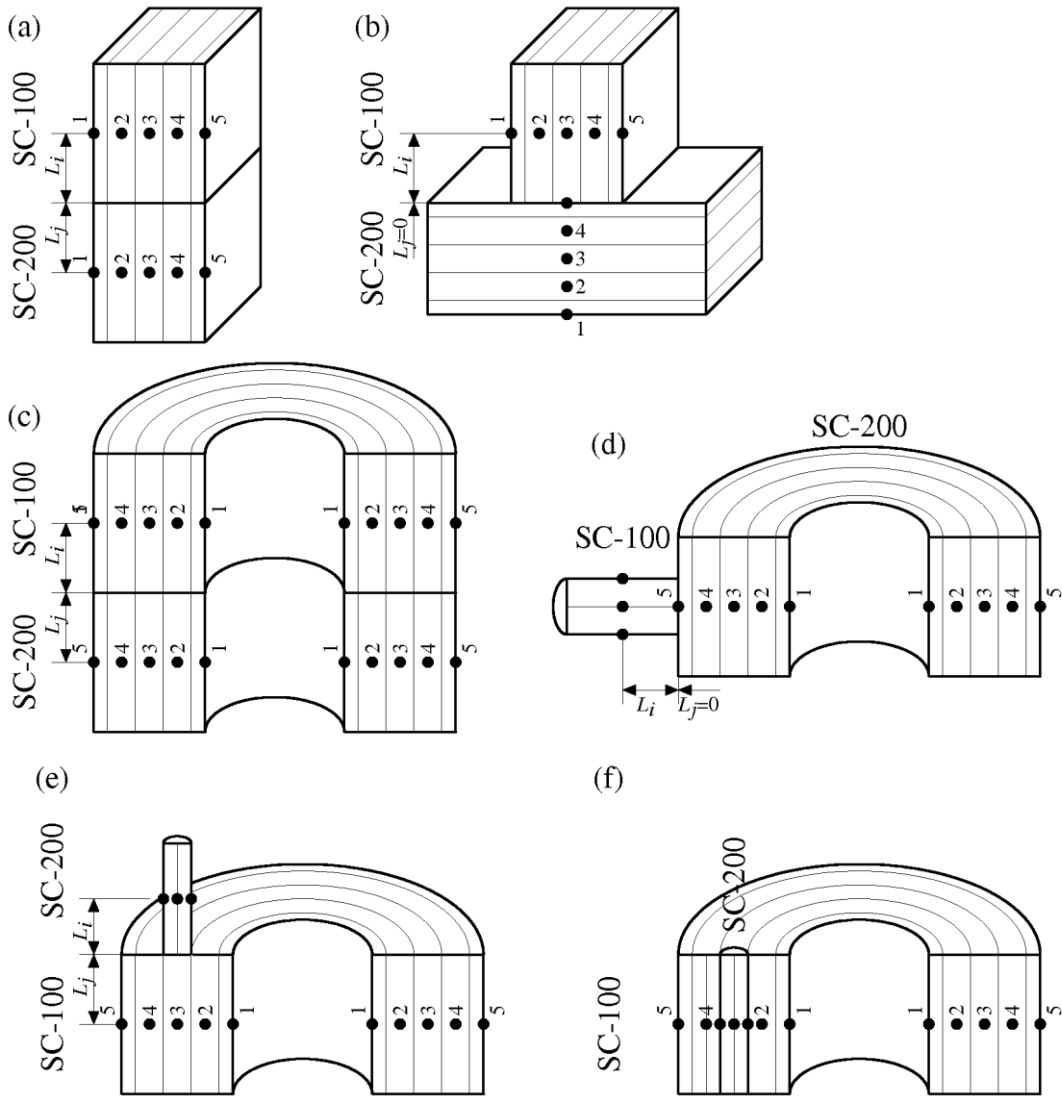


Figure 2-25 Axial conduction, direct contact between different SC

Cases (b) and (d) - all cells (axial) to one cell (direct contact)

```
* SC-100: heat transfer to SC-200
* - all cells from SC-100 transfer heat to cell 5 of SC-200
* - "axial" heat transfer for SC-100, normal conduction heat flow in SC-200
* - axial conduction length: L = 0.5 m for SC-100, L=0.0 m for SC-200
* - contact h = TF-900
*
*          SC  Cell-i  Cell-j   L-i   L-j   h
390100 1 200      0      5     0.5   0.0  900 * Input for SC-100
```

alternatively the following input may be defined for SC-200:

```
*          SC  Cell-i  Cell-j   L-i   L-j   h
390200 1 100      5      0     0.0   0.5  900 * Input for SC-200
*
```

If both records are present, then an error "double specification of axial transfer" - will be encountered.

Case (e) - all cells (axial) to one cell (direct contact)

```
* SC-100: heat transfer to SC-200
* - all cells from SC-200 transfer heat to cell 3 of SC-100
* - "axial" heat transfer - perpendicular to the normal conduction heat flow
* - conduction length: L = 0.5 m for SC-100, L=0.3 m for SC-200
* - contact h = TF-900
*
*          SC  Cell-i  Cell-j   L-i   L-j   h
390100 1 200      3      0     0.5   0.3  900 * Input for SC-100
```

Case (f) - single cell to single cell heat transfer

```
* SC-100: heat transfer to SC-200
* - outer cell of SC-200 transfer heat to cell 3 of SC-100
* - "radial" heat transfer
* - conduction length: L = 0.0 m for SC-100, L=0.0 m for SC-200
* - contact h = TF-900
*
*          SC  Cell-i  Cell-j   L-i   L-j   h
390100 1 200      3      3     0.0   0.0  900 * Input for SC-100
```

Example of pebble reactor. Inlet pipes passing through s reflector structure - Figure 2-26.

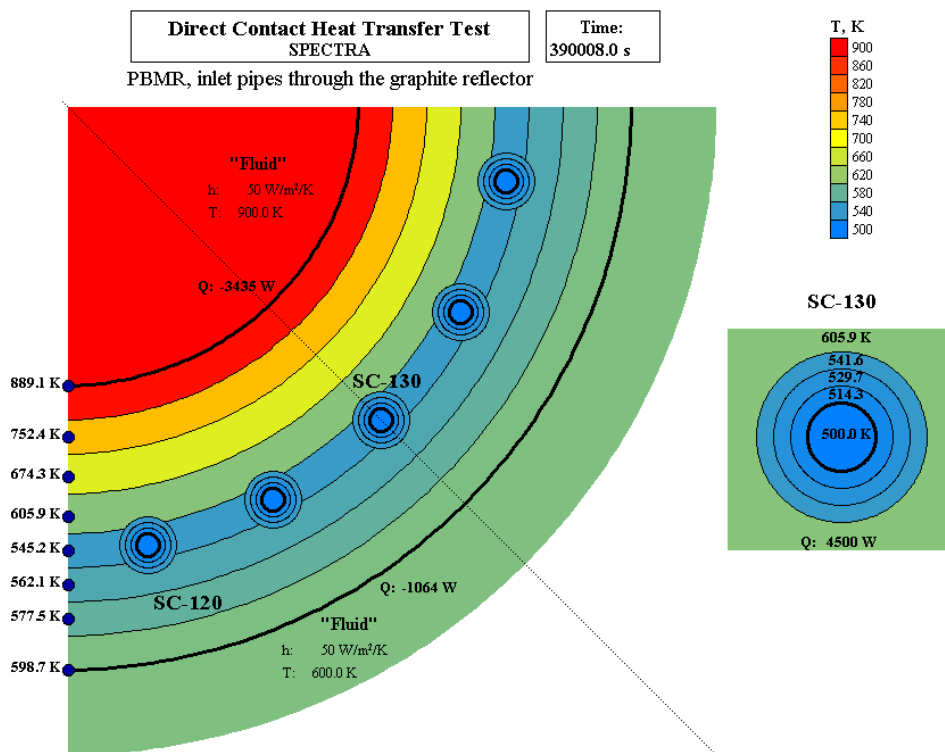


Figure 2-26 Example of SC-to-SC transfer (see Volume 3, PBMR-IP)

Example input, linking SC-130, which represents space around the inlet channels and SC-120, which represents the reflector, is shown below. This example case is discussed further in Volume 3.

```

*
*      SC   i j  L-i  L-j   h  A1  A2
390130 1 120 3 5 0.01  0.00 200 0  0 * Axial heat transfer to SC-120, contact h = TF-200

605200 h-c(1), W/m/K
600200  0.0 10000.0
    
```

Example of pebble reactor. pebble bed effective conductivity - Figure 2-27.

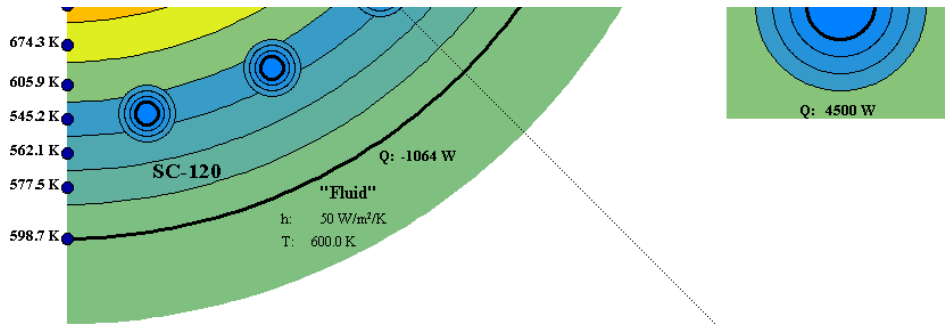


Figure 2-27 Example of pebble bed heat transfer

Example input, linking SC-130, which represents the inner pebble ring, and SC-120, which represents the outer pebble ring, is shown below. This example case is discussed further in Volume 3.

```
*
      SC   i j  L-i  L-j    h  A1 A2
390130 1 120 3 5 0.01  0.00 200 0  0 * Axial heat transfer to SC-120, contact h = TF-200
```

Example of prismatic reactor geometry. Effective conductivity for block-to-block transfer - Figure 2-28.

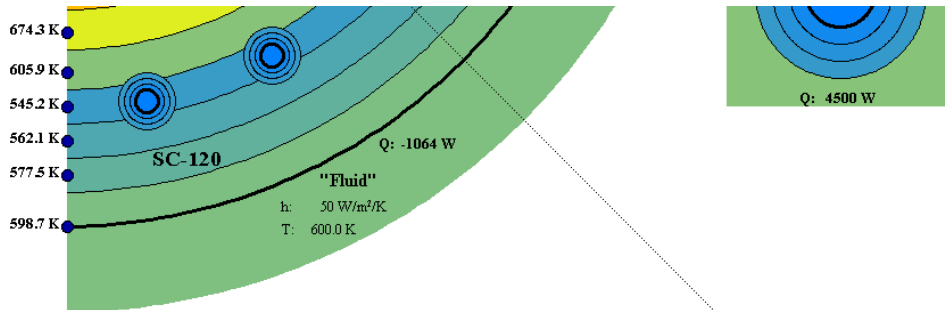


Figure 2-28 Example of prismatic block heat transfer

Example input, linking SC-130, which represents the inner prismatic block, and SC-120, which represents the outer prismatic block, is shown below. This example case is discussed further in Volume 3.

```
*
      SC   i j  L-i  L-j    h  A1 A2
390130 1 120 3 5 0.01  0.00 200 0  0 * Axial heat transfer to SC-120, contact h = TF-200
```


SPECTRA Code Manuals - Volume 2: User's Guide

The heat transfer from the upper surface of the roof (SC-003) is modelled using the Tabular Functions TF-001 and TF-002. The lower part of the floor (SC-004) is insulated.

The SC input data for the example problem is shown below. Note that the surface areas of SC-003 and SC-004, which are equal to 200π , were entered with a fair accuracy. This was done to be consistent with the view factors, needed when the thermal radiation models are applied for this configuration (see section 2.6.9).

```
*
* ----- SC-001
305001 Outer wall, upper part
300001 2      5.0  15.0  7.5  0  * Main data : GEO,LEN,X0,ELEV,VER
310001 0.05   1  0.0  358.0  20 * Cell data : DX, MAT, Q, T
321001 001    * Left side : Vol
322001 000 0 005 006 * Right side: Vol, H, HTC, Tfluid
*
* ----- SC-002
305002 Inner wall, upper part
300002 2      5.0   4.0  7.5  0  * Main data : GEO,LEN,X0,ELEV,VER
310002 0.05   1  0.0  358.0  20 * Cell data : DX, MAT, Q, T
321002 000 0 003 004 * Left side : Vol, H, HTC, Tfluid
322002 002    * Right side: Vol
*
* ----- SC-003
305003 Roof
300003 1 628.31853 0.0 10.5 1 * Main data : GEO,LEN,X0,ELEV,VER
310003 0.05   1  0.0  358.0  20 * Cell data : DX, MAT, Q, T
321003 000 0 001 002 * Left side : Vol, H, HTC, Tfluid
322003 001    * Right side: Vol
*
* ----- SC-004
305004 Floor
300004 1 628.31853 0.0 -0.5 -1 * Main data : GEO,LEN,X0,ELEV,VER
310004 0.05   1  0.0  358.0  20 * Cell data : DX, MAT, Q, T
321004 000    * Left side : Vol
322004 001    * Right side: Vol
*
* ----- SC-005
305005 Outer wall, lower part
300005 2      5.0  15.0  2.5  0  * Main data : GEO,LEN,X0,ELEV,VER
310005 0.05   1  0.0  358.0  20 * Cell data : DX, MAT, Q, T
321005 001    * Left side : Vol
322005 000 0 005 006 * Right side: Vol, H, HTC, Tfluid
*
* ----- SC-006
305006 Inner wall, lower part
300006 2      5.0   4.0  2.5  0  * Main data : GEO,LEN,X0,ELEV,VER
310006 0.05   1  0.0  358.0  20 * Cell data : DX, MAT, Q, T
321006 000 0 003 004 * Left side : Vol, H, HTC, Tfluid
322006 001    * Right side: Vol
*
* ----- Tabular Functions
*      x      y
600001 0.0    2000.00 * drywell-to-roof heat transfer coefficient
600002 0.0    415.00  * drywell (above roof) temperature
600003 0.0    2000.00 * drywell-to-inner wall heat transfer coefficient
600004 0.0    415.00  * drywell (left inner wall) temperature
600005 0.0     5.00   * outer wall-to-atmosphere heat transfer coefficient
600006 0.0    308.00  * atmosphere temperature
```

Example 2

As a second example a reactor core is modelled. The core consists of one hot rod and one average rod, each of them is represented by five 1-D Solid Heat Conductors in the axial direction (Figure 2-30). The hot rod is represented by SC-101 through SC-105. The average rod is represented by SC-201 through SC-205. The fuel regions and the common fuel regions are in such case defined as follows:

- Fuel regions (total reactor core):
SC-101, SC-102, SC-103, SC-104, SC-105, SC-201, SC-202, SC-203, SC-204, SC-205
- Common fuel regions:
 - Common region 1 (hot rod):
SC-101, SC-102, SC-103, SC-104, SC-105
 - Common region 2 (average rod):
SC-201, SC-202, SC-203, SC-204, SC-205

The hot rod and the average rod, shown in Figure 2-30, are made of 6 nodes. Nodes 1 - 4 represent the fuel, node 5 represents the gap, node 6 represents the cladding. This is the case for all SC-s in Figure 2-30. This is not a formal requirement; i.e. the gap node number may be different for different fuel regions or even for the same common fuel region. The only requirement is that all nodes representing the same gap must have the same thickness.

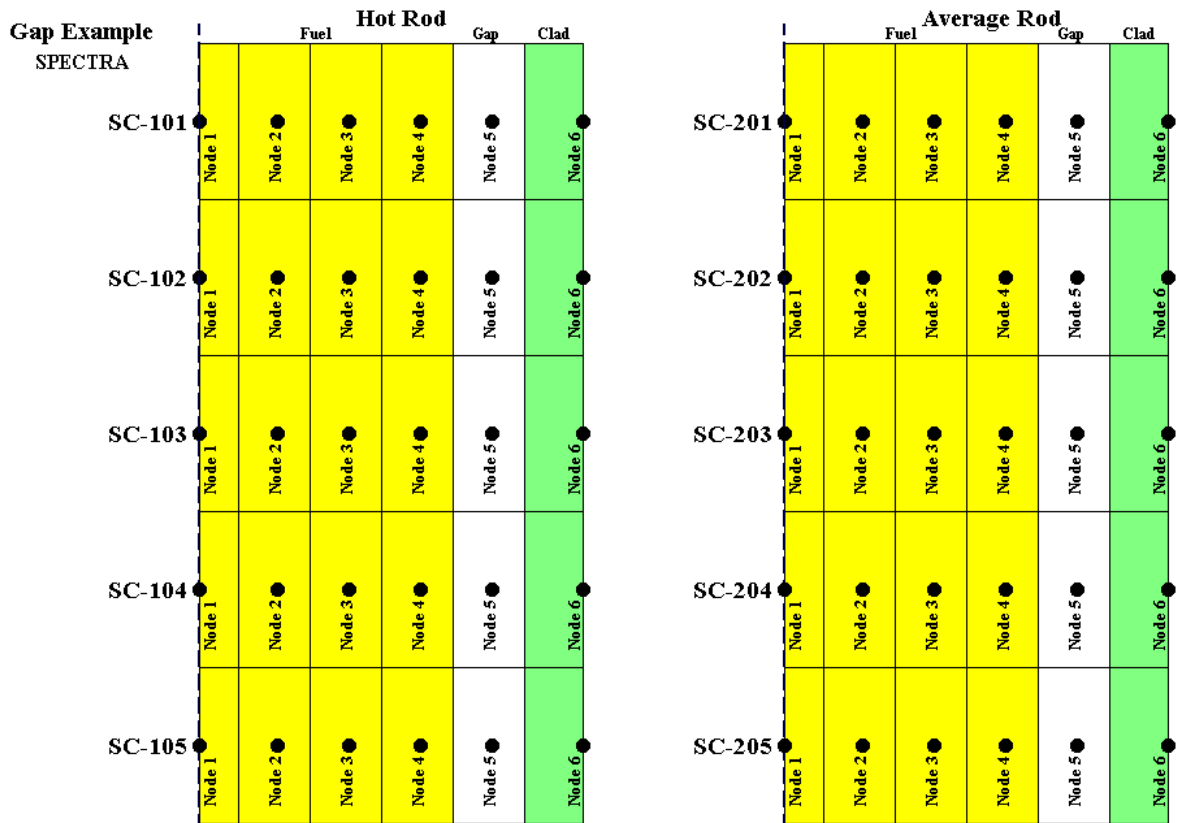


Figure 2-30 Example model for fuel and gap calculations

Listing of the input defining the fuel regions, the gap and all Solid Heat Conductors, is provided below.

SPECTRA Code Manuals - Volume 2: User's Guide

```

* ===== FUEL REGIONS AND GAP MODEL DATA =====
*
* FUEL REGION DEFINITION
* Region: 1          2          3          4          5
* SC Node Gap SC Node Gap SC Node Gap SC Node Gap SC Node Gap
340000 1 101 0 1 1 102 0 1 1 103 0 1 1 104 0 1 1 105 0 1
*
* Region: 6          7          8          9          10
* SC Node Gap SC Node Gap SC Node Gap SC Node Gap SC Node Gap
340000 1 201 0 1 1 202 0 1 1 203 0 1 1 204 0 1 1 205 0 1
*
* COMMON REGIONS
340201 1 2 3 4 5 * Hot rod
340202 6 7 8 9 10 * Average rod
*
* GAP DATA
*
341001 * GAP 1 - USE DEFAULTS
*
* ===== SC 1-D SOLID HEAT CONDUCTOR DATA =====
*
305101 Hot rod, Level 1
305102 Hot rod, Level 2
305103 Hot rod, Level 3
305104 Hot rod, Level 4
305105 Hot rod, Level 5
*
* N
302101 1 * Hot rod, Level 1
302102 1 * Hot rod, Level 2
302103 1 * Hot rod, Level 3
302104 1 * Hot rod, Level 4
302105 1 * Hot rod, Level 5
*
* GEO L X0 ELEV VER POWER
300101 2 0.5 0.0 2.25 0 1000 100 * Hot rod, Level 1
300102 2 0.5 0.0 1.75 0 1000 100 * Hot rod, Level 2
300103 2 0.5 0.0 1.25 0 1000 100 * Hot rod, Level 3
300104 2 0.5 0.0 0.75 0 1000 100 * Hot rod, Level 4
300105 2 0.5 0.0 0.25 0 1000 100 * Hot rod, Level 5
*
* Fuel
* dx mat power T nodes
310101 0.0005 101 1.0 500.0 1 * Hot rod, Level 1
310102 0.0005 101 1.0 500.0 1 * Hot rod, Level 2
310103 0.0005 101 1.0 500.0 1 * Hot rod, Level 3
310104 0.0005 101 1.0 500.0 1 * Hot rod, Level 4
310105 0.0005 101 1.0 500.0 1 * Hot rod, Level 5
*
* Fuel
* dx mat power T nodes
310101 0.001 101 1.0 500.0 3 * Hot rod, Level 1
310102 0.001 101 1.0 500.0 3 * Hot rod, Level 2
310103 0.001 101 1.0 500.0 3 * Hot rod, Level 3
310104 0.001 101 1.0 500.0 3 * Hot rod, Level 4
310105 0.001 101 1.0 500.0 3 * Hot rod, Level 5
*
* Gap
* dx mat power T nodes
310101 0.001 001 0.01 500.0 1 * Hot rod, Level 1
310102 0.001 001 0.01 500.0 1 * Hot rod, Level 2
310103 0.001 001 0.01 500.0 1 * Hot rod, Level 3
310104 0.001 001 0.01 500.0 1 * Hot rod, Level 4
310105 0.001 001 0.01 500.0 1 * Hot rod, Level 5
*
* Cladding
* dx mat power T nodes
310101 0.001 102 0.01 500.0 1 * Hot rod, Level 1
310102 0.001 102 0.01 500.0 1 * Hot rod, Level 2
310103 0.001 102 0.01 500.0 1 * Hot rod, Level 3
310104 0.001 102 0.01 500.0 1 * Hot rod, Level 4
310105 0.001 102 0.01 500.0 1 * Hot rod, Level 5

```

SPECTRA Code Manuals - Volume 2: User's Guide

```

*
*      Right CV
322101 100          * Hot rod, Level 1
322102 100          * Hot rod, Level 2
322103 100          * Hot rod, Level 3
322104 100          * Hot rod, Level 4
322105 100          * Hot rod, Level 5
*
305201 Average rod, Level 1
305202 Average rod, Level 2
305203 Average rod, Level 3
305204 Average rod, Level 4
305205 Average rod, Level 5
*
*      N
302201 1000 * Average rod, Level 1
302202 1000 * Average rod, Level 2
302203 1000 * Average rod, Level 3
302204 1000 * Average rod, Level 4
302205 1000 * Average rod, Level 5
*
*      GEO L   X0   ELEV VER   POWER
300201 2  0.5  0.0  2.25  0   500 100 * Average rod, Level 1
300202 2  0.5  0.0  1.75  0   500 100 * Average rod, Level 2
300203 2  0.5  0.0  1.25  0   500 100 * Average rod, Level 3
300204 2  0.5  0.0  0.75  0   500 100 * Average rod, Level 4
300205 2  0.5  0.0  0.25  0   500 100 * Average rod, Level 5
*
*      Fuel
*      dx   mat  power  T   nodes
310201 0.0005 101   1.0 500.0   1 * Hot rod, Level 1
310202 0.0005 101   1.0 500.0   1 * Hot rod, Level 2
310203 0.0005 101   1.0 500.0   1 * Hot rod, Level 3
310204 0.0005 101   1.0 500.0   1 * Hot rod, Level 4
310205 0.0005 101   1.0 500.0   1 * Hot rod, Level 5
*
*      Fuel
*      dx   mat  power  T   nodes
310201 0.001  101   1.0 500.0   3 * Hot rod, Level 1
310202 0.001  101   1.0 500.0   3 * Hot rod, Level 2
310203 0.001  101   1.0 500.0   3 * Hot rod, Level 3
310204 0.001  101   1.0 500.0   3 * Hot rod, Level 4
310205 0.001  101   1.0 500.0   3 * Hot rod, Level 5
*
*      Gap
*      dx   mat  power  T   nodes
310201 0.001  001   0.01 500.0   1 * Hot rod, Level 1
310202 0.001  001   0.01 500.0   1 * Hot rod, Level 2
310203 0.001  001   0.01 500.0   1 * Hot rod, Level 3
310204 0.001  001   0.01 500.0   1 * Hot rod, Level 4
310205 0.001  001   0.01 500.0   1 * Hot rod, Level 5
*
*      Cladding
*      dx   mat  power  T   nodes
310201 0.001  102   0.01 500.0   1 * Hot rod, Level 1
310202 0.001  102   0.01 500.0   1 * Hot rod, Level 2
310203 0.001  102   0.01 500.0   1 * Hot rod, Level 3
310204 0.001  102   0.01 500.0   1 * Hot rod, Level 4
310205 0.001  102   0.01 500.0   1 * Hot rod, Level 5
*
*      Right CV
322201 100          * Average rod, Level 1
322202 100          * Average rod, Level 2
322203 100          * Average rod, Level 3
322204 100          * Average rod, Level 4
322205 100          * Average rod, Level 5
*
*
605100 Power table
*      t (s)   Relative power  No.
600100 -1000.0   1.0           1

```


2.4 2-D Solid Heat Conductor Input Data

2.4.1 Records: 400XXX, 2-D Solid Heat Conductor Main Data

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

- W-1 (I) : IGEOTC Geometry type, (-).
 IGEOTC = 1 : rectangular geometry,
 IGEOTC = 2 : cylindrical geometry,
 Acceptable range: 1, 2.
 Default value: none.
- W-2 (R) : SIZETC Size of solid conductor. The interpretation depends on the geometry type.
 IGEOTC = 1 : length (z-coordinate) of the 2-D structure, (m),
 IGEOTC = 2 : not used.
 Acceptable range: $0.0 < SIZETC \leq 10^{10}$.
 Default value: none.
- W-3 (R) : X0TC Left side coordinate. The interpretation depends on the geometry type.
 IGEOTC = 1 : not used,
 IGEOTC = 2 : inner radius of the cylinder, (m),
 Acceptable range: $0.0 \leq X0TC \leq 10^{10}$.
 Default value: 0.0 .
- W-4 (R) : ELEVTC Elevation of highest point of the conductor, (m). In case of a horizontal cylinder this is the elevation of the cylinder axis - Figure 2-31.
 Acceptable range: all real numbers (note that the elevations of these boundary cells that transfer heat to Control Volumes must lie within the elevations of the corresponding Control Volumes).
 Default value: 0.0 .
- W-5 (I) : IVERTC Vertical orientation of conductor, (-), see Figure 2-31.
 Rectangular geometry:
 IVERTC = 0 : x-y surface is horizontal, z-coordinate is vertical
 IVERTC = 1 : x-y surface is vertical, z-coordinate is horizontal, y-coordinate is vertical down
 Cylindrical geometry:
 IVERTC = 0 : vertical cylinder (z-coordinate is vertical)
 IVERTC = 1 : horizontal cylinder (z-coordinate is horizontal)
 Acceptable range: 0, 1
 Default value: 0

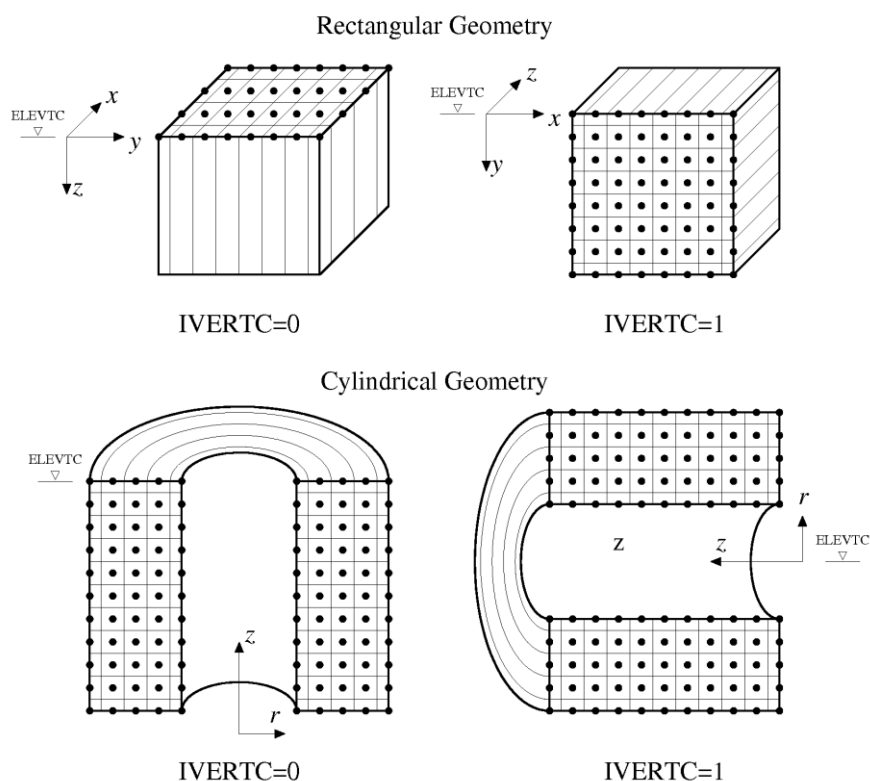


Figure 2-31 Vertical orientations of 2-D Solid Heat Conductors

- W-6 (R) : POWRTC Internal power source, (W). In order to obtain the current internal source, the value of POWRTC is multiplied by the time dependent multiplier defined by IPOWTC (word 7) and by the constant multiplier POWMTC (word 9), if present.
Acceptable range: $-10^{10} \leq \text{POWRTC} \leq 10^{10}$.
Default value: 0.0 .
- W-7 (I) : IPOWTC Pointer to a Tabular Function which defines the internal power multiplier. If the number is equal to zero, then internal power source is constant, and equal to POWRTC (Word 6). If the number is positive, then the internal power multiplier will be defined by the Tabular Function IPOWTC. If it is negative, the multiplier will be defined by the Control Function $|\text{IPOWTC}|$. No lower or upper limit is imposed on the value obtained from Tabular or Control Function (thus negative power source is allowed). If there is no internal power source (POWRTC=0.0) then IPOWTC must also be equal to zero.
Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.
Default value: 0 .
- W-8 (R) : HINCTC Inclination of nearly horizontal tubes, (degree). Tubes that have small inclination should be modelled as horizontal (IVERTC=1, see Word 5 above) with HINCTC $> 0.0^\circ$. The value is used by the condensation model.
Acceptable range: $0.0^\circ \leq \text{HINCTC} \leq 20.0^\circ$.

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 0.0° .

W-9 (R) : POWMTC Constant power multiplier. The constant power multiplier is introduced to have an easy way of defining for example axial power profile.
Acceptable range: $-10^{10} \leq \text{POWMTC} \leq 10^{10}$
Default value: 1.0

2.4.2 Records: 401000, TC Groups - General Data

W-1 (I) : KGRPTC Default TC group number. TC groups are introduced for editing; at the end of input processing volumes and masses of all materials is printed for each TC group. TC groups may be used to check the volumes and masses of materials in primary system, secondary system, etc.
Acceptable range: $1 \leq \text{KGRPTC} \leq 10$
Default value: 1

2.4.3 Records: 401XXX, Initial and Transient Temperatures

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

This record is optional. All entries from this record have their default values, recommended for general application.

W-1 (I) : INTTC Initial temperature calculation indicator.
1: Initial temperature distribution is calculated. If this option is selected, the program calculates the temperature distribution performing conduction calculation with a large ($\Delta t=10^{99}$ s) time step. In rare cases convergence failure may be encountered when performing the initial step. Usually it is good to ignore the convergence failure, since the calculated initial temperatures are typically better than could be obtained by manual initialization. The convergence failure can be ignored, by setting IACSFL (Word 8 in record 920000 - see section 2.16.5).
2: Input values (Words 4 in records 310XXX) are used. Use this option also if temperatures should be read from an Initial Condition File - ICF (section 2.16.3).
Acceptable range: 1, 2.
Default value: 2 .

W-2 (R) : ITYPTC Transient temperature calculation indicator.
1: Temperatures are time independent; that means the initial temperatures are kept through the transient.
2: Transient temperatures are calculated from the conduction equation (normal TC type).
Acceptable range: 1, 2.
Default value: 2 .

SPECTRA Code Manuals - Volume 2: User's Guide

W-3 (I) : IGRPTC TC group number. TC groups are introduced for editing; at the end of input processing volumes and masses of all materials is printed for each TC group. TC groups may be used to check the volumes and masses of materials in primary system, secondary system, etc.
Acceptable range: $1 \leq \text{IGRPTC} \leq 10$
Default value: KGRPTC (defined in record 401000)

2.4.4 Records: 402XXX, Multiplicity of the 2-D Solid Heat Conductor

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

W-1 (R) : XMLTTC Multiplicity of the 2-D solid conductor. This is the number of solid conductors that are identical to the conductor XXX. If XMLTTC < 0 then multiplicity will be time-dependent and defined by a Control Function with reference number $|\text{XMLTTC}|$.
Acceptable range: $0.0 < \text{XMLTTC} < 10^{10}$ or CF reference number
Default value: 1.0 .

2.4.5 Records: 405XXX, Name of the 2-D Solid Heat Conductor

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

W-1 (A) : NAMETC User defined name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.
Acceptable range: any string of up to 50 characters.
Default value: 50 "underline" characters: " _ " .

2.4.6 Records: 410XXX, Number of Cells of the 2-D Solid Heat Conductor

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

W-1 (I) : NCLXTC Number of cells in x-direction (horizontal direction in rectangular geometry and radial direction in cylindrical geometry).
Acceptable range: $2 \leq \text{NCLXTC} \leq 51$. (The maximum value is 51 rather than 50 because it is convenient to use odd number of cells rather than even. Since the first and the last cell is often half filled - see example 1 in

SPECTRA Code Manuals - Volume 2: User's Guide

- (3) *Acceptable range:* $0.0 < \text{CELYTC}(2) \leq 10^{10}$.
 Default value: none.

. . . etc. until all NCLYTC cell sizes are specified.

2.4.9 Records: 413XXX, Cell Types

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

W-1 (I) : L Row number in *y*-direction. The following data must specify NCLXTC values of cell types in the *y*-row number L
 Acceptable range: $1 \leq L \leq \text{NCLYTC}$.
 Default value: none.

W-2 (I) : IT00TC Cell type for cell (1,L), (*x*-row 1, *y*-row L), (-).
 (1,L) The input entry IT00TC consists of four digits; each digit specifies the filling of each of the four quarter-cells.
 IT00TC = *abcd*, where:
 a - upper-left quarter-cell.
 b - upper-right quarter-cell.
 c - lower-left quarter-cell.
 d - lower-right quarter-cell.
 Each of the digits is equal to 0 if the quarter cell is empty, and equal to 1 if the quarter-cell is filled with material.
 Acceptable range: (see Figure 2-32)
 0000 (empty cell), 1111 (full cell)
 0001, 0010, 0100, 1000 (quarter-cells)
 0011, 0101, 1010, 1100 (half-cells)
 1110, 1101, 1011, 0111 (three-quarter-cells)
 1001, 0110 (two separate quarter-cells)
 For each quarter-cell of a given cell, it is required that a filled quarter-cell must be adjacent to a filled quarter-cell in the neighboring cell, while an empty quarter cell must be adjacent to an empty quarter-cell in the neighboring cell. For example, the second and the third cell in the top row on the left side of Figure 2-32 cannot be neighboring cells in a real 2-D Heat Conductor. (Note that the left side of Figure 2-32 shows definitions of cell types, arranged in rows of similar cells. The rows do not represent any particular structures, like the ones shown in the Example 1 and 2, on the right side of Figure 2-32.)
 Default value: 0000 .

W-3 (I) : IT00TC(2,1) Cell type for cell (2,L), (*x*-row 2, *y*-row L), (-).

W-4 (I) : IT00TC(3,1) Cell type for cell (3,L), (*x*-row 3, *y*-row L), (-).

... , etc., until all NCLXTC cells are defined for a given row. Figure 2-32 shows definitions of the cell types and two examples of simple 2-D structures, together with the corresponding cell type definitions.

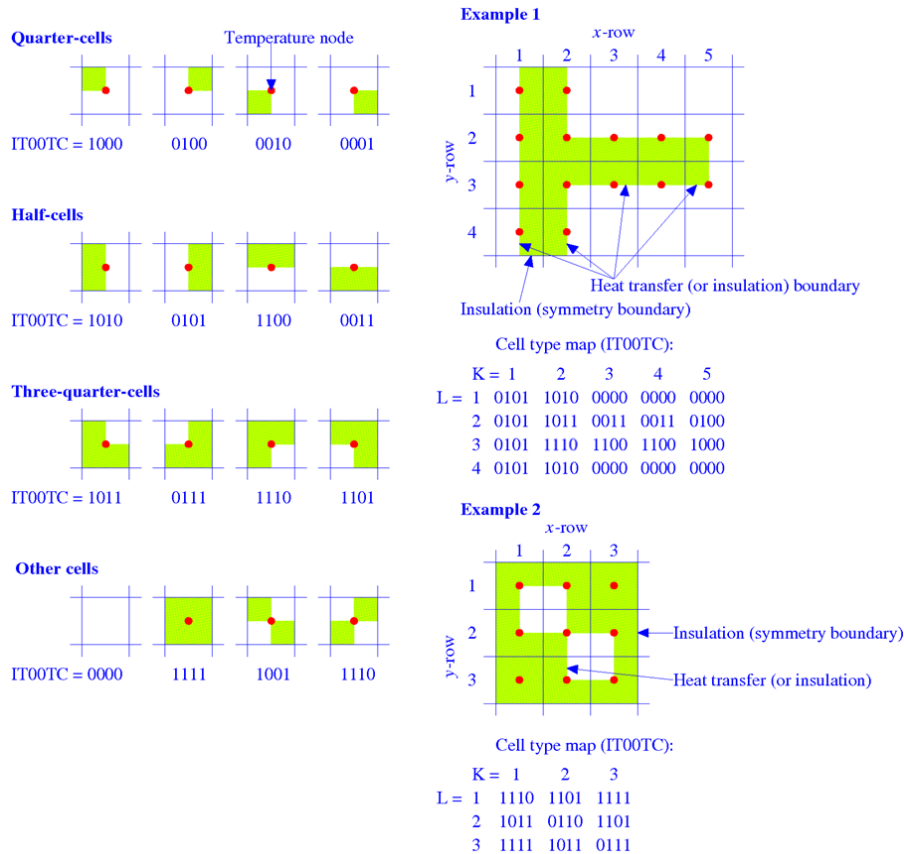


Figure 2-32 Cell type definitions and examples of 2-D structures.

2.4.10 Records: 414XXX, Material Data

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

W-1 (I) : L Row number in y-direction. The following data must specify NCLXTC values of material identifiers for all cells in the y-row number L
Acceptable range: $1 \leq L \leq NCLYTC$.
Default value: none.

W-2 (I) : MATITC Pointer to a material number for cell (1,L), (x-row 1, y-row L), (-).
 (1,L) The cell in x-row 1, y-row L is assumed to be composed of a single material defined by this word.
Acceptable range: must be a valid reference number of a solid material (defined in records 801XXX, 802XXX, 803XXX - see section 2.10). For an empty cell (IT00TC=0000) zero must be entered.

SPECTRA Code Manuals - Volume 2: User's Guide

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used).

- W-1 (I) : L Row number in y -direction. The following data must specify NCLXTC temperatures for all cells in the y -row number L
Acceptable range: $1 \leq L \leq NCLYTC$.
Default value: none.
- W-2 (I) : TCELTC Initial temperature in the cell (1,L), (x -row 1, y -row L), (-).
(1,L) Used only if INTTC=2 (see section 2.4.3).
Acceptable range: $273.0 \leq TCELTC \leq 10,000.0$. For an empty cell (IT00TC=0000) zero must be entered.
Default value: none.
- W-3 (I) : TCELTC Initial temperature in the cell (2,L), (x -row 2, y -row L), (-).
(2,L) Used only if INTTC=2 (see section 2.4.3).
- W-4 (I) : TCELTC Initial temperature in the cell (3,L), (x -row 3, y -row L), (-).
(3,L) Used only if INTTC=2 (see section 2.4.3).

... , etc., until initial temperatures are defined for all NCLXTC cells in a given row.

2.4.13 Records: 420XXX, Boundary Conditions

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. The 2-D Solid Heat Conductor reference numbers, XXX, need not be consecutive. The maximum number of 2-D Solid Heat Conductors is 20 (10 if the RT Package is used). The maximum number of boundary cells for each 2-D Solid Heat Conductor is 200.

- W-1 (I) : K Row number in x -direction. The data in this record defines boundary conditions for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq K \leq NCLXTC$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-2 (I) : L Row number in y -direction. The data in this record defines boundary conditions for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq L \leq NCLYTC$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-3 (I) : IQXBTC Indicator for heat transfer in the x -direction (r in cylindrical geometry).
= -1: heat transfer in the x -direction not allowed.
= +1: heat transfer in the x -direction allowed.
The use of IQXBTC and IQYBTC (below) allows some flexibility in the definition of boundary conditions for the cells which have boundaries in

SPECTRA Code Manuals - Volume 2: User's Guide

both x and y directions (such as for example the quarter-cells, or the three-quarter-cells, shown in Figure 2-32).

Acceptable range: IQXBTC = -1, or IQXBTC = +1.

Default value: +1.

- W-4 (I) : IQYBTC Indicator for heat transfer in the y -direction (z in cylindrical geometry).
= -1: heat transfer in the y -direction not allowed.
= +1: heat transfer in the y -direction allowed.
The use of IQYBTC and IQXBTC (above) allows some flexibility in the definition of boundary conditions for the cells which have boundaries in both x and y directions (such as for example the quarter-cells, or the three-quarter-cells, shown in Figure 2-32).
Acceptable range: IQYBTC = -1, or IQYBTC = +1.
Default value: +1.
- W-5 (I) : IVLBTC Control Volume number for convective heat transfer. The value specifies the Control Volume, which is associated with the boundary cell (K, L), (x -row K, y -row L). If zero is entered, then the boundary cell surface is either insulated, or the convective heat transfer coefficient and the fluid temperature are specified by Tabular or Control Functions (defined by words 6 and 7 below). If IVLBTC > 0, then heat is transferred to/from the CV using the standard heat and mass transfer package (see Volume 1). It is also possible to overrule the use of the standard heat and mass transfer package, and use a Tabular or Control Function (defined by word 6 below) to determine the heat transfer coefficient. Also the fluid temperature can be altered by a Tabular or a Control Function, by using the Word 7 below. In such case the value obtained from the Tabular or Control Function will be taken with weighting factor of 0.5, and the true (Control Volume) fluid temperature will be taken with the weighting factor of 0.5. If the heat transfer coefficient or the fluid temperature are defined by Tabular or Control Functions, then only heat transfer will occur on the surface, mass transfer (boiling/condensation) will not be calculated.
Acceptable range: must be a valid reference number of a Control Volume, if non-zero.
Default value: 0 .
- W-6 (I) : IHTBTC Pointer to a Tabular or Control Function defining the convective heat transfer coefficient (HTC) at the surface of the boundary cell (K, L), (x -row K, y -row L). If zero then the HTC is calculated by the code for the thermal-hydraulic conditions taken from the volume IVLBTC (Word 1). If the value is positive, the heat transfer coefficient will be defined by the Tabular Function IHTBTC. If it is negative, it will be defined by the Control Function $|IHTBTC|$. The units of the quantities obtained from the Tabular or Control Function are assumed to be (W/m²/K). If the obtained value is negative, it will be set to zero. If IHTBTC ≠ 0 then the fluid temperature, needed to calculate the boundary heat flux, is taken as:
- if IVLBTC > 0 then the fluid temperature in Control Volume IVLBTC is used.
 - if ITPBTC ≠ 0 then the fluid temperature is given by a Tabular or Control Function, defined by ITPBTC (word 4 below).

- if IVLBTC=0 and ITPBTC=0 then the fluid temperature is set to 300 K.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-7 (I) : ITPBTC Pointer to a Tabular or Control Function defining the fluid temperature at the boundary cell (K, L), (x-row K, y-row L). If the value is positive, the fluid temperature will be defined by the Tabular Function ITPBTC. If it is negative, it will be defined by the Control Function $|ITPBTC|$. The units of quantity obtained from the Tabular or Control Function are assumed to be (K). If the obtained value is negative, it will be set to zero. If ITPBTC \neq 0 and IVLBTC $>$ 0 (heat transfer to a Control Volume), then the value obtained from the Tabular or Control Function will be used with the weighting factor of FIN TTC. The true fluid temperature (from Control Volume) will be used with the weighting factor of 1.0-FIN TTC. Boiling and condensation models will be disabled by setting CSFBTC to -1.0 and ICNBTC to -4. In the past the input combination of IPTBTC \neq 0 and IVLBTC $>$ 0 was used to perform temperature averaging for heat exchangers. Currently it is not recommended to use this method. A more elaborate temperature averaging model has been developed, and is available through input records 425XXX (see section 2.4.14).

Acceptable range: must be a valid reference number of a Tabular, or a Control Function, if non-zero.

Default value: 0.

W-8 (I) : IQRBTC Indicator for non-convective heat flux at the boundary cell (K, L), (x-row K, y-row L). The heat flux defined by this pointer is used only on the uncovered part of the cell (above water level). With this pointer a user can model in a simple way radiative heat transfer. If the net enclosure thermal radiation model is used, and this cell surface is associated with one of the radiating surfaces (section 2.6.3), then this parameter must not be used. The meaning is as follows:

IQRBTC $>$ 1000:

A simple radiation model between the cell (K, L) surface and atmosphere gas is used to determine the non-convective heat transfer. The grey gas model is used, the atmosphere is assumed to be opaque (the reason for assuming opaque atmosphere is discussed in Volume 3). The heat flux is equal to:

$$q = \varepsilon(T_w) \sigma (T_w^4 - T_g^4)$$

where $\varepsilon(T_w)$ is the wall emissivity, σ is the Stefan-Boltzmann constant, T_w , T_g are the wall and gas temperatures respectively. The emissivity is obtained from the Tabular Function number: (IQRBTC - 1000). The argument for the Tabular Function is the wall surface temperature, (K).

0<IQRBTC<1000:

The heat flux is obtained from the Tabular Function number IQRBTC. The units of the quantities obtained from the Tabular Function are

positive. Best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DFCBTC should be equal to: for internal flow - hydraulic diameter; for external flow - width (rectangular wall).

Acceptable range: $0.0 < \text{DFCBTC} < 10^{10}$.

Default value: RECTANGULAR geometry (IGEOTC=1):
x-coordinate total length, if cell has horizontal boundary surface, y-coordinate total length, if cell has vertical boundary surface (or vertical and horizontal).

CYLINDRICAL geometry (IGEOTC=2):
inner diameter ($2.0 \times \text{ROTC}$) for the inner cylindrical surfaces; outer diameter for the outer cylindrical surfaces as well as the flat surfaces.

W-13 (I) : IFBBTC Configuration indicator for film boiling. The value is used only when IVLBTC is positive. The meaning of this variable is as follows:

- 0 vertical surface,
- ± 1 horizontal cylinder,
- 1 horizontal plate, facing down,
- +1 horizontal plate, facing up.

Acceptable range: $-1 \leq \text{IFBBTC} \leq +1$.

Default value: depend on boundary surface orientation. If the cell has the boundary surface in both vertical and horizontal directions (such as for example the quarter-cells, or the three-quarter-cells, shown in Figure 2-32), then the surface is interpreted as vertical.

W-14 (R) : DFBBTC Characteristic dimension for film boiling, (m). The value is used only when IVLBTC is positive. A best estimate value is provided for each geometrical configuration. Thus the value need not be entered or may be entered as zero. The value of DFBBTC should be equal to: for vertical walls - height; for horizontal plates - width; for cylinders and spheres - diameter.

Acceptable range: $0.0 < \text{DFCBTC} < 10^{10}$.

Default value: height, for rectangular geometry, inner or outer diameter for the cylindrical geometry cells.

W-15 (I) : ICNBTC Configuration indicator for condensation. The value is used only when IVLBTC is positive. The meaning of this variable is as follows:

- 4 condensation model disabled (the same for ICNBTC < -4)
 - 3 condensation on horizontal wall facing up,
 - 2 condensation on horizontal wall facing down,
 - 1 condensation inside horizontal tubes,
 - 0 condensation on vertical walls,
 - 1 condensation on outside surface of horizontal tube.
 - ≥ 2 condensation on outside surface of horizontal tube bank.
- ICNBTC is equal to the number of vertical rows of tubes.

Acceptable range: all integers.

Default value: depends on the boundary surface orientation. If the cell has the boundary surface in both vertical and

horizontal directions (such as for example the quarter-cells, or the three-quarter-cells, shown in Figure 2-32), then the surface is interpreted as vertical.

- W-16 (R) : DCNBTC Characteristic dimension for condensation, (m). The value is used only when IVLBTC is positive. The value of DCNBTC should be equal to: for vertical walls (or cylinders) - wall height; inside horizontal tubes - inner diameter; outside surface of horizontal tubes or tube banks - outer diameter; horizontal walls facing up - maximum film thickness (equilibrium thickness of water layer with free fall of liquid at the edges of the wall). The condensation type is defined by ICNBTC (word 15). In case of condensate flow through a stack of cells the characteristic dimension of the cell number k in the stack (counting from the top) should be defined as follows:

$$DCNBTC(k) = \left(\frac{z_{BOT}(k)^{5/4} - z_{TOP}(k)^{5/4}}{z_{BOT}(k) - z_{TOP}(k)} \right)^4$$

where: $z_{BOT}(k)$ distance from the bottom of the cell (K, L) to the top of the stack, (m),
 $z_{TOP}(k)$ distance from the top of the cell (K, L) to the top of the stack, (m).

If the height of each cell in the stack is identical then the above formula reduces to:

$$DCNBTC(k) = \left(k^{5/4} - (k-1)^{5/4} \right)^4 \frac{H}{N}$$

where: H - total height of the wall, (m),
 N - number of cells in the stack.

The ratio: (H/N) is the height of a single conductor in the stack. Note that only for $k=1$ DCNBTC is equal to the physical height of the conductor, (H/N) . For $k>1$ DCNBTC is greater than (H/N) . For $k=N$ DCNBTC is always greater than the total wall height, H .

Acceptable range: $0.0 < DCNBTC < 10^{10}$.

Default value: depends on boundary surface orientation. If the cell has the boundary surface in both vertical and horizontal directions (such as for example the quarter-cells, or the three-quarter-cells, shown in Figure 2-32), then the surface is interpreted as vertical.

- W-17 (R) : CSFBTC The constant C_{sf} in the Rohsenow equation for nucleate boiling (see Volume 1). The values of C_{sf} for different surfaces are given in table below. Entering a negative value will disable the full boiling model.
Acceptable range: all reals.
Default value: 0.013 .

Table 2-17 Values of C_{sf} for Rohsenow correlation.

Surface type	C_{sf}	Surface type	C_{sf}
Nickel	0.0060	Platinum	0.0130
Ground and polished stainless steel	0.0080	Brass	0.0060
Teflon pitted stainless steel	0.0058	Polished copper	0.0128
Chemically etched stainless steel	0.0133	Lapped copper	0.0147
Mechanically polished stainless steel	0.0132	Scored copper	0.0068

- W-18 (I) : MCFBTC Critical heat flux model selection. The value is used only when IVLBTC > 0.
- 1 Zuber pool boiling correlation with Ivey-Morris correction for subcooling.
 - 2 Combination of model based on USSR Academy of Sciences CHF look-up tables for high flow, with Zuber and Ivey-Morris for low flow.
 - 3 Combination of Biasi correlation for high flow, with Zuber and Ivey-Morris for low flow.
 - 4 Groeneveld (1986) look-up tables.
 - <0 CHF is calculated by a user-defined Control Function with the number |MCFBTC|.
- Acceptable range:* 1, 2, 3 or reference to a Control Function
Default value: 2.
- W-19 (I) : MNCBTC Selection of model for the influence of non-condensable gases for condensation. The value is used only when IVLBTC is positive and ICNBTC is greater than -2. The meaning of this variable is as follows:
- 1 Kuhn-Shrock-Petersen (KSP) correlations - recommended for condensation on the inside surface of tubes,
 - 2 Ogg correlations,
 - 3 Modified Ogg correlations - recommended for condensation on the outside surface of tubes, plates, etc.
- Acceptable range:* 1, 2, 3.
Default value: 3.
- W-20 (R) : CFDBTC Indicator of condensate film drainage behavior.
- If the value is positive then CFDBTC is the height of the cell. The elevation of the lowermost point of this surface is equal to the elevation of the cell center minus CFDBTC/2.0. The drainage from this surface is either deposited in the pool of a CV (if the lowest point of the surface is immersed in pool), or converted to droplets and suspended in the atmosphere of a CV as "rain" drops (if the lowest point of the surface is not immersed in the pool).
- If the value is negative then the drainage is assumed to be deposited on a surface of another (lower) cell of the same 2-D Solid Conductor. The absolute value of CFDBTC must then be equal to the number of a boundary cell at the bottom of the stack. Note that the boundary cell number must be used. The cell numbers and boundary cell numbers are internally assigned by the program, and therefore the user must look-up the boundary cell number in the boundary cell numbering map, printed in the SPECTRA output of the TC data.

The use of the drainage parameter, CFDBTC, and the condensation characteristic dimension, DCNBTC, in case of individual and stacked conductors is illustrated in Figure 2-33 (see also Volume 3). The half-cell size all cells is assumed to be 0.05 m. The appropriate values of DCNBTC and CFDBTC are shown in Table 2-18.

Acceptable range: if $CFDBTC < 0.0$ then the boundary cell No. $|CFDBTC|$ must be connected to a Control Volume (not necessarily equal to IVLBTC), if $CFDBTC > 0.0$ then the bottom elevation of the left surface (center point elevation minus $CFDBTC/2.0$) must be within the boundary Control Volume.

Default value: the default value is set to twice the distance between the center point of the left surface and the bottom of the boundary Control Volume. That value will result in deposition of condensate always in the pool. This is done to avoid numerical problems, and time step reduction, when condensate is converted into droplets.

W-21 (I) : IHDBTC Indicator of CV flow direction relative to the cell (K, L). Used only for rectangular geometry (IGEOTC=1). The meaning is:

For vertical TC's (IVERTC=0):

0: CV horizontal flow is parallel, $v_{TC} = (v_{CV,ver}^2 + v_{CV,hor}^2)^{1/2}$,

1: CV horizontal flow is perpendicular, $v_{TC} = v_{CV,ver}$.

For horizontal SC's (IVERSC > 0):

0: CV vertical flow is parallel, $v_{TC} = (v_{CV,ver}^2 + v_{CV,hor}^2)^{1/2}$,

1: CV vertical flow is perpendicular, $v_{TC} = v_{CV,ver}$.

For cylindrical geometry always:

$v_{TC} = (v_{CV,ver}^2 + v_{CV,hor}^2)^{1/2}$,

Acceptable range: 0, 1 .

Default value: 0 .

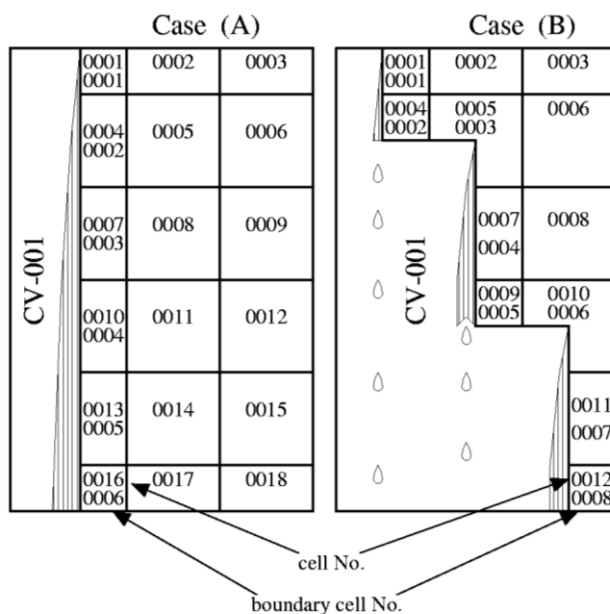


Figure 2-33 Condensation example cases (A) and (B). The half cell size is 0.05 m.

Table 2-18 Values of DCNBTC and CFDBTC for the example cases (A) and (B).

Bnd. Cell	Case (A)		Case (B)	
	DCNBTC	CFDBTC	DCNBTC	CFDBTC
1	$((0.05^{5/4} - 0.00^{5/4}) / (0.05 - 0.00))^4 = 0.050$	-0006	$((0.05^{5/4} - 0.00^{5/4}) / (0.05 - 0.00))^4 = 0.050$	-0002
2	$((0.15^{5/4} - 0.05^{5/4}) / (0.15 - 0.05))^4 = 0.236$	-0006	$((0.15^{5/4} - 0.05^{5/4}) / (0.15 - 0.05))^4 = 0.236$	0.05
3	$((0.25^{5/4} - 0.15^{5/4}) / (0.25 - 0.15))^4 = 0.484$	-0006	$((0.05^{5/4} - 0.00^{5/4}) / (0.05 - 0.00))^4 = 0.050$	-0005
4	$((0.35^{5/4} - 0.25^{5/4}) / (0.35 - 0.25))^4 = 0.730$	-0006	$((0.15^{5/4} - 0.05^{5/4}) / (0.15 - 0.05))^4 = 0.236$	-0005
5	$((0.45^{5/4} - 0.35^{5/4}) / (0.45 - 0.35))^4 = 0.975$	-0006	$((0.20^{5/4} - 0.15^{5/4}) / (0.20 - 0.15))^4 = 0.426$	0.05
6	$((0.50^{5/4} - 0.45^{5/4}) / (0.50 - 0.45))^4 = 1.159$	0.05	$((0.05^{5/4} - 0.00^{5/4}) / (0.05 - 0.00))^4 = 0.050$	-0008
7	-	-	$((0.15^{5/4} - 0.05^{5/4}) / (0.15 - 0.05))^4 = 0.236$	-0008
8	-	-	$((0.20^{5/4} - 0.15^{5/4}) / (0.20 - 0.15))^4 = 0.426$	0.05

W-22 (I) : **THTBTC** Contact angle, θ , (degree). Used to determine the diameter of bubbles created during nucleate boiling: $D = 0.0208 \cdot \theta \cdot (\sigma/g/(\rho_{liq} - \rho_{gas}))^{(1/2)}$.
Acceptable range: $10^\circ \leq \text{THTBTC} \leq 180^\circ$.
Default value: 96° .

W-23 (R) : **XRBBTC** Multiplier for convective heat transfer, X_{RB} .
XRBBTC < 0.0: HTC is multiplied by |XRBBTC| in both natural and force convection. It may be used to obtain a conservative estimation of heat transfer.
XRBBTC > 0.0: HTC is multiplied by XRBBTC only in case of turbulent forced convection (FC-TUR), internal flow (IFCBTC = -1). It is intended to allow the user to define a rod bundle multiplier in forced convection:

$$Nu_{tur} = X_{RB} \cdot 0.023 \cdot Re^{0.8} \cdot Pr^{0.4}$$

Appropriate values for parallel flow and cross-flow may be found in literature. The ratio of pitch over diameter is a good approximation (see Volume 1, description of forced convection correlations):

$$X_{RB} = P / D$$

For tube arrangements other than equilateral triangle pitch, the multiplier is given by:

$$X_{RB} = \left(\frac{P_1 \cdot P_2}{D^2} \right)$$

Note that the rod bundle multiplier may be different for different fluids. For example, for the liquid metals the value may even show different tendency (see Volume 1, description of liquid metals correlations):

$$X_{RB} = 1 - \exp[-3.8 \cdot (P/D - 1)]$$

Acceptable range: $0.0 \leq |\text{XRBBTC}| \leq 10^6$

Default value: **XRBBHT**
(global activator, defined in the record 810020)

W-24 (I) : **IHCBTC** Selection of heat transfer correlation for alternative fluid.

Acceptable range: one of the correlations defined in records 843XXX or 843YYY
Default value: rectangular: 1, cylindrical: 2.

2.4.14 Records: 425XXX, Heat Exchanger Temperature Averaging

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. These records may be used to model a heat exchanger. If these records are used, then an averaging procedure will be applied to calculate the representative fluid temperature at the TC cell surface. The representative fluid temperature will be equal to the weighted average of the inlet and outlet fluid temperatures. Note that if the temperature averaging is not used, then the representative fluid temperature is always equal to the fluid temperature in the boundary volume, which means it is equal to the outlet temperature. As shown in Volume 3, when the temperature-averaging concept is not used, a large number of nodes (~100) may be required to obtain accurate results. With the temperature averaging the same accuracy may be obtained using only a few nodes. An example of the temperature averaging is shown below - see Figure 2-34 and the corresponding discussion.

Inlet Junction Data:

- | | | |
|-----------|---------------|--|
| W-1 (I) : | I1 | Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for which the temperature averaging data defined in this record will be applied. The temperature averaging data will be applied for the boundary cells IBC: $I1 \leq IBC \leq I2$.
<i>Acceptable range:</i> must be an existing boundary cell number.
<i>Default value:</i> none. |
| W-2 (I) : | I2 | Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for which the temperature averaging data defined in this record will be applied. The temperature averaging data will be applied for the boundary cells IBC: $I1 \leq IBC \leq I2$.
<i>Acceptable range:</i> must be an existing boundary cell number. $I2 \geq I1$.
<i>Default value:</i> none. |
| W-3 (I) : | JTABTC
(1) | Junction reference number of the inlet Junction on the “primary” side (the side of the heat exchanger adjacent to cells I1 - I2).
<i>Acceptable range:</i> must be a Junction connected to the boundary Control Volume of all cells I1 - I2, if non-zero.
<i>Default value:</i> none. |
| W-4 (R) : | WTABTC
(1) | Limiting mass flow in the inlet Junction JTABTC(1) for full temperature averaging (W_{TAL} in Figure 2-16 (a)). Applied when there is a flow through JTABTC(1) into IVLBTC and there is no flow through KTABTC(1) - <u>normal flow direction on both primary and secondary side</u> . The temperature of the fluid entering through the Junction JTABTC(1) will be used with maximum weighting factor if the mass flow at the Junction is larger than WTABTC(1) ($W_{JN} > WTABTC(1)$). Generally speaking, WTABTC(1) is a flow for which the temperature distribution in the boundary Control Volume is approximately linear, provided that there is flow in through JTABTC(1) and there is no flow |

425001	2	2	021	100.0	012	1.0E+6	1	022	1.0E+6	012	100.0	1	* Secondary
425001	4	4	021	100.0	012	1.0E+6	1	022	1.0E+6	012	100.0	1	* Secondary
425001	6	6	021	100.0	012	1.0E+6	1	022	1.0E+6	012	100.0	1	* Secondary
425001	8	8	021	100.0	012	1.0E+6	1	022	1.0E+6	012 <td 100.0	1	* Secondary	
425001	10	10	021	100.0	012	1.0E+6	1	022	1.0E+6	012	100.0	1	* Secondary

Compared to the 1-D heat conductors, the extra input includes cell identifiers I1, I2, and the “other side” cell identifier, LTABTC.

Using the cell identifiers I1, I2 one can specify a cell range and therefore limit the amount of input. In the present example it is impossible to take advantage of that because no consecutive cells can be found transferring heat to the same Control Volume. Therefore the input above consists of five lines for each heat exchanger side. If the cells were numbered differently (by horizontal rows rather than vertical) only two lines would be needed, first with I1=1, I2=5, specifying data for the primary side (CV-10), and second with I1=6, I2=10, specifying data for the secondary side (CV-20). The user however, cannot affect the cell numbering. The cells are numbered internally by the SPECTRA code. The code optimizes the numbering scheme in order to minimize the computational effort, i.e. to minimize the size of the band diagonal matrix that needs to be solved for a 2-D Solid Heat Conductor (see Volume 1). In the case shown in Figure 2-34 the band size is smaller (2) when cells are numbered vertically, than it would be (5) if the cells were numbered horizontally.

In the present example cell 10 is used arbitrarily as the secondary side identifier. This choice is arbitrary; it could be any of the cells facing CV-20 (cells 2, 4, 6, 8). For the primary side identifier the cell 1 is used; again it could be any of the cells facing CV-10 (3, 5, 7, 9).

Note that the limiting flow for T-A is affected by the multipliers CMN1TC, CMN2TC, defined in record 460XXX (section 2.4.18). Generally one should make sure that the limiting flows, W_{TA} , approximately fulfil the relation:

$$(W_{TA} c_p)_{primary} \approx (W_{TA} c_p)_{secondary}$$

The multipliers will then assure proper temperature averaging in case the flow on the primary side becomes very different from the flow on the secondary side.

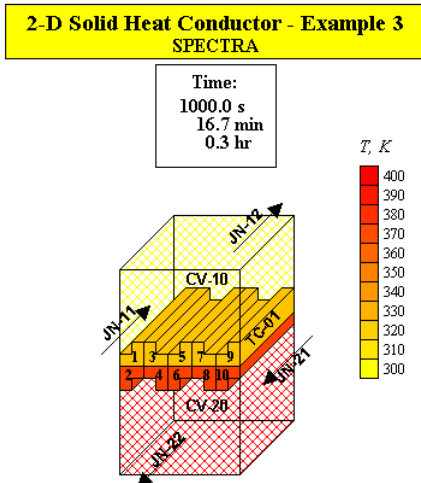


Figure 2-34 Temperature averaging for a 2-D Solid Heat Conductor.

2.4.15 Records: 450XXX, Boundary Fluid Temperature Calculation

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record describes the boundary fluid temperature calculation in case of intensive boiling. This record is optional. All entries from this record have their default values, recommended for general application.

- W-1 (I) : K Row number in x -direction. The data in this record defines boundary conditions for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq K \leq NCLXTC$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-2 (I) : L Row number in y -direction. The data in this record defines boundary conditions for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq L \leq NCLYTC$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-3 (I) : IBPTTC Indicator for boundary fluid temperature calculation for pool-bubble flow. Typically the pool temperature is used as boundary fluid temperature for Solid Heat Conductors. In case of intensive boiling the program assumes that bubbles rise up in a plume of relatively warm water (see Volume 1). The water temperature in this plume is equal to the local saturation temperature, and is therefore higher than the pool average temperature, which is no higher than the saturation temperature at the pool surface pressure. The indicator IBPTTC defines how the program should determine whether the TC surface will be exposed to the warm plume or to the relatively cold pool outside the plume. Three factors may be used by the program: the void fraction factor, f_a , the temperature factor, f_T , and the submergence factor, f_Z . Those factors are defined as follows:

a) The void fraction factor, f_a :

$$f_a = \begin{cases} 0.0 & \text{if } \alpha \leq \alpha_1 \\ (3 - 2X)X^2 & \text{if } \alpha_1 < \alpha < \alpha_2 \\ 1.0 & \text{if } \alpha \geq \alpha_2 \end{cases}$$

where α is the average void fraction in the pool, X is the interpolation factor, equal to: $X = (\alpha - \alpha_1) / (\alpha_2 - \alpha_1)$, and the boundary values of void fractions, α_1 , α_2 , are defined below (words 2 and 3). Note that the cubic interpolation is used, which ensures continuity of the function as well as its first derivative.

b) The surface temperature factor, f_T :

$$f_T = \begin{cases} 0.0 & \text{if } T_{TC} \leq T_{int} + \Delta T_1 \\ (3 - 2X)X^2 & \text{if } T_{int} + \Delta T_1 < T_{TC} < T_{int} + \Delta T_2 \\ 1.0 & \text{if } T_{TC} \geq T_{int} + \Delta T_2 \end{cases}$$

where T_{TC} is the surface temperature of the Solid Heat Conductor, T_{int} is the liquid temperature at the pool-bubble interphase, X is the interpolation factor, equal to:

$$X = (T_{TC} - (T_{int} + \Delta T_1)) / ((T_{int} + \Delta T_2) - (T_{int} + \Delta T_1)),$$

and the boundary values of ΔT are defined below (words 4 and 5).

c) The surface submergence factor, f_Z :

$$f_Z = \begin{cases} (3 - 2X_1)X_1^2 & \text{if } 0 \leq Z < Z_{bubb} \\ 1.0 & \text{if } Z_{bubb} \leq Z \leq Z_{bubb}Z_{m1} \\ (3 - 2X_2)X_2^2 & \text{if } Z_{bubb}Z_{m1} < Z < Z_{bubb}Z_{m2} \\ 0.0 & \text{if } Z_{bubb}Z_{m2} \leq Z \end{cases}$$

where Z is the TC submergence (equal to the distance between the pool surface and the elevation of the middle point of this part of the TC which is covered by water), Z_{bub} is the submergence of average bubble, X_1 and X_2 are the interpolation factors, equal to:

$$X_1 = Z/Z_{bub},$$

$$X_2 = (Z - Z_{bub} \cdot Z_{m2}) / (Z_{bub} \cdot Z_{m1} - Z_{bub} \cdot Z_{m2}).$$

Values of the multipliers, Z_{m1} and Z_{m2} , are defined below (words 6, 7).

The parameter IBPTTC defines which of the factors described above should be used. The interpretation is as follows:

IBPTTC = -1 : No factors are used. When surface is exposed to a boiling pool, the boundary fluid temperature is always equal to the pool temperature, T_{pool} (approximately equal to the saturation temperature for the pressure at the pool surface).

$$T_{fluid} = T_{pool}$$

IBPTTC = 1 : Only the void fraction factor is taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot f_\alpha$$

where T_{pool} is the pool average temperature, and T_{int} is the liquid temperature at the pool-bubble interphase (thus the warm plume temperature, approximately equal to the saturation temperature for the pressure at the elevation of average bubble).

IBPTTC = 2 : The void fraction factor and the temperature factor are taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot (f_\alpha f_T)$$

SPECTRA Code Manuals - Volume 2: User's Guide

IBPTTC = 3 : The void fraction factor and the submergence factor are taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot (f_{\alpha} f_Z)$$

IBPTTC = 4 : All factors are taken into account. The boundary fluid temperature is calculated as:

$$T_{fluid} = T_{pool} + (T_{int} - T_{pool}) \cdot (f_{\alpha} f_T f_Z)$$

Acceptable range: $-1 \leq \text{IBPTTC} \leq +4$.

Default value: +4. If IWATCV>0 (see section 2.1.31) then the default value is -1.

- W-4 (R) : ALP1TC Upper limit of void fraction to use only the pool temperature as the boundary fluid temperature for the TC surface, α_1 , (-). Used if IBPTTC (word 1 above) is positive. If the average void fraction in the pool is below α_1 then the Solid Heat Conductor surface is not exposed to the warm plume.
Acceptable range: $10^{-5} \leq \text{ALP1TC} \leq 0.1$.
Default value: 10^{-3} .
- W-5 (R) : ALP2TC Lower limit of void fraction to use the warm plume temperature as the boundary fluid temperature for the TC surface, α_2 , (-). Used if IBPTTC (word 1 above) is positive. If the average void fraction in the pool is above α_2 then the Solid Heat Conductor surface can be exposed to the warm plume (depending on other conditions if they are applied).
Acceptable range: $2.0 \cdot \text{ALP1TC} \leq \text{ALP2TC} \leq 0.5$.
Default value: 0.05 .
- W-6 (R) : TSC1TC Upper limit of TC surface superheat to use only the pool temperature as the boundary fluid temperature for the TC surface, ΔT_1 , (K). Used if IBPTTC (word 1 above) is equal to 2 or 4. If the TC surface temperature is lower than the liquid temperature at the pool-bubble interphase (warm plume temperature) plus TSC1TC, then the Solid Heat Conductor surface is not exposed to the warm plume.
Acceptable range: $0.1 \leq \text{TSC1TC} \leq 10.0$.
Default value: 1.0 .
- W-7 (R) : TSC2TC Lower limit of TC surface superheat to use the warm plume temperature as boundary fluid temperature for the TC surface, ΔT_2 , (K). Used if IBPTTC (word 1 above) is equal to 2 or 4. If the TC surface temperature is higher than the liquid temperature at the pool-bubble interphase (warm plume temperature) plus TSC2TC, then the Solid Heat Conductor surface can be exposed to the warm plume (depending on other conditions if they are applied).
Acceptable range: $2.0 \cdot \text{TSC1TC} \leq \text{TSC2TC} \leq 30.0$.
Default value: 3.0 .

SPECTRA Code Manuals - Volume 2: User's Guide

- W-8 (R) : ZSC1TC Lower multiplier on bubble submergence to use the warm plume temperature as the boundary fluid temperature for the TC surface, Z_{m1} , (-). Used if IBPTTC (word 1 above) is equal to 3 or 4. If the TC surface submergence is smaller than the average bubble submergence multiplied by ZSC1TC then the Solid Heat Conductor surface can be exposed to the warm plume (depending on other conditions if they are applied).
Acceptable range: $1.0 \leq ZSC1TC \leq 10.0$.
Default value: 2.0 .
- W-9 (R) : ZSC2TC Upper multiplier on bubble submergence to use only the pool temperature as the boundary fluid temperature for the TC surface, Z_{m2} , (-). Used if IBPTTC (word 1 above) is equal to 3 or 4. If the TC surface submergence is larger than the average bubble submergence multiplied by ZSC2TC then the Solid Heat Conductor surface is not exposed to the warm plume.
Acceptable range: $1.2 \cdot ZSC1TC \leq ZSC2TC \leq 15.0$.
Default value: 4.0 .

2.4.16 Records: 451XXX, Boundary Fluid Velocity Multiplier

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record is optional. The velocity multiplier may be used for to account for own movement of structures, such as for example rotor blades. In such case the relative velocity surface-to-gas velocity is different than the gas velocity in a Control Volume. The user may take into account that difference using a Control Function that depends on the rotational speed, etc.

- W-1 (I) : VLMBTC Velocity multiplier, C_v , for the boundary surface velocity calculation. If a positive value is entered, the velocity multiplier is constant, and equal to this value. If a negative value is entered, the velocity multiplier is obtained from the Control Function equal to $|\text{VLMBTC}|$. An absolute value of the number obtained from the Control Function is used. Furthermore the value is limited to a maximum of 10^{10} .

The fluid velocity at the TC boundary surface is obtained from:

If IHDBTC=0 (Word 21, record 420XXX):

$$v_{TC} = C_v \cdot \sqrt{v_{CV,hor}^2 + v_{CV,ver}^2}$$

If IHDBTC=1, IVERSC=0 (vertical TC, Word 5, record 400XXX):

$$v_{SC} = C_v \cdot v_{CV,ver}$$

If IHDBTC=1, IVERTC≠0 (horizontal TC, Word 5, record 300XXX):

$$v_{SC} = C_v \cdot v_{CV,hor}$$

Acceptable range: $0.0 \leq VLMLSC \leq 10^{10}$

or reference to a Control Function.

Default value: 1.0

2.4.17 Records: 452XXX, Limit for Simultaneous Transfer to Pool and Atmosphere

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$.

- W-1 (I) : K Row number in x -direction. The data in this record defines boundary conditions for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq K \leq \text{NCLXTC}$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-2 (I) : L Row number in y -direction. The data in this record defines boundary conditions for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq L \leq \text{NCLYTC}$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-3 (R) : PMXBTC Critical (maximum) fraction of the boundary surface area covered by pool to allow simultaneous heat transfer to pool and atmosphere. If no value is given, simultaneous heat transfer to pool and atmosphere is always possible. This may lead to too large condensation in some cases. To eliminate it, the user may restrict the simultaneous heat transfer to a situation when the pool-covered fraction is smaller than PMXBTC. This input parameter is similar to CPFPL in the MELCOR code. An interpolation zone is defined. The full transfer to gas occurs when the pool fraction is below 0.9 of the critical value, a linear interpolation is performed in the range between 0.9 and 1.0 times the critical value.
Acceptable range: $0.0 \leq \text{PMXBTC} \leq 1.0$
Default value: 0.0 .

As example of such situation is discussed in Volume 1. As a reference case, a fine nodalization is used (Figure 2-17, left). Coarse nodalization and consequent too slow heat up due to artificial heat transfer from atmosphere to pool through the solid structure is shown in Figure 2-17, middle. This is prevented by using the critical pool fraction of 0.01 (Figure 2-17, right). The heat transfer from atmosphere to pool is practically eliminated. However, a direct heat transfer still exists at the pool-atmosphere interphase. Therefore it is advisable to eliminate the pool-atmosphere heat transfer at the same time (input record 164XXX). This was done in the considered example.

2.4.18 Records: 460000, Global Data: Film Boiling, Slip Ratio, TA, Oxidation

Parameters defined in this record are applied for all 2-D Solid Heat Conductors.

- W-1 (R) : AMFBTC First coefficient in the Simon Minimum Film Boiling correlation, A_{MFB} , (-). SPECTRA selects correlation that gives maximum value of the T_{MFB} .

SPECTRA Code Manuals - Volume 2: User's Guide

therefore the Simon correlation may be deactivated by setting AMFBTC and BMFBTC to small values.

Acceptable range: $0.0 < \text{AMFBTC} \leq 1.0$

Default value: 0.13.

W-2 (R) : BMFBTC Second coefficient in the Simon Minimum Film Boiling correlation, B_{MFB} , (-). SPECTRA selects correlation that gives maximum value of the T_{MFB} , therefore the Simon correlation may be deactivated by setting AMFBTC and BMFBTC to small values.

Acceptable range: $0.0 < \text{BMFBTC} \leq 2.0$

Default value: 0.86.

W-3 (R) : CMFBTC Coefficient in the Berenson Minimum Film Boiling correlation, C_{MFB} , (-). SPECTRA selects correlation that gives maximum value of the T_{MFB} , therefore the Berenson correlation may be deactivated by setting CMFBTC to a small value.

Acceptable range: $0.0 < \text{CMFBTC} \leq 1.0$

Default value: 0.127

W-4 (R) : TFMNTC Minimum value of the Minimum Film Boiling (MFB) temperature minus the Critical Heat Flux (CHF) temperature: $(T_{MFB} - T_{CHF})$, (K). The MFB temperature, calculated from the Simon correlation is limited by this word so that it will never be lower than $T_{CHF} + \text{TFMNTC}$.

Acceptable range: $5.0 \leq \text{TFMNTC} \leq 1000.0$

Default value: 5.0.

W-5 (R) : TFMXTC Maximum value of the Minimum Film Boiling (MFB) temperature minus the Critical Heat Flux (CHF) temperature: $(T_{MFB} - T_{CHF})$, (K). The MFB temperature, calculated from the Simon correlation is limited by this word so that it will never be higher than $T_{CHF} + \text{TFMXTC}$.

Acceptable range: $\text{TFMNTC} \leq \text{TFMXTC} \leq 1000.0$

Default value: 1000.0.

W-6 (R) : XTRBTC Coefficient in the Kalinin Transition Boiling correlation, X_{TB} , (-).

Acceptable range: $0.5 < \text{XTRBTC} \leq 20.0$

Default value: 7.0.

W-7 (R) : ASFBTC Correction for subcooling in the film boiling correlation, A_{SFB} , (-). In case of a subcooled film boiling, the total heat flux is calculated from:

$$q = q_{FB} + A_{SFB} \cdot h_{conv} \cdot (T_{sat} - T_{fluid})$$

where q_{FB} is the saturated film boiling heat flux and h_{conv} is the convective heat transfer coefficient, calculated for the bulk liquid temperature, T_{fluid} .

Acceptable range: $0.0 \leq \text{ASFBTC} \leq 2.0$

Default value: 1.0 (based on comparison with results obtained using RELAP5/MOD3.3).

SPECTRA Code Manuals - Volume 2: User's Guide

W-8 (R) : SMAXTC Maximum value of the slip ratio, (v_{bubb} / v_{pool}), (-). Used for CHF calculations. The slip ratio which is used in the CHF correlation is equal to the minimum of v_{bubb} / v_{pool} and SMAXTC.
Acceptable range: $1.0 \leq \text{SMAXTC} \leq 1000.0$
Default value: 100.0.

W-9 (R) : CMN1TC Multiplier for the first (counter-current) Temperature Averaging (T-A) mode. The nominal flows for the T-A on both primary and secondary side of a heat exchanger are entered in the records 425XXX. If the flows exceed the nominal flows, full T-A is performed. If flows are decreased then also the T-A is decreased - see section 2.4.14. This treatment is approximately correct if flow changes only on one side of the heat exchanger. If the flow changes simultaneously on both sides of the heat exchanger, then T-A should be used for flows much smaller than nominal. This multiplier defines how much the limiting flow (typically taken as the nominal flow) can be decreased when the flow on the other side of a heat exchanger decreases.
 The default value of 0.01 means that in nominal counter-flow conditions full T-A will be performed if the flows decrease down to 1% of the nominal flow, provided that they will decrease simultaneously on both sides of the heat exchanger.

Generally the limiting flow on a given side of a heat exchanger is equal to:

$$W_{TA} = \text{Min} \left[\frac{W_{TA}}{C_{MN1}}, \text{Max} \left(W_{TA} C_{MN1}, W_{TA} \frac{W_{other\ side}}{W_{TA, other\ side}} \right) \right]$$

where W_L is the limiting flow for full T-A, C_{MN1} is the factor CMN1TC, $W_{L, other\ side}$ is the limiting flow for full T-A on the other side, and $W_{other\ side}$ is the current flow on the other side. Note that with this definition, the limiting flow for T-A can be either decreased or increased, and the actual value will always be within the range:

$$W_{TA} C_{MN1} \leq W_{TA} \leq \frac{W_{TA}}{C_{MN1}}$$

The limiting flow will be small when the other side flow is small, and large when the other side flow is large. This is the most appropriate treatment of a heat exchanger, provided that the limiting flows, defined in records 425XXX for both primary and secondary side, fulfil approximately the relation:

$$(W_{TA} C_p)_{primary} \approx (W_{TA} C_p)_{secondary}$$

Acceptable range: $0.001 \leq \text{CMN1TC} \leq 1.0$
Default value: 0.01.

W-10 (R) : CMN2TC Multiplier for the second (co-current) Temperature Averaging (T-A) mode. Works the same as CMN1TC, but in case when the flow is co-current. Default value means that CMN2TC is not used in co-flow

SPECTRA Code Manuals - Volume 2: User's Guide

conditions. It is recommended to disable T-A in co-flow by setting the limiting flow to a large value - see section 2.4.14. In such case the value of CMN2TC is not very important. For consistency it should be equal to 1.0 when T-A is disabled.

Acceptable range: $0.001 \leq \text{CMN2TC} \leq 1.0$

Default value: 1.0.

- W-11 (R) : VGLMTC Gas velocity limit, $v_{g,lm}$ (m/s), to switch off the Temperature Averaging (T-A). Numerical problems may be encountered when T-A is used in case of low velocities and changes of flow direction. To avoid this problems the T-A is turned off when the velocity is smaller than the limit defined by this word. An interpolation zone is defined for gas velocities between VGLMTC and $2 \times \text{VGLMTC}$.

$$X_{TA,eff} = \begin{cases} X_{TA} & \text{if } v_g > 2v_{g,lm} \\ X_{TA} \cdot (v_g - v_{g,lm}) / v_{g,lm} & \text{if } v_{g,lm} < v_g < 2v_{g,lm} \\ 0.0 & \text{if } v_g < v_{g,lm} \end{cases}$$

where X_{TA} is the Temperature Averaging factor for full T-A, $X_{TA,eff}$ is the effective T-A factor, v_g is the gas velocity and $v_{g,lm}$ is the limiting gas velocity, VGLMTC.

Acceptable range: $0.001 \leq \text{VGLMTC} \leq 100.0$

Default value: 1.0

- W-12 (R) : VLLMTC Liquid velocity limit, $v_{l,lm}$ (m/s), to switch off the Temperature Averaging (T-A). Numerical problems may be encountered when T-A is used in case of low velocities and changes of flow direction. To avoid this problems the T-A is turned off when the velocity is smaller than the limit defined by this word. An interpolation zone is defined for liquid velocities between VLLMTC and $2 \times \text{VLLMTC}$.

$$X_{TA,eff} = \begin{cases} X_{TA} & \text{if } v_l > 2v_{l,lm} \\ X_{TA} \cdot (v_l - v_{l,lm}) / v_{l,lm} & \text{if } v_{l,lm} < v_l < 2v_{l,lm} \\ 0.0 & \text{if } v_l < v_{l,lm} \end{cases}$$

where X_{TA} is the Temperature Averaging factor for full T-A, $X_{TA,eff}$ is the effective T-A factor, v_l is the liquid velocity and $v_{l,lm}$ is the limiting liquid velocity, VLLMTC.

Acceptable range: $0.001 \leq \text{VLLMTC} \leq 100.0$

Default value: 0.1

- W-13 (I) : IOXNTC Option for oxidation on surfaces not connected to Control Volumes.
=1: oxidation is calculated on TC surfaces not connected to a CV. It will be assumed that all oxidizing gases are always available at the surface.
=2: oxidation is disabled on TC surfaces not connected to a CV.

Acceptable range: 1, 2

Default value: none

- W-14 (I) : ISEQTC Indicator for multiple oxidation reactions.
=1: all oxidation reactions proceed simultaneously.
=2: dominant reactions: oxidation reactions proceed in sequence, defined in records 480XXX. If there is enough oxidant (gas fraction >

XLIMTC) for the first reaction, only this reaction occurs. If not, second reaction starts, then third, etc. This option is available because, according to [52], reaction with oxygen dominates over reactions with steam and nitrogen.

Acceptable range: 1, 2

Default value: 1

W-15 (R) : XLIMTC Limit for dominant reactions. The default oxidation starvation limits are:
 C1OX = 1.0×10^{-4} : full strength oxidation
 COOX = C1OX / 10.0 = 1.0×10^{-5} : no oxidation
 The default value of XLIMTC was selected approximately in the middle of the interpolation zone, when the dominant reaction strength is reduced roughly by half.
Acceptable range: $1.0 \times 10^{-7} \leq \text{XLIMTC} \leq 1.0 \times 10^{-2}$
Default value: XLIMTC = C1OX / 2.0

W-16 (I) : IMPGTC Implicit/explicit use of gas concentration for oxidation calculations.
 = 1: implicit (end of time step value is used).
 = 2: explicit (beginning of time step value is used).
Acceptable range: 1 or 2
Default value: 1

W17 - (I) IAVETC Method used to calculate average TC temperature. In the SPECTRA output and plot files, the average temperatures are given next to the cell temperatures. This entry defines how the average temperature is obtained.

= 1: volume average:
$$\bar{T} = \frac{\sum_i V_i \cdot T_i}{\sum_i V_i}$$

= 2: mass-average:
$$\bar{T} = \frac{\sum_i M_i \cdot T_i}{\sum_i M_i}$$

Here M_i , V_i , T_i are the mass, volume and temperature of the cell i .

Acceptable range: 1 or 2

Default value: 2

W-18 (I) : IQPLTC Power versus power density as plot parameters - Table 2-26.
 = 1: Power (W) is used as plot parameters: TC-XXX-Qcel-YYYY
 = 2: Power density (W/m³) is used: TC-XXX-qcel-YYYY
Acceptable range: 1 or 2
Default value: 1

2.4.19 Records: 465000, Hydraulic Diameter - TC Versus CV

W-1 (I) : IDHDTC Option to check consistency between the CV hydraulic diameter (DHYDCV) and the TC hydraulic diameter (DFCBTC).
 = 1: consistency is not required. If DFCBTC \neq DHYDCV, then a warning message is issued.
 = 2: consistency is required. If DFCBTC \neq DHYDCV, then an error message is issued.
Acceptable range: 1, 2

Default value: 1

2.4.20 Records: 480XXX, Boundary Cell Oxidation Data

XXX is the Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. These records activate the oxidation model on the boundary cell of a 2-D Solid Heat Conductor. Each surface can have several different oxidation reactions associated with it, for example: a Zircaloy cladding may be oxidized by steam, $Zr+H_2O$, and oxygen, $Zr+O_2$. Maximum number of oxidation reactions is 5.

- W-1 (I) : K Row number in x -direction. The data in this record defines oxidation parameters for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq K \leq NCLXTC$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-2 (I) : L Row number in y -direction. The data in this record defines oxidation parameters for the boundary cell (K, L), (x -row K, y -row L).
Acceptable range: $1 \leq L \leq NCLYTC$. The cell (K, L) must be a boundary cell, i.e. it cannot be an empty cell (IT00TC=0000), or a filled cell (IT00TC=1111).
Default value: none.
- W-3 (R) : XMTBTC Initial thickness of material available for oxidation on the surface of the 2-D Solid Heat Conductor, (m).
Acceptable range: $0.0 \leq XMTBTC \leq$ half of the maximum thickness of TC.
Default value: smaller dimension of the cell (K,L).
- W-4 (R) : XOXBTC Initial thickness of oxidized material on the surface of the 2-D Solid Heat Conductor, (m).
Acceptable range: $0.0 \leq XOXBTC \leq$ half of the maximum thickness of TC.
Default value: 0.0.
- W-5 (I) : IOXBTC(1) Oxidation reaction 1.
 = -1: Zr oxidation by steam, Cathcart model
 = -2: Zr oxidation by steam, Urbanic-Heidrich model
 = -3: Steel oxidation by steam, White model
 = -4: Zr oxidation by O_2 , Benjamin et al. model
 = -5: Graphite oxidation by O_2 , Roes model
 > 0: Oxidation model with user-defined coefficient set, number IOXBTC. The user-defined coefficients are specified in records 8500XX, 8510XX, ..., where XX is the set number (see section 2.14.1).
Acceptable range: $-5 \leq IOXBTC \leq 10$, $IOXBTC \neq 0$. If a positive number is specified, then a user-defined oxidation model must be defined in records 8500XX, 8510XX, ..., with $XX=IOXBTC$.
Default value: none.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-2 (I) : ITFATC Indicator defining how the representative temperature is obtained for the failure calculations.
 =1: use maximum temperature of all TC nodes
 =2: use volume-weighted average temperature
Acceptable range: 1 or 2
Default value: 1
- W-3 (I) : ISFATC Indicator defining which pressures are used for to determine the stress, needed for the failure calculations
 <0: use Control Function number | ISFATC |
 =0: pressure is not used (value is set to 1.0). Stress is constant, and given directly by XSFATC (next word).
 >0: use CV pressure from the CV at the boundary cell ISFATC
Acceptable range: reference to a Control Function or a boundary cell
Default value: 0
- W-4 (R) : XSFATC Ratio of stress and pressure (defined by the word above), (σ/p). For example in case of a tube with the inner diameter D and the thickness t , the relation between the overpressure inside the tube, p , and the stress, σ , (see Figure 2-18):

$$p \cdot D = \sigma \cdot 2t$$

Therefore:

$$\sigma = p \cdot (D/2t)$$

This for this case the ratio is equal to XSFATC = $(D/2t)$.

Acceptable range: XSFATC > 0.0

Default value: none

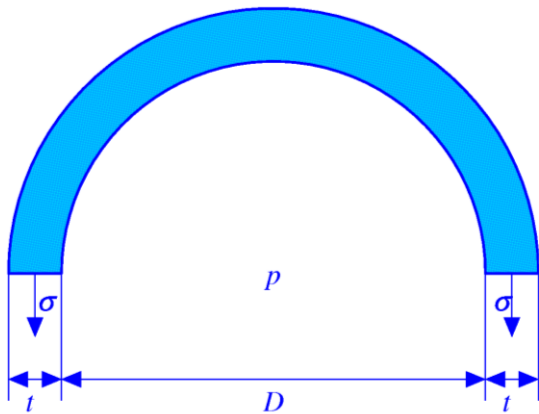


Figure 2-35 Relation between stress and pressure for a tube.

2.4.22 Records: 43Y000, Material Properties Needed for Failure Calculations

Y is the material number, $1 \leq Y \leq 9$. The failure model considers the following three failure mechanisms:

- Ultimate strength failure (failure mode = 1)
- Creep rupture (failure mode = 2)
- Meltdown (failure mode = 3)

Creep rupture is calculated using the method proposed by Larson and Miller [40]. The time to rupture is obtained from the following relation (see Volume 1):

$$\log_{10}(t_r) = \frac{LMP}{T} - C$$

The Larson-Miller parameter, *LMP*, is approximated in SPECTRA by the following correlation:

$$LMP = A - B \cdot \log_{10}(\sigma)$$

The properties for some materials are shown in Table 2-19.

Table 2-19 Failure model data for some frequently used materials

Constants	Material			
	Inconel-600	Steel 304SS	Steel SA106B	Steel SA533B1
<i>A</i>	54,086	58,763	46,129	74,768
<i>B</i>	4,968.5	5,086.4	4,237.9	6,970.9
<i>C</i>	9.44	12.44	9.44	16.44
<i>T_M</i>	1644.0	1671.0	1789.0	1789.0
$\sigma_{U,lowT}$	7.3×10^8	6.4×10^8	5.5×10^8	5.5×10^8
$t_{U,highT}$	634.0	1120.0	515.0	30.0

W-1 (R) : AFATC If a positive number is entered this is the coefficient *A* in the Larson-Miller parameter for creep rupture. If a negative number is entered, then data from Table 2-16 is used. In such case words 2 through 7 are not used. The material identifiers are:
 -1: Inconel-600
 -2: Stainless steel 304SS
 -3: Carbon steel SA106B
 -4: Carbon steel SA533B1
Acceptable range: $10^3 \leq AFATC \leq 10^6$ or $AFATC = -1, -2, -3, -4$
Default value: none

SPECTRA Code Manuals - Volume 2: User's Guide

W-2(R) :	BFATC	Coefficient <i>B</i> in the Larson-Miller parameter for creep rupture. <i>Acceptable range:</i> $10^2 \text{ BFATC} \leq 10^5$ <i>Default value:</i> none
W-3 (R) :	CFATC	Coefficient <i>C</i> in the Larson-Miller parameter for creep rupture. <i>Acceptable range:</i> $1 \leq \text{CFATC} \leq 10^3$ <i>Default value:</i> none
W-4 (R) :	TMFATC	Melting temperature, T_M , (K). <i>Acceptable range:</i> $500 \leq \text{TMFATC} \leq 10,000$ <i>Default value:</i> none
W-6 (R) :	USFATC	Low temperature ultimate strength, $\sigma_{U,lowT}$, (Pa). <i>Acceptable range:</i> $10^6 \leq \text{USFATC} \leq 10^{10}$ <i>Default value:</i> none
W-7 (R) :	TUFATC	High temperature ultimate strength parameter, $t_{U,highT}$, (s). <i>Acceptable range:</i> $1 \leq \text{TUFATC} \leq 10^4$ <i>Default value:</i> none

2.4.23 Record: 490XXX, Axial Conduction and Direct Contact Conduction

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record activates the axial heat transfer process for this 2-D Solid Heat Conductor. The maximum number of axial heat transfer processes is 100 (10 for 1-D Solid Heat Conductors).

The axial heat conduction or direct contact heat transfer between two structures, i (the “current solid heat conductor”, XXX) and j (the “other solid heat conductor”), is considered - Figure 2-36. The heat transfer between the two solid heat conductors is calculated from:

$$Q_{i-j} = A_{i-j} \frac{T_i - T_j}{R_{i-j}}$$

- Q_{i-j} heat transferred between the solid heat conductors i and j , (W)
- A_{i-j} area of contact between the solid heat conductors i and j , (m²)
- T_i temperature of the solid heat conductor i (local or averaged - see Word 2 below), (K)
- T_j temperature of the solid heat conductor j (local or averaged - see Word 2 below), (K)
- R_{i-j} thermal resistance for the axial heat flow between the solid conductors i and j , (m²-K/W)

The thermal resistance for the heat flow is obtained from:

$$R_{i-j} = \frac{L_i}{k_i} + \frac{1}{h_{i-j}} + \frac{L_j}{k_j}$$

- L_i length for axial conduction in the solid heat conductor i (input parameter X1AXTC)
- k_i thermal conductivity in the solid heat conductor i
- L_j length for axial conduction in the solid heat conductor j (input parameter X2AXTC)
- k_j thermal conductivity in the solid heat conductor j
- h_{i-j} heat transfer coefficient at the point of contact of solid heat conductors i and j

- W-1 (I) : J1AXTC First indicator of the other solid heat conductor (j).
 =1: 1-D Solid Heat Conductor (SC)
 =2: 2-D Solid Heat Conductor (TC)
 Acceptable range: 1 or 2
 Default value: none

- W-2 (I) : J2AXTC Second indicator of the other solid heat conductor (j).
 if J1AXTC=1: SC reference number
 if J1AXTC=2: TC reference number
 Acceptable range: must be a valid reference number of SC or TC
 Default value: none

- W-3 (I) : I1AXTC Cell number for axial or direct contact heat conduction through the
 current solid heat conductor, i .

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 1.0

- W-10 (I) : MHAXTC Parameter affecting direct contact conduction:
=1: IHAXTC defines the heat transfer coefficient, $h_{i,j}$ (W/m²-K)
=2: IHAXTC defines the resistance, $1/h_{i,j}$ (m²-K/W)
Acceptable range: 1 or 2
Default value: 1
- W-11 (I) : M1AXTC Pointer to a material number which defines thermal conductivity in the current solid heat conductor. If zero or no value is specified the conductivity of the actual material, defined in the records 410XXX, is used. If a positive value is defined then the thermal conductivity of the material M1AXTC is used. For example, in case of a pebble bed model, the actual material should represent the true material of a pebble, to get a correct surface-to-center temperature difference. M1AXTC should be an artificial material, which is used to define the effective conductivity of the pebble bed, for example from Zehner-Schlunder or Robold correlation (see Volume 3, test PBR-k-eff).
Acceptable range: must be a valid reference number of a solid material, defined in records 801XXX, 802XXX, 803XXX - see section 2.10).
Default value: 0
- W-12 (I) : M2AXTC Pointer to a material number which defines thermal conductivity in the other solid heat conductor. If zero or no value is specified the conductivity of the actual material, defined in the records 410XXX, is used. If a positive value is defined then the thermal conductivity of the material M2AXTC is used. For example, in case of a pebble bed model, the actual material should represent the true material of a pebble, to get a correct surface-to-center temperature difference. M2AXTC should be an artificial material, which is used to define the effective conductivity of the pebble bed, for example from Zehner-Schlunder or Robold correlation (see Volume 3, test PBR-k-eff).
Acceptable range: must be a valid reference number of a solid material, defined in records 801XXX, 802XXX, 803XXX - see section 2.10).
Default value: 0
- W-13 (I) : L1AXTC Option used for the direct contact transfer (I1AXTC > 0 and I2AXTC > 0) in the current solid heat conductor.
=0: Cell-to-cell direct contact. The temperature T_i is taken from the cell I1AXTC. The calculated heat is removed/added to the cell I1AXTC.
=1: Global radial transfer. The temperature T_i is equal to the average temperature of the linked Solid Heat Conductors (mass-averaged or volume-averaged, depending of IAVETC). The calculated heat is distributed over all cells, proportionally to the cell volume or cell mass. The input parameter I1AXTC is used only to determine the area for the heat transfer. This option is intended to model the effective conductivity of the pebble bed or prismatic blocks (see Volume 3, tests PBR-k-eff, PMR-k-eff).
Acceptable range: 0 or 1
Default value: 0

SPECTRA Code Manuals - Volume 2: User's Guide

- W-14 (I) : L2AXTC Option used for the direct contact transfer (I1AXTC > 0 and I2AXTC > 0) in the other solid heat conductor.
=0: Cell-to-cell direct contact. The temperature T_j is taken from the cell I2AXTC. The calculated heat is removed/added to the cell I2AXTC.
=1: Global radial transfer. The temperature T_j is equal to the average temperature of the other solid heat conductor (mass-averaged or volume-averaged, depending of IAVETC). The calculated heat is distributed over all cells, proportionally to the cell volume or cell mass. The input parameter I2AXTC is used only to determine the area for the heat transfer. This option is intended to model the effective conductivity of the pebble bed or prismatic blocks (see Volume 3, tests PBR-k-eff, PMR-k-eff).
Acceptable range: 0 or 1
Default value: 0
- W-15 (R) : AXAXTC Area of heat transfer, (m²). If zero or no value is entered, then the area is calculated as the smaller value of the cell areas (multiplicity included):

$$A_{HT} = \text{MIN} (A_{cell,TC-1} \times A1AXTC , A_{cell,TC-2} \times A2AXTC)$$

If a positive value is entered, then the heat transfer area is equal to the entered value:

$$A_{HT} = AXAXTC$$

Acceptable range: $0.0 \leq AXAXTC \leq 10^{10}$
Default value: 0.0
- W-16 (I) : KAXTC Sequential number of the axial heat transfer process. If no value or zero is entered, then the data are read sequentially - the first record 490XXX in the input file is interpreted as containing the first axial transfer process, the second record with this number the second heat transfer process, etc.
Acceptable range: I = 1, 2, ..., 6
Default value: none

SPECTRA Code Manuals - Volume 2: User's Guide

Examples are shown in Figure 2-36. Further examples and discussion is included in Volume 3.

Figure 2-36 Cases (a) and (c) - cell-to-cell axial heat conduction

```
*
* Rectangular geometry - Case (a)
* - "axial" heat transfer - perpendicular to the normal conduction heat flow
* - conduction length: L = 0.05 m
* - contact h = TF-210
* All cells of TC-220 to all cells of TC-210
* All cells of TC-220 to all cells of TC-230
*      TC   i j L-i L-j   h   A-frac
490220 2 210 0 0 0.05 0.05 210   1.0 * Axial heat transfer to TC-210
490220 2 230 0 0 0.05 0.05 210   1.0 * Axial heat transfer to TC-230
*
* Cylindrical geometry - Case (b)
* - "axial" heat transfer - perpendicular to the normal conduction heat flow
* - conduction length: L = 0.05 m
* - contact h = TF-210
* Cells of level 1 of TC-210 to level 2 of TC-230 and level 1 of TC-230 to level 2 of TC-250
*      TC   i j L-i L-j   h   A-frac
490210 2 230 -1 -2 0.05 0.05 210   1.0 * Axial heat transfer to TC-230
490230 2 250 -1 -2 0.05 0.05 210   1.0 * Axial heat transfer to TC-230
```

Figure 2-36 Cases (b) and (d) - all cells (axial) to one cell (direct contact)

```
* TC-220: heat transfer to TC-210 - Case (b)
* - all cells from TC-220 transfer heat to cell 0101 of TC-210
* - "axial" heat transfer for TC-220, normal conduction heat flow in TC-210
* - axial conduction length: L = 0.05 m for TC-220, L=0.0 m for TC-210
* - contact h = TF-220
*      TC   i j L-i L-j   h   A-frac
490220 2 210 0 0101 0.05 0.0 210   1.0 * Axial heat transfer to TC-220
*
* TC-220: heat transfer to TC-210 - Case (d)
* - level 5 cells from TC-220 transfer heat to cell 0101 of TC-210
* - "axial" heat transfer for TC-220, normal conduction heat flow in TC-210
* - axial conduction length: L = 0.05 m for TC-220, L=0.0 m for TC-210
* - contact h = TF-220
*      TC   i j L-i L-j   h   A-frac
490220 2 210 -5 0101 0.05 0.00 0   1.0 * TC-220 - Axial heat transfer to TC-210

*      HOLE 01: LOWER LEFT, X-CELLS 04-06, Y-CELLS 09-11
*      SC   i j L-i L-j   h   A1-frac   A2-frac
490120 1 122 0409 2 0.0 0.0 0   100.0   0.125
490120 1 122 0509 2 0.0 0.0 0   100.0   0.125
490120 1 122 0609 2 0.0 0.0 0   100.0   0.125
490120 1 122 0410 2 0.0 0.0 0   100.0   0.125
490120 1 122 0610 2 0.0 0.0 0   100.0   0.125
490120 1 122 0411 2 0.0 0.0 0   100.0   0.125
490120 1 122 0511 2 0.0 0.0 0   100.0   0.125
490120 1 122 0611 2 0.0 0.0 0   100.0   0.125
```

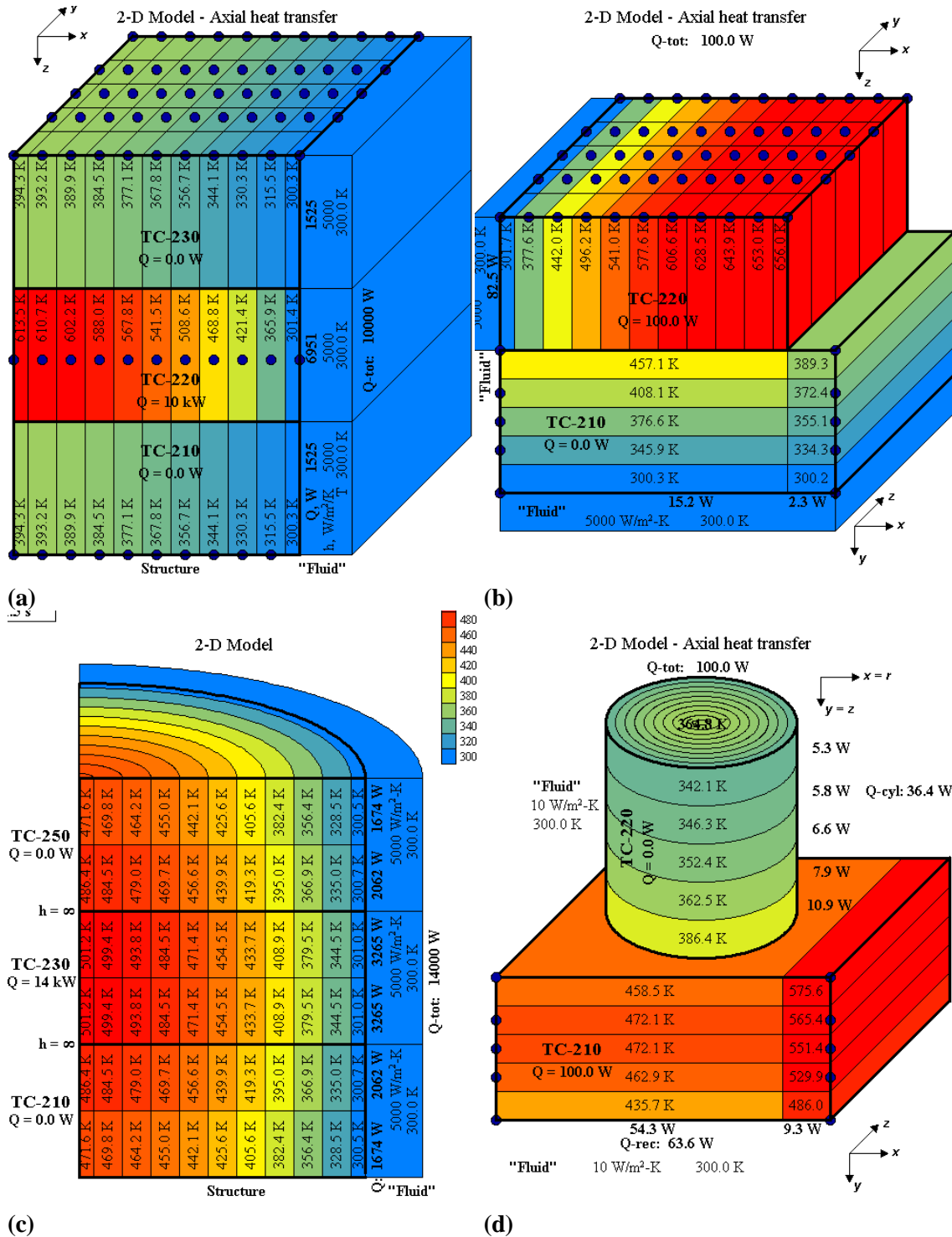


Figure 2-36 Axial conduction, direct contact between different TC

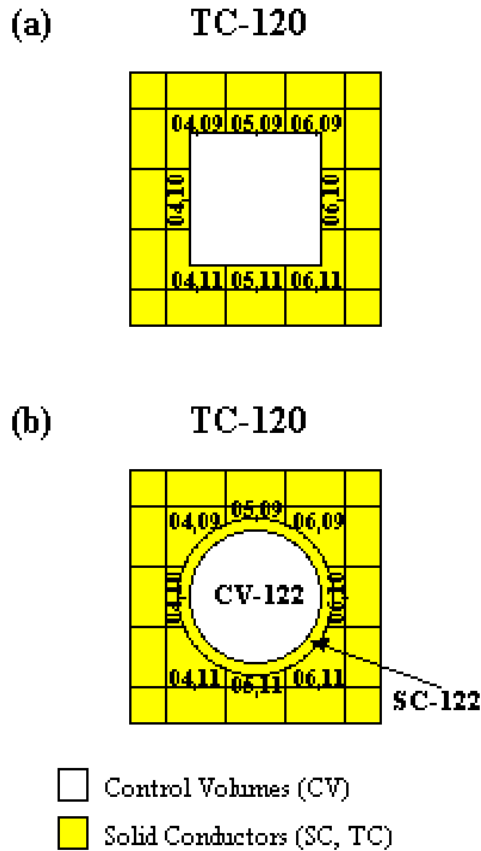


Figure 2-37 Axial conduction, example of TC-SC transfer

2.4.24 Record: 499000, Interpolation Factor for Boundary Temperature

W-1 (R) : FINTTC Interpolation factor. Used only if a boundary surface is linked to a Control Volume (IVLBTC>0) and at the same time the boundary fluid temperature is defined by a Tabular or Control Function (ITPBTC≠0). In such case the value obtained from the Tabular or Control Function is taken with the weighting factor of FINTTC and the temperature in the Control Volume is taken with the weighting factor of 1.0 – FINTTC.
 Acceptable range: $0.0 < FINTTC \leq 1.0$
 Default value: 0.5

2.4.25 Example of the 2-D Solid Heat Conductor Input Data

As an example problem a simple geometry, shown as the Example Problem 2 in Figure 2-32, is considered. The geometry is shown again below, in Figure 2-38.

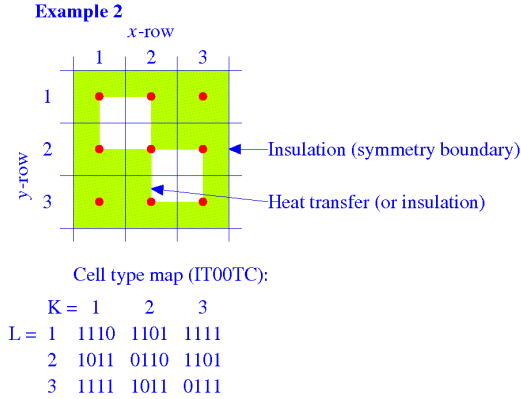


Figure 2-38 Example of 2-D Solid Heat Conductor.

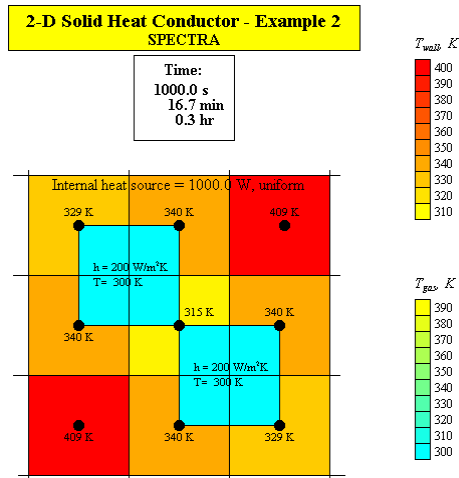


Figure 2-39 Results of the 2-D test case - stationary conditions.

The example consists of a simple structure with insulation (symmetry) at the external boundaries. At the internal boundaries a fixed heat transfer coefficient of $100.0 \text{ W}/(\text{m}^2\text{K})$, and a constant fluid temperature of 300 K is used. The heat transfer coefficient is defined using TF-001, while the fluid temperature is specified using TF-002. The half-cell size is 0.01 m . Therefore the size of the structure is 0.6 m in both x and y direction. The length of the structure (the third, z , dimension) is 1.0 m . There is a uniform internal heat source of $Q=1000.0 \text{ W}$.

The input deck is shown below. Results of this test case, obtained for a stationary state, are shown in Figure 2-39.

*
405100 Steady state with heat source - rectangular, 2-D

SPECTRA Code Manuals - Volume 2: User's Guide

```
400100 1 1.0 0.0 0.0 0 1.0E+3 * Main data : GEO,L,X0,ELEV,VER,POWER (W),
401100 2 * USE ENTERED TEMPERATURES
410100 3 3 * NUMBER OF CELLS
* X-CELL SIZES
* 1 2 3
411100 0.01 0.01 0.01
* Y-CELL SIZES
* 1 2 3
412100 0.01 0.01 0.01
*
* TC MAP
* 1 2 3
413100 1 1110 1101 1111
413100 2 1011 0110 1101
413100 3 1111 1011 0111
*
* TC CELL MATERIAL
* 1 2 3
414100 1 1 1 1
414100 2 1 1 1
414100 3 1 1 1
*
* TC CELL POWER
* 1 2 3
415100 1 1.0 1.0 1.0
415100 2 1.0 1.0 1.0
415100 3 1.0 1.0 1.0
*
* TC CELL TEMPERATURES
* 1 2 3
416100 1 300. 300. 300.
416100 2 300. 300. 300.
416100 3 300. 300. 300.
*
* BOUNDARY CONDITIONS
* K L X Y CV HTC T
420100 1 1 0 0 000 001 002 *
420100 1 2 0 0 000 001 002 *
420100 2 1 0 0 000 001 002 *
420100 2 2 0 0 000 001 002 *
420100 2 3 0 0 000 001 002 *
420100 3 2 0 0 000 001 002 *
420100 3 3 0 0 000 001 002 *
*
* ===== Tabular Functions
*
* TF-001 - constant htc of 200 W/m/K
*
* time htc
600001 0.0 200.0
*
* TF-002 - constant temperature of 300 K
*
* time temp
600002 0.0 300.0
*
```

2.5 MCCI Input Data

2.5.1 Records: 440000, MCCI Main Data

The MCCI model may be activated with this record and the main MCCI data defined. Note that MCCI is always using a cell network of 2-D Solid Heat Conductor. Therefore it must be defined in the input. If more than one TC is defined, the first one is used for MCCI. The TC must be a vertical cylinder.

- W-1 (I) : IMMCTC MCCI model activator:
 = 0 : not active,
 = 1 : active, liquid flow calculated from Navier-Stokes equation
 = 2 : active, simplified calculation
Acceptable range: 0, 1, 2
Default value: 0
- W-2 (I) : ICTPTC Concrete type:
 = 0 : user-defined,
 = 1 : Basaltic aggregate concrete [35],
 = 2 : Limestone common sand 1 [57],
 = 3 : Limestone common sand 2 [35] ,
 = 4 : Siliceous 1 [57],
 = 5 : Siliceous 2 [35],
Acceptable range: 0, 1, 2, 3, 4, 5
Default value: 0
- W-3 (I) : ITSCTC Reference to a Tabular Function defining the solidus line, i.e. the solidus temperature versus concrete weight fraction in a UO₂-concrete mixture. Data for several concrete types, obtained from [58], is shown in Figure 2-40. The figure was digitized and the appropriate data files are available in the folder with SPECTRA inputs (input file: Z-INPUTS\TC\MCCI\Model\TLIQSOL).
Acceptable range: must be a reference to a valid Tabular Function
Default value: none
- W-4 (I) : ITLCTC Reference to a Tabular Function defining the liquidus line, i.e. the liquidus temperature versus concrete weight fraction in a UO₂-concrete mixture.
Acceptable range: must be a reference to a valid Tabular Function
Default value: none
- W-5 (I) : ICCMTC Material number of concrete.
Acceptable range: must be a reference to a valid material defined in the MP Package
Default value: none
- W-6 (I) : ICMMTC Material number of corium.
Acceptable range: must be a reference to a valid material defined in the MP Package
Default value: none

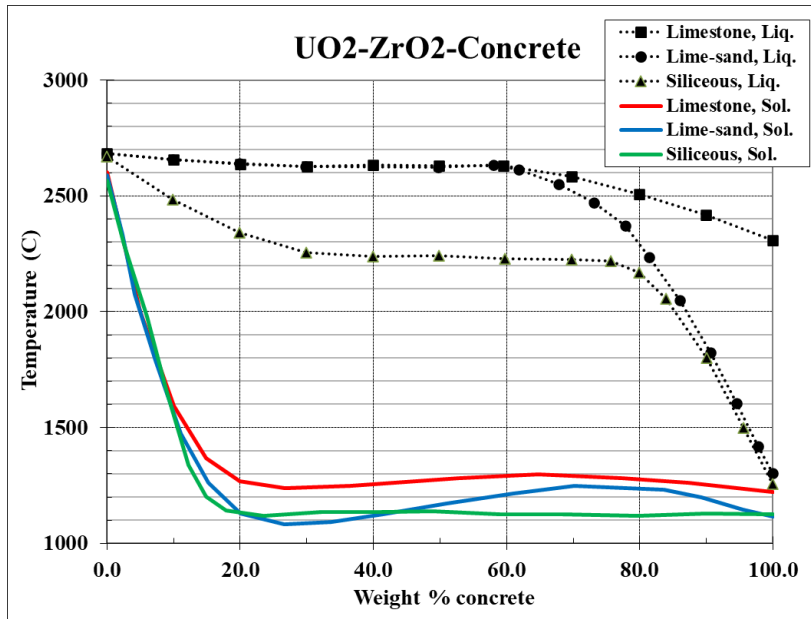


Figure 2-40 Solidus and liquidus temperature for corium/concrete mixtures [58] (digitized)

- W-7 (R) : ZRCMTC Oxidic corium composition. Oxidic corium is assumed to be composed of UO₂ and ZrO₂. ZRCMTC is the molar (volume) fraction of ZrO₂ in corium.
Acceptable range: 0.0 ≤ ZRCMTC ≤ 1.0
Default value: 0.385 [58]
 (a small number <10⁻⁵⁰, sets the value to 0.0)
- W-8 (R) : XMETTC Mass of metallic material related to the mass of oxidic corium. This is the total mass of metals: Fe, Cr, Ni, and unoxidized Zr, divided by the total mass of UO₂ +ZrO₂.
Acceptable range: 0.0 ≤ XMETTC ≤ 1.0
Default value: 0.2
 (a small number <10⁻⁵⁰, sets the value to 0.0)
- W-9 (R) : XMFETC Mass fraction of Fe in the metallic material.
Acceptable range: 0.0 ≤ XMFETC ≤ 1.0
Default value: 0.74
 (a small number <10⁻⁵⁰, sets the value to 0.0)
- W-10 (R) : XMCRTC Mass fraction of Cr in the metallic material.
Acceptable range: 0.0 ≤ XMCRTC ≤ 1.0
Default value: 0.18
 (a small number <10⁻⁵⁰, sets the value to 0.0)

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 837.3 for X=1 [59], 1.0 for X=2 and 3

W-3 (R) : TCLMTC Thermal conductivity of liquid material X, (W/m-K). For UO₂ and ZrO₂ a temperature-dependent correlation from [60] is used, with TCLMTC being a user-defined multiplier:

$$\begin{aligned} \text{UO}_2: & \quad k = 1.64 + 4.74 \times 10^{-2} \times T \times \exp(-1.45 \times 10^4/T) \times \text{TCLMTC} \\ \text{ZrO}_2: & \quad k = 2.11 + 4.46 \times T \times \exp(-2.75 \times 10^4/T) \times \text{TCLMTC} \end{aligned}$$

Acceptable range: $0.01 \leq \text{TCLMTC} \leq 1000.0$

Default value: 1.1 for X=1 [58], 1.0 for X=2 and 3

W-4 (R) : VSLMTC Dynamic viscosity of liquid material X, (kg/m-s). For UO₂ and ZrO₂ a temperature-dependent correlation from [59] is used, with VSLMTC being a user-defined multiplier:

$$\begin{aligned} \text{UO}_2: & \quad \mu = 0.52 \times \exp(8.26 \times 10^3/T) \times \text{VSLMTC} \\ \text{ZrO}_2: & \quad \mu = 0.32 \times \exp(8.79 \times 10^3/T) \times \text{VSLMTC} \end{aligned}$$

Acceptable range: $0.01 \leq \text{VSLMTC} \leq 1000.0$

Default value: 0.3 for X=1 [58], 1.0 for X=2 and=3

for X = 2 and 3 (UO₂ and ZrO₂):

W-5 (R) : HFUSTC Heat of fusion, (J/kg).
Acceptable range: $0.0 < \text{HFUSTC} \leq 1.0 \times 10^7$
Default value: 2.18×10^5 for X = 2, 2.60×10^5 for X = 3 [60]

W-6 (R) : TLIQTC Melting temperature, (K). The value must be consistent with the value defined in the function ITLCTC.
Acceptable range: $1000.0 \leq \text{TLIQTC} \leq 9000.0$
Default value: 3113 for X = 2, 2990 for X = 3 [60]

for X = 1 (concrete):

W-5 (R) : HABLTC Ablation enthalpy, (J/kg).
Acceptable range: $0.0 < \text{HABLTC} \leq 1.0 \times 10^7$
Default value: defined for the built-in concrete types (ICTPTC>0)

W-6 (R) : TLIQTC Liquidus temperature, (K). The value must be consistent with the value defined in the function ITSCTC.
Acceptable range: $1000.0 \leq \text{TLIQTC} \leq 9000.0$
Default value: defined for the built-in concrete types (ICTPTC>0)

W-7 (R) : TSOLTC Solidus temperature, (K). The value must be consistent with the value defined in the function ITLCTC.
Acceptable range: $400.0 \leq \text{TSOLTC} \leq 5000.0$
Default value: defined for the built-in concrete types (ICTPTC>0)

SPECTRA Code Manuals - Volume 2: User's Guide

- W-8 (R) : TABLTC Ablation temperature, (K).
Acceptable range: $400.0 \leq \text{TABLTC} \leq 5000.0$
Default value: defined for the built-in concrete types (ICTPTC>0)
- W-9 (R) : RABLTC Ablation temperature ratio, $\text{RABLTC} = (T_{abl}-T_{sol})/(T_{liq}-T_{sol})$. Default value should be used. The input is intended for eventual sensitivity calculations.
Acceptable range: $0.0 \leq \text{RABLTC} \leq 1.0$
Default value: $\text{RABLTC} = (T_{abl}-T_{sol})/(T_{liq}-T_{sol})$

Properties from several sources: [58], [59], [60], are presented in Table 2-20. In some cases different values were given in different references. In those cases the default values were taken from [60]. The user may wish to perform a sensitivity calculation using the alternative sources shown in the table (or other sources). Further discussion on the liquid properties is provided in Volume 1.

Table 2-20 Properties of relevant materials in liquid state

	Concrete	UO₂	ZrO₂	Reference
ρ (kg/m ³)	2200 2306	8860 10960	5150 5600	[58], sec. 3.5, p.33 [59], MP-RM
C_p (J/kg-K)	837.3	503.0	544.3	[59], MP-RM
k (W/m-K)	1.10	3.05	2.49	[58], sec. 3.5, p.35
μ (kg/m-s)	0.3 (LCS) 1.5 (L)	-	-	[58], sec. 3.5, p.33 [58], sec. 3.5, p.33
H (J/kg)	-	2.74E5 2.18E5	7.07E5 2.60E5	[59], MP-RM [60]
T_m (K)	-	3113 3200	2990 3000	[59], MP-RM [60]

2.5.3 Records: 4402XX, Concrete Composition

The concrete composition is defined with this record. XX is the substance number, $\text{XX} \leq 15$.

- W-1 (R) : CCOMTC Mass fraction of substance XX - see Table 2-21 for substance numbers.
Acceptable range: $0.0 \leq \text{CCOMTC} \leq 1.0$
Default value: defined for the built-in concrete types (ICTPTC>0)

The concrete composition as well as the main properties for the built-in concrete types are shown in Table 2-21.

Table 2-21 Built-in concrete composition and properties.

NO.	Substance	Concrete composition, mass fractions (%)				
		Basaltic aggregate	Limestone c. sand 1	Limestone c. sand 2	Siliceous 1	Siliceous 2
1	CO ₂	1.5	30.46	21.15	10.0	0
2	H ₂ O	5.68	4.46	4.7	3.78	4.0
3	K ₂ O	5.39	0.56	1.22	0.83	0
4	Na ₂ O	1.8	0.32	0.08	0.68	0
5	TiO ₂	1.05	0.14	0.18	0.16	0
6	SiO ₂	54.84	22.0	35.806	61.34	65.0
7	CaO	8.82	26.4	31.3	17.2	0
8	MgO	6.16	11.7	0.48	0.87	0
9	Al ₂ O ₃	6.32	2.54	3.6	3.61	20.0
10	Fe ₂ O ₃	6.26	1.42	1.44	1.53	0
11	Cr ₂ O ₃	0	0	0.014	0	0
12	CaCO ₃	0	0	0	0	3.0
13	Ca(OH) ₂	0	0	0	0	8.0
14	MnO	0	0	0.03	0	0
15	SO ₃	0	0	0	0	0
T(solidus) (K)		1350	1392	1420	1403	1350
T(liquidus) (K)		1650	1568	1670	1523	1650
T(ablation) (K)		1450	1500	1500	1450	1450
density ρ (kg/m ³)		2340	2340	2340	2340	2400
Abl. enth. ΔH (J/kg)		2.8×10 ⁶	2.4×10 ⁶	2.4×10 ⁶	1.95×10 ⁶	1.95×10 ⁶
X(ablation)		0.333	0.614	0.320	0.392	0.333
Source		[59] (CAV-UG)	[57]	[59] (CAV-UG)	[57]	[59] (CAV-UG)

2.5.4 Records: 440300, Model Coefficients

W-1 (R) : CRAMTC Coefficient in Ramacciotti correlation [61] for two-phase viscosity:

$$\mu_2 = \mu_1 \exp(2.5 \times \text{CRAMTC} \times \phi)$$

If a negative value is entered, then Kunitz correlation is used (Figure 2-41):

$$\mu_2 = \mu_1 (1 + 0.5 \times \phi) / (1 + \phi)^4$$

Here μ_1 is the liquid viscosity, μ_2 is the two-phase viscosity and ϕ is the solid fraction in the mixture.

Acceptable range: $0.1 \leq \text{CRAMTC} \leq 10.0$ or < 0.0
(note: [59] recommends 4.0 - 8.0)

Default value: 4.0

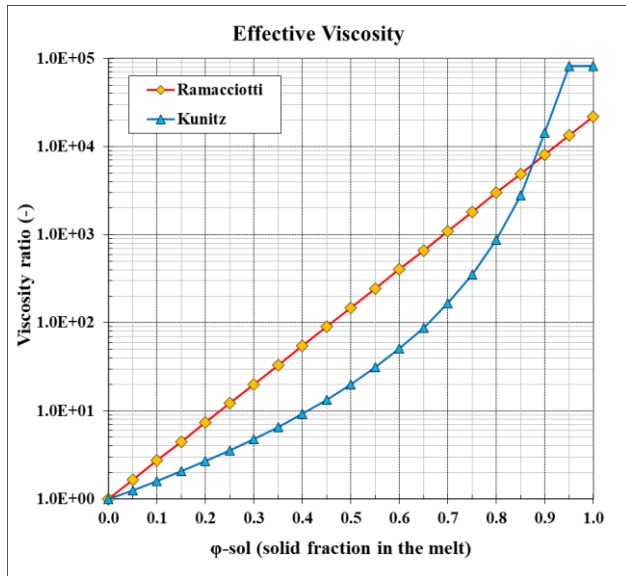


Figure 2-41 Comparison of Ramacciotti and Kunitz correlations.

- W-2 (R) : XRAPTC Radial erosion parameter. Fraction of ablated concrete that is removed from a cell (replaced by corium) in a time step. If the entered value is smaller than the minimum set by mass balance, which is equal to the ratio of degassed mass to the ablated mass ($XRAPTC = V_{deg}/V_{abl}$), the latter will be used. A large value may be used to speed up removal of ablated concrete from a cell.
Acceptable range: $0.0 \leq XRAPTC \leq 0.9$
Default value: 0.0
- W-3 (R) : XZAPTC Axial erosion parameter. Fraction of ablated concrete that is removed from a cell (replaced by corium) in a time step. If the entered value is smaller than the minimum set by the mass balance, which gives the value equal to the ratio of degassed mass to the ablated mass ($XZAPTC = V_{deg}/V_{abl}$), the latter will be used. A large value may be used to speed up removal of ablated concrete from a cell.
Acceptable range: $0.0 \leq XZAPTC \leq 0.9$
Default value: 0.0
- W-4 (R) : XDISTC Maximum dissolution of ablated concrete in corium. If zero or no value is entered, the value is calculated from the ratio of degassed mass and the ablated mass as follows: $XDISTC = 1 - V_{deg}/V_{abl}$.
Acceptable range: $0.1 \leq XDISTC \leq 0.9$ or $XDISTC = 0.0$
Default value: $1.0 - V_{deg}/V_{abl}$
- W-5 (R) : IDEPTC Indicator for corium depression calculation in simplified model (IMMCTC=2).
 =1: depression not calculated
 =2: depression calculated
Acceptable range: 1 or 2
Default value: 2

W-6 (R) : IRSQTC Indicator for reaction sequence.
 =1: all reactions proceed simultaneously
 >1: reactions proceed in a sequence, following [58]: "Zr is oxidized first, and Si, Cr, and Fe follow". The relative strength of reaction is proportional to 10^X , where $X = 1 - \text{IRSQTC}$. The sequential effect becomes stronger with increasing value of IRSQTC.
 Acceptable range: 1, 2, 3, 4
 Default value: 3

2.5.5 Records: 441001, Initial Velocities, Horizontal (Radial) Direction

The initial velocities in molten cells or partially molten cells are defined with this record. The values are used only if IMMCTC=1.

W-1 (I) : L Row number in y (axial) direction. The following data must specify NCLXTC-1 velocities in the y-row number L.
 Acceptable range: $1 \leq L \leq \text{NCLYTC}$
 Default value: none

W-2 (R) : VELXTC Initial velocity (m/s), cell (1,L)
 (1,L) Acceptable range: $-100.0 \leq \text{VELXTC} \leq 100.0$
 Default value: 0.0

W-3 (R) : VELXTC Initial velocity (m/s), cell (2,L)
 (2,L) Acceptable range: $-100.0 \leq \text{VELXTC} \leq 100.0$
 Default value: 0.0

... , etc. until velocities are defined for all cells (NCLXTC-1 velocities should be entered).

2.5.6 Records: 441002, Initial Velocities, Vertical (Axial) Direction

The initial velocities in molten cells or partially molten cells are defined with this record. The values are used only if IMMCTC=1.

W-1 (I) : L Row number. The following data must specify NCLXTC velocities in the y-row number L.
 Acceptable range: $1 \leq L \leq \text{NCLYTC} - 1$
 Default value: none

W-2 (R) : VELYTC Initial velocity (m/s), cell (1,L)
 (1,L) Acceptable range: $-100.0 \leq \text{VELYTC} \leq 100.0$
 Default value: 0.0

W-3 (R) : VELYTC Initial velocity (m/s), cell (2,L)
 (2,L) Acceptable range: $-100.0 \leq \text{VELYTC} \leq 100.0$
 Default value: 0.0

... , etc. until velocities are defined for all cells (NCLXTC-1 velocities should be entered).

2.5.7 Records: 441003, Initial Porosities

The initial porosities are defined with this record.

- W-1 (I) : L Row number. The following data must specify NCLXTC porosities in the y-row number L.
Acceptable range: $1 \leq L \leq \text{NCLYTC}$
Default value: none
- W-2 (R) : POROTC Initial porosity (-), cell (1,L)
(1,L) *Acceptable range:* $0.0 \leq \text{POROTC} \leq 1.0$
Default value: 0.0
- W-3 (R) : POROTC Initial porosity (-), cell (2,L)
(2,L) *Acceptable range:* $0.0 \leq \text{POROTC} \leq 1.0$
Default value: 0.0

... , etc. until porosities are defined for all cells (NCLXTC porosities should be entered).

2.5.8 Records: 441004, Initial Concrete Fractions

The initial concrete fractions are typically defined by the code using the cell material data and the input parameter ICCMTC (record 440000), as follows:

- XCONTC = 1.0 if the material number in the cell is equal to ICCMTC
- XCONTC = 0.0 otherwise

It is possible to define different initial conditions using this record.

- W-1 (I) : L Row number. The following data must specify NCLXTC fractions in the y-row number L.
Acceptable range: $1 \leq L \leq \text{NCLYTC}$
Default value: none
- W-2 (R) : XCONTC Initial concrete fraction (-), cell (1,L)
(1,L) *Acceptable range:* $0.0 \leq \text{XCONTC} \leq 1.0$
Default value: 1.0 if the cell material = ICCMTC, 0.0 otherwise
- W-3 (R) : XCONTC Initial concrete fraction (-), cell (2,L)
(2,L) *Acceptable range:* $0.0 \leq \text{XCONTC} \leq 1.0$
Default value: 1.0 if the cell material = ICCMTC, 0.0 otherwise

... , etc. until concrete fractions are defined for all cells (NCLXTC fractions should be entered).

2.5.9 Records: 441005, Initial Ablated Concrete Fractions

The initial ablated concrete fractions are typically set as zero. It is possible to define different initial ablated fractions using this record.

W-1 (I) : L Row number. The following data must specify NCLXTC fractions in the y-row number L.
Acceptable range: $1 \leq L \leq \text{NCLXTC}$
Default value: none

W-2 (R) : XABLTC Initial ablated concrete fraction (-), cell (1,L)
 (1,L) *Acceptable range:* $0.0 \leq \text{XCONTC} \leq 1.0$
 Default value: 1.0 if the cell material = ICCMTC, 0.0 otherwise

W-3 (R) : XABLTC Initial ablated concrete fraction (-), cell (2,L)
 (2,L) *Acceptable range:* $0.0 \leq \text{XCONTC} \leq 1.0$
 Default value: 1.0 if the cell material = ICCMTC, 0.0 otherwise

. . . , etc. until concrete fractions are defined for all cells (NCLXTC porosities should be entered).

2.6 Thermal Radiation Input Data

2.6.1 Records: 500Y00, Thermal Radiation Model Selection

Y = 1, ..., 9, is the radiating system number. Up to 9 systems are allowed. The numbering must be consecutive. Each system may consist of up to 90 radiating surfaces. Surfaces radiate among each other within each system. There is no direct radiation between surfaces belonging to different radiating systems.

W-1 (I) : MODRAD Radiation model. MODRAD = 1 - radiation in grey enclosure with non-absorbing/non-emitting gas. MODRAD = 2 - radiation in grey enclosure with absorbing/emitting gas. The radiation model is used only if the number of radiating surfaces, entered on the records 510YXX, is greater than 1. Application of the thermal radiation model often involves significant effort, needed to prepare the view factor and beam length data. For cases when thermal radiation is less important, a simple wall-gas radiation model is available for Solid Heat Conductors (see sections 1.3.6, 1.3.7).

Acceptable range: 1, 2

Default value: 2

W-2 (I) : IWTRAD Selector of option for radiating surfaces covered by water.
= 1: do not radiate to water. Stop calculations if more than 10% of any radiating surface is covered by water.
= 2: the water-covered part of the surface radiates to the water pool. The global energy remains conserved. The thermal radiation is completely deactivated if more than 50% of all surfaces is covered with water.
= 3: the water-covered part does not radiate. The global energy is, in general, not conserved (with this option the global energy is conserved only if the water-covered fraction is the same for all radiating surfaces). The thermal radiation is completely deactivated if more than 50% of all surfaces is covered with water.

Acceptable range: 1, 2, 3

Default value: 2

W-3 (R) : XWTRAD Minimum fraction of fluid volume occupied by water to switch off the thermal radiation model. Used only for RADMOD =2 (enclosure with participating gas). If the water level in a volume representing an enclosure is higher than XWTRAD times the volume height, the thermal radiation model is switched off for this particular enclosure.

Acceptable range: $0.1 \leq XWTRAD \leq 1.0$

Default value: 0.9

2.6.2 Records: 505Y00, Radiating System Name

Y = 1, ..., 9, is the radiating system number.

W-1 (A) : NAMETR User defined name of the radiating system Y, length up to 50 characters. The name is read as a 50-character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.
Acceptable range: any string of up to 50 characters.
Default value: 50 "underline" characters: "_".

2.6.3 Records: 510YXX, Radiating Surface Data

Y = 1, ..., 9, is the radiating system number. The numbering of radiating systems must be consecutive. XX is the reference number of a radiating surface. XX need not be consecutive. The maximum number of radiating surfaces in each radiating system is 90.

Data on those records associate radiating surfaces with the surfaces of 1-D or 2-D Solid Heat Conductors.

W-1 (I) : ISCRAD Number of 1-D Solid Heat Conductor (if ITCRAD=0, see Word 4 below), or a 2-D Solid Heat Conductor (if ITCRAD>0) for the surface XXX. If ITCRAD=0, then ISCRAD < 0 indicates the left surface of the 1-D Solid Conductor | ISCRAD |, while ISCRAD > 0 indicates the right surface of Solid Conductor number ISCRAD as the radiating surface XXX. If ITCRAD>0, then ITCRAD indicates the boundary cell number of the 2-D Solid Heat Conductor ISCRAD, as the radiating surface XXX. When ITCRAD=0, ISCRAD < 0, then the left boundary heat flux for the 1-D Solid Conductor | ISCRAD | cannot be specified using Tabular or Control Functions; IQRLSC must be equal to zero (see section 2.3.11). When ITCRAD=0, ISCRAD > 0, then the right boundary heat flux for the 1-D Solid Conductor ISCRAD cannot be specified using Tabular or Control Functions; IQRRSC must be equal to zero (see section 2.3.12). When ITCRAD>0, then the heat flux for the cell number ITCRAD of the 2-D Solid Conductor ISCRAD cannot be specified using Tabular or Control Functions; IQRBTC must be equal to zero (see section 2.4.13).

Only one radiating surface may be associated with a given SC or TC surface. Both left and right surfaces of a SC can be associated with radiating surfaces, belonging to the same or to different radiating systems. Multiple boundary cell surfaces of a TC can be associated with radiating surfaces, belonging to the same or to different radiating systems.

Acceptable range: must be a valid reference number of a 1-D or a 2-D Solid Heat Conductor.

Default value: none.

W-2 (I) : IESRAD Pointer to a Tabular Function or a Control Function that defines the surface emissivity. If the number is positive then the emissivity of the

surface XXX will be calculated using the Tabular Function IESRAD. The argument for the Tabular Function IESRAD will always be the surface temperature. The emissivity will therefore not be equal to the value of the Tabular Function itself, because Tabular Function values are always printed as functions of time. If the number is negative then the emissivity will be defined by the value of Control Function |IESRAD|. If the value obtained from Tabular Function or Control Function is smaller than 10^{-5} , then it will be set to 10^{-5} . If it is larger than 1.0 it will be set to 1.0. If no value is entered, or the entered value is equal to zero, then the emissivity is set to 1.0 (black surface).

Acceptable range: must be a valid reference number of a Tabular or a Control Function.

Default value: 0.

W-3 (I) : IPLRAD Activates pool radiation option for this surface (only for 1-D Conductors)

If IPLRAD = 0 then the pool option is deactivated. In this case the treatment of radiating surface is defined by IWTRAD (Word 2 in record 500Y00).

If IPLRAD > 0 then the pool in the Control Volume adjacent to the surface will participate in radiation heat transfer. When IPLRAD > 0 then the surface XXX is considered as a "floor", that can be covered by water. The following conditions must be met to use the pool radiation option:

- The elevation of the surface must be equal to the bottom elevation of the corresponding Control Volume: $IVLLSC(|ISCRAD|)$ if $ISCRAD < 0$, or $IVLRSC(ISCRAD)$ if $ISCRAD > 0$.

- The geometry must be rectangular: $IGEOSC(|ISCRAD|) = 1$.

- The surface must be horizontal: $IVERSC(|ISCRAD|) = \pm 1$.

- The surface area must be the same as the bottom (segment number 1) cross section area of the corresponding Control Volume:

$ASEGCV(1,IV) = SIZEVC(|ISCRAD|)$, where IV is the Control Volume number: $IVLLSC(|ISCRAD|)$ or $IVLRSC(ISCRAD)$, depending on the sign of ISCRAD.

If the above conditions are met then the radiative heat exchange for this surface is calculated as follows:

- If the pool liquid level exceeds the surface elevation by more than $\Delta Z = 10^{-3}$ m, then the surface temperature is set to the pool temperature, the emissivity is set to the liquid water emissivity (0.96 - [14], page 15-23):

$$T = T_{POOL},$$

$$\varepsilon = 0.96.$$

where T_{POOL} is the pool temperature. The calculated radiant heat flux is deposited in the pool.

- If the pool level is below 10^{-3} m, temperature and emissivity is linearly interpolated between the pool values and the radiation surface values:

$$T = T_{POOL} \Delta Z / 10^{-3} + T_{SC} (10^{-3} - \Delta Z) / 10^{-3}$$

$$\varepsilon = 0.96 \Delta Z / 10^{-3} + \varepsilon_{SC} (10^{-3} - \Delta Z) / 10^{-3}$$

where: T_{SC} is the surface temperature equal to the left or right temperature of the Solid Conductor |ISCRAD|, and ε_{SC} is the emissivity obtained from the Tabular Function or the Control Function

|IESRAD|. The obtained heat flux is partitioned between pool and Solid Conductor:

$$Q_{POOL} = Q_{TOT} \Delta Z / 10^{-3}, \quad Q_{SC} = Q_{TOT} (10^{-3} - \Delta Z) / 10^{-3}.$$

where Q_{POOL} is heat deposited in the water pool, Q_{SC} is the heat deposited at the surface of the Solid Conductor |ISCRAD|, and Q_{TOT} is the total heat flux calculated for this surface by the radiation heat exchange model.

The surface area of the pool is assumed to be always equal to the area of the surface XXX. This may not be true if Control Volume consists of several segments with different cross section areas. In that case calculations will still be performed but a warning message will be issued. It is recommended to use a single-segment Control Volume in case the pool radiation option is activated.

Acceptable range: the pool option is available only for 1-D Solid Heat Conductors.

Default value: 0.

W-4 (I) : ITCRAD Boundary cell number of the 2-D Solid Heat Conductor (defined by ISCRAD - Word 1 above) associated with this radiating surface. Used only if a 2-D Solid Heat Conductor should be associated with this surface. If a 1-D Solid Heat Conductor should be associated with this surface, then the number must be zero.

Acceptable range: must be a valid boundary cell number if non-zero.

Default value: 0.

2.6.4 Records: 520YXX, View Factors

Y = 1, ..., 9, is the radiating system number. The numbering of radiating systems must be consecutive. XX is the reference number of a radiating surface. XX need not be consecutive. The maximum number of radiating surfaces in each radiating system is 90.

The data on records 520YXX give view factors from the surface XX to all other surfaces belonging to the system Y. Several records with the same number may be entered. The data is read sequentially.

W-1 (R) : VFCRAD View factor from the surface YXX to the surface Y01, $F_{YXX \rightarrow Y01}$. This is the fraction of the total power emitted by the surface YXX that reaches the surface Y01.

Acceptable range: $0.0 \leq VFCRAD \leq 1.0$.

Default value: none.

W-2 (R) : VFCRAD View factor from the surface YXX to the surface Y02, $F_{YXX \rightarrow Y02}$. The II-th word on the record gives the view factor from the surface YXX to the surface YII. NSFRAD numbers must be entered. Several records with the same number may be used. The records are read sequentially in the order they appear in the input deck.

Acceptable range: $0.0 \leq VFCRAD \leq 1.0$.

Default value: none.

... VFCRAD until NSFRAD(Y) numbers are entered.

Conservation of energy in a system of radiating surfaces depends on the fact whether the reciprocity relation and closure relation is fulfilled with good accuracy. The reciprocity relation is:

$$A_i F_{i \rightarrow j} = A_j F_{j \rightarrow i}$$

where A_i is the surface area, m^2 , of the i -th radiating surface. The closure relation is:

$$\sum_{j=1}^N F_{i \rightarrow j} = 1.0$$

where N is the total number of radiating surfaces within a given radiating system, NSFRAD(Y). The program checks if those relations are fulfilled with an accuracy of at least 8 decimal places. Therefore view factors must be carefully evaluated before the radiation model can be activated.

2.6.5 Records: 530YXX, Beam Lengths

$Y = 1, \dots, 9$, is the radiating system number. The numbering of radiating systems must be consecutive. XX is the reference number of a radiating surface. XX need not be consecutive. The maximum number of radiating surfaces in each radiating system is 90.

The data on records 530YXX give average beam lengths between the surface XX and all other surfaces belonging to the system Y. Several records with the same number may be entered. The data is read sequentially.

- W-1 (R) : XBLRAD Average beam length between the surface YXX and the surface Y01, $L_{YXX \rightarrow Y01}$. This number is used to determine the gas emissivity and absorptivity on the path between surface YXX and Y01.
Acceptable range: XBLRAD = 0.0, if the corresponding view factor, VFCRAD, is equal to zero;
 $10^{-10} \leq XBLRAD \leq 10^{10}$, if the corresponding view factor, VFCRAD, is positive.
Default value: none.
- W-2 (R) : XBLRAD Average beam length between the surface YXX and the surface Y02, $L_{YXX \rightarrow Y02}$. The II-th word on the record gives the beam length between the surface YXX and the surface YII. NSFRAD numbers must be entered. Several records with the same number may be used. The records are read sequentially in the order they appear in the input deck.
Acceptable range: XBLRAD = 0.0, if the corresponding view factor, VFCRAD, is equal to zero;
 $10^{-10} \leq XBLRAD \leq 10^{10}$, if the corresponding view factor, VFCRAD, is positive.
Default value: none.
- ... XBLRAD until NSFRAD numbers are entered.

2.6.6 Records: 531YXX, Beam Lengths for Multiple CV Paths

Y = 1, ..., 9, is the radiating system number. The numbering of radiating systems must be consecutive. XX is the reference number of a radiating surface. XX need not be consecutive. The maximum number of radiating surfaces in each radiating system is 90.

The data on records 531YXX give average beam lengths for cases when beam passes through several Control Volumes. If a set of volumes is specified for radiation path between surfaces *i* and *j*, then exactly the same set of volumes must be supplied for the path between surfaces *j* and *i*. In fact it is better to specify data for one direction only (for example *i* → *j*). In such case the code will assume the same volumes and beam length for the "return" path (*j* → *i*). If the beam length on the path *i* → *j* are different then the lengths on the path *j* → *i*, then a warning message is printed but such input is accepted for calculations. It may be used if gas emissivity is close to 1.0 and all radiation is absorbed on the in the vicinity of the radiating surface.

W-1 (I) : JJ Surface number. The following entries define beam lengths on the path between surface YXX and YJJ.
Acceptable range: JJ must be a valid surface number in the system Y.
Default value: none.

W-2 (I) : ICV(1) Control Volume number.
Acceptable range: ICV(1) must be a valid Control Volume number.
Default value: none.

W-3 (R) : YBLRAD(1) Average beam length in the Control Volume ICV(1).
Acceptable range: YBLRAD(1) > 0.0, Sum of all values of YBLRAD(i) must be the same as the total beam length, XBLRAD, entered in the record 530YXX.
Default value: none.

W-4 (I) : ICV(2) Control Volume number.
Acceptable range: ICV(2) must be a valid Control Volume number.
Default value: none.

W-5 (R) : YBLRAD(2) Average beam length in the Control Volume ICV(2).
Acceptable range: YBLRAD(2) > 0.0, Sum of all values of YBLRAD(i) must be the same as the total beam length, XBLRAD, entered in the record 530YXX.
Default value: none.

... until all beam lengths are defined. The maximum number of Control Volumes on a single radiation beam path is 10.

2.6.7 Records: 5400XX, Radiation Properties of Gases

XX = 01, 02, ... , NGAS is the ID number of the gas. The number of gases is the same as in the gas property main data base. The following built-in gases are built-in:

1 = H₂, 2 = He, 3 = H₂O, 4 = N₂, 5 = O₂, 6 = CO₂

SPECTRA Code Manuals - Volume 2: User's Guide

The radiation properties of gases are defined in this record. The same radiation properties of gases are used for all radiating systems. This record is optional. All entries from this record have their default values, recommended for general application.

W-1 (R) : EMSMAX Gas emissivity at infinite path length, ε_{∞} . This number is also used as a selector of the gas emissivity correlation. If the value is: $0.0 < \text{EMSMAX} \leq 1.0$ the emissivity for gas i ($i=\text{XXX}$) is calculated from the following correlation:

$$\varepsilon_i = \varepsilon_{i,\infty} \left\{ 1 - \exp [-(a_i + b_i T) (p_i L)^{c_i}] \right\}$$

where $\varepsilon_{i,\infty}$, a_i , b_i , c_i are user input constants.

EMSMAX=0.0: gas does not participate in radiative heat transfer.

EMSMAX>0.0: maximum emissivity = EMSMAX, gray gas model is applied for spectral overlap: $\Delta\varepsilon_g = \varepsilon_{H_2O} \cdot \varepsilon_{CO_2}$ (see Volume 1)

EMSMAX<0.0: recommended Kostowski correlations are used for steam and CO₂. The correlation for spectral overlap, $\Delta\varepsilon_g = f(T, p_{H_2O}, p_{CO_2})$, described in Volume 1, is used, with the limit set by the gray gas model: $\Delta\varepsilon_g \leq \varepsilon_{H_2O} \cdot \varepsilon_{CO_2}$.

Note! For gases other than steam and CO₂ EMSMAX < 0 gives the same effect as EMSMAX = 0.0, no emission/absorption. Note that if zero is entered then the default value is assumed which for steam and CO₂ is: -1, and leads to Kostowski correlations. If the emissivity of these gases needs to be switched off then a small positive value, 10^{-90} , should be entered.

Acceptable range: $0.0 \leq \text{EMSMAX} \leq 1.0$ or EMSMAX = -1.0

Default value: -1.0, if XX = 3 (H₂O) or XX = 6 (CO₂),
0.0, for all other gases.

W-2 (R) : AEMISG Constant a_i in general equation for gas emissivity. Used only if EMSMAX is greater than zero for this gas.

Acceptable range: AEMISG ≥ 0.0 .

Default value: 0.0.

W-3 (R) : BEMISG Constant b_i in general equation for gas emissivity. Used only if EMSMAX is greater than zero for this gas. The values of $a_i + b_i T$ must be positive to obtain physically correct results. Input processing subroutines check if the condition is fulfilled for up to 2200 K, that means: $a_i + b_i 2200 \geq 0.0$. The calculation procedures ensure that the sum $a_i + b_i T$ is never negative. If a negative value is obtained it will be set to zero.

Acceptable range: BEMISG $\geq -\text{AEMISG}/2200.0$.

Default value: 0.0.

W-4 (R) : CEMISG Constant c_i in general equation for gas emissivity. Used only if EMSMAX is greater than zero for this gas.

Acceptable range: CEMISG ≥ 0.0 .

Default value: 0.0.

W-5 (R) : XABSPG Exponent, n, in gas absorptivity correlation. Absorptivity is calculated from the following correlation:

$$a_g = \left(\frac{T_g}{T_w} \right)^n \varepsilon_g \left(T_w, pL \frac{T_w}{T_g} \right)$$

where:

T_g	-	gas temperature, (K),
T_w	-	wall temperature, (K),
pL	-	optical length, (Pa m),
ε_g	-	gas emissivity calculated at wall temperature and optical length multiplied by the ratio (T_w/T_g), (-),
n	-	constant defined by user = XABSPG.

The value of XABSPG is used only if the gas is participating in the radiative heat transfer, that means if EMSMAX > 0.0 (for all gases), or if EMSMAX < 0.0 (for steam and CO₂).

Acceptable range: $0.0 \leq \text{XABSPG} \leq 1.0$.

Default value: 0.45, if XXX = 3 (H₂O),
 0.65, if XXX = 6 (CO₂),
 0.50, for all other gases.

2.6.8 Records: 541000, Radiation Properties of Aerosols

The radiation properties of aerosols are defined in this record. The same radiation properties of aerosols are used for all radiating systems. This record is optional. Note: in order to take the aerosol radiation into account, the parameters present in this record must be defined, as described below.

The emissivity of a mixture of gases and aerosol particles is obtained from:

$$\varepsilon_{mix} = 1 - (1 - \varepsilon_{aer}) \cdot \prod_{k=1}^{N_{gas}} (1 - \varepsilon_k)$$

The aerosol emissivity is calculated from (see Volume 1):

$$\varepsilon_{aer} = 1 - \exp \left[-L \cdot \sum_{i=1}^{N_{size}} n_i \cdot \left(\frac{\pi D_i^2}{4} \right) \cdot (a_{aer} + b_{aer} T^{c_{aer}}) \right]$$

ε_{aer}	emissivity of aerosols, (-)
L	radiation beam length, (m)
n_i	density of aerosol size section i , (1/m ³)
D_i	diameter of aerosol size section i , (m)
T	temperature, (K)
N_{size}	number of aerosol size sections
$a_{aer}, b_{aer}, c_{aer}$	user-defined constants, entered in this record

SPECTRA Code Manuals - Volume 2: User's Guide

In absence of a more detailed data, a simple way to take the aerosol emissivity into account is to use the following values of the model constants: $a_{aer} = 1.0$, $b_{aer} = 0.0$, $c_{aer} = 0.0$. In such case the aerosol emissivity is equal to:

$$\varepsilon_{aer} = 1 - \exp \left[-L \cdot \sum_{i=1}^{N_{sig}} n_i \cdot \left(\frac{\pi D_i^2}{4} \right) \right]$$

- W-2 (R) : AAERTR Constant a_{aer} in the equation for the aerosol emissivity. If the value is zero then the aerosol emissivity is not taken into account.
Acceptable range: AAERTR \geq 0.0
Default value: 0.0
- W-3 (R) : BAERTR Constant b_{aer} in the equation for the aerosol emissivity.
Acceptable range: BAERTR \geq 0.0
Default value: 0.0.
- W-4 (R) : CAERTR Constant c_{aer} in the equation for the aerosol emissivity.
Acceptable range: $-10.0 \leq$ CAERTR \leq 10.0 .
Default value: 0.0.

2.6.9 Example of Thermal Radiation Input Data

As an example problem the radiative heat transfer inside a cylindrical space, partly filled with liquid water is considered. The geometrical configuration is shown in Figure 2-42. A single Control Volume is used, which is filled with liquid water up to the height of H_{pool} . The remaining, gas filled part of the CV, has the height of H_{gas} .

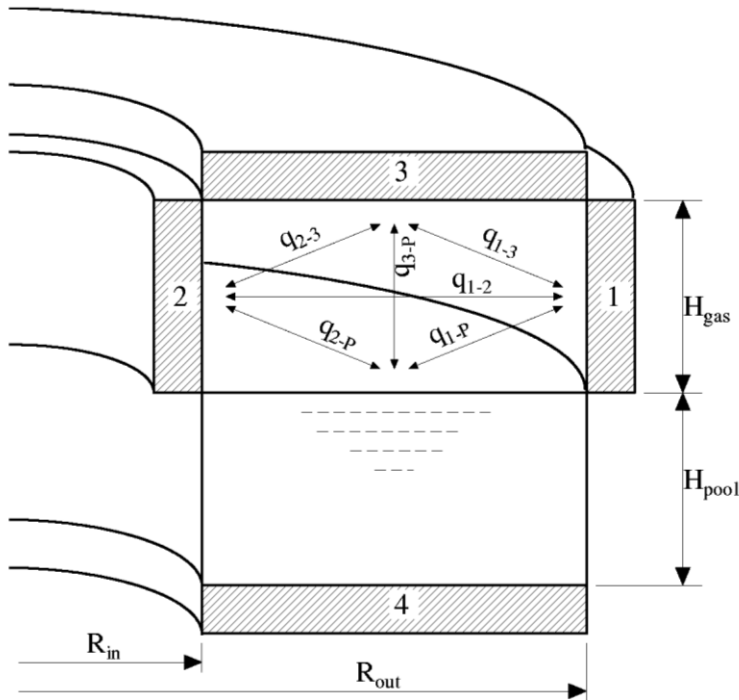


Figure 2-42 Geometrical configuration for Thermal Radiation example problem.

Four solid conductors are used to model the walls, ceiling and floor of the volume (see example problem in section 2.3.39). SC-001 is a cylindrical Heat Conductor, which represents the outer wall, above the liquid level. The inner radius of this wall is equal to the outer radius of the cylindrical space, R_{out} . The height is equal to the height of gas space, H_{gas} . SC-002 represents the inner wall. The outer radius of this SC is equal to R_{in} . SC-003 is a rectangular conductor, which represents the ceiling. SC-004 represents the floor. Additional conductors may be used in the model to represent the cylindrical walls below the liquid level, (as in the example problem shown in section 2.3.39), but are not considered here since they will not participate in radiation heat transfer.

The thermal radiation input is created in three steps:

- I First, the surfaces which will be allowed to participate in radiation heat transfer are chosen and associated with the appropriate SC surfaces. In this problem the following associations are made:
 - Surface: 1 - SC-1, left side,
 - Surface: 2 - SC-2, right side,
 - Surface: 3 - SC-3, right side (this must be the lower side of SC-3. The right side is the lower one if $IVERSC = 1$ for this SC, see section 2.3.39),
 - Surface: 4 - SC-4, right side (this must be the upper side of SC-4. The right side is the upper one if $IVERSC = -1$ for this SC, see section 2.3.39).

For the surface 4 the pool radiation option is chosen. The SC is considered as a floor for the pool. When the pool is present the radiative flux will be deposited at the pool surface. If there is no pool in the CV then the right surface of SC-4 will participate in radiation heat transfer. The area of SC-4 must be equal to the cross section area of the CV, so that the view factors calculated based on surface area of SC-4 are appropriate for the pool surface too. If the pool level changes during the calculations it may partly cover the SC-1 and SC-2. Still the radiation heat transfer areas and the view factors will remain the same. The view factors are not recalculated during transient. Consequently the areas must remain the same to avoid violation of radiant energy conservation.

- II Second, view factors must be calculated. The view factors must be supplied with good accuracy (see Volume 1). For the considered geometry the view factors may be calculated using the formulae shown in [14] (page 15-46):

View factor from the outer wall to the inner wall is equal to:

$$F_{1 \rightarrow 2} = \frac{1}{X} - \frac{1}{\pi X} \cdot \left[\arccos\left(\frac{b}{a}\right) - \frac{1}{2Y} \cdot \left(\sqrt{(a+2)^2 - (2X)^2} \cdot \arccos\left(\frac{b}{aX}\right) + b \cdot \arcsin\left(\frac{1}{X}\right) - \frac{\pi a}{2} \right) \right]$$

View factor from the outer wall to the outer wall itself is equal to:

$$F_{1 \rightarrow 1} = 1 - \frac{1}{X} + \frac{2}{\pi X} \cdot \arctan\left(\frac{2\sqrt{X^2 - 1}}{Y}\right) - \frac{Y}{2\pi X} \cdot \left[\frac{\sqrt{4X^2 + Y^2}}{Y} \cdot \arcsin\left(\frac{4(X^2 - 1) + Y^2 / X^2 \cdot (X^2 - 2)}{Y^2 + 4 \cdot (X^2 - 1)}\right) - \arcsin\left(\frac{X^2 - 2}{X^2}\right) + \frac{\pi}{2} \cdot \left(\frac{\sqrt{4X^2 + Y^2}}{Y} - 1\right) \right]$$

The meaning of the symbols in the above equations is as follows:

$$X = R_{out}/R_{in}$$

$$Y = H_{gas}/R_{in}$$

$$a = Y^2 + X^2 - 1$$

$$b = Y^2 - X^2 + 1$$

Due to symmetry the values of $F_{1 \rightarrow 3}$ and $F_{1 \rightarrow 4}$ are equal. Thus once $F_{1 \rightarrow 2}$ and $F_{1 \rightarrow 1}$ are known the values of $F_{1 \rightarrow 3}$ and $F_{1 \rightarrow 4}$ are obtained as:

$$F_{1 \rightarrow 3} = F_{1 \rightarrow 4} = \frac{1}{2} \cdot (1 - F_{1 \rightarrow 2} - F_{1 \rightarrow 1})$$

The remaining view factors are obtained using the reciprocity ($A_i F_{i \rightarrow j} = A_j F_{j \rightarrow i}$) and the closure ($\sum F_{i \rightarrow j} = 1$) relations.

SPECTRA Code Manuals - Volume 2: User's Guide

For the example problem the following data were assumed: $R_{in} = 5$ m, $R_{out} = 15$ m, $H_{gas} = 5$ m. The resulting view factors are:

- $F_{1 \rightarrow 1} = 0.117156532$
- $F_{1 \rightarrow 2} = 0.092480799$
- $F_{1 \rightarrow 3} = F_{1 \rightarrow 4} = 0.395181335$

Values of other view factors, calculated using the reciprocity and closure relations, are shown in the listing below.

Note that the surface area of rectangular conductors (3 and 4), which is equal to 628.31853 (=200 π), must be entered with the accuracy corresponding to the accuracy of view factors (see section 2.3.39). For the cylindrical SC the program calculates the area internally using the length and radius.

III The last step is to calculate the mean beam lengths. The exact values may be obtained by rather complicated integration. However there is no need to calculate beam lengths with very good accuracy. They are used to obtain gas emissivity/absorptivity. This is done by correlations, which have, at best, the accuracy of two decimal places. Here a simplified method, described below, is used to obtain the mean beam lengths.

The mean beam lengths for all paths except $L_{1 \rightarrow 1}$, are calculated by multiplying the distance between the centres of surfaces by a constant factor, greater than one, $(1 + \varphi)$. The $L_{1 \rightarrow 1}$ length was estimated by multiplying the maximum possible beam length by the factor $(1 - \varphi)$.

$$\begin{aligned}
 L_{1 \rightarrow 2} &= (1 + \varphi) \cdot (R_{out} - R_{in}) \\
 L_{3 \rightarrow 4} &= (1 + \varphi) \cdot H_{gas} \\
 L_{1 \rightarrow 3} &= (1 + \varphi) \cdot \frac{1}{2} \cdot \sqrt{H_{gas}^2 + (R_{out} - R_{in})^2} = L_{1 \rightarrow 4} \\
 L_{1 \rightarrow 1} &= (1 - \varphi) \cdot 2 \cdot \sqrt{R_{out}^2 - R_{in}^2}
 \end{aligned}$$

The other lengths were calculated assuming that $L_{i \rightarrow j} = L_{j \rightarrow i}$. The value of φ was taken as 0.3. The calculated beam lengths are shown in the printout below.

The average value of the beam length for an enclosure is calculated by the program internally, as:

$$L_{ave} = \frac{\sum_{i=1}^N \sum_{j=1}^N A_i \cdot F_{i \rightarrow j} \cdot L_{i \rightarrow j}}{\sum_{i=1}^N \sum_{j=1}^N A_i \cdot F_{i \rightarrow j}}$$

where: A_i - area of surface i , (m^2),
 $F_{i \rightarrow j}$ - view factor between surface i and j , (-),
 $L_{i \rightarrow j}$ - mean beam length between surface i and j , (m).

The average value is compared with an "engineering estimation" of mean beam length in an enclosure, which is ([14] page 15-65):

SPECTRA Code Manuals - Volume 2: User's Guide

$$L_{eng} = \frac{4V}{A}$$

where: V - total volume of the enclosure, (m³)
 A - total surface area of the enclosure, = ΣA_i , (m²)

In the presented example the L_{ave} is equal to 7.60, while L_{eng} is equal to 7.93. Another possibility of calculating the beam lengths is to calculate L_{eng} and then use this value for all $L_{i \rightarrow j}$.

A program to calculate view factors and beam lengths in a cylindrical enclosure, using the formulae shown above on is provided in: \Z-INPUTS\TR\CyIVF. SPECTRA input for the example problem is shown below. The default gas radiation models are used in the presented example.

```

*
* ----- Thermal radiation data
*
505100 Cylindrical system with radiation to pool
500100 2 * radiation model : absorbing/emitting medium
*
510101 1 7 0 * TR-101 = SC-001, left surface
510102 2 7 0 * TR-102 = SC-002, right surface
510103 3 7 0 * TR-103 = SC-003, right surface
510104 4 7 1 * TR-104 = SC-004, right surface, pool option
*
* View factors, F(i->j)
* \j      j=1      j=2      j=3      j=4
* i\
520101 0.117156532 0.092480799 0.395181335 0.395181335
520102 0.277442397 0.000000000 0.361278801 0.361278801
520103 0.296386001 0.090319700 0.000000000 0.613294299
520104 0.296386001 0.090319700 0.613294299 0.000000000
*
* Beam lengths, L(i->j)
* \j      j=1  j=2  j=3  j=4
* i\
530101 19.8 13.0 7.3 7.3
530102 13.0 0.0 7.3 7.3
530103 7.3 7.3 0.0 6.5
530104 7.3 7.3 6.5 0.0

```

2.7 Tabular Function Input Data

2.7.1 Records: 605XXX, Tabular Function Name

XXX is the Tabular Function reference number, $001 \leq XXX \leq 999$. The TF reference numbers need not be consecutive. The maximum number of Tabular Functions is 999.

W-1 (A) : NAMETF User defined name, length up to 50 characters. The name is read as a 50-character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.
Acceptable range: any string of up to 50 characters.
Default value: 50 "underline" characters: "_".

2.7.2 Records: 601XXX, Scaling Factor and Additive Constant

XXX is the Tabular Function reference number, $001 \leq XXX \leq 999$. The TF reference numbers need not be consecutive. The maximum number of Tabular Functions is 999.

W-1 (R) : SCLFTF Scaling factor, S . The value defined by the tabulated data points, or interactively by the user, is multiplied by this factor.
Acceptable range: all real numbers.
Default value: 1.0 (a small number $<10^{-50}$, sets the value to 0.0).

W-2 (R) : ADDCTF Additive constant, A . The value of this constant is added to the value defined by the tabulated data points, or interactively by the user. The value of Tabular Function is:

$$TF(t) = f(t) \cdot S + A$$

Acceptable range: all real numbers.
Default value: 0.0 .

2.7.3 Records: 602XXX, Lower and Upper Limits, Rate Change Limits

XXX is the Tabular Function reference number, $001 \leq XXX \leq 999$. The TF reference numbers need not be consecutive. The maximum number of Tabular Functions is 999.

W-1 (R) : VMINTF Minimum value of Tabular Function: $TF(t) \geq VMINTF$.
Acceptable range: $-10^{99} \leq VMINTF \leq +10^{99}$
Default value: -10^{99} (a small number $<10^{-50}$, sets the value to 0.0)

W-2 (R) : VMAXTF Maximum value of Tabular Function: $TF(t) \leq VMAXTF$.
Acceptable range: $-10^{99} \leq VMAXTF \leq +10^{99}$

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: $+10^{99}$ (a small number $<10^{-50}$, sets the value to 0.0)

- W-3 (R) : DDDTTF Maximum rate of change in case of decreasing value of TF:
 $d TF(t) / dt \geq \text{DDDTTF}$.
Acceptable range: $-10^{99} \leq \text{DDDTTF} \leq 0.0$
Default value: -10^{99} (a small number $<10^{-50}$, sets the value to 0.0)
- W-4 (R) : DIDTTF Maximum rate of change in case of increasing value of TF:
 $d TF(t) / dt \leq +\text{DIDTTF}$.
Acceptable range: $0.0 \leq \text{DIDTTF} \leq +10^{99}$
Default value: $+10^{99}$ (a small number $<10^{-50}$, sets the value to 0.0)

2.7.4 Records: 603XXX, Rate Change Limits for Generating Message

XXX is the Tabular Function reference number, $001 \leq \text{XXX} \leq 999$. A message is written to the message file (and optionally screen) if the TF value or the rate of change exceeds the values defined in this record.

- W-1 (R) : VMNMTF Minimum limit for messaging. Message is generated if:
 $TF(t) < \text{VMNMTF}$.
Acceptable range: $-10^{99} \leq \text{VMNMTF} \leq +10^{99}$
Default value: -10^{99}
- W-2 (R) : VMAXTF Maximum limit for messaging. Message is generated if:
 $TF(t) > \text{VMAXTF}$.
Acceptable range: $-10^{99} \leq \text{VMAXTF} \leq +10^{99}$
Default value: $+10^{99}$
- W-3 (R) : DDDMTF Rate of change in case of decreasing value of TF.
Message is generated if the rate of change is $d TF(t) / dt < \text{DDDMTF}$.
Acceptable range: $-10^{99} \leq \text{DDDMTF} \leq 0.0$
Default value: -10^{99}
- W-4 (R) : DIDMTF Rate of change in case of increasing value of TF.
Message is generated if the rate of change is $d TF(t) / dt > +\text{DIDMTF}$.
Acceptable range: $0.0 \leq \text{DIDMTF} \leq +10^{99}$
Default value: $+10^{99}$

2.7.5 Records: 610XXX, Interpolation Type, Interactive Type

XXX is the Tabular Function reference number, $001 \leq \text{XXX} \leq 999$. The TF reference numbers need not be consecutive. The maximum number of Tabular Functions is 999.

- W-1 (I) : INTKTF The absolute value determines the type of interpolation, while the sign determines whether this TF is an interactive function
 $\text{INTKTF} > 0$

Non-interactive TF - the value of the TF is always determined by the table, entered in the input deck.

INTKTF < 0

Interactive Tabular Function - this type of TF is useful in the simulation mode. At any time of calculations the TF value may be modified in the file *.TFD (see section 3.6). The value that needs to be specified in the *.TFD file is simply the TF number and the value that it should take. Therefore, to set the value of TF-120 to 521.0 one needs to type (or the simulation tool needs to send) the following line in the *.TFD file:

```
120      521.0
```

If there is no data for the TF in the *.TFD file, then the value of the function will be determined by the table present in the input deck. If the value is present in the *.TFD file, then the value of TF will change, the rate of change being limited by the DDDTTF and DIDTTF, until it reaches the value designated in *.TFD file, provided that it is not outside the limits given by VMINTF, VMAXTF. The TF will stay at that value for as long as it is present in the *.TFD file. If the value in the *.TFD value should change, the TF will start changing to reach the new value, again respecting the limits set by DDDTTF, DIDTTF, VMINTF, VMAXTF. If the value disappears from the *.TFD file, then the TF will start changing to reach the value prescribed for it by the tabulated data pairs, again respecting the limits set by DDDTTF, DIDTTF, VMINTF, VMAXTF.

The type of interpolation is used only when the TF is using the data table, not the value from the *.TFD file (in other words, when the *.TFD file does not contain a value of this TF). The possible types of interpolations are (see Figure 2-43):

|INTKTF|=1: linear interpolation (continuous function).

|INTKTF|=3: cubic interpolation ("smooth" function - continuous function and it's first derivative).

Acceptable range: -3, -1, +1, +3 .

Default value: -1 .

2.7.6 Records: 611XXX, Automatic Reset Option for Interactive TF

XXX is the Tabular Function reference number, $001 \leq XXX \leq 999$. The TF reference numbers need not be consecutive. The maximum number of Tabular Functions is 999.

W-1 (R) : RSETTF Automatic reset for interactive TF. If the value of an interactive Tabular Function has been specified in the *.TFD file, it is being used until a new value is specified or the current value is removed. In order to switch back to the TF data tabulated in the input deck, one must remove all definitions of given TF from the TFD file. This can be done automatically using the automatic reset option.

=0.0: automatic reset option not used

>0.0: automatic reset to the tabulated TF after the time of RSETTF (s) since the function has been specified in the *.TFD file. This option removes the definition of the given TF from the *.TFD file after specified amount of seconds elapses.

Acceptable range: RSETTF \geq 0.0
Default value: 0.0

2.7.7 Records: 600XXX, Tabular Function Data Records

XXX is the Tabular Function reference number, $001 \leq XXX \leq 999$. The TF reference numbers need not be consecutive. The maximum number of Tabular Functions is 999.

Each data record contains one data pair. The total number of data pairs may not exceed 20,000, for a single Tabular Function.

W-1 (R) : TBFUNX Value of the independent variable, point I. In case of Tabular Functions the independent variable is always time (s). If the user wishes to use tables for which the independent variable is other than time, he must use Control Functions (section 2.8).

Acceptable range: Values of TBFUNX must increase. Thus the value for a given point must be greater than the previous value (TBFUNX for the previous point).

Default value: none.

W-2 (R) : TBFUNY Value of the dependent variable, point I. The value of the Tabular Function XXX, $f(t)$, at time equal to $t = \text{TBFUNX}$. Note that in case of interactive TF the values tabulated in the input deck may be overridden by the numbers entered by the user (or a simulation tool) in the file *.TFD.

Acceptable range: all real numbers.

Default value: none.

W-3 (I) : I Point number. If no value, or zero is entered, then the data points are read sequentially - the first record in the input is interpreted as containing the first point (I=1), then I=2, etc.

Acceptable range: $0 < I \leq 20,000$.

Default value: none.

2.7.8 Examples of Tabular Function Input and Use of *.TFD

The example input of the Tabular Function data defines two Tabular Functions. TF-001 uses linear interpolation between the data points. TF-002 uses cubic interpolation between the data points. Both Tabular Functions are defined by seven data points. Negative value of the TF type means that the interactive option is used, and the TF value may be redefined during calculations in the *.TFD file. The limits of 0.0 and 99.0 are imposed on the values read from the *.TFD file.

```
605001    Example 1 of Tabular Function
601001    1.0   0.0    * Scaling factor, Additive constant
602001    0.0  99.0    * Limits
610001    -1            * Interactive, Linear Interpolation TF
*
*            Time    Value
600001    5.0    0.10    *
```


SPECTRA Code Manuals - Volume 2: User's Guide

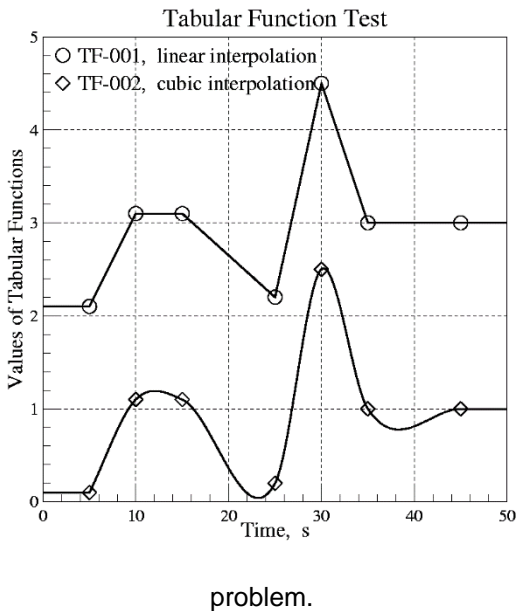
```

600001 10.0 1.10 *
600001 15.0 1.10 *
600001 25.0 0.20 *
600001 30.0 2.50 *
600001 35.0 1.00 *
600001 45.0 1.00 *
*
605002 Example 2 of Tabular Function
601002 1.0 0.0 * Scaling factor, Additive constant
602002 0.0 99.0 * Limits
610002 -3 * Interactive, Cubic Interpolation TF
*
* Time Value
600002 5.0 2.10 *
600002 10.0 3.10 *
600002 15.0 3.10 *
600002 25.0 2.20 *
600002 30.0 4.50 *
600002 35.0 3.00 *
600002 45.0 3.00 *

```

Figure 2-43 shows the values of TF-001 and TF-002, as well as the data points. The data points are shown using markers. The values of TF-001 and TF-002, calculated for times between 0 and 50 s, are marked by lines.

The cubic interpolation ensures continuity of the first derivative in all range except for the boundary (first and last) data points. In those points the derivative "jumps" to zero, since flat lines are used outside the data points. The discontinuity was programmed on purpose, because this formulation is considered safer for practical use. The cubic interpolation subroutine is used in SPECTRA, among others, for the calculation of water properties. In this case the applied formulation allows to obtain



correct behavior of the interpolated functions in the region close to the freezing point. The fact that the functions won't be smooth if the temperature drops below the freezing point has no practical meaning. If the user wishes to avoid this discontinuity, he can do that by specific definition of the data points near the boundary, as shown below.

The last two data points of TF-002 were given the same value. It is seen in Figure 2-43 that the discontinuity of the derivative, clearly seen at the left boundary of this function, is not present at the right boundary.

Figure 2-43 Values of Tabular Functions (lines) and data points (markers) for the two Tabular Functions, defined in the example problem.

By including the point numbers (Word 3) the data can be entered in an arbitrary order. For example, the two definitions shown below are equivalent:

```

605001 Example 1 of Tabular Function
601001 1.0 0.0 * Scaling factor, Additive constant
602001 0.0 99.0 * Limits
610001 -1 * Interactive, Linear Interpolation TF
*

```

SPECTRA Code Manuals - Volume 2: User's Guide

```
*      Time  Value  Point
600001  5.0    0.10   1   *
600001 10.0    1.10   2   *
600001 15.0    1.10   3   *
600001 25.0    0.20   4   *
600001 30.0    2.50   5   *
600001 35.0    1.00   6   *
600001 45.0    1.00   7   *

605001  Example 1 of Tabular Function
601001  1.0    0.0    * Scaling factor, Additive constant
602001  0.0  99.0    * Limits
610001  -1      * Interactive, Linear Interpolation TF
*
*      Time  Value  Point
600001 45.0    1.00   7   *
600001  5.0    0.10   1   *
600001 35.0    1.00   6   *
600001 10.0    1.10   2   *
600001 15.0    1.10   3   *
600001 25.0    0.20   4   *
600001 30.0    2.50   5   *
```

Both sets of records shown above define the same function.

The data present in the *.TFD file may have two formats:

- Arbitrary number of pairs, for example:
120 1.0 200 1.5 250 -5.0
The above record will set (immediately as it appears in the *.TFD file) the following values: TF-120=1.0, TF-200=1.5, TF-250=-5.0
- Three input parameters, single TF definition with TIMEON. For example:
120 1.0 1000.0
The above record will set TF-120=1.0 at the time = TIMEOF =1000.0 s (or immediately if the current time is larger than 1000.0 s.
Another example. The following records:
120 1.0 1000.0
120 2.0 2000.0
120 5.0 3000.0
will set the value of TF-120 to 1.0 at t = 1000.0 s, to 2.0 at t = 2000.0 s, and finally to 5.0 at t = 5000.0 s.

Note that the maximum amount of data pairs that can be defined in a single line is 20. This means up to 20 Tabular Function values can be specified in a single record, if the first format (immediate action) is used.

2.8 Control Function Input Data

2.8.1 Records: 700XXX, Control Function Main Data

XXX is the Control Function reference number, $001 \leq XXX \leq 999$. The CF reference numbers need not be consecutive. The maximum number of Control Functions is 999.

- W-1 (I) : IGRPCF First identifier defining the type of Control Function - see Table 2-22.
Acceptable range: $1 \leq \text{IGRPCF} \leq 3$.
Default value: none.
- W-2 (I) : INUMCF Second identifier defining the type of Control Function, Table 2-22.
Acceptable range: $1 \leq \text{INUMCF} \leq 9$, if IGRPCF = 1,
 $1 \leq \text{INUMCF} \leq 16$, if IGRPCF = 2,
 $1 \leq \text{INUMCF} \leq 5$, if IGRPCF = 3.
Default value: none.
- W-3 (R) : SCLFCF Scaling factor, *S*. The result of the function defined by previous two integers is multiplied by this factor.
Acceptable range: all real numbers
Default value: 1.0 (a small number $< 10^{-50}$, sets the value to 0.0)
- W-4 (R) : ADDFCF Additive constant, *A*. The value of this constant is added to the calculated value of the function. The value of Control Function is:

$$CF(t) = f(x_1, x_2, \dots) \cdot S + A$$

Acceptable range: all real numbers

Default value: 0.0 .

2.8.2 Records: 701XXX, Initial Value

XXX is the Control Function reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : INTCF Initial value calculation indicator.
1: Initial value is calculated.
2: Input value (Word 2 below) is used. Use this option also when the initial value should be read from an Initial Condition File - ICF (section 2.16.3).
Acceptable range: 1, 2. For integral type CF the initial value must be specified, therefor INTCF must be equal to 2
Default value: 1 for all CF types except integral, 2 for integral.
- W-2 (R) : CONFUN Initial value of the Control Function.
Acceptable range: $-10^{99} \leq \text{CONFUN} \leq +10^{99}$.
Default value: 0.0 .

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-22 Types of Control Functions.

Group and No.		Function type	Number of arguments	FORTRAN definition
IGRPCF	INUMCF			
1	1	Add / subtract	≤ 100	$f = a_1 + (-) a_2 + (-) \dots + (-) a_n$
	2	Multiply / divide	≤ 100	$f = a_1 \cdot (/) a_2 \cdot (/) \dots \cdot (/) a_n$
	3	Power function	2	$f = a_1 ** a_2$ if $a_1 > 0$ $f = - a_1 ** a_2$ if $a_1 < 0$
	4	Selected argument	4	IF (a_1 .LT. a_2) THEN $f = a_3$ ELSE $f = a_4$ ENDIF
	5	General tabular function	≤ 100	see example in section 2.8.6
	6	Hysteresis	3	see example in section 2.8.11
	7	Derivative	1	$f = (a_1 - a_1^0) / \Delta t$
	8	Integral	1	$f = f^0 + a_1 \cdot \Delta t$
	9	Random number	1	$f = \text{rnd}() \cdot S(a_1) + A(a_1)$
2	1	Absolute value	1	$f = \text{DABS}(a_1)$
	2	Minimum value	≤ 100	$f = \text{DMIN1}(a_1, a_2, \dots, a_n)$
	3	Maximum value	≤ 100	$f = \text{DMAX1}(a_1, a_2, \dots, a_n)$
	4	Square root	1	$f = \text{DSQRT}(a_1)$
	5	Exponent	1	$f = \text{DEXP}(a_1)$
	6	Natural logarithm	1	$f = \text{DLOG}(a_1)$
	7	Decimal logarithm	1	$f = \text{DLOG10}(a_1)$
	8	Sine	1	$f = \text{DSIN}(a_1)$
	9	Cosine	1	$f = \text{DCOS}(a_1)$
	10	Tangent	1	$f = \text{DTAN}(a_1)$
	11	Arc sine	1	$f = \text{DASIN}(a_1)$
	12	Arc cosine	1	$f = \text{DACOS}(a_1)$
	13	Arc tangent	1	$f = \text{DATAN}(a_1)$
	14	Hyperbolic sine	1	$f = \text{DSINH}(a_1)$
	15	Hyperbolic cosine	1	$f = \text{DCOSH}(a_1)$
	16	Hyperbolic tangent	1	$f = \text{DTANH}(a_1)$
3	1	Error function	1	$f = \text{DERF}(a_1)$
	2	Complementary error f.	1	$f = \text{DERFC}(a_1)$
	3	Gamma function	1	$f = \text{DGAMMA}(a_1)$
	4	Log gamma function	1	$f = \text{DLGAMA}(a_1)$
	5	Reactor Kinetics	1	see Volume 1

2.8.5 Records: 705XXX, Control Function Name

XXX is the Control Function reference number, $001 \leq XXX \leq 999$.

W-1 (A) : NAMECF User defined name, length up to 50 characters. The name is read as a 50-character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.

Acceptable range: any string of up to 50 characters.

Default value: 50 "underline" characters: "_".

2.8.6 Records: 708XXX, Y-Coordinate Points for 2-D Tabular Functions

XXX is the Control Function reference number, $001 \leq XXX \leq 999$.

A General Tabular Function is one of the types of a Control Function (IGRPCF=1, INUMCF=5, - see Table 2-22). The main difference between a Tabular Function (section 2.7) and a General Tabular Function from the CF Package is the argument type. In case of a TF the argument is always time. This allows excluding all TF from the main iteration loop to obtain implicit solution (the implicit values of all TF is known; they are tabulated versus time, so the value at any given time point is readily available). On the other hand the General Tabular Function type of a CF (IGRPCF=1, INUMCF=5, - see Table 2-22) may use any variable from the SPECTRA data base as an argument. Since the implicit value of its argument may not be available at the start of the time step, this CF, like all other CF, is included in the main iteration loop to obtain implicit solution (the implicit treatment of CF may be altered by setting argument calculation on explicit - record 709XXX, or by the implicit solution indicator - record 715000).

There are two kinds of a General Tabular Function:

- A simple, one-dimensional general Tabular Function. This function has two arguments. The first argument defines an independent variable for this function. The second argument is a reference number of a Tabular Function from the TF data base. An example is shown below.

```
605105 Tabular Function TF-123
*      x      f(x)
600105 300.0   0.0
600105 400.0   1.0
*
705105 1-D General Tabular Function
*      Group  Number      Fact.  Const.
700105   1      5          1.0    0.0   * Type      : General TF
*      Arguments
* Pointers: (1) (2) (3) (4) Fact.  Const.
710105   1    123 14   1    1.0    0.0 * Use CV-123-Temp-atms as argument
710105   6     105 1   0    1.0    0.0 * Use table TF-105
```

In the above example Tabular Function, TF-105 and a General Tabular Function, CF-105, are defined. The value of TF-105 will be equal to zero for times $t < 300.0$ s, increase linearly to 1.0 during $300.0 < t < 400.0$ s, and remain equal to 1.0 afterwards. The value of CF-105 will be equal to zero when the atmosphere temperature in CV-123 is below $T < 300.0$ K, increase

SPECTRA Code Manuals - Volume 2: User's Guide

linearly to 1.0 with the temperature increasing between $300.0 < T < 400.0$ K, and remain equal to 1.0 for higher temperatures.

- A two-dimensional Tabular Function, $F(x,y)$, may be created, where x is the first argument and y is the second argument. In this case the general Tabular Function should be defined by a number of TFs, each TF defining the value of function versus the argument x for one value of the argument y . The y -arguments are defined in this record. An example of a 2-D function is shown below.

```

605101 Efficiency versus flow, pump speed of 20 rev/s
*      x      f(x)
600101 0.05   0.30
600101 0.2    0.60
600101 0.5    0.72
600101 0.8    0.80
600101 1.0    0.75
600101 1.1    0.70
*
605102 Efficiency versus flow, pump speed of 40 rev/s
*      x      f(x)
600102 0.05   0.40
600102 0.1    0.60
600102 0.2    0.70
600102 0.5    0.82
600102 1.0    0.85
600102 1.1    0.81
*
605103 Efficiency versus flow, pump speed of 50 rev/s
*      x      f(x)
600103 0.05   0.50
600103 0.1    0.70
600103 0.2    0.80
600103 0.35   0.90
600103 1.0    0.92
600103 1.1    0.88
*
705100 2-D General Tabular Function
*      Group  Number      Fact.  Const.
700100 1       5         1.0   0.0   * Type      : General TF
*      y1     y2     y3
708100 20.0  40.0  50.0 * y-coordinate data points (pump speeds)
*      Arguments
* Pointers: (1) (2) (3) (4) Fact. Const.
710100 2 500 37 2 1.0 0.0 * x-argument: JN-500, pump flow (pool)
710100 6 101 1 0 1.0 0.0 * uses TF-101 for y = y1
710100 6 102 1 0 1.0 0.0 * uses TF-102 for y = y2
710100 6 103 1 0 1.0 0.0 * uses TF-103 for y = y3
710100 2 500 36 2 1.0 0.0 * y-argument: JN-500, pump speed (pool)

```

The above example defines the pump efficiency, as a function of pump volumetric flow and pump speed. During the calculations a 2-D interpolation is performed to find the value of a function.

For example, suppose that during the execution the CF-100 (pump efficiency) should be calculated for the Volumetric flow of $V = 0.15$ m³/s and speed of 45 rev/s. First the x -coordinate interpolations are performed; the calculated values are (see the data values above):

$$\begin{aligned} \omega = 40.0 \text{ rev/s} & \quad \text{TF-102 } (x=0.15) = 0.65 \\ \omega = 50.0 \text{ rev/s} & \quad \text{TF-103 } (x=0.15) = 0.75 \end{aligned}$$

Now the linear interpolations between the two points shown above is performed, to give:

$$\omega = 45.0 \text{ rev/s} \quad \text{CF-100 } (x=0.15, y=45.0) = 0.70$$

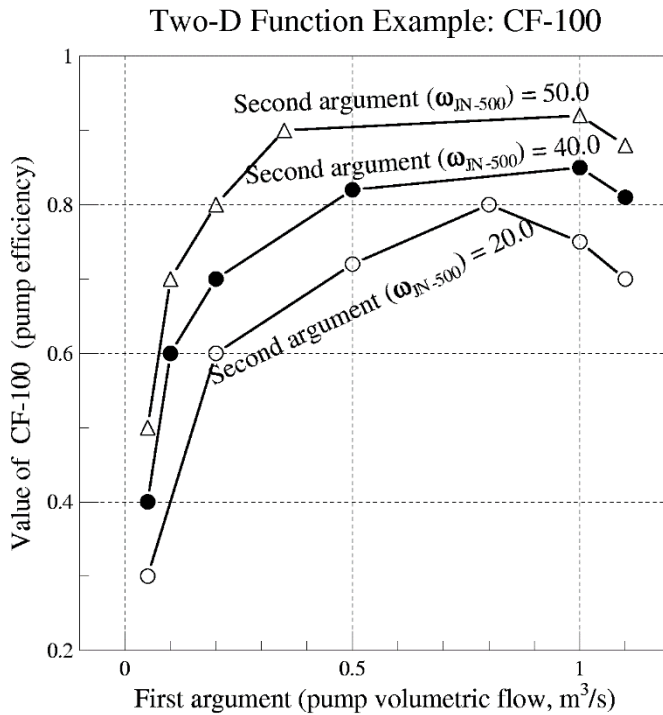


Figure 2-44 Example of a 2-D General Tabular Function

The y-coordinate data points are defined by the following data words:

- W-1 (R) : ARG2CF The first y-coordinate value for the 2-D interpolation.
 (1) Acceptable range: any real.
 Default value: none.
- W-2 (R) : ARG2CF The second y-coordinate value for the 2-D interpolation.
 (2) Acceptable range: ARG2CF(2) > ARG2CF(1).
 Default value: none.

... until all arguments are entered. The number of y-coordinate data points must be the same as the number of Tabular Functions used with this CF. The first argument for the general Tabular Function defines an independent variable for the x-coordinate. The last argument defines an independent variable for the y-coordinate. All other arguments are pointing to Tabular Functions. Since the total number of arguments of any CF is limited to 100, and the first and last argument are defining the independent variables, therefore the maximum number of Tabular Functions (and simultaneously the maximum number of y-coordinate data points) is 98.

2.8.7 Records: 709000, Implicit/Explicit Use of Arguments - Global Activator

This records specifies the implicit/explicit use of CF arguments for all Control Function. The values can be redefined for each individual CF using the records 709XXX.

W-1 (A) : IMARCF Indicator defining the method of using CF arguments.
IMARCF = 1: Implicit (use end of time step value).
IMARCF = 2: Explicit (use beginning of time step value, if such
value is available).

By default the implicit method is used. If convergence problems are observed for Control Functions, then the explicit method should be used. Note that not all variables are kept at the two levels: new time step and old time step. Those variables for which the old time step value is available and the explicit method may be used, are marked by the symbol **I/E** in Table 2-23 through Table 2-32. Those for which only implicit method is available are marked by the symbol **I/-**.
Acceptable range: 1 or 2 .
Default value: 1 .

This records specifies default values of the friction model parameters. The default values can be redefined for each individual junction in the records 210XXX.

2.8.8 Records: 709XXX, Implicit/Explicit Use of Arguments

This records specifies the implicit/explicit use of CF arguments for Control Function with reference number XXX, 001 ≤ XXX ≤ 999.

W-1 (A) : IMARCF Indicator defining the method of using CF arguments.
IMARCF = 1: Implicit (use end of time step value).
IMARCF = 2: Explicit (use beginning of time step value, if such
value is available).

By default the implicit method is used. If convergence problems are observed for Control Functions, then the explicit method should be used. Note that not all variables are kept at the two levels: new time step and old time step. Those variables for which the old time step value is available and the explicit method may be used, are marked by the symbol **I/E** in Table 2-23 through Table 2-32. Those for which only implicit method is available are marked by the symbol **I/-**.
Acceptable range: 1 or 2 .
Default value: 1 .

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: none.

W-3 (I) : IARG3C Third pointer for Control Function argument. This pointer defines the type of parameter (variable name). The values of IARG3C and their interpretation are shown in Table 2-23 through Table 2-32.

Acceptable range: $0 \leq \text{IARG3C} \leq 131$; if IARG1C=1,
 $1 \leq \text{IARG3C} \leq 47$; if IARG1C=2,
 $0 \leq \text{IARG3C} \leq 43$; if IARG1C=3,
 $0 \leq \text{IARG3C} \leq 59$; if IARG1C=4,
 $1 \leq \text{IARG3C} \leq 8$; if IARG1C=5,
 $\text{IARG3C} = 1$; if IARG1C=6,
 $0 \leq \text{IARG3C} \leq 25$; if IARG1C=7,
 $1 \leq \text{IARG3C} \leq 323$; if IARG1C=8,
 $1 \leq \text{IARG3C} \leq 8$; if IARG1C=9.

Default value: none.

W-4 (I) : IARG4C Fourth pointer for Control Function argument. For example, if the Control Volume temperature is needed (IARG1C = 1, IARG3C = 14; see Table 2-23) then this pointer specifies whether the temperature of the atmosphere gas (IARG4C =1), atmosphere droplets (=2), pool liquid (=3), or pool bubbles (=4), is used. If the Solid Heat Conductor Temperature is needed (IARG1C = 3, IARG3C = 16; see Table 2-23) then this pointer specifies the node number. The values of IARG4C, their interpretation and acceptable range, are shown in Table 2-23 through Table 2-32.

Acceptable range: indicated in Table 2-23 through Table 2-32.

Default value: none.

W-5 (R) : SCLACF Scaling factor for the CF argument. The value of the argument, defined by previous four integers, $a(t)$, is multiplied by this factor.

Acceptable range: all real numbers.

Default value: 1.0 (a small number $<10^{-50}$, sets the value to 0.0)

W-6 (R) : ADDACF Additive constant for the CF argument. The value of this constant is added to the calculated value of the argument. The argument value, used by the Control Function is:

$$\text{Arg}_i(t) = a_i(t) \cdot \text{SCLACF}_i + \text{ADDACF}_i$$

Acceptable range: all real numbers.

Default value: 0.0 .

W-7 (I) : I Argument number. If no value, or zero is entered, then the argument data are read sequentially - the first record in the input is interpreted as containing the first argument (I=1), then I=2, etc.

Acceptable range: $0 < I \leq 100$.

Default value: none.

Additional pointers for the Radioactive Particle Transport Package

SPECTRA Code Manuals - Volume 2: User's Guide

- W-8 (I) : IARG5C Fifth pointer for Control Function argument. This pointer is used for some parameters in the Radioactive Particle Transport Package - Table 2-28. For example, if the gravitational deposition velocity of aerosol particles is needed (IARG1C = 8, IARG3C = 53 or 74, see Table 2-28) then this pointer specifies the aerosol size section number. (Note that in this case the fourth pointer specifies the boundary cell number). The values of IARG5C, their interpretation and acceptable range, are shown in Table 2-28.
Acceptable range: indicated in Table 2-28.
Default value: none.
- W-9 (I) : IARG6C Sixth pointer for Control Function argument. This pointer is used for some parameters in the Radioactive Particle Transport Package - Table 2-28. For example, if the deposited fractions in given F_a -section (adhesion force section) is needed (IARG1C = 8, IARG3C = 65 or 86, see Table 2-28) then this pointer specifies F_a -section number. (Note that in this case the fifth pointer specifies the aerosol size section number and the fourth pointer specifies the boundary cell number). The values of IARG6C, their interpretation and acceptable range, are shown in Table 2-28.
Acceptable range: indicated in Table 2-28.
Default value: none.

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-23 List of arguments available for Control Functions, variables available in Control Volume Data Base.

Pointer 1: IARG1C = 1, Control Volume Data Base
 Pointer 2: IARG2C = CV reference number

Code name: CV
 Code name: three digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
Stratification data				
1		Density Stratification Parameter	CV-123- <u> </u> DSP-0000	I/E
2		Thermal Stratification Parameter	CV-123- <u> </u> TSP-0000	I/E
3		Pool Stratification Parameter	CV-123- <u> </u> PSP-0000	I/E
4	-	Atmosphere temperature, bottom of CV or pool surface, K	CV-123-Tatb-0000	I/E
5		Atmosphere temperature, top of CV, K	CV-123-Tatt-0000	I/E
6		Pool temperature, bottom of CV, K	CV-123-Tplb-0000	I/E
7		Pool temperature, pool surface, K	CV-123-Tpls-0000	I/E
Pool surface dat				
8		Pool level related to the bottom of CV, m	CV-123-Zpls-0000	I/E
9		Velocity (upwards) of the pool surface, m/s	CV-123-Vpls-0000	I/E
10	-	Area of the pool surface, m ²	CV-123-Apls-0000	I/-
11		Volumetric fraction of droplets at the pool surface	CV-123-Dpls-0000	I/E
12		Volumetric fraction of bubbles at the pool surface	CV-123-Bpls-0000	I/E
Thermodynamic data				
13		Pressure, Pa	CV-123-Pres-atms	I/E
14		Temperature, K	CV-123-Temp-drop	I/E
15		Saturation temperature, K	CV-123-Tsat-pool	I/E
16	1=atms	Saturation pressure, Pa	CV-123-Psat-bubb	I/-
17	2=drop	Volumetric fraction of dispersed in continuous comp.	CV-123-VolF-atms	I/-
18	3=pool	Mass fraction of dispersed in continuous comp.	CV-123-MasF-drop	I/-
19	4=bubb	Volume, m ³	CV-123-Volm-pool	I/E
20		Mass, kg	CV-123-Mass-atms	I/E
21		Total internal energy, J	CV-123-Enrg-drop	I/E
22		Vertical velocity (atms drop: down; pool bubb: up), m/s	CV-123-Vvrt-pool	I/E
23		Horizontal velocity, m/s	CV-123-Vhor-bubb	I/E
Fluid property data				
24		Density, m ³ /s	CV-123-Dens-atms	I/E
25		Specific internal energy, J/kg	CV-123-SEnr-drop	I/-
26		Specific enthalpy, J/kg	CV-123-Enth-pool	I/E
27	1=atms	Viscosity, kg/m/s	CV-123-Visc-bubb	I/-
28	2=drop	Thermal conductivity, W/m/K	CV-123-Tcon-atms	I/-
29	3=pool	Specific heat at constant pressure, c _p , J/kg/K	CV-123- <u> </u> Cp-drop	I/E
30	4=bubb	Specific heat at constant volume, c _v , J/kg/K	CV-123- <u> </u> Cv-pool	I/E
31		Prandtl number	CV-123- <u> </u> Pr-bubb	I/-
32		Thermal expansion coefficient, 1/K	CV-123-Beta-atms	I/-
33	1, 4	Diffusion coefficient, m ² /s	CV-123-DifC-atms	I/-
34	2, 3	Surface tension, N/m	CV-123-Sigm-drop	I/-
Atmosphere and bubble gas data				
35		Atmosphere, mass of given gas, kg	CV-123- <u> </u> Mag-H2- <u> </u>	I/E
36	1=H ₂	Atmosphere, gas partial pressure, Pa	CV-123-PPag-He- <u> </u>	I/-
37	2=He	Atmosphere, mass fraction of given gas	CV-123-CMag-H2O- <u> </u>	I/E
38	3=H ₂ O	Atmosphere, volume fraction of gas	CV-123-CVag-N2- <u> </u>	I/E
39	4=N ₂	Bubbles, mass of given gas, kg	CV-123- <u> </u> Mpg-O2- <u> </u>	I/E
40	5=O ₂	Bubbles, gas partial pressure, Pa	CV-123-PPpg-CO2- <u> </u>	I/-
41	6=CO ₂	Bubbles, mass fraction of given gas	CV-123-CMpg-H2- <u> </u>	I/E
42		Bubbles, volume fraction of gas	CV-123-CVpg-He- <u> </u>	I/E
43	1=atms 2=bubb	Relative humidity	CV-123-RHum-atms CV-123-RHum-bubb	I/-
Dispersed component - particle data (bubbles and droplets)				
44		Number of particles in a continuous component of a CV	CV-123-P_No-drop	I/E
45	1=drop	Average position (bubb: from bottom, drop: from top), m	CV-123-P_Po-bubb	I/E
46	2=bubb	Average diameter of a single particle, m	CV-123-P_Di-drop	I/-
47		Average volume of a single particle, m ³	CV-123-P_Vo-bubb	I/-
Mass sources - Junction source data				
48	1=atms	Total mass source from all JN into a CV, kg/s	CV-123-WmJN-atms	I/-
49	2=drop 3=pool 4=bubb	Enthalpy source associated with the mass source, J/s	CV-123-HmJN-drop	I/-
50	consec	Diameter of created droplets, m	CV-123-DdJN-0001	I/-
51	JN	Diameter of created bubbles, m	CV-123-DbJN-0002	I/-
52	number	Droplet source strength, drop/s	CV-123-SdJN-0003	I/-
53	in CV	Bubble source strength, bubb/s	CV-123-SbJN-0004	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

continued.

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
Mass source data - 1-D Solid Heat Conductor source data				
54	1=atms	Total mass source from all SC mass transfer	CV-123-WmSC-atms	I/-
55	2=drop 3=pool 4=bubb	(boiling, condensation) in a CV, kg/s Enthalpy source associated with the mass source, J/s	CV-123-HmSC-drop	I/-
56	consec	Diameter of created droplets, m	CV-123-DdSC-0001	I/-
57	SC	Diameter of created bubbles, m	CV-123-DbSC-0002	I/-
58	number	Droplet source strength, drop/s	CV-123-SdSC-0003	I/-
59	in CV	Bubble source strength, bubb/s	CV-123-SbSC-0004	I/-
Mass source data - Non-equilibrium mass transfer data				
60	1=atms	Total mass source from all non-equilibrium processes,	CV-123-WmNE-atms	I/-
61	2=drop 3=pool 4=bubb	(flashing, fogging) in a CV, kg/s Enthalpy source associated with the mass source, J/s	CV-123-HmNE-drop	I/-
62		Diameter of created droplets, m	CV-123-DdNE-0000	I/-
63	-	Diameter of created bubbles, m	CV-123-DbNE-0000	I/-
64		Droplet source strength, drop/s	CV-123-SdNE-0000	I/-
65		Bubble source strength, bubb/s	CV-123-SbNE-0000	I/-
Mass source data - Inter-phase mass transfer data				
66	1=atms	Total mass source from all inter-phase processes,	CV-123-WmIN-atms	I/E
67	2=drop 3=pool 4=bubb	(evaporation, condensation) in a CV, kg/s Enthalpy source associated with the mass source, J/s	CV-123-HmIN-drop	I/-
68	1=pool	Inter-phase area, m ²	CV-123-A_IN-pl>a	I/E
69	-atms	Mass flux at the inter-phase, kg/s/m ²	CV-123-W_IN-dp>a	I/-
70	2=drop	Heat flux at the inter-phase, W/m ²	CV-123-QhIN-pl>b	I/-
71	-atms	Enthalpy flux due to mass transfer, W/m ²	CV-123-QmIN-pl>a	I/-
72	3=bubb -pool	Liquid temperature at the inter-phase, K	CV-123-TlIN-dp>a	I/-
Mass source data - De-entrainment data				
73	1=atms	Total mass source from all de-entrainment processes,	CV-123-WmDE-atms	I/-
74	2=drop 3=pool 4=bubb	(droplet, bubble; vertical horizontal) in a CV, kg/s Enthalpy source associated with the mass source, J/s	CV-123-HmDE-drop	I/-
75	1=drop vert. 2=drop hor. 3=bubb vert.	Mass transfer fluxes from individual processes, kg/s	CV-123-WiDE-dp>v CV-123-WiDE-dp>h CV-123-WiDE-bb>v	I/-
Mass source data - Tabular mass sources				
76	1=atms	Total mass source from all tabular mass sources	CV-123-WmMS-atms	I/-
77	2=drop 3=pool 4=bubb	in a CV, kg/s Enthalpy source associated with the mass source, J/s	CV-123-HmMS-drop	I/-
78	consec	Diameter of created droplets, m	CV-123-DdMS-0001	I/-
79	source	Diameter of created bubbles, m	CV-123-DbMS-0002	I/-
80	number	Droplet source strength, drop/s	CV-123-SdMS-0003	I/-
81	in CV	Bubble source strength, bubb/s	CV-123-SbMS-0004	I/-
Energy source data				
82		Total energy source due to convection from all SC, W	CV-123-Q_SC-atms	I/-
83	1=atms	Total energy source due to radiation from all SC, W	CV-123-Qrad-drop	I/-
84	2=drop	Total energy source due to inter-phase processes, W	CV-123-Q_IN-pool	I/-
85	3=pool	Total energy source for pool due to bubble collapse, W	CV-123-Qcol-bubb	I/-
86	4=bubb	Total energy source due to tabular energy sources, W	CV-123-Q_ES-atms	I/-
87		Work, ($\rho \cdot dV/dt$), W	CV-123-PdVT-drop	I/-
Bubble collapse data for Junction flows				
88		Bubble collapse time, s	CV-123-TcJN-0001	I/-
89	consec	Bubble flow time, s	CV-123-TfJN-0002	I/-
90	JN	Pool bypass fraction	CV-123-PsJN-0003	I/-
91	number	Heat transfer coefficient during bubble collapse, W/m ² K	CV-123-HtJN-0004	I/-
92		Heat flux, W/m ²	CV-123-QtJN-0005	I/-
Bubble collapse data for Solid Heat Conductors				
93		Bubble collapse time, s	CV-123-TcSC-0001	I/-
94	consec	Bubble flow time, s	CV-123-TfSC-0002	I/-
95	SC	Pool bypass fraction	CV-123-PsSC-0003	I/-
96	number	Heat transfer coefficient during bubble collapse, W/m ² K	CV-123-HtSC-0004	I/-
97		Heat flux, W/m ²	CV-123-QtSC-0005	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

continued.

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
Bubble collapse data for the tabular mass sources				
98		Bubble collapse time, s	CV-123-TcMS-0001	I/-
99	consec	Bubble flow time, s	CV-123-TfMS-0002	I/-
100	source	Pool bypass fraction	CV-123-PsMS-0003	I/-
101	number	Heat transfer coefficient during bubble collapse, W/m ² K	CV-123-HtMS-0004	I/-
102		Heat flux, W/m ²	CV-123-QtMS-0005	I/-
Summed quantities - individual gas masses (second pointer, IARG2C=000)				
103	1=H ₂ 2=He 3=H ₂ O	Sum of masses of a given gas in the atmosphere of all CV in the model, kg	CV-000-MagT-H2__ CV-000-MagT-He__ CV-000-MagT-H2O__	I/-
104	4=N ₂ 5=O ₂ 6=CO ₂	Sum of masses of a given gas in the pool bubbles of all CV in the model, kg	CV-000-MpgT-N2__ CV-000-MpgT-O2__ CV-000-MpgT-CO2__	I/-
Summed quantities - component data (second pointer, IARG2C=000)				
105	1=atms 2=drop	Sum of the volumes occupied by a given component in all CV in the model, m ³	CV-000-VolT-atms	I/-
106	3=pool	Sum of the masses of a given component in all CV, kg	CV-000-MasT-drop	I/-
107	4=bubb	Sum of the energies of a given component in all CV, kg	CV-000-EnrT-pool	I/-
Summed quantities - overall data (second pointer, IARG2C=000)				
108		Sum of the volumes occupied by all components in all CV in the model, m ³	CV-000-VolX-0000	I/-
109		Sum of the masses of all components in all CV, kg	CV-000-MasX-0000	I/-
110	-	Sum of the energies of all components in all CV, kg	CV-000-EnrX-0000	I/-
111		Mass error, kg	CV-000-ErrM-0000	I/-
112		Energy error, J	CV-000-ErrE-0000	I/-
Hydrogen burn data				
113		Igniter temperature, K	CV-123-Tign-0000	I/-
114		Maximum temperature of all structures present in CV, K	CV-123-Twal-0000	I/-
115		Gas temperature, K	CV-123-Tgas-0000	I/-
116		Gas velocity, m/s	CV-123-Vgas-0000	I/-
117		Gas flammability, 0 = inflammable 1 = slow deflagration expected if ignited 2 = FTD expected 3 = detonation expected	CV-123-Flam-0000	I/-
118	-	Burn mode, 0 = no burn 1 = slow deflagration in progress 2 = FTD in progress 3 = detonation in progress	CV-123-Burn-0000	I/E
119		Flame velocity, m/s	CV-123-Vflm-0000	I/E
120		H ₂ consumption rate, kg/s	CV-123-mH2-0000	I/-
121		O ₂ consumption rate, kg/s	CV-123-mO2-0000	I/-
122		H ₂ O production rate, kg/s	CV-123-mH2O-0000	I/-
123		Heat produced due to burn, W	CV-123-Qbrn-0000	I/-
124		Time of start of burn (zero if no burn), s	CV-123-Tbrn-0000	I/-
125		Length flame has propagated since start of burn, m	CV-123-Prop-0000	I/-
126		H ₂ fraction expected at the end of the burn	CV-123-Feob-0000	I/-
127		Shock wave pressure, Pa	CV-123-PshW-0000	I/-
128		Critical elevation (stratified volumes)	CV-123-Zcrt-0000	I/-
129	1=H ₂ 2=He 3=H ₂ O 4=N ₂ 5=O ₂ 6=CO ₂	Gas volume fractions at the critical elevation	CV-123-Ccrt-H2__ CV-123-Ccrt-He__ CV-123-Ccrt-H2O__ CV-123-Ccrt-N2__ CV-123-Ccrt-O2__ CV-123-Ccrt-CO2__	I/-
Oxidation data				
130	1=H ₂ 2=He 3=H ₂ O	Mass source due to oxidation reactions in a CV, kg/s	CV-123-WmOX-H2__ CV-123-WmOX-He__ CV-123-WmOX-H2O__	I/-
131	4=N ₂ 5=O ₂ 6=CO ₂	Specific enthalpy of oxidizing gases, J/kg	CV-123-HmOX-N2__ CV-123-HmOX-O2__ CV-123-HmOX-CO2__	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

continued - Homogeneous Control Volumes

Pointer 1: IARG1C = 1, Control Volume Data Base

Code name: CV

Pointer 2: IARG2C = CV reference number

Code name: three digits

Pointers 3, 4		Description	Code Name Example	Impl/Expl
IARG3C	IARG4C			
Stratification data				
Thermodynamic data				
13	3	Volume center pressure, Pa	CV-123-Pres-pool	I/E
17	1	Void fraction, -, (volume fraction of gas)	CV-123-VolF-atms	I/-
18	1	Mass fraction of gas, -	CV-123-MasF-atms	I/-
14	1=gas 3=liq	Temperature, K	CV-123-Temp-atms	I/E
15		Saturation temperature, K	CV-123-Tsat-pool	I/E
16		Saturation pressure, Pa	CV-123-Psat-atms	I/-
19		Volume, m ³	CV-123-Volm-pool	I/E
20		Mass, kg	CV-123-Mass-atms	I/E
21		Total internal energy, J	CV-123-Enrg-pool	I/E
22		Vertical velocity (gas down; pool bubb: up), m/s	CV-123-Vvrt-atms	I/E
23		Horizontal velocity, m/s	CV-123-Vhor-pool	I/E
Fluid property data				
24	1=gas 3=liq	Density, m ³ /s	CV-123-Dens-atms	I/E
25		Specific internal energy, J/kg	CV-123-SEnr-pool	I/-
26		Specific enthalpy, J/kg	CV-123-Enth-atms	I/E
27		Viscosity, kg/m/s	CV-123-Visc-pool	I/-
28		Thermal conductivity, W/m/K	CV-123-Tcon-atms	I/-
29		Specific heat at constant pressure, c _p , J/kg/K	CV-123-__Cp-pool	I/E
30		Specific heat at constant volume, c _v , J/kg/K	CV-123-__Cv-atms	I/E
31		Prandtl number	CV-123-__Pr-pool	I/-
32		Thermal expansion coefficient, 1/K	CV-123-Beta-atms	I/-
33		1=gas	Diffusion coefficient, m ² /s	CV-123-DifC-atms
34	3=liq	Surface tension, N/m	CV-123-Sigm-pool	I/-

Other parameters (IARG3C > 35) are available as for heterogeneous Control Volumes but only parameters with the suffixes: -atms and -pool are available, with -atms meaning the gas phase and -pool meaning the liquid phase. Parameters with the suffixes: -bubb -drop are not available, except for bubble or droplet diameter and volume, CV-xxx-P_Di-bubb, CV-xxx-P_Di-drop, CV-xxx-P_Vo-bubb, CV-xxx-P_Vo-drop.

Apart from the -bubb -drop, the following plot parameters are not available and should not be used for the homogeneous CV:

Volume fraction of liquid CV-xxx-VolF-pool (use: 1.0 - CV-xxx-VolF-atms)

Mass fraction of liquid CV-xxx-MasF-pool (use: 1.0 - CV-xxx-MasF-atms)

The pool level can be used. It gives the collapsed liquid level in a homogeneous CV:

Pool level: CV-xxx-Zpls-0000 collapsed liquid level.

The volume-center Control Volume pressure is available as the plot parameter: CV-XXX-Pres-pool. The plot parameter: CV-XXX-Pres-atms gives the pressure at the collapsed liquid level in CV (in a gas-filled CV this is the pressure at the CV bottom; in a liquid-filled CV this is the pressure at the CV top).

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-24 List of arguments available for Control Functions, variables available in Junction Data Base.

Pointer 1: IARG1C = 2, Junction Data Base

Code name: JN

Pointer 2: IARG2C = JN reference number

Code name: three digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
Component data				
1		Velocity, m/s	JN-234-Velo-atms	I/E
2		Mass flow, kg/s	JN-234-Flow-drop	I/E
3	1=atms	Flow area, m ²	JN-234-Area-pool	I/E
4	2=drop	Temperature, K	JN-234-Temp-bubb	I/-
5	3=pool	Density, kg/m ³	JN-234-Dens-atms	I/-
6	4=bubb	Specific enthalpy, J/kg	JN-234-Enth-drop	I/-
7		Specific heat at constant pressure, c _p , J/kg/K	JN-234-__Cv-pool	I/-
8		Specific heat at constant volume, c _v , J/kg/K	JN-234-__Cp-bubb	I/-
Gas composition data				
9	1=H ₂	Atmosphere gas - mass fraction of given gas	JN-234-CMag-H2__	I/-
10	2=He	Atmosphere gas - volume fraction of given gas	JN-234-CVag-He__	I/-
11	3=H ₂ O	Pool bubbles - mass fraction of given gas	JN-234-CMpg-H2O__	I/-
12	4=N ₂	Pool bubbles - volume fraction of given gas	JN-234-CVpg-N2__	I/-
	5=O ₂			
	6=CO ₂			
Overall data				
13		Flow area of gas (atmosphere + bubbles), m ²	JN-234-Agas-0000	I/-
14		Flow area of liquid (pool + droplets), m ²	JN-234-Aliq-0000	I/-
15		Total flow area, m ²	JN-234-Area-0000	I/E
16		Mass flow of gas (atmosphere + bubbles), kg/s	JN-234-Wgas-0000	I/-
17		Mass flow of liquid (pool + droplets), kg/s	JN-234-Wliq-0000	I/-
18	-	Total mass flow, kg/s	JN-234-Wtot-0000	I/-
19		Average enthalpy of gas (atmosphere & bubbles), J/kg	JN-234-Hgas-0000	I/-
20		Average enthalpy of liquid (pool & droplets), J/kg	JN-234-Hliq-0000	I/-
21		Average enthalpy of fluid (gas & liquid), J/kg	JN-234-Htot-0000	I/-
22		Average velocity of gas (atmosphere & bubbles), m/s	JN-234-Vgas-0000	I/-
23		Average velocity of liquid (pool & droplets), m/s	JN-234-Vliq-0000	I/-
24	1=H ₂	Average gas composition (atmosphere & bubbles)	JN-234-Cgas-H2__	I/-
	2=He	NOTE:	JN-234-Cgas-He__	I/-
	3=H ₂ O	If diffusion parameters are requested (input record	JN-234-Cgas-H2O__	I/-
	4=N ₂	256000, LDIFUN=2), then this parameter is replaced by:	JN-234-Cgas-N2__	I/-
	5=O ₂	Volume transfer rate due to diffusion, m ³ /s, e.g.:	JN-234-Cgas-O2__	I/-
	6=CO ₂	JN-234-VDif-H2	JN-234-Cgas-CO2__	I/-
Valve data				
25	-	Fraction open	JN-234-FrOp-0000	I/-
Critical flow data				
26	-	Critical flow indicator	JN-234-__ICF-0000	I/-
27	-	Critical mass flux, kg/m ² /s	JN-234-__Gcrt-0000	I/-
Atmosphere and pool data				
28		Pressure at JN elevation, upstream (from) CV, Pa	JN-234-__P-F-atms	I/E
29	1=atms	Pressure at JN elevation, downstream (to) CV, Pa	JN-234-__P-T-pool	I/E
30	2=pool	Reynolds number	JN-234-__Re-atms	I/-
31		Wall friction factor	JN-234-__ff-pool	I/-
32		Form loss factor (K-factor), (-)	JN-234-Kfac-atms	I/-
33		Pool level in JN, m	JN-234-Zpol-0000	I/-
34	-	Ratio of c _p /c _v for gas (atmosphere & bubbles)	JN-234-CpCv-0000	I/-
35		Density of gas (atmosphere & bubbles), kg/m ³	JN-234-Rgas-0000	I/-
Pump/compressor/turbine data				
36		Pump/compressor/turbine speed, rev/s	JN-234-PSpd-atms	I/-
37		Pump/compressor/turbine volumetric flow, m ³ /s	JN-234-PVfl-pool	I/E
38	1=atms	Pump/compressor/turbine pressure ratio	JN-234-PRpr-atms	I/E
39	2=pool	Pump/compressor/turbine pressure head, Pa	JN-234-PHef-pool	I/-
40		Pump/compressor/turbine degradation factor (surge)	JN-234-PHdf-atms	I/-
41		Pump/compressor/turbine efficiency	JN-234-PEff-pool	I/E
42		Pump/compressor/turbine power into fluid, W	JN-234-QPmp-atms	I/E
43		Pump/compressor/turbine total power into fluid, W	JN-234-QPmp-0000	I/E
44	-	Pump/compressor/turbine friction power, =4π ² C _f ω ³ , W	JN-234-Qfrp-0000	I/-
45		Pump/compressor/turbine fluid plus friction power, W	JN-234-QPfp-0000	I/-
46	1=atms	Reduced flow divided by a function of reduced speed:	JN-234-Vred-atms	I/-
	2=pool	$V_R / (\omega R^{a-b})^{1/c}$, -	JN-234-Vred-pool	I/-
Friction pressure loss + Local pressure loss				
47	1=atms	Single phase pressure loss (friction + local), [Pa]	JN-234-DPfr-atms	I/-
	2=pool	$dP(f+K) = (K + fL/D)(\rho v^2/2)$	JN-234-DPfr-pool	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-25 List of arguments available for Control Functions,
variables available in 1-D Solid Heat Conductor Data Base.

Pointer 1: IARG1C = 3, 1-D Solid Heat Conductor Data Base Code name: SC

Pointer 2: IARG2C = SC reference number Code name: three digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
SC surface data				
1	-1=left +1=right	Fraction of the surface immersed in the pool of a CV	SC-345-Pool-left	I/-
2	cell No or 0	Internal heat generation, W, in a cell of a single SC or total SC (including multiplicity) when IARG4C=0 If IQPLSC=2, power density (W/m ³) (SC-345-qcel-0001)	SC-345-Qcel-0001	I/-
Fluid data at SC surfaces				
3	<0=left	Fluid temperature, K	SC-345-Tfld-l-at	I/-
4	>0=right	Heat transfer coefficient, W/m ² /K (for fins->19)	SC-345-HTC-l-pl	I/-
5	1 =atms	Convective heat flux, W/m ² (for fins->20)	SC-345-Fcnv-l-rp	I/-
6	2 =pool	Convective heat, W (total, including multiplicity)	SC-345-Qcnv-r-at	I/-
7	3 =repr	Fluid velocity, m/s (only 1 and 2 for IARG4C)	SC-345-Vfld-r-pl	I/-
Thermal radiation data				
8	-1=left	Radiative heat flux, W/m ²	SC-345-Frad-left	I/-
9	+1=right	Radiative heat, W (total, including multiplicity)	SC-345-Qrad-righ	I/-
Local gas or particle concentrations at the SC surface				
10	<0=left >0=right 1 =H ₂ 2 =He 3 =H ₂ O	Volume fraction of gas or particle type	SC-345-Vfrc-H2_l SC-345-Vfrc-H2O1 SC-345-Vfrc-CO2l SC-345-Vfrc-dp.l SC-345-Vfrc-bb.l	I/E
11	4 =N ₂ 5 =O ₂ 6 =CO ₂ 7 =drop 8 =bubb	Mass fraction of gas or particle type	SC-345-Mfrc-H2_r SC-345-Mfrc-H2Or SC-345-Mfrc-CO2r SC-345-Mfrc-dp.r SC-345-Mfrc-bb.r	I/E
Condensation and boiling data				
12		Condensate film thickness, m	SC-345-Dcnd-left	I/-
13	-1=left	Critical heat flux, W/m ²	SC-345-qCHF-righ	I/-
14	+1=right	Condensation mass transfer rate, kg/m ² /s	SC-345-Mcnd-left	I/-
15		Boiling mass transfer rate, kg/m ² /s	SC-345-Mboi-righ	I/-
Mesh cell data				
16	cell No. or 0	Cell temperature, K or volume-averaged SC temperature when IARG4C=0	SC-345-Tcel-0001	I/E
Extended surfaces (fins, spines) data				
17		Efficiency of fins	SC-345-EffF-l-at	I/-
18	<0=left	Enhancement of heat & mass transfer due to fins	SC-345-EnhF-l-pl	I/-
19	>0=right	True heat transfer coefficient, W/m ² /K (do not use 4)	SC-345-HTCF-r-at	I/-
20	1 =atms	True heat flux, W/m ² (do not use 5)	SC-345-qcnF-r-pl	I/-
21	2 =pool	True mass flux, kg/m ² /s	SC-345-MmtF-l-at	I/-
22		True enthalpy flux due to mass flux, W/m ²	SC-345-HmtF-l-pl	I/-
23		Fin average temperature based on fin efficiency, K	SC-345-Tfin-r-at	I/-
Summed quantities (second pointer, IARG2C=000)				
24		Sum of convective heat of all SC, W	SC-000-QcnS-0000	I/-
25		Sum of integrated convective heat of all SC, J	SC-000-QcnI-0000	I/-
26	-	Sum of radiative heat of all SC, W	SC-000-QrdS-0000	I/-
27		Sum of integrated radiative heat of all SC, J	SC-000-QrdI-0000	I/-
28		Sum of convective + radiative heat of all SC, W	SC-000-QttS-0000	I/-
29		Sum of integrated convective+radiative heat all SC, W	SC-000-QttI-0000	I/-
Oxidation data				
30		Thickness of the un-oxidized material, m	SC-345-XMtl-left	I/E
31		Thickness of the oxide layer, m	SC-345-XOxd-righ	I/E
32	-1=left +1=right	Total gas consumption rate due to oxidation, kg/m ² /s (for multiple reactions sum of all reacting gases)	SC-345-W1OX-left	I/-
33		Total gas generation rate, kg/m ² /s (for multiple reactions sum of all produced gases)	SC-345-W2OX-righ	I/-
34		Total heat generation due to oxidation reactions, W/m ²	SC-345-Qoxi-left	I/-
Failure data (or graphite ignition parameters - see below)				
35		Cumulative damage, (-)	SC-345-CDam-0000	I/E
36	-	Time to failure, (s)	SC-345-TtFl-0000	I/-
37		Failure mode, (-) (1=u.strength, 2=creep, 3=meltdown)	SC-345-Fail-0000	I/-
38		Time of failue (if occurred, zero otherwise)	SC-345-ToFl-0000	I/-
Gap data				
39		Gap thickness, (m)	SC-345-xGap-0000	I/-
40	-	Gap conductance, (W/m ² -K)	SC-345-hGap-0000	I/-
41		Gap left (fuel outer surface) temperature (K)	SC-345-Tfue-0000	I/-
42		Gap right (clad inner surface) temperature (K)	SC-345-Tcld-0000	I/-
BDC data				
43	-1=left +1=right	BDC heat flux, W/m ²	SC-345-qBDC-left	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

Notes:

(1) For IARG3C = 3 through 6 the user can request three values

- atmosphere
- pool
- representative

Definition of the representative values is provided in Volume 1, section: "Representative Boundary Conditions". The representative values are recommended for general use. In the case of 2-D Solid Heat Conductors only the representative values are available for IARG3C = 3 through 6.

(2) If the graphite oxidation model of Roes is used (IOXLSC/IOXRSC=-5), the graphite ignition criterion is calculated from the correlation shown in Volume 1. In such case the ignition parameters may be plotted using IARG3C = 35 through 38. This is possible only if the failure model is not simultaneously used. In such case the plot parameters are defined as follows:

Graphite ignition parameters				
35		Ignition temperature (K), left surface	SC-345-CDam-0000	I/E
36	-	Time when the ignition temperature was exceeded (s)	SC-345-TtF1-0000	I/-
37		Ignition temperature (K), right surface	SC-345-Fail-0000	I/-
38		Time when the ignition temperature was exceeded (s)	SC-345-ToF1-0000	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-26 List of arguments available for Control Functions, variables available in 2-D Solid Heat Conductor Data Base.

Pointer 1: IARG1C = 4, 2-D Solid Heat Conductor Data Base Code name: TC
 Pointer 2: IARG2C = TC reference number Code name: three digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
TC surface (boundary cell) data				
1	boundary cell No.	Fraction of the surface immersed in the pool of a CV	TC-456-Pool-0001	I/-
2	cell No or 0	Internal heat generation, W, in a cell of a single TC or total TC (including multiplicity) when IARG4C=0 If IQPLTC=2, power density (W/m ³) (TC-456-qcel-0001)	TC-456-Qcel-0001	I/-
Fluid data at TC surfaces (boundary cells)				
3	boundary cell No.	Fluid temperature, K	TC-456-Tfld-0001	I/-
4		Heat transfer coefficient, W/m ² /K	TC-456-HTC-0002	I/-
5		Convective heat flux, W/m ²	TC-456-Fcnv-0003	I/-
6		Convective heat, W (total, including multiplicity)	TC-456-Qcnv-0004	I/-
7		Fluid velocity, m/s	TC-456-Vfld-0005	I/-
Thermal radiation data at TC surfaces (boundary cells)				
8	boundary cell No.	Radiative heat flux, W/m ²	TC-456-Frad-0001	I/-
9		Radiative heat, W (total, including multiplicity)	TC-456-Qrad-0002	I/-
Local steam concentrations at the TC surfaces (boundary cells)				
10	boundary cell No.	Volume fraction of steam at the boundary cell surface	TC-456-Vfrc-0001	I/E
11		Mass fraction of steam at the boundary cell surface	TC-456-Mfrc-0002	I/E
Condensation and boiling data at TC surfaces (boundary cells)				
12	boundary cell No.	Condensate film thickness, m	TC-456-Dcnd-0001	I/-
13		Critical heat flux, W/m ²	TC-456-qCHF-0002	I/-
14		Condensation mass transfer rate, kg/m ² /s	TC-456-Mcnd-0003	I/-
15		Boiling mass transfer rate, kg/m ² /s	TC-456-Mboi-0004	I/-
Mesh cell data				
16	cell No. or 0	Cell temperature, K (*) or volume-averaged SC temperature when IARG4C=0	TC-456-Tcel-0001	I/E
Summed quantities (second pointer, IARG2C=000)				
17	-	Sum of convective heat of all TC, W	TC-000-QcnT-0000	I/-
18		Sum of integrated convective heat of all TC, J	TC-000-QcnI-0000	I/-
19		Sum of radiative heat of all TC, W	TC-000-QrdT-0000	I/-
20		Sum of integrated radiative heat of all TC, J	TC-000-QrdI-0000	I/-
21		Sum of convective + radiative heat of all TC, W	TC-000-QttT-0000	I/-
22		Sum of integrated convective+radiative heat all TC, W	TC-000-QttI-0000	I/-
Oxidation data at TC surfaces (boundary cells)				
23	boundary cell No.	Thickness of the un-oxidized material, m	TC-456-XMtl-0001	I/E
24		Thickness of the oxide layer, m	TC-456-XOxd-0002	I/E
25		Total gas consumption rate due to oxidation, kg/m ² /s (for multiple reactions sum of all reacting gases)	TC-456-W1OX-0003	I/-
26		Total gas generation rate, kg/m ² /s (for multiple reactions sum of all produced gases)	TC-456-W2OX-0004	I/-
27		Total heat generation due to oxidation reactions, W/m ²	TC-456-Qoxi-0005	I/-
Failure data				
28	-	Cumulative damage, (-)	TC-456-CDam-0000	I/E
29		Time to failure, (s)	TC-456-TtFl-0000	I/-
30		Failure mode, (-) (1=u.strength, 2=creep, 3=meltdown)	TC-456-Fail-0000	I/-
31		Time of failue (if occurred, zero otherwise)	TC-456-ToFl-0000	I/-
Gap data				
32	axial level No	Gap thickness, (m)	TC-456-xGap-0001	I/-
33		Gap conductance, (W/m ² -K)	TC-456-hGap-0002	I/-
34		Fuel surface (gap left) temperature (K)	TC-456-Tfue-0003	I/-
35		Cladding surface (gap right) temperature (K)	TC-456-TclD-0004	I/-
BDC data				
36	boundary cell No.	BDC heat flux, W/m ²	TC-456-qBDC-0001	I/-

(*) Note: in the case of cell temperatures (IARG3C=16), the cell numbers are as follows.
 - For plotting: xyyy, where xx is the column number and yy is the row number.
 - For Control Functions: internal cell number printed in the *.OUT file, e.g.:

=TC= TC-100, CELL NUMBERING MAP

```

\ K:  1  2  3  4  5  6  7  8  9 10
L \  -----
1  0001 0002 0003 0004 0005 0006 0007 0008 0009 0010
2  0011 0012 0013 0014 0015 0016 0017 0018 0019 0020
3  0021 0022 0023 0024 0025 0026 0027 0028 0029 0030
    
```

In this example, the cell number 26 has the plotting number (in the *.PLT file) of 0603.

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3,4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
MCCI data (MC)				
The second pointer must refer to the first TC in the model if more TCs are present				
MCCI data per cell				
37	cell No.	X-velocities, (m/s)	TC-456-VelX-0001	I/E
38		Y-velocities, (m/s)	TC-456-VelY-0001	I/E
39		Porosity of the cell, (-)	TC-456-Poro-0001	I/E
40		Concrete fraction in a cell, (-)	TC-456-XCon-0001	I/E
41		Corium fraction in a cell, (-)	TC-456-XCor-0002	I/-
42		Liquid fraction in a cell, (-)	TC-456-XLiq-0003	I/-
43		Ablated fraction in a cell, (-)	TC-456-XAbl-0004	I/E
Metals in corium				
44	0	Total mass of metals in corium (kg)	TC-456-MMet-0000	I/E
45		Total mass of Fe in corium (kg)	TC-456-MMFe-0000	I/E
46		Total mass of Cr in corium (kg)	TC-456-MMcr-0000	I/E
47		Total mass of Ni in corium (kg)	TC-456-MMni-0000	I/E
48		Total mass of Zr in corium (kg)	TC-456-MMZr-0000	I/E
Concrete ablation				
49	-	Volume of ablated concrete (m ³)	TC-456-VAbl-0000	I/E
50		Mass of ablated concrete (kg)	TC-456-MAbl-0000	I/E
Gas release due to MCCI				
51	-	Total mass of H ₂ O released, (kg)	TC-456-MH2O-0000	I/E
52		Total mass of H ₂ released, (kg)	TC-456-MH2_-0000	I/E
53		Total mass of CO ₂ released, (kg)	TC-456-MCO2-0000	I/E
54		Total mass of CO released, (kg)	TC-456-MCO_-0000	I/E
55	-	Release rate of H ₂ O, (kg/s)	TC-456-RH2O-0000	I/E
56		Release rate of H ₂ , (kg/s)	TC-456-RH2_-0000	I/E
57		Release rate of CO ₂ , (kg/s)	TC-456-RCO2-0000	I/E
58		Release rate of CO, (kg/s)	TC-456-RCO_-0000	I/E
Heating data				
59	-	Heating rate by chemical reactions, (W)	TC-456-QChe-0000	I/E
60		Power used for concrete ablation, (W)	TC-456-QAbl-0000	I/E
61		Integrated heating rate by chemical reactions, (J)	TC-456-EChe-0000	I/E
62		Integrated power used for concrete ablation, (J)	TC-456-EAbl-0000	I/E
Maximum ablation data (m)				
63	-	Maximum ablation in radial (horizontal) direction, (m)	TC-456-RAbl-0000	I/-
64		Maximum ablation in axial (vertical) direction, (m)	TC-456-ZAbl-0000	I/-
Concrete and corium masses and volumes				
65		Total volume of concrete, (m ³)	TC-456-VCon-0000	I/-
66		Total mass of concrete, (kg)	TC-456-MCon-0000	I/-
67		Total volume of corium, (m ³)	TC-456-VCor-0000	I/-
68		Total mass of corium, (kg)	TC-456-MCor-0000	I/-
69		Total volume of concrete lost due to de-gassing, (m ³)	TC-456-VGas-0000	I/-
70		Total mass of concrete lost due to de-gassing, (kg)	TC-456-MGas-0000	I/E
71		Total volume of corium increase to oxidation, (m ³)	TC-456-VOxi-0000	I/-
72		Total mass of corium increase to oxidation, (kg)	TC-456-MOxi-0000	I/E

Table 2-27 List of arguments available for Control Functions, variables available in Thermal Radiation Data Base.

Pointer 1: IARG1C = 5, Thermal Radiation Data Base

Code name: TR

Pointer 2: IARG2C = TR system No. / surface reference No.

Code name: one digit / two digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
TR surface data				
1	-	Surface temperature, K	TR-511-Tsrf-0000	I/-
2		Surface emissivity	TR-512-Esrf-0000	I/-
3		Radiative heat flux, W/m ²	TR-513-Fsrf-0000	I/-
4		Radiative heat, W	TR-514-Qsrf-0000	I/-
Gas radiative properties				
5	j=other surface	Gas emissivity from current (511) to j (512) surface	TR-511-Egas-0512	I/-
6	surface	Gas absorptivity from current (513) to j (514) surf.	TR-513-Agas-0514	I/-
7	j=above	Gas emissivity from (511) to (512) through CV 01	TR-511-Eg01-0512	I/-
8	IARG5C: CV path	Gas absorptivity from (513) to (514) through CV 02	TR-513-Ag02-0514	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-28 List of arguments available for Control Functions, variables available in Radioactive Particle Transport Data Base.

Pointer 1: IARG1C = 8, Radioactive P. Transport Data Base Code name: RT (IARG1C=CV/JN/SC/TC/RT)
 Pointer 2: IARG2C = CV, JN, SC, or TC reference number Code name: three digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
PART I - AEROSOL DATA				
Control Volume related data (CV)				
Keep in mind that although these are CV related parameters, the pointer 1 is equal to 8 and not 1 IARG1C=8				
Airborne aerosols and aerosols suspended in the CV pool - sources and masses				
1		External (TF/CF) source of airborne aerosols, (kg/s)	CV-123-ASEm-0001	I/-
2		External (TF/CF) source of airborne aer. (part/m ³ -s)	CV-123-ASEp-0002	I/-
3		Release source of airborne aerosols, (kg/s)	CV-123-ASRm-0003	I/-
4		Release source of airborne aerosols, (part/m ³ -s)	CV-123-ASRp-0004	I/-
5		Airborne aerosol source due to all JN flows, (kg/s)	CV-123-ASJm-0005	I/-
6		Airborne aer. source due to all JN flows, (part/m ³ -s)	CV-123-ASJp-0001	I/-
7	Size section number	External (TF/CF) source of pool aerosols, (kg/s)	CV-123-PSEm-0002	I/-
8		External (TF/CF) source of pool aerosols, (part/m ³ -s)	CV-123-PSEp-0003	I/-
9		Release source of pool aerosols, (kg/s)	CV-123-PSRm-0004	I/-
10		Release source of pool aerosols, (part/m ³ -s)	CV-123-PSRp-0005	I/-
11		Pool aerosol source due to all JN flows, (kg/s)	CV-123-PSJm-0001	I/-
12		Pool aerosol source due to all JN flows, (part/m ³ -s)	CV-123-PSJp-0002	I/-
13		Airborne aerosol mass, (kg)	CV-123-Maer-0003	I/E
14		Airborne aerosol density, (part/m ³)	CV-123-Daer-0004	I/E
15		Airborne aerosol heat source (W)	CV-123-Qaer-0005	I/-
16		Airborne aerosol activity, (Bq)	CV-123-Aaer-0001	I/-
Airborne aerosols - data summed for all size sections				
17		Airborne aerosol mass, all size sections, (kg)	CV-123-SMae-0000	I/-
18	-	Airborne aerosol density, all size sections (part/m ³)	CV-123-SDae-0000	I/E
19		Airborne aerosol heat source, all size sections, (W)	CV-123-SQae-0000	I/-
20		Airborne aerosol activity, all size sections, (Bq)	CV-123-SAae-0000	I/-
Deposition and resuspension data for CV pool surface				
21		Deposition velocity, gravitational, (m/s)	CV-123-VdgP-0001	I/-
22		Deposition velocity, Brownian, (m/s)	CV-123-VdbP-0002	I/-
23		Deposition velocity, thermophoretic, (m/s)	CV-123-VdtP-0003	I/-
24		Deposition velocity, diffusiophoretic, (m/s)	CV-123-VddP-0004	I/-
25		Deposition velocity, turbulent impaction, (m/s)	CV-123-VdiP-0005	I/-
26		Deposition velocity, effective, (m/s)	CV-123-VdeP-0001	I/-
27	Size section number	Deposition rate for CV pool surface, (kg/s)	CV-123-DRPL-0002	I/-
28		Resuspension rate for CV pool surface, (kg/s)	CV-123-RRPL-0003	I/-
29		Deposition rate, total including SC/TC, (kg/s)	CV-123-Depm-0004	I/-
30		Deposition rate, total including SC/TC, (part/m ³ -s)	CV-123-Depp-0005	I/-
31		Resuspension rates total including SC/TC, (kg/s)	CV-123-Resm-0001	I/-
32		Resuspension rates total including SC/TC, (part/m ³ -s)	CV-123-Resp-0002	I/-
33		Pool aerosol mass, (kg)	CV-123-MaeP-0003	I/E
34		Pool aerosol density, (part/m ³)	CV-123-DaeP-0004	I/E
35		Pool aerosol heat source (W)	CV-123-QaeP-0005	I/-
36		Pool aerosol activity, (Bq)	CV-123-AaeP-0001	I/-
Aerosols suspended in the CV pool - data summed for all size sections				
37		Pool aerosol mass, all size sections, (kg)	CV-123-SMaP-0000	I/-
38	-	Pool aerosol density, all size sections (part/m ³)	CV-123-SDaP-0000	I/-
39		Pool aerosol heat source, all size sections, (W)	CV-123-SQaP-0000	I/-
40		Pool aerosol activity, all size sections, (Bq)	CV-123-SAaP-0000	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3,4,5,6		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
<i>Junction related data (JN)</i>				
Keep in mind that although these are JN related parameters, the pointer 1 is equal to 8 and not 2 IARG1C=8				
<i>Junction area data</i>				
41	-	Area reduction due to aerosol deposition, (m2)	JN-234-Ared-0000	I/-
42		Mass flow of atmosphere aerosols, (kg/s)	JN-234-WmAf-0000	I/-
43	>0: sec.	Mass flow of pool aerosols, (kg/s)	JN-234-WmPf-0001	I/-
44	number	Efficiency of filter, (-)	JN-234-EffF-0002	I/-
45		Mass deposited on the filter, (kg)	JN-234-MdpF-0003	I/E
46	(42, 43:	Number of particles deposited on the filter, (-)	JN-234-NdpF-0004	I/-
47	=0:total	Heat of aerosols deposited on the filter, (W)	JN-234-QdpF-0005	I/-
48	flow)	Activity of aerosols deposited on the filter, (W)	JN-234-AdpF-0001	I/-
49		Deposited aerosol mass, all size sections, (kg)	JN-234-SMdf-0000	I/-
50	-	Deposited aerosol density, all size sec., (part/m2)	JN-234-SNdf-0000	I/-
51		Deposited aerosol heat source, all size sections, (W)	JN-234-SQdf-0000	I/-
52		Deposited aerosol activity, all size sections, (Bq)	JN-234-SAdf-0000	I/-
<i>1-D Solid Heat Conductor related data (SC)</i>				
Keep in mind that although these are SC related parameters, the pointer 1 is equal to 8 and not 3 IARG1C=8				
<i>SC surface deposition data for different size sections</i>				
53		Deposition velocity, gravity, size sec. No., (m/s)	SC-345-Vg01-0001	I/-
54		Deposition velocity, Brownian, size sec. No., (m/s)	SC-345-Vb02-0002	I/-
55	Surface	Deposition velocity, thermophoretic, sec. No., (m/s)	SC-345-Vt03-0001	I/-
56	number:	Deposition velocity, diffusio-phoretic, sec. No. (m/s)	SC-345-Vd04-0002	I/-
57	1=left	Deposition velocity, turbulent, size sec. No., (m/s)	SC-345-Vi05-0001	I/-
58	2=right	Deposition velocity, effective, size sec. No., (m/s)	SC-345-Ve01-0002	I/-
59	IARG5C:	Deposition rate for SC surface, size sec. No., (kg/s)	SC-345-DR02-0001	I/E
60	size sec	Resuspension rate for SC surface, sec. No., (kg/s)	SC-345-RR03-0002	I/-
61	=01-N _{sec}	Deposited aerosol mass, size sec. No., (kg)	SC-345-Md04-0001	I/E
62		Deposited aerosol density, size sec. No., (part/m2)	SC-345-Dd05-0002	I/E
63		Deposited aerosol heat source, size sec. No., (W)	SC-345-Qd01-0001	I/-
64		Deposited aerosol activity, size sec. No., (Bq)	SC-345-Ad02-0002	I/-
65	Surface number: 1=left 2=right IARG5C: size sec =01-N _{sec} IARG6C: F _a -sec.= =01-99	Deposited frac. in F _a -sec. No. (01), size sec. No.(03)	SC-345-0103-0001	I/-
<i>SC surface deposition - size sections independent data</i>				
66	Surface	Deposited aerosol mass, all size sections, (kg)	SC-345-SMd1-0001	I/-
67	number:	Deposited aerosol density, all size sec., (part/m2)	SC-345-SDd1-0002	I/-
68	1=left	Deposited aerosol heat source, all size sections, (W)	SC-345-SQd1-0001	I/-
69	2=right	Deposited aerosol activity, all size sections, (Bq)	SC-345-SAd1-0002	I/-
70		Thickness of deposited aerosol layer, (m)	SC-345-Tdp1-0001	I/-
71	Surface number	If IARG5C = 0: Deposition rate due to inertial impaction, (kg/s) If IARG5C > 0: Inertial impaction efficiency, size section No. (01)	SC-345-DrI1-0002	I/-
72	Surface	Reduction of atms. heat transfer due to deposition, %	SC-345-Ared-0001	I/-
73	number	Reduction of pool heat transfer due to deposition, %	SC-345-Pred-0002	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
<i>2-D Solid Heat Conductor related data (TC)</i>				
Keep in mind that although these are TC related parameters, the pointer 1 is equal to 8 and not 4 IARG1C=8				
TC surface deposition data for different size sections				
74		Deposition velocity, gravity, size sec. No., (m/s)	TC-456-Vg01-0001	I/-
75		Deposition velocity, Brownian, size sec. No., (m/s)	TC-456-Vb02-0002	I/-
76	Boundary	Deposition velocity, thermophoretic, sec. No., (m/s)	TC-456-Vt03-0003	I/-
77	cell	Deposition velocity, diffusiophoretic, sec. No. (m/s)	TC-456-Vd04-0004	I/-
78	number	Deposition velocity, turbulent, size sec. No., (m/s)	TC-456-Vi05-0005	I/-
79		Deposition velocity, effective, size sec. No., (m/s)	TC-456-Ve01-0006	I/-
80	IARG5C:	Deposition rate for TC surface, size sec. No., (kg/s)	TC-456-DR02-0007	I/E
81	size sec	Resuspension rate for TC surface, sec. No., (kg/s)	TC-456-RR03-0008	I/-
82	=01-N _{sec}	Deposited aerosol mass, size sec. No., (kg)	TC-456-Md04-0009	I/E
83		Deposited aerosol density, size sec. No., (part/m ²)	TC-456-Dd05-0010	I/E
84		Deposited aerosol heat source, size sec. No., (W)	TC-456-Qd01-0011	I/-
85		Deposited aerosol activity, size sec. No., (Bq)	TC-456-Ad02-0012	I/-
86	Boundary cell number IARG5C: size sec =01-N _{sec} IARG6C: F _a -sec.= =01-99	Deposited frac. in F _a -sec. No.(01), size sec. No.(03)	TC-456-0103-0013	I/-
TC surface deposition - size sections independent data				
87		Deposited aerosol mass, all size sections, (kg)	TC-456-SMd2-0001	I/-
88	Boundary	Deposited aerosol density, all size sec., (part/m ²)	TC-456-SDd2-0002	I/-
89	cell	Deposited aerosol heat source, all size sections, (W)	TC-456-SQd2-0003	I/-
90	number	Deposited aerosol activity, all size sections, (Bq)	TC-456-SAd2-0004	I/-
91		Thickness of deposited aerosol layer, (m)	TC-456-Tdp2-0005	I/-
92	Boundary cell number	If IARG5C = 0: Deposition rate due to inertial impaction, (kg/s) If IARG5C > 0: Inertial impaction efficiency, size section No. (01)	TC-456-DrI2-0006 TC-456-IE01-0006	I/- I/-
93	Boundary	Reduction of atms. heat transfer due to deposition, %	TC-456-Ared-0007	I/-
94	cell no.	Reduction of pool heat transfer due to deposition, %	TC-456-Pred-0008	I/-
<i>Global parameters - Summed aerosol masses (RT)</i>				
95		Total mass of airborne aerosols in all CV, (kg)	RT-000-GMae-0000	I/-
96		Summed density of airborne aerosols, (part/m ³)	RT-000-GDae-0000	I/-
97		Total heat of airborne aerosols, (W)	RT-000-GQae-0000	I/-
98		Total activity of airborne aerosols, (Bq)	RT-000-GAae-0000	I/-
99		Total mass of pool aerosols in all CV, (kg)	RT-000-GMaP-0000	I/-
100		Summed density of pool aerosols, (part/m ³)	RT-000-GDaP-0000	I/-
101		Total heat of pool aerosols, (W)	RT-000-GQaP-0000	I/-
102	-	Total activity of pool aerosols, (Bq)	RT-000-GAaP-0000	I/-
103		Total mass of filter aerosols in all CV, (kg)	RT-000-GMdF-0000	I/-
104		Summed density of filter aerosols, (part/m ³)	RT-000-GDdF-0000	I/-
105		Total heat of filter aerosols, (W)	RT-000-GQdF-0000	I/-
106		Total activity of filter aerosols, (Bq)	RT-000-GAdF-0000	I/-
107		Total mass deposited on all SC, (kg)	RT-000-GMd1-0000	I/-
108		Summed density of SC deposited aerosols, (part/m ²)	RT-000-GDd1-0000	I/-
109		Total heat of SC deposited aerosols, (W)	RT-000-GQd1-0000	I/-
110		Total activity of SC deposited aerosols, (Bq)	RT-000-GAd1-0000	I/-
111		Total mass deposited on all TC, (kg)	RT-000-GMd2-0000	I/-
112		Summed density of TC deposited aerosols, (part/m ²)	RT-000-GDd2-0000	I/-
113		Total heat of TC deposited aerosols, (W)	RT-000-GQd2-0000	I/-
114		Total activity of TC deposited aerosols, (Bq)	RT-000-GAd2-0000	I/-
<i>Global parameters - Total aerosol mass and overall error (RT)</i>				
115		Sum of CV, SC, TC aerosol masses, M _{tot} , (kg)	RT-000-Mtot-0000	I/-
116	-	Integrated aerosol sources + initial mass, M _{src} , (kg)	RT-000-Msrc-0000	I/-
117		Aerosol mass error (M _{tot} - M _{src})/M _{tot} , (-)	RT-000-Merr-0000	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
PART II - RADIOACTIVE FISSION PRODUCT DATA				
<i>Core data (RT)</i>				
118		In-core mass at location L (L = IARG2C), (kg)	RT-001-MCor-0101	I/E
119	isotope	No. of nuclides at location L, (nucl.)	RT-001-NCor-0102	I/E
120	No.:0XXY	Decay heat of isotope XXY at location L, (W)	RT-001-QCor-0103	I/-
121		Activity of isotope XXY at location L, (Bq)	RT-001-ACor-0104	I/-
122	XX=chain	Gap mass of isotope XXY at location L, (kg)	RT-001-MGap-0111	I/E
123	Y=isot.	Gap fraction (gap mass divided by in-core mass), (-)	RT-001-FGap-0112	I/-
124		Released mass of isotope XXY at location L, (kg)	RT-001-MRel-0113	I/E
<i>Control Volume related data (CV) - Isotopes in CV atmosphere</i>				
Keep in mind that although these are CV related parameters, the pointer 1 is equal to 8 and not 1 IARG1C=8				
125	FP	Mass of FP vapor in atmosphere of CV, (kg)	CV-123-MVap-0001	I/-
126	vapor	Pressure of FP vapor in atmosphere of CV, (Pa)	CV-123-PVap-0002	I/-
127	number	Saturation pressure of FP vapor, (Pa)	CV-123-PsVp-0003	I/-
128	isotope	Mass of isotope XXY as vapor in CV atms., (kg) (000)	CV-000-MIAi-0101	I/E
129	No.:0XXY	No. of nuclides of XXY in atmosphere of CV, (nucl/m ³)	CV-123-NIAi-0102	I/E
130	XX=chain	Decay heat of XXY in atmosphere of CV, (W)	CV-123-QIAi-0103	I/-
131	Y=isot.	Activity of XXY in atmosphere of CV, (Bq)	CV-123-AIAi-0104	I/-
132		Mass of all isotopes as vapor in atms. of CV, (kg)	CV-123-MIAt-0000	I/-
133	-	No. of all nuclides in atmosphere of CV, (nucl/m ³)	CV-123-NIAt-0000	I/-
134		Decay heat of all nuclides in atmosphere of CV, (W)	CV-123-QIAt-0000	I/-
135		Activity of all nuclides atmosphere of CV, (Bq)	CV-123-AIAt-0000	I/-
136		External (TF/CF) source of isotope XXY, (kg/s)	CV-123-ESAm-0111	I/-
137		External (TF/CF) source of isotope XXY, (nucl/s)	CV-123-ESAn-0112	I/-
138		Core release source of isotope XXY, (kg/s)	CV-123-RSAm-0113	I/-
139		Core release source of isotope XXY, (nucl/s)	CV-123-RSAn-0114	I/-
140	isotope	Source of isotope XXY due to all JN flows, (kg/s)	CV-123-FSAm-0115	I/-
141	No.:0XXY	Source of isotope XXY due to all JN flows, (nucl/s)	CV-123-FSNn-0116	I/-
142	XX=chain	Total removal of XXY due to all adsorptions, (kg/s)	CV-123-AdAm-0121	I/E
143	Y=isot.	Total removal of XXY due to all adsorptions, (nucl/s)	CV-123-AdAn-0122	I/-
144		Total source of XXY due to all desorptions, (kg/s)	CV-123-DeAm-0123	I/E
145		Total source of XXY due to all desorptions, (nucl/s)	CV-123-DeAn-0124	I/-
146		Saturation mass of isotope XXY in atms. of CV, (kg)	CV-123-Msat-0131	I/-
147		Condensation mass transfer rate of XXY, (kg/s)	CV-123-Cond-0132	I/-
<i>Control Volume related data (CV) - Isotopes on aerosols in CV atmosphere</i>				
148	FP	Total mass, sorbed vapor (11), size sec.No.(01), (kg)	CV-123-MT01-0011	I/E
149	vapor	Penetrated mass, sorbed vap.(12), size.No.(02), (kg)	CV-123-MP02-0012	I/E
150	number	Sorption flux, vapor (13), size sec.No.(03), (kg/m ² -s)	CV-123-SF03-0013	I/-
151		C _{rev} of vapor (14) on size sec.No.(04), (kg/m ²)	CV-123-Cr04-0014	I/E
152	IARG5C:	Available sites, vapor (15) size sec.No.(05), (kg/m ²)	CV-123-Cx05-0015	I/-
153	size sec	C _{rev} of vapor (16) on size sec. No. (01), (nucl/m ²)	CV-123-Nr01-0016	I/E
154	=01-N _{sec}	Available sites, vapor (17) size sec.No.(02) (nucl/m ²)	CV-123-Nx02-0017	I/-
155	isotope No.:0XXY IARG5C: size sec =01-N _{sec}	No. of nuclides of XXY (321) on size sec. No. (05), (nucl/m ²)	CV-123-NA05-0321	I/E
156	isotope	Mass of isotope XXY on all size sec., (kg) (000)	CV-000-MAAi-0102	I/-
157	No.:0XXY	No. of nuclides of XXY on all size sec., (nucl)	CV-123-NAAi-0102	I/-
158	XX=chain	Decay heat of XXY on all size sec., (W)	CV-123-QAAi-0103	I/-
159	Y=isot.	Activity of XXY on all size sec., (Bq)	CV-123-AAAi-0104	I/-
160		Mass of all isotopes on all size sec. (kg)	CV-123-MAAt-0000	I/-
161	-	No. of all nuclides on all size sec., (nucl)	CV-123-NAAt-0000	I/-
162		Decay heat of all nuclides on all size sec., (W)	CV-123-QAAt-0000	I/-
163		Activity of all nuclides on all size sec., (Bq)	CV-123-AAAt-0000	I/-

(000) The second pointer may be zero instead of CV number; in such case the parameter gives the total mass for all Control Volumes.

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3, 4, 5		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
<i>Control Volume related data (CV) - Isotopes in CV pool</i>				
Keep in mind that although these are CV related parameters, the pointer 1 is equal to 8 and not 1 IARG1C=8				
164		Pool-gas mass transfer rate, (kg/s)	CV-123-FmPA-0101	I/-
165	isotope No.:0XXY	Pool-gas nuclide transfer rate, (nucl/s)	CV-123-FnPA-0101	I/-
166		Mass of isotope XXY as vapor in CV pool, (kg) (000)	CV-000-MIPi-0101	I/E
167	XX=chain	No. of nuclides of XXY in pool of CV, (nucl/m ³)	CV-123-NIPi-0102	I/E
168	Y=isot.	Decay heat of XXY in pool of CV, (W)	CV-123-QIPi-0103	I/-
169		Activity of XXY in pool of CV, (Bq)	CV-123-AIPi-0104	I/-
170		Mass of all isotopes as vapor in pool of CV, (kg)	CV-123-MIPt-0000	I/-
171	-	No. of all nuclides in pool of CV, (nucl/m ³)	CV-123-NIPt-0000	I/-
172		Decay heat of all nuclides in pool of CV, (W)	CV-123-QIPt-0000	I/-
173		Activity of all nuclides pool of CV, (Bq)	CV-123-AIPt-0000	I/-
174		External (TF/CF/RK) source of isotope XXY, (kg/s) (*)	CV-123-ESPM-0111	I/-
175		External (TF/CF/RK) source of isotope XXY (nucl/s) (*)	CV-123-ESPN-0112	I/-
176	isotope	Core release source of isotope XXY, (kg/s)	CV-123-RSPm-0113	I/-
177	No.:0XXY	Core release source of isotope XXY, (nucl/s)	CV-123-RSPn-0114	I/-
178		Source of isotope XXY due to all JN flows, (kg/s)	CV-123-FSPm-0115	I/-
179	XX=chain Y=isot.	Source of isotope XXY due to all JN flows, (nucl/s)	CV-123-FSPn-0116	I/-
180		Total removal of XXY due to all adsorptions, (kg/s)	CV-123-AdPm-0121	I/E
181		Total removal of XXY due to all adsorptions, (nucl/s)	CV-123-AdPn-0122	I/-
182		Total source of XXY due to all desorptions, (kg/s)	CV-123-DePm-0123	I/E
183		Total source of XXY due to all desorptions, (nucl/s)	CV-123-DePn-0124	I/-
<i>Control Volume related data (CV) - Isotopes on aerosols deposited in CV pool</i>				
184	FP	Total mass, sorbed vapor (11), size sec.No.(01), (kg)	CV-123-MT01-1011	I/E
185	vapor	Penetrated mass, sorbed vap.(12), size.No.(02), (kg)	CV-123-MP02-1012	I/E
186	number	Sorption flux, vapor (13), size sec.No.(03), (kg/m ² -s)	CV-123-SF03-1013	I/-
187		C _{rev} of vapor (14) on size sec.No.(04), (kg/m ²)	CV-123-Cr04-1014	I/E
188	IARG5C:	Available sites, vapor (15) size sec.No.(05), (kg/m ²)	CV-123-Cx05-1015	I/-
189	size sec =01-N _{sec}	C _{rev} of vapor (16) on size sec. No. (01), (nucl/m ²)	CV-123-Nr01-1016	I/E
190		Available sites, vapor (17) size sec.No.(02) (nucl/m ²)	CV-123-Nx02-1017	I/-
191	isotope No.:1XXY IARG5C: size sec =01-N _{sec}	No. of nuclides of XXY (321) on size sec. No.(05) (nucl/m ²)	CV-123-NA05-1321	I/E
192	isotope	Mass of isotope XXY on all size sec. (kg) (000)	CV-000-MAPi-0102	I/-
193	No.:0XXY	No. of nuclides of XXY on all size sec., (nucl)	CV-123-NAPi-0102	I/-
194	XX=chain	Decay heat of XXY on all size sec., (W)	CV-123-QAPi-0103	I/-
195	Y=isot.	Activity of XXY on all size sec., (Bq)	CV-123-AAPi-0104	I/-
196		Mass of all isotopes on all size sec. (kg)	CV-123-MAPt-0000	I/-
197	-	No. of all nuclides on all size sec., (nucl)	CV-123-NAPt-0000	I/-
198		Decay heat of all nuclides on all size sec., (W)	CV-123-QAPt-0000	I/-
199		Activity of all nuclides on all size sec., (Bq)	CV-123-AAPt-0000	I/-
<i>Control Volume related data (CV) - Exposure and doses</i>				
200		Exposure rate, γ -rays, ((C/kg)/s)	CV-123-ExyC-0000	I/-
201		Exposure rate, γ -rays, (R/s)	CV-123-ExyR-0000	I/-
202		Dose rate, γ -rays, (Gy/s)	CV-123-DsyG-0000	I/-
203	-	Dose rate, γ -rays, (rad/s)	CV-123-DsyR-0000	I/-
204		Dose rate, β -rays, (Gy/s)	CV-123-DsbG-0000	I/-
205		Dose rate, β -rays, (rad/s)	CV-123-DsbR-0000	I/-
206		Dose equivalent rate, (Sv/s)	CV-123-DsES-0000	I/-
207		Dose equivalent rate, (rem/s)	CV-123-DsER-0000	I/-

(*) In case of circulating fuel, the sources are calculated by the RK package, including the delayed neutron precursors.

(000) The second pointer may be zero instead of a CV number; in such case the parameter gives the total mass for all Control Volumes.

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3, 4, 5		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
<i>Junction related data (JN)</i>				
Keep in mind that although these are JN related parameters, the pointer 1 is equal to 8 and not 2 IARG1C=8				
208		Flow of isotope XXY with atmosphere, (kg/s)	JN-234-WIsA-0101	I/-
209	isotope No.:0XXY	Flow of isotope XXY with pool, (kg/s)	JN-234-WIsP-0102	I/-
210		Mass of isotope XXY on vapor filter, (kg) (000)	JN-000-MVf1-0111	I/E
211	XX=chain	No. of nuclides of XXY on vapor filter, (nucl)	JN-234-NVf1-0112	I/E
212	Y=isot.	Decay heat of XXY on vapor filter, (W)	JN-234-QVf1-0113	I/-
213		Activity of XXY on vapor filter, (Bq)	JN-234-AVf1-0114	I/-
214	isotope No.:0XXY IARG5C: size sec =01-N _{sec}	No. of nucl. of XXY on aerosol filter, size sec. No. (05), (nucl)	JN-234-NF05-0112	I/E
215	isotope	Mass of XXY on aerosol filter, all sizes, (kg) (000)	JN-000-MAf1-0111	I/-
216	No.:0XXY	No. of nuclides of XXY on aerosol filter, (nucl)	JN-234-NAf1-0112	I/-
217	XX=chain	Decay heat of XXY on aerosol filter, (W)	JN-234-QAf1-0113	I/-
218	Y=isot.	Activity of XXY on aerosol filter, (Bq)	JN-234-AAf1-0114	I/-

(000) The second pointer may be zero instead of a JN number; in such case the parameter gives the total mass for all Junctions.

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3,4,5,6		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
<p><i>1-D Solid Heat Conductor related data (SC) - Sorbed isotopes</i></p> <p>Keep in mind that although these are SC related parameters, the pointer 1 is equal to 8 and not 3 IARG1C=8</p>				
219	FP vapor number	Total mass of sorbed vapor, (kg)	SC-345-MTot-0001	I/-
220		Penetrated mass of sorbed vapor, (kg)	SC-345-MPen-0002	I/-
221	Cell No. IARG5C: Vapor No =01-N _{vap}	Concentration of penetrated vapor No.(12), (kg/m ³)	SC-345-CV12-0001	I/E
222	Surf.No.	Sorption flux of vapor No.(11), (kg/m ² -s)	SC-345-SF11-0001	I/-
223	1=left	Desorption flux (pool) of vapor No.(12), (kg/m ² -s)	SC-345-DF12-0002	I/-
224	2=right	C _{rev} of vapor No.(13), (kg/m ²)	SC-345-Cr13-0001	I/E
225	IARG5C:	Available sites for vapor No.(14), (kg/m ²)	SC-345-Cx14-0002	I/-
226	Vapor No	C _{rev} of vapor No.(15), (nucl/m ²)	SC-345-Nr15-0001	I/E
227	=01-N _{vap}	Available sites for vapor No.(16), (nucl/m ²)	SC-345-Nx16-0002	I/-
228	isotope	Sorbed mass of isotope XXY, (kg) (000)	SC-000-MIsi-0102	I/E
229	No.:0XXY	No. of nuclides of sorbed isotope XXY, (nucl/m ²)	SC-345-NIsi-0102	I/E
230	XX=chain	Decay heat of sorbed isotope XXY, (W)	SC-345-QIsi-0103	I/-
231	Y=isot.	Activity of sorbed isotope XXY, (Bq)	SC-345-AIsi-0104	I/-
232		Mass of all sorbed isotopes (kg)	SC-345-MIst-0000	I/-
233	-	No. of nuclides of all sorbed isotopes, (nucl/m ²)	SC-345-NIst-0000	I/-
234		Decay heat of all sorbed isotopes, (W)	SC-345-QIst-0000	I/-
235		Activity of all sorbed isotopes, (Bq)	SC-345-AIst-0000	I/-
<p><i>1-D Solid Heat Conductor related data (SC) - Isotopes on aerosols deposited in SC surfaces</i></p>				
236	Surf.No.	Mass of sorbed vap. No.(12) size sec. No.(7), (kg)	SC-345-MT12-7001	I/E
237	1=left	Penetrated mass, vap. No.(13) size sec. No.(8), (kg)	SC-345-MP13-8002	I/E
238	2=right	Sorption flux, vap. No.(01) size sec.No.(9), (kg/m ² -s)	SC-345-SF01-9001	I/-
239	IARG5C:	Desorp. flux, vap. No.(02) size sec. No.(10), (kg/m ² -s)	SC-345-DF02-A001	I/-
240	size sec	C _{rev} , vap. No.(03) size sec. No.(11), (kg/m ²)	SC-345-Cr03-B002	I/E
241	=1-N _{sec}	Available sites, vap. No.(04) sec. No.(12), (kg/m ²)	SC-345-Cx04-C001	I/-
242	IARG6C:	C _{rev} , vap. No.(05) size sec. No.(13) (nucl/m ²)	SC-345-Nr05-D002	I/E
243	Vapor No =01-N _{vap}	Available sites, vap. No.(06) sec. No.(14) (nucl/m ²)	SC-345-Nx06-E001	I/-
244	Surf.No. 1=left 2=right IARG5C: size sec =1-N _{sec} IARG6C: isotope No.:XXY	No. of nuclides of isotope No. (101) on aerosols size sec. No.(15), (nucl/m ²)	SC-345-Y101-F001	I/E
245	Surf.No. 1=left	Mass of isotope No. (101) on all size sec. (kg) (000)	SC-000-M101-0000	I/-
246	2=right	No. of nuclides of No. (102) on all size sec., (nucl)	SC-345-N102-0002	I/-
247	IARG5C:	Decay heat of isotope No. (103) on all size sec., (W)	SC-345-Q103-0001	I/-
248	isotope No.:XXY	Activity of isotope No. (104) on all size sec., (Bq)	SC-345-A104-0002	I/-
249	Surf.No.	Mass of all isotopes on all size sec. (kg)	SC-345-MAIt-0001	I/-
250	1=left	No. of all nuclides on all size sec., (nucl)	SC-345-NAIt-0002	I/-
251	2=right	Decay heat of all nuclides on all size sec., (W)	SC-345-QAIt-0001	I/-
252		Activity of all nuclides on all size sec., (Bq)	SC-345-AAIt-0002	I/-

(000) The second pointer may be zero instead of a SC number; in such case the parameter gives the total mass for all Solid Heat Conductors (also boundary cell number must be zero for IARG2C=245).

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3,4,5,6		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
2-D Solid Heat Conductor related data (TC) - Sorbed isotopes Keep in mind that although these are TC related parameters, the pointer 1 is equal to 8 and not 4 IARG1C=8				
253	FP vapor number	Total mass of sorbed vapor, (kg)	TC-456-MTot-0001	I/-
254		Penetrated mass of sorbed vapor, (kg)	TC-456-MPen-0002	I/-
255	Cell No. IARG5C: Vapor No =01-N _{vap}	Concentration of penetrated vapor No.(12), (kg/m ³)	TC-456-CV12-0001	I/E
256	Boundary cell No.	Sorption flux of vapor No.(11), (kg/m ² -s)	TC-456-SF11-0121	I/-
257		Desorption flux (pool) of vapor No.(12), (kg/m ² -s)	TC-456-DF12-0122	I/-
258		C _{rev} of vapor No.(13), (kg/m ²)	TC-456-Cr13-0123	I/E
259	IARG5C:	Available sites for vapor No.(14), (kg/m ²)	TC-456-Cx14-0124	I/-
260	Vapor No	C _{rev} of vapor No.(15), (nucl/m ²)	TC-456-Nr15-0125	I/E
261	=01-N _{vap}	Available sites for vapor No.(16), (nucl/m ²)	TC-456-Nx16-0126	I/-
262	isotope	Sorbed mass of isotope XXY, (kg) (000)	TC-000-MIsi-0102	I/E
263	No.:0XXY	No. of nuclides of sorbed isotope XXY, (nucl/m ²)	TC-456-NIsi-0102	I/E
264	XX=chain	Decay heat of sorbed isotope XXY, (W)	TC-456-QIsi-0103	I/-
265	Y=isot.	Activity of sorbed isotope XXY, (Bq)	TC-456-AIsi-0104	I/-
266		Mass of all sorbed isotopes (kg)	TC-456-Mist-0000	I/-
267	-	No. of nuclides of all sorbed isotopes, (nucl/m ²)	TC-456-NIst-0000	I/-
268		Decay heat of all sorbed isotopes, (W)	TC-456-QIst-0000	I/-
269		Activity of all sorbed isotopes, (Bq)	TC-456-AIst-0000	I/-
2-D Solid Heat Conductor related data (TC) - Isotopes on aerosols deposited in SC surfaces				
270	Boundary cell No.	Mass of sorbed vap. No.(12) size sec. No.(7), (kg)	SC-345-MT12-7001	I/E
271		Penetrated mass, vap. No.(13) size sec. No.(8), (kg)	SC-345-MP13-8002	I/E
272	IARG5C:	Sorption flux, vap. No.(01) size sec. No.(9), (kg/m ² -s)	SC-345-SF01-9003	I/-
273	size sec	Desorp. flux, vap. No.(02) size sec. No.(10), (kg/m ² -s)	SC-345-DF02-A004	I/-
274	=1-N _{sec}	C _{rev} , vap. No.(03) size sec. No.(11), (kg/m ²)	SC-345-Cr03-B005	I/E
275	IARG6C:	Available sites, vap. No.(04) sec. No.(12), (kg/m ²)	SC-345-Cx04-C006	I/-
276	Vapor No	C _{rev} , vap. No.(05) size sec. No.(13) (nucl/m ²)	SC-345-Nr05-D007	I/E
277	=01-N _{vap}	Available sites, vap. No.(06) sec. No.(14) (nucl/m ²)	SC-345-Nx06-E008	I/-
278	Boundary cell No. IARG5C: size sec =1-N _{sec} IARG6C: isotope No.:XXY	No. of nuclides of isotope No. (101) on aerosols size sec. No.(15), (kg) (boundary cell 023), (nucl/m ²)	TC-456-Y101-F023	I/E
279	Boundary cell No.	Mass of isotope No. (101) on all size sec. (kg) (000)	TC-000-M101-0000	I/-
280		No. of nuclides of No. (102) on all size sec., (nucl)	TC-456-N102-0332	I/-
281	IARG5C:	Decay heat of isotope No. (103) on all size sec., (W)	TC-456-Q103-0333	I/-
282	isotope No.:XXY	Activity of isotope No. (104) on all size sec., (Bq)	TC-456-A104-0334	I/-
283		Mass of all isotopes on all size sec. (kg)	TC-456-MAIt-0341	I/-
284	Boundary cell No.	No. of all nuclides on all size sec., (nucl)	TC-456-NAIt-0342	I/-
285		Decay heat of all nuclides on all size sec., (W)	TC-456-QAIt-0343	I/-
286		Activity of all nuclides on all size sec., (Bq)	TC-456-AAIt-0344	I/-

(000) The second pointer may be zero instead of a TC number; in such case the parameter gives the total mass for all Solid Heat Conductors (also boundary cell number must be zero for IARG2C=279).

SPECTRA Code Manuals - Volume 2: User's Guide

continued

Pointers 3,4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
<i>Global parameters - Isotopes in atmosphere and pool of all CV-s, sorbed by all SC-s and TC-s (RT)</i>				
287		Mass of all isotopes, atms of all CV-s, (kg)	RT-000-MIAG-0000	I/-
288		No. of all nuclides, atms of all CV-s, (nucl)	RT-000-NIAG-0000	I/-
289		Decay heat of all nuclides, atms of all CV-s, (W)	RT-000-QIAG-0000	I/-
290		Activity of all nuclides, atms of all CV-s, (Bq)	RT-000-AIAG-0000	I/-
291		Mass of all isotopes, pool of all CV-s, (kg)	RT-000-MIPG-0000	I/-
292		No. of all nuclides, pool of all CV-s, (nucl)	RT-000-NIPG-0000	I/-
293		Decay heat of all nuclides, pool of all CV-s, (W)	RT-000-QIPG-0000	I/-
294	-	Activity of all nuclides, pool of all CV-s, (Bq)	RT-000-AIPG-0000	I/-
295		Mass of all isotopes on all SC-s, (kg)	RT-000-MSCG-0000	I/-
296		No. of all nuclides on all SC-s, (nucl)	RT-000-NSCG-0000	I/-
297		Decay heat of all nuclides on all SC-s, (W)	RT-000-QSCG-0000	I/-
298		Activity of all nuclides on all SC-s, (Bq)	RT-000-ASCG-0000	I/-
299		Mass of all isotopes on all TC-s, (kg)	RT-000-MTCG-0000	I/-
300		No. of all nuclides on all TC-s, (nucl)	RT-000-NTCG-0000	I/-
301		Decay heat of all nuclides on all TC-s, (W)	RT-000-QTCG-0000	I/-
302		Activity of all nuclides on all TC-s, (Bq)	RT-000-ATCG-0000	I/-
<i>Global parameters - Isotopes on aerosols in all CV-s, deposited on all SC-s and TC-s (RT)</i>				
303		Mass of all isotopes, aerosols in all CV-s, (kg)	RT-000-MAAG-0000	I/-
304		No. of all nuclides, aerosols in all CV-s, (nucl)	RT-000-NAAG-0000	I/-
305		Decay heat of all nuclides, aerosols in all CV-s, (W)	RT-000-QAAG-0000	I/-
306		Activity of all nuclides, aerosols in all CV-s, (Bq)	RT-000-AAAG-0000	I/-
307		Mass of all isotopes, pool-aerosols in all CV-s, (kg)	RT-000-MAPG-0000	I/-
308		No. of all nuclides, pool-aerosols in all CV-s, (nucl)	RT-000-NAPG-0000	I/-
309		Decay heat of all nuclides, pool-aer.in all CV-s, (W)	RT-000-QAPG-0000	I/-
310	-	Activity of all nuclides, pool-aer. in all CV-s, (Bq)	RT-000-AAPG-0000	I/-
311		Mass of all isotopes, aerosols on all SC-s, (kg)	RT-000-MASG-0000	I/-
312		No. of all nuclides, aerosols on all SC-s, (nucl)	RT-000-NASG-0000	I/-
313		Decay heat of all nuclides, aerosols on all SC-s, (W)	RT-000-QASG-0000	I/-
314		Activity of all nuclides, aerosols on all SC-s, (Bq)	RT-000-AASG-0000	I/-
315		Mass of all isotopes, aerosols on all TC-s, (kg)	RT-000-MATG-0000	I/-
316		No. of all nuclides, aerosols on all TC-s, (nucl)	RT-000-NATG-0000	I/-
317		Decay heat of all nuclides, aerosols on all TC-s, (W)	RT-000-QATG-0000	I/-
318		Activity of all nuclides, aerosols on all TC-s, (Bq)	RT-000-AATG-0000	I/-
<i>Global parameters - Total number of nuclides and overall error (RT)</i>				
319		Total number of nuclides of all isotopes, N_{tot} , (nucl)	RT-000-Ntot-0000	I/-
320	-	Integrated sources + initial masses, N_{src} , (nucl)	RT-000-Nsrc-0000	I/-
321		Relative error $(N_{tot} - N_{src})/N_{tot}$, (-)	RT-000-Nerr-0000	I/-
<i>Reactor Kinetics for Circulating Fuel (RT)</i>				
322	-	Volume of active core, (m^3)	RT-000-RVol-0000	I/-
323		Reactivity feedback from the core volume change, (β)	RT-000-ReVo-0000	I/-

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-31 List of arguments available for Control Functions, variables available in Control Function Data Base.

Pointer 1: IARG1C = 7, Control Function Data Base Code name: CF
 Pointer 2: IARG2C = CF reference number Code name: three digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
CF data				
1	-	Value of the Control Function	CF-789-Valu-0000	I/E

Table 2-32 List of arguments available for Control Functions, variables available in Numerical Solver Data Base.

Pointer 1: IARG1C = 9, Numerical Solver Data Base Code name: SL
 Pointer 2: IARG2C = Not used - must be equal to zero Code name: three digits

Pointers 3, 4		Description	Code Name Examples	Impl/Expl
IARG3C	IARG4C			
Material property data				
1		Current model time, s	SL-000-Time-0000	I/-
2		Current time step, s	SL-000- _Dt-0000	I/-
3		Current CPU time (processor usage), s	SL-000- _CPU-0000	I/-
4	-	Warp factor (model time / CPU time)	SL-000-Warp-0000	I/-
5		Current run time (clock time), s	SL-000-RunT-0000	I/-
6		Run time ratio (run time / model time)	SL-000-RunR-0000	I/-
7		Local warp factor (within the last plot interval)	SL-000-WarL-0000	I/-
8		Local run ratio (within the last plot interval)	SL-000-RunL-0000	I/-

2.8.10 Records: 715000, Implicit Solution of All Control Functions

The Control Functions are always included in the main iteration loop to obtain implicit solution. Therefore the CF values are (like all other parameters in the implicit solution) controlled by the SPECTRA Numerical Solver. The main iteration is finished after all end-of-time-step values assumed and calculated are in agreement, according to the Solver criteria). In some cases the Control Functions are last to converge. In such case a warning message is printed by the Solver, advising the user to ignore the CF convergence criteria. In most cases the CF accuracy is sufficient even when the CF convergence is ignored by the Solver.

W-1 (A) : IMPLCF Indicator defining the CF convergence
 IMPLCF = 1: CF convergence criteria must be satisfied in order to complete the iteration.
 IMPLCF = 2: CF convergence criteria are ignored. When all other parameters are converged, then the iteration is completed even if the CF convergence is not yet satisfactory.
 Acceptable range: 1 or 2 .
 Default value: 1 .

2.8.11 Examples of Control Function Input Data

MAXIMUM

The function CF-100 below calculates the maximum temperature of a 1-D Solid Heat Conductor SC-123.

```

705100 Maximum temperature of SC-123
*      (The "Max" CF)      Scale      Additive
*      Group  Number      Fact.      Const.
700100  2      3      1.0      0.0 *
*      Arguments
* Pointers: (1) (2) (3) (4) * (1) (2) (3) (4)
710100  3 123 16 1 * SC data base, SC-123, Cell temperature, Cell No. 1
710100  3 123 16 2 * SC data base, SC 123, Cell temperature, Cell No. 2
710100  3 123 16 3 * SC data base, SC 123, Cell temperature, Cell No. 3
710100  3 123 16 4 * SC data base, SC 123, Cell temperature, Cell No. 4
710100  3 123 16 5 * SC data base, SC 123, Cell temperature, Cell No. 5
710100  3 123 16 6 * SC data base, SC 123, Cell temperature, Cell No. 6
710100  3 123 16 7 * SC data base, SC 123, Cell temperature, Cell No. 7
710100  3 123 16 8 * SC data base, SC 123, Cell temperature, Cell No. 8
710100  3 123 16 9 * SC data base, SC 123, Cell temperature, Cell No. 9
    
```

IF-THEN-ELSE

CF-182 is an example of an IF-THEN-ELSE function. The function CF-182 checks the rotational speed of the pump JN-100, and computes the pump status signal, as:

- if the pump speed is less than 1.0 rev/s, then the status signal is 0.0 (off),
- if the pump speed is larger than 1.0 rev/s then the status signal is 1.0 (on).

In order to obtain a constant value a “dummy” variable is used. The dummy variable is the current time step (pointers: 9 0 2 0). The value of the dummy variable is multiplied by zero, and the required constant is added. Note that the multipliers of 1.0E-90 were used whenever zero was desired. This must be done to prevent the program from assigning the default multiplier of 1.0, which is done when no value is entered or the entered value is zero.

```

705182 STATUS: Gas Pump (SGP)
*      Group  Number      Fact.      Const.
700182  1      4      1.0      0.0 * Type : IF-THEN-ELSE
709182  2
*      Arguments
* Pointers: (1) (2) (3) (4) Fact. Const.
710182  2 100 35 1 1.0 0.0 * IF ( JN-100 pump speed <
710182  9 0 2 0 1.0E-90 1.0 * < 1.0 rev/s )
710182  9 0 2 0 1.0E-90 0.0 * THEN signal = 0.0
710182  9 0 2 0 1.0E-90 1.0 * ELSE signal = 1.0
    
```

Below, another example of the IF-THEN-ELSE function is given. This time the function defines the control rod reactivity after scram. The scram signal is given by the function CF-901. When the scram signal is received, the control rods start moving down with a delay of 0.1 s. The control rod reactivity is tabulated as a function of time after scram as TF-900. Note that if a TF is used within an IF-THEN-ELSE function and the TF is not an interactive type, then the argument for the TF is always the current time minus the time when the corresponding IF-THEN-ELSE was last becoming true.

```

705900 Control rod reactivity
*      Group  Number      Fact.      Const.
    
```

SPECTRA Code Manuals - Volume 2: User's Guide

```

700900 1      4      1.0      0.0      * Type : IF-THEN-ELSE
709900 2
* Arguments
* Pointers: (1) (2) (3) (4) Fact. Const.
710900 7 901 1 0 1.0 0.0 * IF ( CF-901 (scram signal) <
710900 9 0 2 0 1.0E-90 1.0 * < 1.0 )
710900 9 0 2 0 1.0E-90 0.0 * THEN rod reactivity is zero
710900 6 900 1 0 1.0 0.0 * ELSE use TF-900 to define rod reactivity
*
605900 Control rod reactivity after scram
* Fact. Const.
601900 1.0 0.0 * Scaling
602900 -30.0 0.0 0.0 0.0 * Limits: Min, Max, dTF/dt
610900 1 * Type: NON-INTERACTIVE !! otherwise the program will use
* the actual value of TF and not TF(t-t0)
*
* Time after scram Reactivity ($)
600900 0.0 0.0
600900 0.1 0.0
600900 0.2 -1.0
600900 0.3 -30.0

```

Apart from reactor scram, such function may be useful to model pump trip with pump coastdown curve versus time, etc.

HYSTERESIS

An example of the hysteresis function type 1, shown in Figure 2-45, is shown below.

```

705200 Example of a Hysteresis Function Type 1
* Group Number Fact. Const.
700200 1 6 1.0 0.0 * Type : Hysteresis
* Arguments
* Pointers: (1) (2) (3) (4) Fact. Const.
710200 1 333 13 1 1.0E-6 0.0 * uses CV-333 pressure (in MPa) as an argument
710200 6 201 1 0 1.0 0.0 * uses TF-201 as a definition of the first point
710200 6 202 1 0 1.0 0.0 * uses TF-202 as a definition of the second point
*
605201 Hysteresis point 1
* x f(x)
600201 0.0 2.5 * single data pair means hysteresis type 1
*
605202 Hysteresis point 2
* x f(x)
600202 0.0 3.7 * single data pair means hysteresis type 1

```

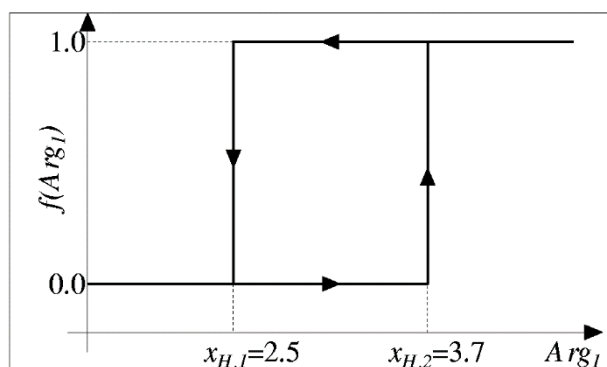


Figure 2-45 Hysteresis function type 1

SPECTRA Code Manuals - Volume 2: User's Guide

An example of the hysteresis function type 2, shown in Figure 2-45, is shown below.

```
705300 Example of a Hysteresis Function Type 2
*   Group   Number      Fact.   Const.
700300     1       6         1.0     0.0   * Type    : Hysteresis
*   Arguments
* Pointers: (1) (2) (3) (4) Fact. Const.
710300     1    333 13     1 1.0E-6 0.0 * uses CV-333 pressure (in MPa) as an argument
710300     6    301  1     0 1.0     0.0 * uses TF-301 as the Forward function
710300     6    302  1     0 1.0     0.0 * uses TF-302 as the Reverse function
*
605301 Forward function
*   x       f(x)
600301  2.0   0.0 * multiple data pair means hysteresis type 2
600301  3.0   0.0
600301  4.0   1.0
*
605302 Reverse function
*   x       f(x)
600302  2.0   0.0 * multiple data pair means hysteresis type 2
600302  3.0   1.0
600302  4.0   1.0
```

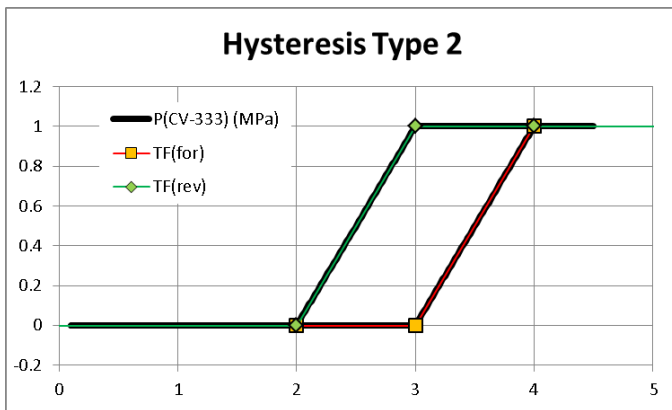


Figure 2-46 Hysteresis function type 2

GENERAL TABULAR FUNCTIONS

Examples of general tabular functions, including a 1-D and a 2-D function, are shown in section 2.8.6.

2.9 Reactor Kinetics Input Data

In order to activate the reactor kinetics model, a Control Function "reactor kinetics" (group number 3, type number 5 - see section 2.8.1, Table 2-22) must be present in the input deck. The reactor power, calculated by the Reactor Kinetics Package, is assigned to this Control Function. The reactor kinetics Control Function has one argument: the problem time. The value of the CF is the total reactor power (fission+decay) in case of normal (solid) fuel. In case of circulating fuel (IFTORK=2), the reactor kinetics function gives only the fission power, since in such case the decay power is calculated by the RT Package and is automatically added to the pool of Control Volumes. Furthermore, in case of circulating fuel, the following steps are taken:

- If the power source for a Control Volume, ITESCV, is defined through the "reactor kinetics" the power is added to the pool of CV only, never to the atmosphere.
- The value obtained from the reactor kinetics Control Function is used if the CV has sufficient amount of liquid, i.e. if the liquid fraction in CV is more than the limit XFULRK (record 748000).
- If the pool occupies less than XFULRK of the CV volume, the source obtained from the reactor kinetics Control Function is interpolated to obtain zero in case of empty volume, i.e. it is multiplied by $(V_{pool}/V_{CV})/XFULRK$. Here V_{pool} is the pool volume in CV and V_{CV} is the total volume of CV. This is done to automatically reduce the power generated in the pool of a CV when the pool is removed from this CV.

If the nodal point kinetics is used, then the total reactor power is available in the "reactor kinetics" Control Function, while the node-specific power is given in the subsequent Control Functions. For example, if the reactor kinetics function is defined as CF-100 and the nodal point kinetics model is used with 10 nodes, then the power is available as:

- CF-100 total reactor power,
 - CF-101 power in the node 1,
 - CF-102 power in the node 2,
 - CF-103 power in the node 3,
 - CF-104 power in the node 4,
 - CF-105 power in the node 5,
 - CF-106 power in the node 6,
 - CF-107 power in the node 7,
 - CF-108 power in the node 8,
 - CF-109 power in the node 9,
 - CF-110 power in the node 10.

The functions 101 through 110 must be present in the input deck and they must also be the "reactor kinetics" type (group number 3, type number 5)

2.9.1 Record: 750000, Reactor Kinetics Main Data

W-1 (R) : PNGTRK Prompt neutron generation time, Λ , (s). If a negative value is entered, the generation time is computed from the Control Function |PNGTRK|. The value obtained from the Control Function is restricted to the range of: 10^{-7} - 1.0.
Acceptable range: $10^{-7} \leq \text{PNGTRK} \leq 1.0$.
or reference to a Control Function

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: $A = (v\Sigma_f v_n)^{-1}$
(all variables in this formula are defined below).

W-2 (R) : SIGFRK Macroscopic fission cross section, Σ_f , (1/m). No default value is provided. A value for given reactor type must be entered (see example in 2.9.21 below).
Acceptable range: $10^{-4} \leq \text{SIGFRK} \leq 10^3$
Default value: none.

W-3 (R) : XNPFRK Number of neutrons generated per fission, ν , (-).
Acceptable range: $1.0 \leq \text{XNPFRK} \leq 5.0$.
Default value: 2.5 ([1], sections 1.5.1, 1.5.2).

W-4 (R) : QFISRK Heat released per fission, q_f , (J).
Acceptable range: $1.0 \cdot 10^{-13} \leq \text{QFISRK} \leq 1.0 \cdot 10^{-9}$.
Default value: $3.09 \cdot 10^{-11}$
Note that 1 MeV = $1.602 \cdot 10^{-13}$ J. The default value is equal to 192.9 MeV, based on [5], 2, table 2-5.

W-5 (R) : CTHNRK Constant in thermal neutron velocity calculation, C_n . Thermal neutron velocity, v_n , is calculated from:

$$v_n = C_n \sqrt{T}$$

where T is temperature, determined by the word 6 below.

Acceptable range: $10.0 \leq \text{CTHNRK} \leq 1000.0$.

Default value: 128.0 ([5], equation 9-10).

W-6 (I) : ITN1RK Indicator for thermal neutron temperature calculation.
= 0: T is constant and equal to 400.0 K. This yields thermal neutron velocity of 2560 m/s.
= 1: T is equal to the moderator temperature, defined by weighting factors, described in 2.9.19.
= 2: T is equal to the fuel temperature, defined by weighting factors, described in section 2.9.18.
= 3: T is equal to the value of Tabular Function No. ITN2RK (Word 7 below).
= 4: T is equal to the value of Control Function No. ITN2RK (Word 7 below).

Acceptable range: $0 \leq \text{ITN1RK} \leq 4$.

Default value: 0.

W-7 (I) : ITN2RK Indicator for thermal neutron temperature calculation.
if ITN1RK = 3: ITN2RK is a Tabular Function number,
if ITN1RK = 4: ITN2RK is a Control Function number.
Acceptable range: if ITN1RK = 3: valid reference number of a TF,
if ITN1RK = 4: valid reference number of a CF.
Default value: none.

W-8 (R) : EPSRK Fast fission factor, ϵ .
Acceptable range: $1.0 \leq \epsilon \leq 1.20$.

SPECTRA Code Manuals - Volume 2: User's Guide

		<i>Default value:</i>	1.02 ([5], chapter 3).
W-9 (R) :	PRESRK	Resonance escape probability, p .	
		<i>Acceptable range:</i>	$0.5 \leq p \leq 1.00$.
		<i>Default value:</i>	0.87 ([5], chapter 3).
W-10 (R) :	PFNLRK	Non-leakage probability for fast neutrons, P_{FNL} , (-).	
		<i>Acceptable range:</i>	$0.5 \leq P_{FNL} \leq 1.0$.
		<i>Default value:</i>	0.97 ([5], chapter 3).
W-11 (R) :	PTNLRK	Non-leakage probability for thermal neutrons, P_{TNL} , (-).	
		<i>Acceptable range:</i>	$0.5 \leq P_{TNL} \leq 1.0$.
			$P_{FNL} \cdot P_{TNL} \geq 1/v$ or $\geq 1/(v \cdot p \cdot \epsilon)$, depending on the value of IPERRK (word 13).
		<i>Default value:</i>	0.99 ([5], chapter 3).
W-12 (R) :	QDMLRK	Multiplier on decay heat (for decay heat see sections 2.9.25, 2.9.36).	
		<i>Acceptable range:</i>	$0.0 \leq QDMLRK \leq 5.0$.
		<i>Default value:</i>	1.0 .
W-13 (I) :	IPERRK	Indicator defining how the reactivity effect due to isotope concentration changes is calculated (note: the reactivity effect due to isotope concentration changes can be disabled by using the input parameter IREIRK, record 748000):	
		=1:	do not include $p\epsilon$ in reactivity effect calculation. In this case the reactivity effect is proportional to $1/(v \cdot P_{FNL} \cdot P_{TNL})$ - Volume 1),
		=2:	include $p\epsilon$ in reactivity effect calculation; in this case the reactivity effect is proportional to $1/(v \cdot p \cdot \epsilon \cdot P_{FNL} \cdot P_{TNL})$.
		<i>Acceptable range:</i>	IPERRK = 1 or 2.
		<i>Default value:</i>	1 .
W-14 (R) :	SIGMRK	Minimum value of Σ_f , (1/m). Calculations are stopped if the macroscopic fission cross section is smaller than this number.	
		<i>Acceptable range:</i>	$0.0 \leq SIGMRK \leq 10^{-5}$
		<i>Default value:</i>	10^{-6}

2.9.2 Record: 750XXX, Nodal Point Kinetics - Main Data

This record defines data for the nodal point kinetics model. XXX is the node number, i . The maximum number of nodes is NRKMAX = 50. This record defines the node specific values of the first two inputs in the record 750000:

- W-1, the prompt neutron generation time, PNGTRK(i) and
- W-2, the macroscopic fission cross section, SIGFRK(i).

The remaining input entries defined in the record 750000 (W-3 through W-14) are used for all nodes.

W-1 (R) : PNGTRK(i) Prompt neutron generation time, Λ_i , (s), for the node $i = XXX$. If a negative value is entered, the generation time is computed from the

SPECTRA Code Manuals - Volume 2: User's Guide

Control Function |PNGTRK(i)|. The value obtained from the Control Function is restricted to the range of: 10^{-7} - 1.0.

Acceptable range: $10^{-7} \leq \text{PNGTRK} \leq 1.0$.

or reference to a Control Function

Default value: PNGTRK defined in the record 750000

W-2 (R) : SIGFRK(i) Macroscopic fission cross section, Σ_{fi} , (1/m), for the node $i = \text{XXX}$.

Acceptable range: $10^{-4} \leq \text{SIGFRK}(i) \leq 10^3$

Default value: SIGFRK defined in the record 750000

The following input entries must be defined for the nodal point kinetics.

W-3 (R) : DCXNRK(i) Diffusion coefficient D_i , (m), in the node $i = \text{XXX}$. The diffusion coefficient is equal to:

$$D_i = \frac{1}{3\Sigma_{tr,i}}$$

Here $\Sigma_{tr,i}$ is the macroscopic transport cross section (1/m).

If a value < 1.0 is entered, then the diffusion coefficient is constant and equal to the input value. If the value is ≥ 1.0 then the value is defined by a Tabular Function with the number DCXNRK. The argument for the Tabular Function is the node temperature, (K). The values obtained from the Tabular Function are internally limited to the range between 10^{-6} and 1.0.

Acceptable range: $10^{-30} \leq \text{DCPKRK}(i) < 1.0$

or a reference to a valid Tabular Function

Default value: none

W-4 (R) : DNXNRK(i) Thickness, d_i , (m), of the node $i = \text{XXX}$.

Acceptable range: $10^{-2} \leq \text{DNPCKRK}(i) \leq 10^2$

Default value: none

W-5 (R) : ANXNRK(i) Cross section area between the nodes $i-1$ and i , A_i , (m^2).

Acceptable range: $0.0 \leq \text{ANXNRK}(i) \leq 10^4$

Default value: none

The nodal point kinetics discretization is shown in Figure 2-47. The nomenclature is as follows:

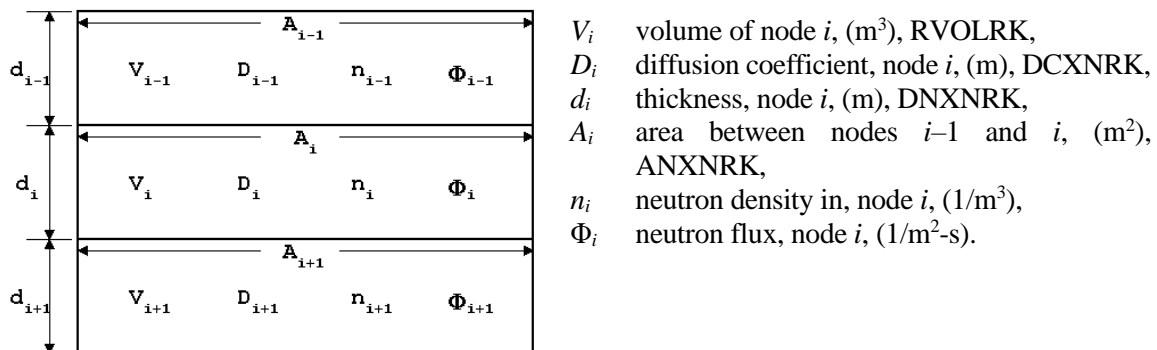


Figure 2-47 Discretization in the nodal point kinetics model

if ININRK=1:

W-2 (R) : XCNNRK Convergence criterion. Used if INONRK=1. Calculations are stopped automatically, if maximum value of the relative change of neutron density in all nodes is smaller than this value:

$$XMXNRK = \text{Max} \left(\frac{1}{n_i} \frac{dn_i}{dt} \right) = \text{Max} \left(\frac{1}{n_i} \frac{\Delta n_i}{\Delta t} \right) < XCNNRK$$

n_i neutron density (1/m³) in the node i

Δn_i change of neutron density (1/m³) over a time step

Δt time step size (s)

If INONRK=1, the relative change $(1/n_i)(dn_i/dt)$ is printed in the output file and the calculation is stopped when the maximum value $<XCNNRK$. If the maximum value is larger than $XCNNRK$ until the end of the run, an error message is printed in the diagnostics file.

Acceptable range: $0.0 \leq XCNNRK \leq 10^{-5}$

Default value: 10^{-7}

a small number $<10^{-50}$, sets the value to 0.0; setting the value to 0.0 prevents the run from stopping

if ININRK=2:

W-2 (R) : XCNNRK End-time for applying power control (s). The PI controller will be used only for time $t < XCNNRK$.

Acceptable range: any real number

Default value: 0.0

if ININRK=1 or 2:

W-3 (R) : POWORK Target total power, (W). Used if INONRK=1.

Acceptable range: within 10% of the default, if non-zero

Default value: described below

The user defines the fission power in every node in the record 751XXX, PINIRK(i). The total fission power is obtained as:

$$SPOWRK = \sum_i PINIRK(i)$$

If the Isotope Transformation model is used, then the decay power summed in all nodes is added to the fission power.

$$SQDPRK = \sum_i QDTPRK(i)$$

The node decay power, QDTPRK(i), is calculated as selected by the indicator ICITRK (input record 740000). Finally, the default value of the target power is equal to:

$$POWORK = SPOWRK + SQDPRK$$

W-4 (I) : IRPLRK Reactivity versus multiplication factor as plot parameters - Table 2-29.

= 1: reactivity is used as plot parameters: RK-000-Reac-0000

= 2: multiplication factors are used as plot parameters

point kinetics: $k_{eff} = RK-000-Keff-0000$

nodal kinetics: $k_{\infty} = RK-000-Kinf-0000$

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: 1 or 2
Default value: point kinetics: 1
nodal kinetics: 2

2.9.5 Record: 751000, Volume, Initial Fission Power and Initial Reactivity Data

- W-1 (R) : RVOLRK Total reactor volume (fuel + moderator), V_R , (m^3).
Acceptable range: RVOLRK > 0.0.
Default value: none.
- W-2 (R) : PINIRK Initial fission power, (W) (do not include the decay power).
Acceptable range: PINIRK \geq 0.0.
Default value: 0.0.
- W-3 (R) : RINIRK Initial reactivity, ($\$$). Here 1\$ = sum of the global DNP yields for all groups, $\sum[BTDNRK(i)]$ - section 2.9.12. The actual initial reactivity that is used (and can be plotted) will be converted based on the actual DNP yields calculated for the current fuel composition and the individual DNP yields, defined as input parameters BIDNRK.
Acceptable range: all real numbers.
Default value: 0.0.
- W-4 (I) : IINIRK Indicator for the initial reactivity calculation:
=1: Initial reactivity is given by RINIRK.
=2: Initial reactivity is given by the Control Function ICINIRK. The Control Rod reactivity is included, i.e. the initial reactivity will be equal to the value of the Control Function ICINIRK, independently of the initial value of the Control Rod reactivity, defined in the record 760000.
=3: Initial reactivity is given by the Control Function ICINIRK. The Control Rod reactivity is excluded, i.e. the initial reactivity will be equal to the value of the Control Function ICINIRK plus the initial value of the Control Rod reactivity, defined in the record 760000.
Acceptable range: 1, 2, 3
Default value: 1
- W-5 (I) : ICNIRK Control Function defining the initial reactivity, ($\$$) if the value of IINIRK is equal to 2 or 3.
Acceptable range: a reference number of a Control Function if IINIRK is equal to 2 or 3. Zero if IINIRK is equal to 1.
Default value: 0

2.9.6 Record: 751XXX, Nodal Point Kinetics - Volume, etc. Data

This record defines data for the nodal point kinetics model. XXX is the node number, i . The maximum number of nodes is NRKMAX = 50. This record defines the node-specific values, which for the point kinetics model are defined in the record 751000.

W-1 (R) : RVOLRK(i) Total reactor volume (fuel + moderator), V_R , (m^3), for the node $i = XXX$.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: RVOLRK > 0.0.

Default value: none.

W-2 (R) : PINIRK(*i*) Initial fission power, (W) (do not include the decay power), for the node *i* = XXX.

Acceptable range: PINIRK ≥ 0.0.

Default value: 0.0.

W-3 (R) : RINIRK(*i*) Initial reactivity, (\$), for the node *i* = XXX.

Acceptable range: all real numbers.

Default value: 0.0.

W-4 (I) : IINIRK(*i*) Indicator for the initial reactivity calculation for the node *i* = XXX:

=1: Initial reactivity is given by RINIRK(*i*).

=2: Initial reactivity is given by the Control Function ICINIRK(*i*). The Control Rod reactivity is included, i.e. the initial reactivity will be equal to the value of the Control Function ICINIRK(*i*), independently of the initial value of the Control Rod reactivity, defined in the record 760XXX.

=3: Initial reactivity is given by the Control Function ICINIRK(*i*). The Control Rod reactivity is excluded, i.e. the initial reactivity will be equal to the value of the Control Function ICINIRK(*i*) plus the initial value of the Control Rod reactivity, defined in the record 760XXX.

Acceptable range: 1, 2, 3

Default value: 1

W-5 (I) : ICNIRK(*i*) Control Function defining the initial reactivity, (\$), for the node *i* = XXX. Only used if the value of IINIRK(*i*) is equal to 2 or 3.

Acceptable range: must be a valid reference number of a Control Function if IINIRK(*i*) is equal to 2 or 3.

Default value: 0

2.9.7 Record: 755000, External Neutron Source Data

W-1 (I) : ISRCRK Pointer to a Tabular or Control Function that defines the external neutron source, *S*. If the number is positive then the source will be defined by a Tabular Function with the number: ISRCRK. If the number is negative then the source will be defined by a Control Function with the number: |ISRCRK|. The units obtained from the Tabular or Control Function are assumed to be (neutrons/s). The volumetric source, *S_v*, is equal to: $S_v = S/V_R$, where *V_R* is the reactor volume, defined in record 751000 (2.9.5).

Acceptable range: must be a valid reference number of a tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used.

Default value: 0.

2.9.8 Record: 755XXX, Nodal Point Kinetics - External Neutron Source Data

This record defines data for the nodal point kinetics model. XXX is the node number, i . The maximum number of nodes is NRKMAX = 50. This record defines the node-specific values, which for the point kinetics model are defined in the record 755000.

- W-1 (I) : ISRCRK(i) Pointer to a Tabular or Control Function that defines the external neutron source, S , for the node $i = \text{XXX}$. If the number is positive then the source will be defined by a Tabular Function with the number: ISRCRK. If the number is negative then the source will be defined by a Control Function with the number: $|\text{ISRCRK}|$. The units obtained from the Tabular or Control Function are assumed to be (neutrons/s). The volumetric source, S_V , is equal to: $S_V = S/V_R$, where V_R is the reactor volume, defined in record 751XXX.
- Acceptable range:* must be a valid reference number of a tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used.
- Default value:* 0.

2.9.9 Record: 760000, Control Rod Reactivity Data

- W-1 (I) : IREARK(1) Pointer to a Tabular or Control Function that defines the reactivity. If the number is positive then the reactivity will be defined by a Tabular Function with the number: IREARK(1). If the number is negative then the reactivity will be defined by a Control Function with the number: $|\text{IREARK}(1)|$. The units obtained from the Tabular or Control Function are assumed to be (\$). Here 1\$ = sum of the global DNP yields for all groups, $\sum[\text{BTDNRK}(i)]$ - section 2.9.12.
- Acceptable range:* must be a valid reference number of a tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used.
- Default value:* 0.
- W-2 (I) : IREARK(2) Pointer to a Tabular or Control Function that defines the reactivity. If the number is positive then the reactivity will be defined by a Tabular Function with the number: IREARK(2). If the number is negative then the reactivity will be defined by a Control Function with the number: $|\text{IREARK}(2)|$. The units obtained from the Tabular or Control Function are assumed to be (\$). Here 1\$ = sum of the global DNP yields for all groups, $\sum[\text{BTDNRK}(i)]$ - section 2.9.12.
- Acceptable range:* must be a valid reference number of a tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used.
- Default value:* 0.

... until all reactivity tables are defined. The maximum number of reactivity tables is 50.

2.9.10 Record: 760XXX, Nodal Point Kinetics - Control Rod Reactivity Data

This record defines data for the nodal point kinetics model. XXX is the node number, i . The maximum number of nodes is $NRKMAX = 50$. This record defines the node-specific values, which for the point kinetics model are defined in the record 760000.

W-1 (I) : IREARK(1, i) Pointer to a Tabular or Control Function that defines the reactivity for the node $i = XXX$. If the number is positive, the reactivity will be defined by a Tabular Function with the number: IREARK(1). If the number is negative then the reactivity will be defined by a Control Function with the number: $|IREARK(1)|$. The units obtained from the Tabular or Control Function are assumed to be (\$). Here 1\$ = sum of the global DNP yields for all groups, $\sum[BTDNRK(i)]$ - section 2.9.12.

Acceptable range: must be a valid reference number of a tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used.

Default value: 0.

W-2 (I) : IREARK(2, i) Pointer to a Tabular or Control Function that defines the reactivity for the node $i = XXX$. If the number is positive, the reactivity will be defined by a Tabular Function with the number: IREARK(2). If the number is negative then the reactivity will be defined by a Control Function with the number: $|IREARK(2)|$. The units obtained from the Tabular or Control Function are assumed to be (\$). Here 1\$ = sum of the global DNP yields for all groups, $\sum[BTDNRK(i)]$ - section 2.9.12.

Acceptable range: must be a valid reference number of a tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used.

Default value: 0.

... until all reactivity tables are defined. The maximum number of reactivity tables is 50.

2.9.11 Record: 761000, Power Control

This record defines the automatic power control, used to keep the reactor power constant in one of the following situations.

- When the CV/JN/... packages are deactivated, and the constant reactor power option is requested (IRKSL=2 in the record 900XXX).
- When the nodal point kinetics model is used and the initialization option is requested (INONRK=1 in the record 750999).
- When INONRK=2 in the record 750999.

The power control is performed by the Solver by inserting or removing reactivity, according to the following formula:

$$R(t) = CPCVRK \times \left(\frac{Q_{tar} - Q(t)}{Q_{tar}} \right) + CICVRK \times \int_{t_0}^t \left(\frac{Q_{tar} - Q(t')}{Q_{tar}} \right) dt'$$

SPECTRA Code Manuals - Volume 2: User's Guide

where $R(t)$ is the control system reactivity, (β), and Q_{tar} it the target power, (W), equal to the reactor power at the time when:

- CV/JN/... packages become inactive (when IRKSL=2),
- Start of the calculations (when INONRK=1).

W-1 (I) : CPCVRK Constant in the proportional part of the PI reactor power controller.
Acceptable range: $10^{-6} \leq \text{CPCVRK} \leq 10^{+1}$
Default value: 1.0

W-2 (I) : CICVRK Constant in the integral part of the PI reactor power controller.
Acceptable range: $10^{-6} \leq \text{CPCVRK} \leq 10^{+1}$
Default value: 1.0

2.9.12 Record: 770XXX, Delayed Neutron Precursor Data

XXX = 001, 002, ... , NDNGRK, is the number of the delayed neutron precursor group. The maximum number of delayed neutron precursor groups is 10. SPECTRA contains data for eight groups of delayed neutrons, which is being used if no data is entered. Thus, by default NDNGRK is equal to 8. If records 770XXX are entered, then the NDNGRK is equal to the largest value of XXX. For XXX = 1 through 8 any of the entries described below may be entered as zero to use the built-in value.

W-1 (R) : BTDNRK Yield of the group XXX, $\beta_{i=XXX}$, (-).
Acceptable range: $10^{-6} \leq \text{BTDNRK} \leq 10^{-2}$
Default value: values for U-235, shown in the example below

W-2 (R) : DCDNRK Decay constant of the group XXX, $\lambda_{i=XXX}$, (1/s).
Acceptable range: $10^{-4} \leq \text{DCDNRK} \leq 10^2$
Default value: values for U-235, shown in the example below

Example:

In the example below, the delayed neutron precursors are defined using the data for thermal fission of U-235:

```
*          DELAYED NEUTRON DATA
*          BTDNRK (-)   DCDNRK (1/s)
770001    2.145E-04     1.24667E-02
770002    1.001E-03     2.82917E-02
770003    5.915E-04     4.25244E-02
770004    1.281E-03     1.33042E-01
770005    2.151E-03     2.92467E-01
770006    5.850E-04     6.66488E-01
770007    5.265E-04     1.63478E+00
770008    1.495E-04     3.55460E+00
```

Using the following inputs, the user may define individual yield fractions, specific to all fissile isotopes in the problem. If the input entries are present, there must be exactly the same values as the number of fissile isotopes (isotopes with positive fission cross section, SFITRK>0.0) present in the RK Package. Zeroes may be entered; in such case the value will be set to the average yield, BTDNRK.

W-3 (R) : BIDNRK(1) Individual yield of the group XXX from the first fissile isotope.
Acceptable range: $0.0 \leq \text{BIDNRK}(1) \leq 10^{-2}$

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: BTDNRK

W-4 (R) : BIDNRK(2) Individual yield of the group XXX from the first fissile isotope.

Acceptable range: $0.0 \leq \text{BIDNRK}(2) \leq 10^{-2}$

Default value: BTDNRK

[. . .] until the yields are defined for all fissile isotopes.

Example:

In the example below, the fission yields of delayed neutron precursors are defined for:

- U-235, Pu-239, and Pu-241.

Assuming that all default fuel chains are present, the fissile isotopes are:

- U-233, U-235, U-239, Pu-239, Pu-241.

The following input defines individual yields for U-233 and Pu-239, based on the available data (see Volume 1). It is assumed that the values for U-239 are the same as for U-235 (defined as BTDNRK), while the values for Pu-241 are assumed to be the same as for Pu-239.

```

*          DELAYED NEUTRON DATA                individual yields (BIDNRK)
*          BTDNRK (-)   DCDNRK (1/s)           U-233      U-235  U-239  Pu-239      Pu-241
770001    2.145E-04     1.24667E-02           8.580E-05  0      0      6.930E-05  6.930E-05
770002    1.001E-03     2.82917E-02           4.004E-04  0      0      3.234E-04  3.234E-04
770003    5.915E-04     4.25244E-02           2.366E-04  0      0      1.911E-04  1.911E-04
770004    1.281E-03     1.33042E-01           5.122E-04  0      0      4.137E-04  4.137E-04
770005    2.151E-03     2.92467E-01           8.606E-04  0      0      6.951E-04  6.951E-04
770006    5.850E-04     6.66488E-01           2.340E-04  0      0      1.890E-04  1.890E-04
770007    5.265E-04     1.63478E+00           2.106E-04  0      0      1.701E-04  1.701E-04
770008    1.495E-04     3.55460E+00           5.980E-05  0      0      4.830E-05  4.830E-05
    
```

The actual yields will be determined based on the current fuel composition, using the values of BIDNRK. The value of BTDNRK is serving only as a definition of the default value. The correctness of input may be checked in the *.OUT file, where it is printed below the isotope data, in the following block:

=RK= INDIVIDUAL FISSION YIELDS FOR 8 DELAYED NEUTRON PRECURSOR

Group	INDIVIDUAL FOR FISSION ISOTOPES, BIDNRK:					
	GLOBAL BTDNRK	U-233	U-235	U-239	Pu-239	Pu-241
1	2.14500E-04	8.58000E-05	2.14500E-04	2.14500E-04	6.93000E-05	6.93000E-05
2	1.00100E-03	4.00400E-04	1.00100E-03	1.00100E-03	3.23400E-04	3.23400E-04
3	5.91500E-04	2.36600E-04	5.91500E-04	5.91500E-04	1.91100E-04	1.91100E-04
4	1.28100E-03	5.12200E-04	1.28100E-03	1.28100E-03	4.13700E-04	4.13700E-04
5	2.15100E-03	8.60600E-04	2.15100E-03	2.15100E-03	6.95100E-04	6.95100E-04
6	5.85000E-04	2.34000E-04	5.85000E-04	5.85000E-04	1.89000E-04	1.89000E-04
7	5.26500E-04	2.10600E-04	5.26500E-04	5.26500E-04	1.70100E-04	1.70100E-04
8	1.49500E-04	5.98000E-05	1.49500E-04	1.49500E-04	4.83000E-05	4.83000E-05
Sum:	6.50000E-03	2.60000E-03	6.50000E-03	6.50000E-03	2.10000E-03	2.10000E-03

Note!

The definition of dollars is always based on the values of BTDNRK; where 1 \$ = sum of the global DNP yields for all groups, $\sum[\text{BTDNRK}(i)]$. The reactivity sources (records 760XXX) and the feedback coefficients (records 784XXX) should always be defined using this value (in the example above it is equal to: 6.78286E-3) - see Volume 3, test cases DNP-1, DNP-2.

2.9.13 Records: 780000, Reactivity Feedback Data – Selection of Independent Variable

W-1 (I) : IRFDRK Indicator determining the independent variable for how the moderator feedback calculation (the moderator feedback data table is defined in records 782XXX). The independent variable is:
=1: Moderator temperature, (K)
=2: Moderator density, (kg/m³)
Acceptable range: 1 or 2.
Default value: 1.

2.9.14 Records: 781XXX, Reactivity Feedback Data - Fuel Temperatures

The reactivity feedback table is defined in records 781XXX, 782XXX, 783XXX, and 784XXX. Record 781XXX contains fuel temperature coordinate data. XXX is the point number in reactivity feedback data tables. The total number of data points in the reactivity feedback data tables may not exceed a maximum of NRFMAX = 50.

W-1 (R) : TFTBRK Fuel temperature coordinate value for reactivity feedback table, at the point XXX, $T_{f,T}(XXX)$, (K).
Acceptable range: Values of TFTBRK must increase. Thus the value for the point XXX must be greater than the value for the point XXX-1.
Default value: none.

2.9.15 Records: 782XXX, Reactivity Feedback Data - Moderator Temperatures/densities

The reactivity feedback table is defined in records 781XXX, 782XXX, 783XXX, and 784XXX. Record 782XXX contains moderator temperature coordinate data. XXX is the point number. The total number of data points may not exceed a maximum of NRFMAX = 50.

W-1 (R) : TMTBRK Moderator temperature or density (depending on the value of IRFDRK defined in the record 780000) coordinate value for reactivity feedback table at point XXX, $T_{m,T}(XXX)$, (K) or (kg/m³).
Acceptable range: Values of TMTBRK must increase. Thus the value for the point XXX must be greater than the value for the point XXX-1.
Default value: none.

2.9.16 Record: 783XXX, Reactivity Feedback Data - Void Fractions

The reactivity feedback table is defined in records 781XXX, 782XXX, 783XXX, and 784XXX. Record 783XXX contains void fraction coordinate data. XXX is the point number. The total number of data points may not exceed a maximum of NRFMAX = 50.

W-1 (R) : VFTBRK Void fraction coordinate value for reactivity feedback table at the point XXX, $\alpha_T(XXX)$, (-).
Acceptable range: Values of VFTBRK must increase. Thus the value for the point XXX must be greater than the value for the point XXX-1.
Default value: none.

2.9.17 Record: 784XXX, Reactivity Feedback Data - Reactivities

The reactivity feedback table is defined in records 781XXX, 782XXX, 783XXX, and 784XXX. Record 784XXX contains reactivity data. XXX is just a record identifying number and does not need to be consecutive. The total number of data points may not exceed a maximum of NRFMAX = 50. If no data is entered, but coordinate values are entered, that means records 781XXX, 782XXX, 783XXX are present in input file, but records 784XXX are not present, then default values are used (see below).

Two formats may be used, namely: independent reactivity table format, with 3 entries per record (Format 2), and full reactivity table format, with four entries per record (Format 1). Data must be entered consistently. Once a given format is chosen, all entries must be given in the same format.

Independent reactivity table format (Format 2):

Using Format 2 three independent reactivity tables are created:

- 1.) $R_{f,T}(i) = f(T_{f,T}(i))$,
- 2.) $R_{m,T}(j) = f(T_{m,T}(j))$, or $f(\rho_{m,T}(j))$,
- 3.) $R_{\alpha,T}(k) = f(\alpha_T(k))$.

The full reactivity table is then created by the code, as a sum of the individual values:

$$R_T(i,j,k) = R_{f,T}(i) + R_{m,T}(j) + R_{\alpha,T}(k).$$

When this format is used reactivity values for all data points must be entered.

W-1 (I) : L Indicator of data type:
 =1: this record contains the fuel temperature reactivity table, $R_{f,T}(T_{f,T})$.
 =2: this record contains the moderator temperature or density reactivity table, $R_{m,T}(T_{m,T})$.
 =3: this record contains the void fraction reactivity table, $R_{\alpha,T}(\alpha_T)$.
Acceptable range: 1, 2, 3.
Default value: none.

W-2 (I) : i, j , or k Point number,
 if L = 1: point number in fuel temperature reactivity table, i ,
 if L = 2: point number in moderator temperature reactivity table, j ,
 if L = 3: point number in void fraction reactivity table, k ,
Acceptable range:
 if L = 1: 1, 2, ..., NTFFRK, where NTFFRK is equal to the number of data points entered in record 781XXX.
 if L = 2: 1, 2, ..., NTMFRK, where NTMFRK is equal to the number of data points entered in record 782XXX.
 if L = 3: 1, 2, ..., NVFFRK, where NVFFRK is equal to the number of data points entered in record 783XXX.
Default value: none.

SPECTRA Code Manuals - Volume 2: User's Guide

$\alpha = 0.0$	R = 0.0 \$
$\alpha = 1.0$	R = -20.0 \$

"Gaps" in reactivity table

When the full reactivity table format is selected, then gaps may be left in the table, that means not all reactivity values need to be entered. The gaps are filled in by the program, using linear interpolation. The interpolation is performed in each of the three "dimensions", between the two closest defined points, bounding the gap from both sides (Figure 2-48). No extrapolation is performed; the defined points must be bounding the point being filled in from both sides. If such points cannot be found in given direction, then interpolation is skipped in this direction.

Therefore up to 3 interpolations may be performed to fill a gap. If three or two interpolations are performed, then an arithmetic average is calculated, and then assigned to the gap - Figure 2-48 (a) and (b). If one interpolation is performed, then the resulting value is assigned to the gap - Figure 2-48 (c). If no interpolation is performed, then an error message is printed and the execution is stopped - Figure 2-48 (d). Only the user defined points are used for interpolation. The points, for which values have been obtained previously by interpolations, are not used in subsequent interpolations.

The method of calculating average value of independent interpolations is used to fill the gaps rather than a full 3-dimensional interpolation (see description of 3-d interpolation below), because in practice it would be difficult to find 8 defined points bounding the gap from all directions. Thus a full 3-d interpolation scheme would often fail because of lack of data. With the applied scheme the interpolation will fail for the first and the last points: ($i=1, j=1, k=1$), ($i=NTFFRK, j=NTMFRK, k=NVFFRK$), so these points must be filled in by the user. But other points, or whole rows of data may be left out and they will be filled in by interpolation.

Linear interpolation in 3-D space to obtain reactivity

Once the reactivity table is filled, the program can start calculations. During calculations reactivity is calculated for actual values of fuel temperature, T_{fuel} , moderator temperature, $T_{mod.}$, and void fraction, α (see sections 2.9.18, 2.9.19, and 2.9.20, for the description how T_{fuel} , $T_{mod.}$ and α are obtained). This is done by performing linear interpolation in a 3-dimensional "space", using eight tabulated points bounding the ($T_{fuel}, T_{mod.}, \alpha$) point from all sides - Figure 2-49. No extrapolation is performed. The end point values are kept outside the tabulated space

The interpolations are performed in the following order (see Figure 2-49). First, four interpolations are performed for the fuel temperature direction. Next, two interpolations are performed in the moderator temperature direction. Finally, the last interpolation is performed in the void fraction direction.

Since all interpolations are linear, the order of interpolations is meaningless. The same end value would be obtained by, for example, performing first four interpolations in $T_{mod.}$, next two interpolations in α , and finally one interpolation in T_{fuel} .

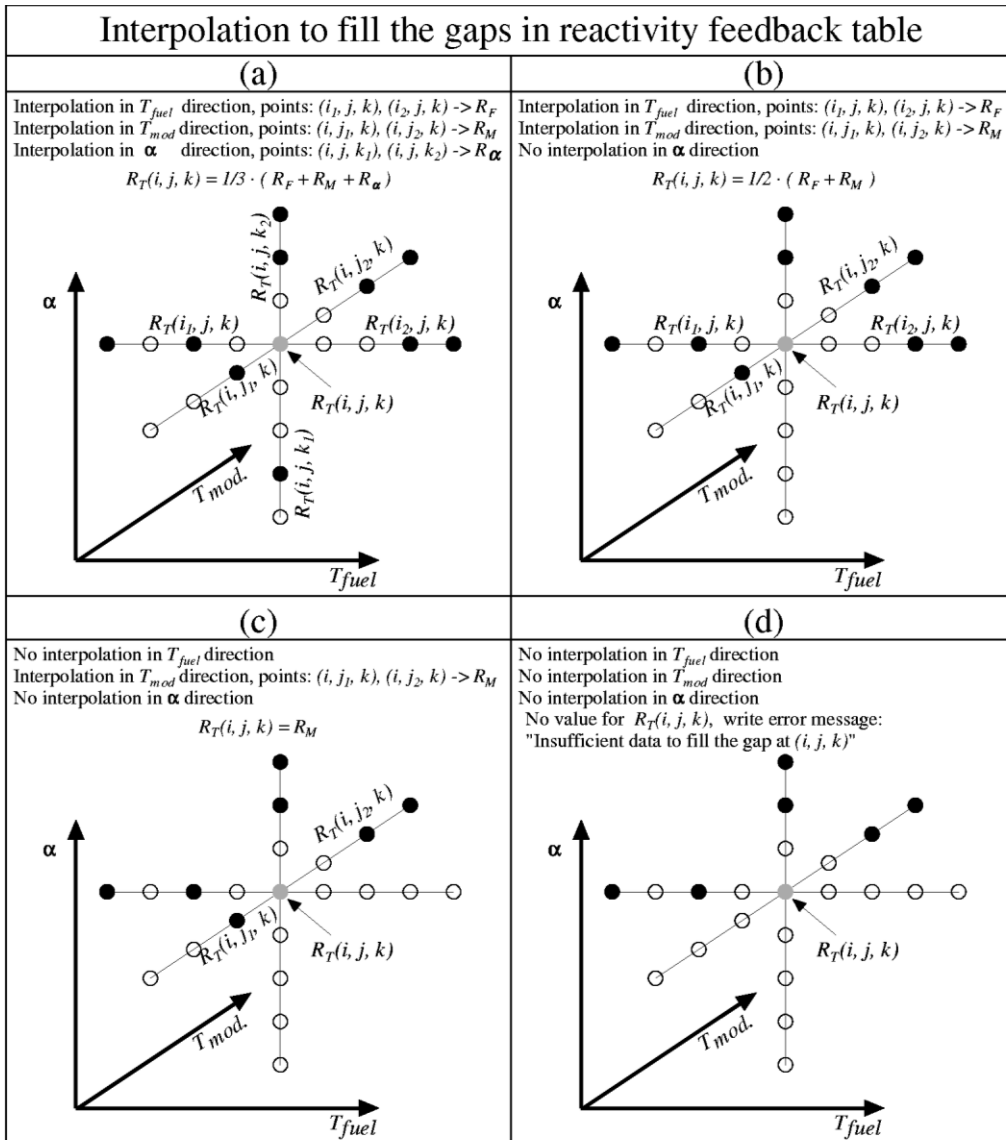


Figure 2-48 Interpolations to fill gaps in the reactivity feedback table.

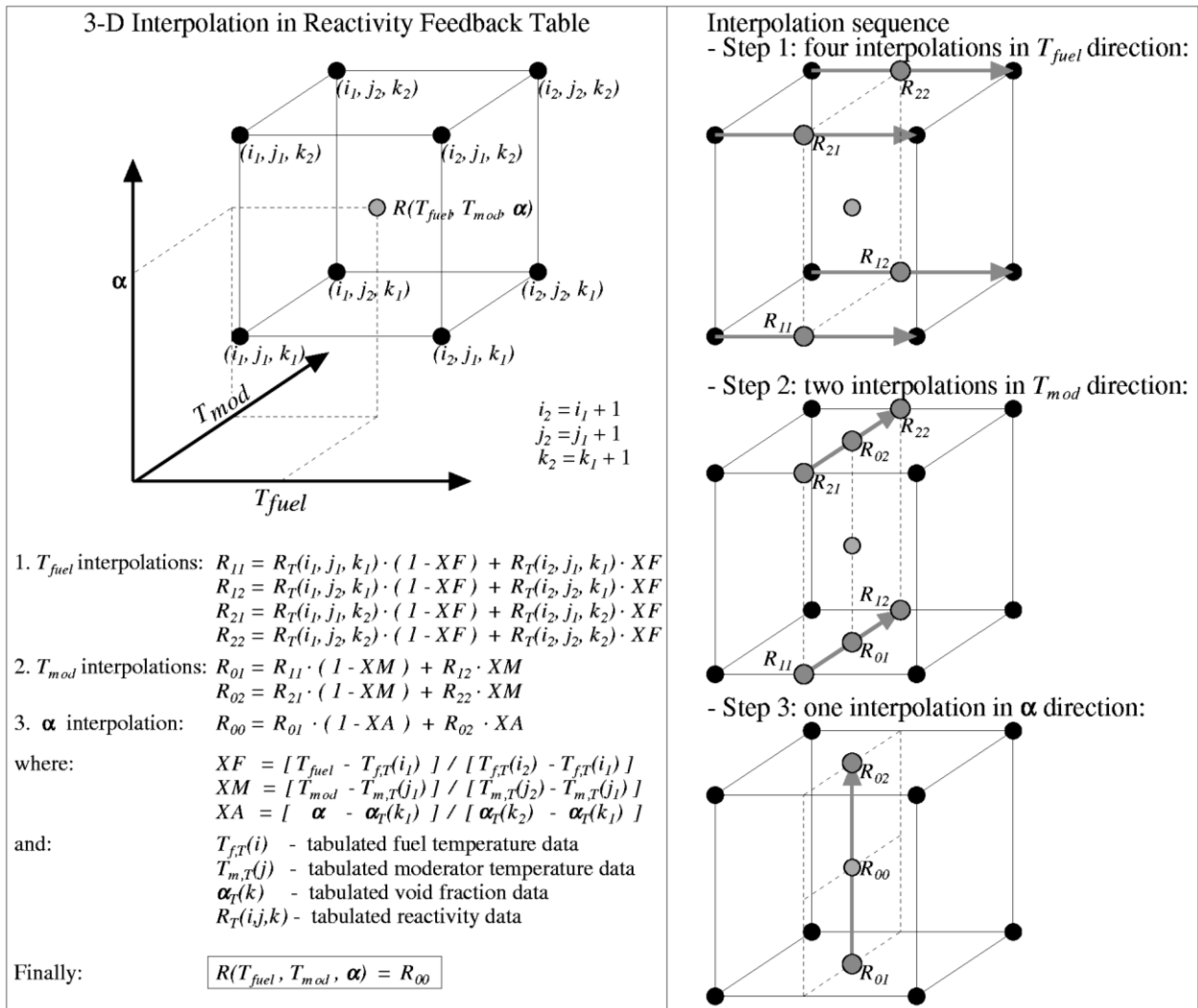


Figure 2-49 Calculating reactivity by 3-D linear interpolation in reactivity feedback table.

2.9.18 Record: 791XXX, Weighting Factors - Fuel Temperatures

The weighting factors are defined in records 791XXX, 792XXX, and 793XXX. Record 791XXX contains fuel temperature weighting factors. The value of XXX is equal to:

- in case of point kinetics: XXX = 000,
- in case of nodal point kinetics: XXX = node number.

W-1 (I) :	ITF1RK	<p>Region indicator 1.</p> <p>= 1: 1-D Solid Heat Conductor temperature defines fuel temperature for this region.</p> <p>= 2: 2-D Solid Heat Conductor temperature defines fuel temperature for this region.</p> <p>= 3: Control Volume pool temperature defines fuel temperature for this region.</p> <p>= 4: Control Volume atmosphere temperature defines fuel temperature for this region.</p> <p><i>Acceptable range:</i> 1, 2, 3, 4 for circulating fuel (IFTORK=2): 3</p> <p><i>Default value:</i> 1.</p>
W-2 (I) :	ITF2RK	<p>Region indicator 2. Defines SC, TC, or CV number for this region.</p> <p>if ITF1RK=1: 1-D Solid Heat Conductor number,</p> <p>if ITF1RK=2: 2-D Solid Heat Conductor number,</p> <p>if ITF1RK=3: Control Volume number,</p> <p>if ITF1RK=4: Control Volume number.</p> <p><i>Acceptable range:</i> must be a valid reference number of a 1-D, 2-D Solid Heat Conductor, or a Control Volume.</p> <p><i>Default value:</i> none.</p>
W-3 (I) :	ITF3RK	<p>Region indicator 3. Defines which mesh cells of a 1-D or 2-D Solid Heat Conductor are within this region.</p> <p>if ITF1RK=1: Starting cell number of a 1-D Heat Conductor.</p> <p>if ITF1RK=2: Starting cell number of a 2-D Heat Conductor.</p> <p>if ITF1RK=3: not used,</p> <p>if ITF1RK=4: not used.</p> <p><i>Acceptable range:</i></p> <p>if ITF1RK=1: $1 \leq \text{ITF3RK} \leq \text{NCELSC}(\text{ITF2RK})$.</p> <p>if ITF1RK=2: $1 \leq \text{ITF3RK} \leq \text{NCELTC}(\text{ITF2RK})$.</p> <p><i>Default value:</i> none.</p>
W-4 (I) :	ITF4RK	<p>Region indicator 4. Defines which mesh cells of a 1-D or 2-D Solid Heat Conductor are within this region.</p> <p>if ITF1RK=1: Last cell number of a 1-D Heat Conductor.</p> <p>if ITF1RK=2: Last cell number of a 2-D Heat Conductor.</p> <p>if ITF1RK=3: not used,</p> <p>if ITF1RK=4: not used.</p> <p><i>Acceptable range:</i></p> <p>if ITF1RK=1: $\text{ITF3RK} \leq \text{ITF4RK} \leq \text{NCELSC}(\text{ITF2RK})$.</p> <p>if ITF1RK=2: $\text{ITF3RK} \leq \text{ITF4RK} \leq \text{NCETSC}(\text{ITF2RK})$.</p> <p><i>Default value:</i> none.</p>

SPECTRA Code Manuals - Volume 2: User's Guide

- W-2 (I) : ITM2RK Region indicator 2. Defines SC number or CV number for this region.
if ITM1RK=1: 1-D Solid Heat Conductor number,
if ITM1RK=2: 2-D Solid Heat Conductor number,
if ITM1RK=3: Control Volume number,
if ITM1RK=4: Control Volume number.
Acceptable range: must be a valid reference number of a 1-D , 2-D
Solid Heat Conductor, or a Control Volume.
Default value: none.
- W-3 (I) : ITM3RK Region indicator 3. Defines which mesh cells of a 1-D or 2-D Solid Heat
Conductor are within this region.
if ITM1RK=1: Starting cell number of a 1-D Heat Conductor.
if ITM1RK=2: Starting cell number of a 2-D Heat Conductor.
if ITM1RK=3: not used,
if ITM1RK=4: not used.
Acceptable range:
if ITM1RK=1: $1 \leq \text{ITM3RK} \leq \text{NCELSC}(\text{ITM2RK})$.
if ITM1RK=2 $1 \leq \text{ITM3RK} \leq \text{NCELTC}(\text{ITM2RK})$.
Default value: none.
- W-4 (I) : ITM4RK Region indicator 4. Defines which mesh cells of a 1-D or 2-D Solid Heat
Conductor are within this region.
if ITM1RK=1: Last cell number of a 1-D Heat Conductor.
if ITM1RK=2: Last cell number of a 2-D Heat Conductor.
if ITM1RK=3: not used,
if ITM1RK=4: not used.
Acceptable range:
if ITM1RK=1: $\text{ITM3RK} \leq \text{ITM4RK} \leq \text{NCELSC}(\text{ITM2RK})$.
if ITM1RK=2: $\text{ITM3RK} \leq \text{ITM4RK} \leq \text{NCETSC}(\text{ITM2RK})$.
Default value: none.
- W-5 (R) : WTMFRK Weighting factor, W_{TM} , for the region defined by the words 1 through 4.
The values will be normalized to 1.0 if all factors are positive. If any
factor is negative, then no normalization is performed and all moderator
temperature/density weighting factors will be used as entered. NOTE: in
such case the value of average moderator temperature/density (RK-000-
Tmod-0000 - Table 2-29) will not have a physical meaning.
Acceptable range: WTMFRK \neq 0.0.
Default value: none.
- W-6 (I) : I Region number. If no value, or zero is entered, then the region data are
read sequentially - the first record in the input is interpreted as containing
the first (lower) region data (I=1), then I=2, etc. The total number of
regions is equal to $\text{NTMWRK} \leq \text{NWFMAX} = 200$
Acceptable range: I = 1, 2, ..., 200
Default value: none

2.9.20 Record: 793XXX, Weighting Factors - Void Fractions

The weighting factors are defined in records 791XXX, 792XXX, and 793XXX. Record 793XXX contains void fraction weighting factors. The value of XXX is equal to:

- in case of point kinetics: XXX = 000,
- in case of nodal point kinetics: XXX = node number (maximum of 50 nodes)

W-1 (I) :	IVF1RK	<p>Region indicator 1.</p> <p>= 1: Local void fraction, α_{SC}, in the pool-covered fraction of a 1-D Solid Heat Conductor surface.</p> <p>= 2: $X_{pool,SC} \cdot \alpha_{SC} + X_{atms,SC}$ Effective local void fraction at a 1-D Solid Heat Conductor surface. $X_{pool,SC}$ is the fraction of surface covered by pool. $X_{atms,SC}$ is the uncovered fraction of surface. α_{SC} is the local void fraction at the pool-covered part of the SC surface.</p> <p>= 3: Local void fraction, α_{TC}, in the pool-covered fraction of a 2-D Solid Heat Conductor boundary cell.</p> <p>= 4: $X_{pool,TC} \cdot \alpha_{TC} + X_{atms,TC}$ Effective local void fraction at a 2-D Solid Heat Conductor boundary cell. $X_{pool,TC}$ is the fraction of cell surface covered by pool. $X_{atms,TC}$ is the uncovered fraction. α_{TC} is the local void fraction at the pool-covered part of the TC cell surface.</p> <p>= 5: Average void fraction, α_{CV}, in a CV pool.</p> <p>= 6: $X_{pool,CV} \cdot \alpha_{CV} + X_{atms,CV}$ Effective void fraction in a Control Volume. $X_{pool,CV}$ is the fraction of CV occupied by pool. $X_{atms,CV}$ is the fraction of CV occupied by atmosphere. α_{CV} is the average void fraction in the pool of CV.</p> <p><i>Acceptable range:</i> 1, 2, 3, 4, 5, and 6.</p> <p><i>Default value:</i> 2.</p>
W-2 (I) :	IVF2RK	<p>Region indicator 2. Defines SC number or CV number for this region.</p> <p>if IVF1RK=1: 1-D Solid Heat Conductor number,</p> <p>if IVF1RK=2: 1-D Solid Heat Conductor number,</p> <p>if IVF1RK=3: 2-D Solid Heat Conductor number,</p> <p>if IVF1RK=4: 2-D Solid Heat Conductor number,</p> <p>if IVF1RK=5: Control Volume number,</p> <p>if IVF1RK=6: Control Volume number.</p> <p><i>Acceptable range:</i> must be a valid reference number of a 1-D, 2-D Solid Heat Conductor, or a Control Volume.</p> <p><i>Default value:</i> none.</p>
W-3 (I) :	IVF3RK	<p>Region indicator 3. Defines which surface of a 1-D Solid Heat Conductor, or which boundary cells of a 2-D Solid Heat Conductor are considered.</p> <p>if IVF1RK=1, 2: IVF3RK = -1: left surface, IVF3RK = +1: right surface.</p> <p>if IVF1RK=3, 4: Starting cell number of a 2-D Heat Conductor.</p> <p>if IVF1RK=5, 6: not used.</p> <p><i>Acceptable range:</i> if IVF1RK=1, 2: -1, or +1. if IVF1RK=3, 4: boundary cell number.</p>

SPECTRA Code Manuals - Volume 2: User's Guide

- Default value:* none.
- W-4 (I) : IVF4RK Region indicator 4. Defines which boundary cells of a 2-D Solid Heat Conductor are within this region.
if IVF1RK=1, 2: not used.
if IVF1RK=3, 4: Last cell number of a 2-D Heat Conductor.
if IVF1RK=5, 6: not used.
Acceptable range:
if IVF1RK=3, 4: $IVF3RK \leq IVF4RK \leq NCETSC(IVF2RK)$.
Default value: none.
- W-5 (R) : WVFMRK Weighting factor, W_{VF} , for the region defined by the words 1 through 4. The values will be normalized to 1.0 if all factors are positive. If any factor is negative, then no normalization is performed and all void fraction weighting factors will be used as entered. NOTE: in such case the value of average void fraction (RK-000-Void-0000 - Table 2-29) will not have a physical meaning.
Acceptable range: WVFMRK \neq 0.0.
Default value: none.
- W-6 (I) : I Region number. If no value, or zero is entered, then the region data are read sequentially - the first record in the input is interpreted as containing the first (lower) region data (I=1), then I=2, etc. The total number of regions is equal to $NVFWRK \leq NWFMAX = 200$
Acceptable range: I = 1, 2, ..., 200
Default value: none

2.9.21 Example of Reactor Kinetics Input Data

Two examples of Reactor Kinetics input are provided below. In the first example the reactivity feedback is defined through independent tables. In the second example the reactivity feedback is defined through a full table.

In the first example the reactor is 50 m³ in size, the initial power is 100 MW. The macroscopic fission cross section is calculated as follows. The fuel consists of 5% enriched uranium. The total mass of uranium in the core is 20 t. The mass of U-235 is equal to 20·0.05 = 1 t = 10³ kg. The number of kmoles is equal to 10³/235 = 4.255. The average molar density is equal to 4.255/50 = 0.0851 kmol/m³. The atomic density is obtained using the Avogadro number (6.022·10²⁶ atoms/kmol): $N = 0.0851 \times 6.022 \cdot 10^{26} = 5.12 \cdot 10^{25}$ atoms/m³. The macroscopic fission cross section is equal to: $\Sigma_f = N \cdot \sigma_f$, where σ_f is the microscopic fission cross-section for U-235, equal to 505 barn = 505·10⁻²⁸ m² (Figure 2-54). The value of Σ_f is equal to:

$$\Sigma_f = N \cdot \sigma_f = 5.12 \cdot 10^{25} \cdot 505 \cdot 10^{-28} = 0.028 \text{ m}^{-1}$$

If there is more than one fissile isotope in the core, then Σ_f is a sum over all individual values, calculated as shown above.

The initial reactivity is zero. Three Tabular Functions (TF-001, TF-002, and TF-003) are used to model three groups of control rods. TF-004 is used to define the external neutron source.

The reactivity feedback is entered using independent reactivity tables input format. Tabular data defining the reactivity feedback from fuel temperature, moderator temperature, and void fraction, are shown in Table 2-33, Table 2-34 and Table 2-35, respectively.

The average fuel temperature is calculated by averaging the Solid Heat Conductor temperatures of SC-001 and SC-002. For both SC-001 and SC-002 mesh cells 1 through 10 are included in average temperature calculation. That means within each of these SC's the average temperature is calculated as cell volume averaged value including cells 1 through 10:

$$T_{SC} = \frac{\sum_{i=1}^{10} V_i T_i}{\sum_{i=1}^{10} V_i}$$

where T_{SC} is the SC average temperature, while T_i and V_i are the temperature and volume respectively of cell i . The weighting factors of 0.6 and 0.4 are assigned to SC-001 and SC-002 respectively, therefore the average fuel temperature is calculated as:

$$T_{fuel} = 0.6 \cdot T_{SC-001} + 0.4 \cdot T_{SC-002} = 0.6 \cdot \left(\frac{\sum_{i=1}^{10} V_i T_i}{\sum_{i=1}^{10} V_i} \right)_{SC-001} + 0.4 \cdot \left(\frac{\sum_{i=1}^{10} V_i T_i}{\sum_{i=1}^{10} V_i} \right)_{SC-002}$$

Table 2-33 Reactivity feedback from fuel temperature.

SPECTRA Code Manuals - Volume 2: User's Guide

<i>i</i>	1	2	3	4
$T_{f,T}(i)$ (K)	300	800	1300	1800
$R_{f,T}(i)$ (\$)	1.00	0.90	0.80	0.70

Table 2-34 Reactivity feedback from moderator temperature.

<i>j</i>	1	2
$T_{m,T}(j)$ (K)	300	900
$R_{m,T}(j)$ (\$)	1.00	0.95

Table 2-35 Reactivity feedback from void fraction.

<i>k</i>	1	2
$\alpha_T(k)$ (K)	0.0	1.0
$R_{a,T}(k)$ (\$)	1.00	0.00

The average moderator temperature is calculated from the pool temperatures in Control Volumes CV-002 and CV-005, with the weighting factors of 0.9 and 0.1 respectively. Therefore:

$$T_{\text{mod}} = 0.9 \cdot T_{\text{pool,CV-002}} + 0.1 \cdot T_{\text{pool,CV-005}}$$

The average moderator void fraction is calculated from the effective local void fraction at the left and right surfaces of SC-001 and SC-002, with the weighting factors of 0.3 at SC-001 surfaces, and 0.2 at SC-002 surfaces. Therefore:

$$\alpha = 0.3 \cdot \alpha_{\text{eff,SC-001-L}} + 0.3 \cdot \alpha_{\text{eff,SC-001-R}} + 0.2 \cdot \alpha_{\text{eff,SC-002-L}} + 0.2 \cdot \alpha_{\text{eff,SC-002-R}}$$

$$\alpha = 0.3 \cdot (X_{\text{pool}} \alpha_{\text{pool}} + X_{\text{atms}})_{\text{SC-001-L}} + 0.3 \cdot (X_{\text{pool}} \alpha_{\text{pool}} + X_{\text{atms}})_{\text{SC-001-R}} +$$

$$+ 0.2 \cdot (X_{\text{pool}} \alpha_{\text{pool}} + X_{\text{atms}})_{\text{SC-002-L}} + 0.2 \cdot (X_{\text{pool}} \alpha_{\text{pool}} + X_{\text{atms}})_{\text{SC-002-R}}$$

where X_{pool} is the fraction of SC surface covered by pool, X_{atms} is the uncovered fraction of SC surface, and α_{pool} is the local bubble fraction at SC surface.

```

*
* ===== CF CONTROL FUNCTION DATA =====
*
705001 REACTOR KINETICS CONTROL FUNCTION
700001 3 5 1.0 0.0 * Type: Reactor Kinetics, Scale=1.0, Add=0.0
710001 9 0 1 0 * Argument: time
*
* ===== RK REACTOR KINETICS DATA =====
*
* PNGTRK SIGFRK
750000 0 0.028 * MACROSCOPIC FISSION CROSS SECTION
* VOL (m3) POWER (W) REAC. ($)
751000 50.0 1.0E8 0.0
755000 4 * EXTERNAL NEUTRON SOURCE (1/s) DEFINED BY TF-004
* ROD 1 ROD 2 ROD 3
760000 1 2 3 * CONTROL ROD REACTIVITY DEFINED BY TF-001, TF-002, TF-003
*
* - REACTIVITY FEEDBACK DATA
*

```

SPECTRA Code Manuals - Volume 2: User's Guide

```
* -- FUEL TEMPERATURE TABLE
781001 300.0 * Tfuel(1)
781002 800.0 * Tfuel(2)
781003 1300.0 * Tfuel(3)
781004 1800.0 * Tfuel(4)
*
* -- MOD. TEMPERATURE TABLE
782001 300.0 * Tmod(1)
782002 900.0 * Tmod(2)
*
* -- VOID FRACTION TABLE
783001 0.0 * void(1)
783002 1.0 * void(2)
*
* -- REACTIVITY TABLE - INDEPENDENT REACTIVITY COEFFICIENT INPUT
*      TYPE      Point      REACTIVITY
*      (1=Tfuel)  No.        ($)
784001 1          1          1.000
784002 1          2          0.900
784003 1          3          0.800
784004 1          4          0.700
*      TYPE      Point      REACTIVITY
*      (2=Tmod.)  No.        ($)
784005 2          1          1.000
784006 2          2          0.950
*      TYPE      Point      REACTIVITY
*      (3=V.Fr.)  No.        ($)
784007 3          1          1.000
784008 3          2          0.000
*
* - WEIGHTING FACTORS
* -- FUEL TEMPERATURE
791000 1 1 1 10 0.6 * SC-001, Temperature in Nodes: 1 - 10, W = 0.6
791000 1 2 1 10 0.4 * SC-002, Temperature in Nodes: 1 - 10, W = 0.4
* -- MODERATOR TEMPERATURE
792000 3 2 0 0 0.9 * CV-002, Pool temperature, W = 0.9
792000 3 5 0 0 0.1 * CV-005, Pool temperature, W = 0.1
* -- VOID FRACTION
793000 2 1 -1 0 0.3 * SC-001, Void fraction at left surf., W = 0.3
793000 2 1 1 0 0.3 * SC-001, Void fraction at right surf., W = 0.3
793000 2 2 -1 0 0.2 * SC-002, Void fraction at left surf., W = 0.2
793000 2 2 1 0 0.2 * SC-002, Void fraction at right surf., W = 0.2
*
```

The second example, shown below, is very similar to the previous one, but in this case only one control rod group is modelled (using TF-001), no external neutron source is present, and the reactivity feedback is defined using full reactivity table format. The data covers a 3-D "space":

$$\begin{aligned} 300 \text{ K} &\leq T_{fuel} \leq 1300 \text{ K}, \\ 300 \text{ K} &\leq T_{mod.} \leq 900 \text{ K}, \\ 0.0 &\leq \alpha \leq 1.0. \end{aligned}$$

The same weighting factors are used, so the average fuel temperature, moderator temperature and void fraction, are calculated as described above.

Note that a Control Function, type "Reactor Kinetics" is entered in both examples. The Reactor Kinetics Package is actually activated by a presence of such Control Function in the input deck. If such CF is not present in the input deck, then the Reactor Kinetics Package will not be used, regardless whether any of the RK data has been entered or not. It should also be remembered that only one such function may be present in the input deck, and that the value of this CF will be equal to the current reactor power. Therefore this CF cannot be used as a CF defining control rod reactivity (section 2.9.9), or CF defining external neutron source (section 2.9.7). Such cases are flagged by the program as input errors.

SPECTRA Code Manuals - Volume 2: User's Guide

```

*
* ===== CF CONTROL FUNCTION DATA =====
*
705001 REACTOR KINETICS CONTROL FUNCTION
700001 3 5 1.0 0.0 * Type: Reactor Kinetics, Scale=1.0, Add=0.0
710001 9 0 1 0 * Argument: time
*
* ===== RK REACTOR KINETICS DATA =====
*
750000 0 0.26 * MACROSCOPIC FISSION CROSS SECTION
751000 50.0 1.0E8 0.0 * V (m3), POWER (W), REAC. ($)
760000 001 * CONTROL ROD REACTIVITY DEFINED BY TF-001
*
* - REACTIVITY FEEDBACK DATA
*
* -- FUEL TEMPERATURE TABLE
781001 300.0 * Tfuel(1)
781002 800.0 * Tfuel(2)
781003 1300.0 * Tfuel(3)
*
* -- MOD. TEMPERATURE TABLE
782001 300.0 * Tmod(1)
782002 900.0 * Tmod(2)
*
* -- VOID FRACTION TABLE
783001 0.0 * void(1)
783002 1.0 * void(2)
*
* -- REACTIVITY TABLE - FULL TABLE INPUT
* Tfuel Tmod. V.Fr. REACTIVITY
* POINT No. POINT No. POINT No. ($)
784001 1 1 1 1.000
784002 1 1 2 0.000
784003 1 2 1 0.950
784004 1 2 2 0.050
*
784005 2 1 1 0.900
784006 2 1 2 -0.100
784007 2 2 1 0.850
784008 2 2 2 -0.150
*
784009 3 1 1 0.800
784010 3 1 2 -0.200
784011 3 2 1 0.750
784012 3 2 2 -0.250
*
* - WEIGHTING FACTORS
*
* -- FUEL TEMPERATURE
791001 1 1 1 10 0.6 * SC-001, Temperature in Nodes: 1 - 10, W = 0.6
791002 1 2 1 10 0.4 * SC-002, Temperature in Nodes: 1 - 10, W = 0.4
*
* -- MODERATOR TEMPERATURE
792001 3 2 0 0 0.9 * CV-002, Pool temperature, W = 0.9
792002 3 5 0 0 0.1 * CV-005, Pool temperature, W = 0.1
*
* -- VOID FRACTION
793001 2 1 -1 0 0.3 * SC-001, Void fraction at left surf., W = 0.3
793002 2 1 1 0 0.3 * SC-001, Void fraction at right surf., W = 0.3
793003 2 2 -1 0 0.2 * SC-002, Void fraction at left surf., W = 0.2
793004 2 2 1 0 0.2 * SC-002, Void fraction at right surf., W = 0.2
*

```

2.9.22 Record: 740000, Isotope Transformation Data - Initial Core Composition

The Isotope Transformation model is a part of the Reactor Kinetics package, and may be used only if the RK package is active.

- W-1 (I) : ICITRK Initial core composition calculation.
1 = only input values. The user can define the initial concentrations of non-fissile isotopes in records 740XXX (section 2.9.24), and fissile isotopes in records 746XXX (section 2.9.28). Use this option also when isotope concentrations should be read from an Initial Condition File - ICF (see section 2.16.3).
2 = equilibrium concentrations are calculated for non-fissile isotopes, unless the initial values are specified in records 740XXX. Concentrations of the isotopes for which there is no removal mechanism (such as decay, neutron absorption) are set to zero, because there is no equilibrium solution (the "equilibrium" concentration would be infinitely large).
3 = equilibrium concentrations are calculated for all isotopes, unless the initial values are specified in records 740XXX (non-fissile) or 746XXX (fissile). Concentrations of the isotopes for which there is no removal mechanism are set to zero.
-1 = suppress the whole isotope transformation model.
Acceptable range: 1, 2, 3, or -1 .
Default value: 2.
- W-2 (I) : IDITRK Request for built-in isotope data (see section 2.9.36). The entry has six-digit format: *fedcba*. For each digit 0 means don't use data.
a≠0 : use built-in data for ²³³U/²³⁵U fuel chain (8 isotopes),
b≠0 : use built-in data for ²³⁹U/²³⁹Pu/²⁴¹Pu fuel chain (8 isotopes),
c≠0 : use built-in data for ¹³⁵Xe chain (3 isotopes),
d≠0 : use built-in data for ¹⁴⁹Sm chain (3 isotopes),
e≠0 : use built-in data for ¹⁵⁷Gd chain (2 isotopes),
f≠0 : use built-in data for 11 decay heat groups.
For example, to use all built in data enter 111111; to use all data except for the gadolinium chain, enter 101111.
Acceptable range: IDITRK ≥ 0.
Default value: 000000.

2.9.23 Records: I05XXX, Isotope Transformation Data - Isotope Names

XXX=001, 002, ..., NIITRK, is the isotope reference number. The isotope reference numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK>0), then the user-defined isotopes must have higher numbers than the built-in isotopes. The recommended numbers are XXX>700. The maximum number of isotopes is 200.

- W-1 (A) : NMITRK User defined name, length up to 7 characters. The name is read as a 7-character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.

Examples of the isotope names are: **U-235**, **Xe-131m**. Note that the name is arbitrary and does not serve as, for example, an indicator of fissile nuclides. Fissile nuclides are identified only by a non-zero fission cross section, entered in record 743XXX (see section 2.9.27).

Acceptable range: any string of up to 7 characters.

Default value: 7 "underline" characters: " ".

2.9.24 Records: 740XXX, Isotope Transformation Data - Initial Isotope Concentrations

XXX=001, 002, ..., NIITRK, is the isotope reference number. The isotope reference numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK>0), then the user-defined isotopes must have higher numbers than the built-in isotopes. The recommended numbers are XXX>700. . The maximum number of isotopes is 200.

W-1 (R) : XIITRK Initial concentration of isotope XXX, $N_{i=XXX}$, ($1/m^3$), or relative concentration of XXX depending on word 2. Only initial concentrations of non-fissile isotopes can be specified here. Fuel initial concentrations are specified in record 746XXX, as mass fractions (see section 2.9.28). If an equilibrium core is specified in record 740000 (see section 2.9.22 above), then the initial concentration entered here overwrites the calculated equilibrium value.

In the case of the nodal point kinetics, the concentration defined here is used in all nodes. The nodal-specific values are printed in the ICF file. The initialization of nodal point kinetics is done by selecting initialization option, INONRK=1, in the record 750XXX. When the initialization run is finished, all initial concentrations are available in the ICF file and may be modified by the user, if needed.

Acceptable range: XIITRK \geq 0.0 .

Default value: 0.0 .

W-2 (I) : IIITRK Reference fissile isotope for definition of initial concentration of isotope XXX.

If IIITRK \leq 0, then XIITRK (word 1 above) is interpreted as initial concentration of isotope XXX, in m^{-3} .

If IIITRK > 0, then XIITRK (word 1 above) is interpreted as initial concentration of isotope XXX relative to the initial concentration of fissile isotope IIITRK. In such case there must exist an isotope IIITRK, with positive fission cross section.

Acceptable range: IIITRK \leq NIITRK .

Default value: 0 .

W-3 (R) : CRITRK Multiplier on reactivity effect of isotope XXX, $C_{R, i=XXX}$, (-). This is a ratio of true reactivity effect of isotope XXX to the value obtained assuming uniform reactor flux distribution (point reactor):

$$CRITRK = \frac{\Delta\rho}{\Delta\rho_{point}}$$

The reactivity change for a point reactor is equal to:

$$\Delta\rho_{point} = -\frac{\Sigma_a}{\nu\Sigma_f}$$

where Σ_a is the absorption cross section of poison, Σ_f is the fission cross section, ν is the number of neutrons produced per fission. For point reactor there is no position independence of cross sections. This is how SPECTRA calculates the reactivity effect. In reality the neutron flux distribution is not uniform, and the cross sections are position dependent. The reactivity effect is approximately given by (see [5], equation 15-35):

$$\Delta\rho = -\frac{\int \Sigma_a(\bar{r})\Phi^2(\bar{r})d^3r}{\nu \int \Sigma_f(\bar{r})\Phi^2(\bar{r})d^3r}$$

where $\Phi(r)$ is the neutron flux. Using perturbation theory a reactivity effect for equilibrium poison concentration can be calculated. It may be shown (see [5], section 15.I.D):

$$\Delta\rho \propto -\frac{\int \Phi^3(\bar{r})d^3r}{\int \Phi^2(\bar{r})d^3r}$$

Thus the value of reactivity worth increases with more non-uniform flux distribution.

Acceptable range: 0.0 < CRITRK ≤ 1000.0

Default value: 1.0

2.9.25 Records: 741XXX, Isotope Transformation Data - Decay Data

XXX=001, 002, ..., NIITRK, is the isotope reference number. The isotope reference numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK>0), then the user-defined isotopes must have higher numbers than the built-in isotopes. The recommended numbers are XXX>700. . The maximum number of isotopes is 200.

W-1 (R) : DCITRK Decay constant, λ , (1/s). If $\lambda = 0.0$, the following data words in this record are ignored.

Acceptable range: DCITRK ≥ 0.0 .

Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36).

W-2 (R) : QDITRK Heat generated per decay, q_d , (J).

Acceptable range: 0.0 ≤ QDITRK ≤ 1.0·10⁻⁹

SPECTRA Code Manuals - Volume 2: User's Guide

- (note that $1 \text{ MeV} = 1.602 \cdot 10^{-13} \text{ J}$).
- Default value:* Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36).
- W-3 (I) : J1 Isotope number of the decay product.
Acceptable range: $J1 \leq \text{NIITRK}$.
Default value: none.
- W-4 (R) : YDITRK Yield fraction of isotope J1 from decay of XXX, (-).
(J1) This number is interpreted as a probability of the fact that a decay of a nuclide of isotope XXX will result in production of a nuclide of isotope J1.
Acceptable range: $\text{YDITRK} \geq 0.0$.
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36). A small number, $<10^{-50}$, sets the built-in value to 0.0.
- W-5 (I) : J2 Isotope number of the decay product.
Acceptable range: $J2 \leq \text{NIITRK}$.
Default value: none.
- W-6 (R) : YDITRK Yield fraction of isotope J2 from decay of XXX, (-).
(J2) This number is interpreted as a probability of the fact that a decay of a nuclide of isotope XXX will result in production of a nuclide of isotope J2.
Acceptable range: $\text{YDITRK} \geq 0.0$.
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36). A small number, $<10^{-50}$, sets the built-in value to 0.0.

... until all decay products are defined.

Note!

If the sum of the decay yield fractions is different than 1.0, then the fractions may be normalized, to give the sum of 1.0. The normalization is requested by the user, through word 1 in record 749000 (section 2.9.34).

2.9.26 Records: 742XXX, Isotope Transformation Data - Absorption Data

XXX=001, 002, ..., NIITRK, is the isotope reference number. The isotope reference numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK>0), then the user-defined isotopes must have higher numbers than the built-in isotopes. The recommended numbers are $\text{XXX} > 700$. The maximum number of isotopes is 200.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-1 (R) : SAITRK Microscopic cross section for neutron capture, σ_c , (barn), for isotope XXX. If $\sigma_c = 0.0$, the following data words in this record are ignored.
Acceptable range: SAITRK ≥ 0.0 .
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36. Note that the values for U-238 and Th-232 depend on resonance absorption and therefore on the fission cross section and the concentrations of all fissile isotopes, as described in section 2.9.36.
- W-2 (I) : J1 Isotope number of the product of neutron capture by XXX.
Acceptable range: J1 \leq NIITRK .
Default value: none.
- W-3 (R) : YAITRK Yield fraction of isotope J1 from neutron capture in XXX, (-).
(J1) This number is interpreted as a probability of the fact that capture of neutron by a nuclide of isotope XXX will result in production of a nuclide of isotope J1.
Acceptable range: YAITRK ≥ 0.0 .
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36). A small number, $<10^{-50}$, sets the built-in value to 0.0.
- W-4 (I) : J2 Isotope number of the product of neutron capture by XXX.
Acceptable range: J2 \leq NIITRK .
Default value: none.
- W-5 (R) : YAITRK Yield fraction of isotope J2 from neutron capture in XXX, (-).
(J2) This number is interpreted as a probability of the fact that capture of neutron by a nuclide of isotope XXX will result in production of a nuclide of isotope J2.
Acceptable range: YAITRK ≥ 0.0 .
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36). A small number, $<10^{-50}$, sets the built-in value to 0.0.

... until all products of neutron capture are defined.

Note!

If the sum of the capture yield fractions is different than 1.0, then the fractions may be normalized, to give the sum of 1.0. The normalization is requested by the user, through word 2 in record 749000 (section 2.9.34).

2.9.27 Records: 743XXX, Isotope Transformation Data - Fission Data

XXX=001, 002, ..., NIITRK, is the isotope reference number. The isotope reference numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK>0), then the user-defined isotopes must have higher numbers than the built-in isotopes. The recommended numbers are XXX>700. . The maximum number of isotopes is 200.

W-1 (R) : SFITRK Microscopic cross section for fission, σ_f , (barn), for isotope XXX. If $\sigma_f = 0.0$, the following data words in this record are ignored.
Acceptable range: SFITRK ≥ 0.0 .
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36).

W-2 (I) : J1 Isotope number of the product of fission of XXX.
Acceptable range: J1 \leq NIITRK .
Default value: none.

W-3 (R) : YFITRK Yield fraction of isotope J1 from fission of XXX, (-).
 (J1) This number is interpreted as a probability of the fact that a nuclide of isotope J1 will be created from fission of XXX.
Acceptable range: YFITRK ≥ 0.0 .
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36). A small number, $<10^{-50}$, sets the built-in value to 0.0.

W-4 (I) : J2 Isotope number of the product of fission of XXX.
Acceptable range: J2 \leq NIITRK .
Default value: none.

W-5 (R) : YFITRK Yield fraction of isotope J2 from fission of XXX, (-).
 (J2) This number is interpreted as a probability of the fact that a nuclide of isotope J2 will be created from fission of XXX.
Acceptable range: YFITRK ≥ 0.0 .
Default value: Default values are available if built-in isotope data is requested in record 740000. The default values for all built-in isotopes are listed below, in section 2.9.36). A small number, $<10^{-50}$, sets the built-in value to 0.0.

... until all fission products are defined.

Note!

If the sum of the fission yield fractions is different than 2.0, then the fractions may be normalized, to give the sum of 2.0. The normalization is requested by the user, through word 3 in record 749000 (section 2.9.34).

2.9.28 Records: 746XXX, Isotope Transformation Data - Fuel Composition

XXX=001, 002, ..., NIITRK, is the isotope number. The maximum number of isotopes is 200. This record specifies initial composition of fuel (mass fractions). At least one positive value must be entered for a fissile isotope. If the sum of all fractions is not equal to 1.0, then the fractions will be normalized, to give the sum of 1.0.

W-1 (R) : FIITRK Mass fraction of fissile isotope XXX in the fuel. If equilibrium fuel concentrations are requested (ICITRK=3, record 740000, section 2.9.22), then concentrations of those isotopes for which initial fractions are zero are calculated from the equilibrium condition, and then all fuel fractions are rescaled to give the sum of one. To avoid using equilibrium concentrations for certain fuels, enter positive small number for these fuels, for example 10^{-30} .

The initial concentrations, in $(1/m^3)$, are calculated using the fissile fractions entered here, and the overall macroscopic fission cross-section, Σ_f , defined in record 750000 (section 2.9.1). To calculate concentrations, N_i , the following relation is used:

$$\Sigma_f = \sum_i N_i \sigma_{f,i} = C \cdot \sum_i f_i \sigma_{f,i}$$

where f_i are the fractions entered in this record, and C is a constant, equal to:

$$C = \frac{\Sigma_f \cdot \sum_i f_i}{\sum_i f_i \sigma_{f,i}}$$

By including the sum of f_i , the above formula automatically takes care that the entered fractions should be normalized to 1.0. Finally, all fuel concentrations are obtained from:

$$N_i = C \cdot f_i.$$

Acceptable range: if isotope XXX does not undergo fission ($\sigma_f = \text{SFITRK} = 0.0$ - section 2.9.27), then FIITRK must be equal to zero; if isotope XXX does undergo fission ($\sigma_f = \text{SFITRK} > 0.0$ - section 2.9.27), then $\text{FIITRK} \geq 0.0$.

Default value: 0.0 .

2.9.29 Record: 747XXX, Isotope Transformation Data - Fuel Removal/Loading Data

The value of XXX is equal to:

- in case of point kinetics: XXX = 000,
- in case of nodal point kinetics: XXX = node number (maximum of 50 nodes).

W-1 (I) : IREMRK Pointer to a Tabular or Control Function that defines relative rate of removal of fuel elements from the core, $R^R = -(1/N_{fe}) \cdot (dN_{fe}/dt)$, (1/s), where N_{fe} is the number of fuel elements in the core. Change of concentration of any isotope i , due to fuel removal function, is given by:

$$\left(\frac{dN_i}{dt} \right)_{R^R} = -N_i C_i R^R$$

where C_i is a constant, defined in records 720XXX (section 2.9.30).

If the number is positive then the relative removal rate will be defined by a Tabular Function with the number: IREMRK. If the number is negative then the relative removal rate will be defined by a Control Function with the number: |IREMRK|. The minimum limit of zero, and the maximum limit of 10^{-3} are imposed on the value obtained from Tabular or Control Function.

Acceptable range: must be a valid reference number of a Tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used here.

Default value: 0.

W-2 (I) : IFILRK Pointer to a Tabular or Control Function that defines first filling function, $R^F(1)$, that defines a relative rate of fuel elements insertion into the core, $R^F(1) = (1/N_{fe}) \cdot (dN_{fe}/dt)$, (1/s), where N_{fe} is the number of fuel elements in the core. Change of concentration of any isotope i , due to the k -th filling function, is given by:

$$\left(\frac{dN_i}{dt} \right)_{R^F(k)} = N_i^F(k) \cdot R^F(k)$$

where $N_i^F(k)$ are the isotope concentrations ($1/m^3$) in the elements loaded to the core with the k -th loading function. The isotope concentrations $N_i^F(k)$ are defined through records 72YXXX, and 73YXXX.

If the number is positive then $R^F(1)$ will be defined by a Tabular Function with the number: IFILRK. If the number is negative then $R^F(1)$ will be defined by a Control Function with the number:

|IFILRK|. The minimum limit of -1.0×10^{-3} , and the maximum limit of $+1.0 \times 10^{-3}$ are imposed on the value obtained from Tabular or Control Function.

Acceptable range: must be a valid reference number of a Tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used here.

Default value: 0.

SPECTRA Code Manuals - Volume 2: User's Guide

W-3 (I) : IFILRK Pointer to a Tabular or Control Function that defines second filling function ($R^F(2)$ - see description of word 2 above).
(2)
Acceptable range: must be a valid reference number of a Tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used here.
Default value: 0.

... until all filling functions are defined. The maximum number of filling functions is 9.

EXAMPLE: The following input (copied from the test case Xe-136-SOL-1) defines loading of U-235 (isotope No. 201) into the core.

```
* fuel load data
*        RR    RF(1)
747000 0    201 *

605201 Loading rate U-235 (1/s)
600201 0.0   2.5518E-8
```

The loading rate is : $R^F = 2.5518E-8$ (1/s). The initial U-235 concentration in the core is printed in the output file:

	Input	Multiplier	
	Initial	on	
	Concentr.	Reactivity	
i	Isotope	[1/m3]	[-]
108	U-235	1.18812E+25	1.00000E+00

The concentration is $N^F = 1.8812E+25$ (1/m³). Therefore the loading rate of U-235 will be equal to: $2.5518E-8 \times 1.8812E+25 = 4.8E+17$ (1/m³-s). The loading functions and the fuel composition for the loading functions are also printed in the output file:

```
=RK= FUEL LOADING FUNCTIONS

NODE LOADING FUNCTION No.
No.    1
1    TF-201
```

[...]

Fuel Composition in Assemblies Being Loaded During Transient

	Mass	Nuclide
	Fraction	Concentration
	[-]	[1/m3]
i	Isotope	
108	U-235	1.00000E+00 1.18812E+25

2.9.30 Records: 720XXX, Isotope Transformation Data - Multipliers for Fuel Removal

XXX=001, 002, ..., NIITRK, is the isotope number. This record specifies multipliers for isotopes that are being removed from the core with the removal function R^R , (see section 2.9.29).

W-1 (R) : CIITRK Value of the multiplier for isotope XXX,
Acceptable range: $0.0 \leq \text{CIITRK} \leq 10.0$.
Default value: 1.0 .

2.9.31 Records: 72YXXX, Isotope Transformation Data - Loaded Fuel Data

XXX=001, 002, ..., NIITRK, is the isotope number. The maximum number of isotopes is 200. Y = 1, ..., 9 is the loading function number, k . This record specifies composition of fuel (mass fractions) in assemblies that are being loaded into the core with the loading function k (see section 2.9.29).

W-1 (R) : FRITRK Mass fraction of fissile isotope XXX in the fuel being loaded into the core with the loading function k , $N_{i=XXX}^F(k=Y)$ (see section 2.9.29). The fuel concentrations, in ($1/m^3$), are calculated from (see section 2.9.28):
 $N_i = C \cdot f_i$.
where f_i are the fractions entered in this record, and C is a constant, calculated as shown in section 2.9.28 (note that C is defined using the initial fuel fractions, entered in records 746XXX, and not the reload fuel fractions entered here). It is important to note that the fractions entered here are not normalized by the program, so any desired concentrations may be obtained for the loaded fuel.
Acceptable range: if isotope XXX does not undergo fission ($\sigma_f =$ SFITRK = 0.0 - section 2.9.27), then FRITRK must be equal to zero; if isotope XXX does undergo fission ($\sigma_f =$ SFITRK > 0.0 - section 2.9.27), then FRITRK \geq 0.0 .
Default value: 0.0 .

2.9.32 Records: 73YXXX, Isotope Transformation Data - Loaded Non-fuel Data

XXX=001, 002, ..., NIITRK, is the isotope number. The maximum number of isotopes is 200. Y = 1, ..., 9 is the loading function number, k . This record specifies concentrations of non-fuel isotopes in assemblies that are being loaded into the core with the loading function k (see section 2.9.29).

W-1 (R) : XRITRK Reload concentration, ($1/m^3$), of isotope XXX being loaded into the core with the loading function k , or relative concentration of XXX, depending on word 2. Only reload concentrations of non-fissile isotopes can be specified here. Fuel concentrations are specified in record 72YXXX, as mass fractions (see section 2.9.31).
Acceptable range: XIITRK \geq 0.0 .
Default value: 0.0 .

W-2 (I) : IRITRK Reference fuel isotope for definition of reload concentration of isotope XXX.
If IRITRK \leq 0, then XRITRK (word 1 above) is interpreted as reload concentration of isotope XXX, in m^{-3} .
If IRITRK > 0, then XRITRK (word 1 above) is interpreted as reload concentration of isotope XXX relative to the reload concentration of fissile isotope IRITRK. In such case there must exist an isotope IRITRK, with positive fission cross section.
Acceptable range: IRITRK \leq NIITRK .
Default value: 0 .

2.9.33 Record: 748000, Point Kinetics Model for Circulating Fuel

The point kinetics model for circulating fuel is intended for applications such as molten salt reactors (MSR). In MSRs the fissile fuel is dissolved in a fluid (molten salt) which circulates in the primary reactor system.

W-1 (I) : IFTORK Fuel type option
1 = *solid fuel*. In such case, standard point kinetics model is used. The delayed neutron precursors are obtained as in the classical point kinetics equation (Volume 1, section 9.2.1):

$$\frac{dC_i(t)}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t)$$

The isotope concentrations are obtained from the isotope transformation model, as shown in Volume 1, section 9.3.1).

2 = *circulating fuel* (e.g. molten salt reactor). Allowed only for alternative fluid (IFLDFL > 1). In such case mapping is necessary (IMAPRK>0). The delayed neutrons must be mapped into the RT Package (see Word 2 below). The RK Package calculates the precursor source as (see Volume 1):

$$S_i(t) = \frac{\beta_i}{\Lambda} n(t)$$

The source is provided to the RT Package, which subsequently calculates transport, decay, as well as eventual other mechanisms such as removal in the filters, etc. The total mass of delayed neutron precursors present at any time in the core, $C_i(t)$, is obtained as a sum of the masses in all core volumes. The core volumes are recognized as these Control Volumes for which a non-zero weighting factor is specified in the records 791XXX, 792XXX, 793XXX.

The fission products, for example the major decay heat producers (group 6) should also be mapped. The RK Package will calculate the source of these isotopes, as described in Volume 1. The source is provided to the RT Package, which subsequently calculates transport, decay, as well as eventual other mechanisms such as removal by filters, etc.

If IFTORK = 2 (circulating fuel), the core region is defined by the fuel temperature feedback weighting factors (record 791XXX). All fuel regions must be defined as Control Volumes (ITF1RK must be set to 3). The source of isotopes (including the delayed neutron precursors), obtained from the RK package as shown above, will be distributed over all volumes with positive weighting factor (WTFPRK>0), as described in Volume 1.

Acceptable range: 1, 2

Default value: 1

SPECTRA Code Manuals - Volume 2: User's Guide

- W-2 (I) : IMAPRK Isotope mapping data. The entry has an eight-digit format: *hgfedcba*. For each digit 0 means don't map the chain. The chains are defined by IDITRK (record 740000, section 2.9.22).
a≠0 : map the ²³³U/²³⁵U chain (8 isotopes) into the RT Package
b≠0 : map the ²³⁹U/²³⁹Pu/²⁴¹Pu chain (8 isotopes) into RT
c≠0 : map the ¹³⁵Xe chain (3 isotopes) into RT
d≠0 : map the ¹⁴⁹Sm chain (3 isotopes) into RT
e≠0 : map the ¹⁵⁷Gd chain (2 isotopes) into RT
f≠0 : map the 11 major decay heat producers chain into RT
g≠0 : map the delayed neutron precursors into RT
h≠0 : map an additional, user-defined chain (if present) into RT
Acceptable range: IMAPRK ≥ 0, if a chain is not active (appropriate digit in IDITRK is zero), the mapping request must not be used for this chain. Mapping is required (IMAPRK>0) for the circulating fuel (IFTORK = 2). Mapping can be requested for solid fuel (IFTORK=1) but in such case there will be no data transfer (sources of isotopes) from the RK to the RT Package. Note: in case of additional, user-defined chain, the molar weight, as well as the vapor class and the release class are not defined in the RK Package. If such chain is mapped (*h*≠0), then those parameters should be defined within the RT Package, using records 880XXY, 885XXY, 886XXY.
Default value: 0
- W-3 (I) : IDSORK Initial distribution of isotopes.
= 1 : isotope concentrations are initially set only in the core volumes, i.e. Control Volumes with positive fuel weighting factor (WTFFRK>0). The concentrations are proportional to the fuel weighting factors, WTFFRK.
= 2 : isotope concentrations are initially set in all Control Volumes belonging to the CV group ICVGRT (Word 4 below). The concentrations are not proportional to the fuel weighting factors, WTFFRK, in the core volumes; the same concentrations are used in all volumes. This option gives best possible approximation of a system that is flowing at the start of the simulation.
= 3 : isotope concentrations of fuel ($\sigma_f > 0$) are initially set in all Control Volumes belonging to the CV group ICVGRT (Word 4 below). The concentrations are not proportional to the fuel weighting factors, WTFFRK. All other isotopes (fission products, including delayed neutron precursors) are initially set only in the core volumes, i.e. Control Volumes with positive fuel weighting factor (WTFFRK>0). The concentrations are proportional to the fuel weighting factors, WTFFRK, in the core volumes. This option gives best possible approximation of a system that is stagnant at the start of the simulation.
= 4 : very similar to option 3, but all isotopes except for the fuel are initially set to zero. This option represent a “cold” (zero-power) non-flow situation.
=-1 : use isotope concentrations from the initial condition file (ICF).
Acceptable range: IDSORK = -1, 1, 2, 3, 4
Default value: 3

SPECTRA Code Manuals - Volume 2: User's Guide

W-4 (I) : ICVGRK CV group (defined in record 101XXX). Initial concentrations of isotopes are set in all Control Volumes belonging to the CV group ICVGRT, if the initial distribution option (IDSORK) is set to 2 or 3.
Acceptable range: ICVGRK ≥ 0
Default value: 1

W-5 (I) : IVRERK Pointer to a Tabular or Control Function that defines the reactivity effect caused by changes of the active core volume in case of circulating fuel. In case of solid fuel (IFTORK=1) the core volume is constant and equal to RVOLRK (input record 751000). In case of circulating fuel (IFTORK=2) the core volume is, in general, time dependent. The core volume is equal to the sum of liquid volumes of the Control Volumes that are defined as the core volumes. The core volumes are defined by a positive fuel weighting factors (WTFFRK>0, record 791XXX).
 When the core volume changes, reactivity will generally change, for example due to different neutron leakage. This effect is taken into account by the present function. The function defines reactivity (in dollars) as a function of relative core volume:

$$R_V [\$] = f \left(\frac{V_R(t)}{V_{REF}} \right)$$

R_V - reactivity effect caused by changes of core volume, (\$) (plot parameter RT-000-ReVo-0000).

$V_R(t)$ - current core volume, m³, (plot parameter RT-000-Rvol-0000).

V_{REF} - reference core volume, m³, (input parameter RVOLRK).

f - function defined by IVRERK. If the number is positive then the reactivity will be defined by a Tabular Function with the number: IVRERK. The argument of this function will be relative volume: $V_R(t)/V_{REF}$. If the number is negative then the reactivity will be defined by a Control Function with the number: |IVRERK|. The units obtained from the Tabular or Control Function are assumed to be (\$).

Acceptable range: must be a valid reference number of a tabular or a Control Function. The "Reactor Kinetics" type CF cannot be used.

Default value: 0.

Note: Typically the reactivity decreases with decreasing core volume. An example of a function defining the reactivity effect is given below:

$V_R(t)/V_{REF}$ (-)	R_V (\$)
0.0	-1.00
1.0	0.00
1.1	+0.10

W-6 (I) : IREIRK Reactivity effect from isotope concentrations.
 =1 : reactivity feedback from isotope concentrations is taken into account
 =2 : reactivity feedback from isotope concentrations is not taken into account. In such case changes of concentrations due to for example thermal expansion of fluid is not taken into account. This option is intended mainly for testing calculations.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: 1, 2

Default value: 1

W-7 (R) : XFULRK Minimum liquid fraction in CV to use full fission power (see parameter ITESCV, record 14YXXX).

Acceptable range: $0.01 \leq \text{XFULRK} \leq 1.0$

Default value: 0.99

W-8 (I) : IRTSRK Source of isotopes defined in the RT Package (non-mapped from RK) in circulating fuel. Typically all isotopes from the RK Package are mapped into the RT Package (see IMAPRK, above; all built-in chains and one user-defined chain may be mapped). However, the user may wish to use the RT chains in the analysis of circulating fuel (see Volume 1, Chapter: Fission Products, section: Isotope Chains). Source of those non-mapped isotopes in the RT Package may be defined for the circulating fuel in a similar way as it is done with the mapped isotopes. The source of isotope i is given by:

$$S_i = \gamma_{f,i} \cdot \sum_{k \in \text{fis}} \sigma_{f,k} N_k \Phi - \sigma_{a,i} N_i \Phi + \sum_{j \neq i} \sigma_{a,j} N_j \Phi \gamma_{a,j \rightarrow i}$$

Here Φ is the neutron flux (1/m²-s), N_k is the concentration (1/m³) of isotope k , $\sigma_{f,k}$ is the fission cross section of isotope k , $\sigma_{a,j}$ is the neutron capture (non-fissile absorption) cross section of isotope j , $\gamma_{f,i}$ is the average yield fraction of isotope i from fission of all fissile isotopes, $\gamma_{a,j \rightarrow i}$ is the yield fraction of isotope i due to neutron capture by isotope j .
Note!

In the RK Package the fission yields are different for each fissile isotope. In the RT Package, no individual fission yields are defined for the built-in isotopes, shown in section 2.15.111. However, if mapping from the RK chains (section 2.9.36) to the RT Package is requested (IMAPRK>0), and the first two chains (the ²³³U / ²³⁵U fuel chain and the ²³⁹U / ²³⁹Pu / ²⁴¹Pu fuel chain) are mapped, then the individual yields are defined for the next three chains: ¹³⁵Xe, ¹⁴⁹Sm, and ¹⁵⁷Gd chains, if they are mapped. The individual yields for those three chains are shown in section 2.9.36. For example, the RK Package defaults for Xe-135 chain are shown in Figure 2-50, left, while the RT Package defaults are shown in Figure 2-50, right.

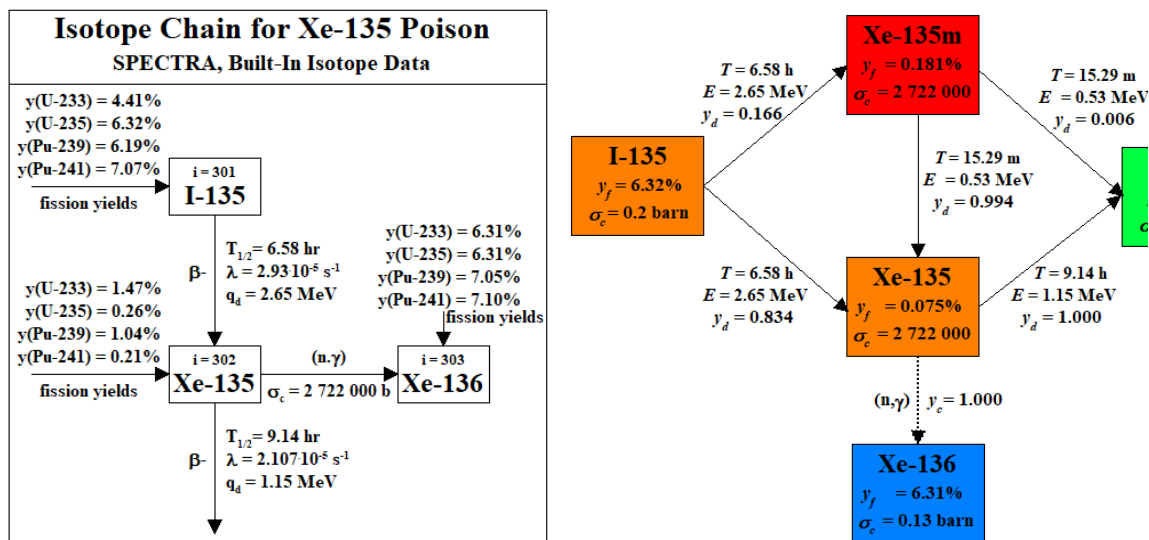


Figure 2-50 Decay chain $M_W = 135$,
 left: RK Package see Volume 1, "Description of the Built-in Isotope Library"
 right: RT Package, see Volume 1, "Isotope Chains (Decay Chains)"

IRTSRK=1 : source of non-mapped isotopes not taken into account
 IRTSRK=2 : source of the non-mapped isotopes taken into account, as described above.

Acceptable range: 1, 2
 Default value: 2

W-9 (I) : IDEPRK Option for calculating isotope concentrations in the core of circulating fuel.
 IDEPRK = 0: only isotopes in the circulating fuel, i.e. CV pool
 IDEPRK = 1 : pool + adsorbed on adjacent structures (SC/TC)
 IDEPRK = 2 : pool + atmosphere (gas space)
 IDEPRK = 3 : pool + atmosphere + adjacent structures
 By adding 10 to IDEPRK, isotopes adsorbed on the aerosol particles are added:
 IDEPRK = 10: + isotopes adsorbed on particles in the CV pool
 IDEPRK = 11 : + pool + particles deposited on adjacent structures
 IDEPRK = 12 : + pool + particles in atmosphere
 IDEPRK = 13 : + pool + atmosphere + adjacent structures
 NOTE: the isotopes located in different parts may have different reactivity worth. Appropriate multipliers are defined by words 11 through 13 below.
 Acceptable range: 0, 1, 2, 3,
 10, 11, 12, 13
 Default value: 0

W-10 (R): RLTVRK Liquid volume fraction in the reactor, $V_{liq}/(V_{liq} + V_{sol})$. The reactor core consists of liquid with dissolved fuel and solid (for example graphite moderator in MSRE). RLTVRK represents the ratio between the liquid volume and the total volume occupied by liquid and solid. For example,

SPECTRA Code Manuals - Volume 2: User's Guide

in case of MSRE, the ratio is 0.225; the graphite volume fraction is 0.775. The core liquid volume is obtained as a sum of pool volumes for all CV-s with positive power fraction, WTCFRK. The formula is:

$$V_{liq} = \sum_{i=1}^N V_{pool}(i)$$

The total core volume (plot parameter RT-000-RVol-0000) is obtained as:

$$V_{core} = \frac{V_{liq}}{RLTVRK} = \frac{1}{RLTVRK} \times \sum_{i=1}^N V_{pool}(i)$$

Acceptable range: $0.01 \leq RLTVRK \leq 1.0$

Default value: 1.0

- | | | |
|------------|--------|--|
| W-11 (R): | RLITRK | Reactivity worth multiplier for isotopes residing in liquid, including. <ul style="list-style-type: none"> <input type="checkbox"/> CV pool (all core volumes), <input type="checkbox"/> adsorbed on particles suspended in CV pool (all core volumes). <p><i>Acceptable range:</i> $10^{-2} \leq RLITRK \leq 10^{+2}$</p> <p><i>Default value:</i> 1.0</p> |
| W-12 (R): | RSITRK | Reactivity worth multiplier for isotopes residing in solids, including <ul style="list-style-type: none"> <input type="checkbox"/> SC/TC (adsorbed on structures adjacent to core volumes), <input type="checkbox"/> adsorbed on particles deposited on SC/TC surfaces (all structures adjacent to the core volumes). <p><i>Acceptable range:</i> $10^{-2} \leq RSITRK \leq 10^{+2}$</p> <p><i>Default value:</i> 1.0</p> |
| W-13 (R): | RGITRK | Reactivity worth multiplier for isotopes residing in gas, including. <ul style="list-style-type: none"> <input type="checkbox"/> CV atmosphere (all core volumes), <input type="checkbox"/> adsorbed on particles airborne in CV atmosphere (all core volumes). <p><i>Acceptable range:</i> $0.0 \leq RGITRK \leq 10^{+2}$</p> <p><i>Default value:</i> 0.0</p> |
| W-14 (I): | IRSLRK | If positive, this is a number of Tabular Function, defining the ratio of solid worth to liquid worth, (RSITRK/RLITRK), versus the ratio of the solid density to the liquid density (N_{SC}/N_{CV}) of isotope JRSLRK, defined below <p><i>Acceptable range:</i> reference to a Tabular Function, if non-zero</p> <p><i>Default value:</i> none</p> |
| W-15 (I) : | JRSLRK | Reference number of the isotope. <p><i>Acceptable range:</i> must be a valid isotope number if IRSLRK > 0
must be zero if IRSLRK = 0</p> <p><i>Default value:</i> none.</p> |
| W-16 (R): | FRSLRK | Ratio of the neutron flux in the solid (graphite) to the liquid (salt). |

$$FRSLRK = \frac{\int_{\text{graphite}} \Phi dV_g}{\int_{\text{salt}} \Phi dV_s}$$

Used to calculate absorption of isotopes, e.g. Xe-135 in graphite. For any isotope i , present in the solid structures of the core, the neutron absorption term is obtained from:

$$\sigma_{c,i} \cdot N_{s,i} \cdot \Phi \cdot FRSLRK$$

Here $\sigma_{c,i}$ is the neutron capture cross section of the isotope i , $N_{s,i}$ is the concentration of the isotope i in the solid, and Φ is the neutron flux, obtained from the reactor kinetics model.

Acceptable range: $10^{-3} \leq FRSLRK \leq 10^{+3}$

Default value: 1.0

- W-17 (I) : ICVURK CV number of the upper plenum. Isotopes that are present in the core are obtained as a sum of all isotopes present in volumes for which positive fuel weighting factor is given. If ICVURK>0 then this number indicates the upper plenum volume. A fraction (FCVURK) of the isotopes present in the upper plenum will affect the core reactivity. This fraction is added to the sum mentioned above.
The main purpose on this and the next entry is to take into account the possibility of delayed neutron precursors in the upper plenum affecting the core reactivity.
Acceptable range: must be a valid reference to a Control Volume, if positive
Default value: none.
- W-18 (R) : FCVURK Fraction of the isotopes present in the upper plenum volume (ICVURK) that are added to the total mass of isotopes present in the core.
The main purpose on this and the previous entry is to take into account the possibility of delayed neutron precursors in the upper plenum affecting the core reactivity.
Acceptable range: $0.0 \leq FCVURK \leq 1.0$
Default value: 0.167 (=1/6, an average fraction that is directed back towards the core)

EXAMPLE OF THE USE OF RLITRK, RSITRK:

In case of MSRE core with fuel salt and graphite moderator, the effective Xe concentration is ([55], sec. 7.2)

$$N = \frac{\int_{salt} N_s \Phi_2^* \Phi_2 dV_s + \int_{graphite} N_g \Phi_2^* \Phi_2 dV_g}{\int_{salt} \Phi_2^* \Phi_2 dV_s + \int_{graphite} \Phi_2^* \Phi_2 dV_g}$$

Here N is the importance-averaged concentration per unit reactor volume, N_s and N_g are the local concentrations per unit volumes of salt and graphite respectively, Φ_2 is the thermal neutron flux. N is the uniform equilibrium concentration of xenon in the reactor, which produces the same reactivity effect as the actual distribution.

This is approximated in SPECTRA by introducing reactivity worth multipliers. The isotope concentrations in liquid (CV pools) are multiplied by RLITRK, while the concentrations in solids (SC/TC) are multiplied by RSITRK:

$$N = \frac{\sum_{CV \in core} N_{CV} \times RLITRK \times V_{CV} + \sum_{SC \in core} N_{SC} \times RSITRK \times V_{SC}}{\sum_{CV \in core} RLITRK \times V_{CV} + \sum_{SC \in core} RSITRK \times V_{SC}}$$

Here N_{CV} and N_{SC} are the isotope concentrations in the core CV pools and core SCs respectively. The theoretical values of the reactivity worth multipliers are:

$$RLITRK = \int_{CV \in core} \Phi_{CV}^* \Phi_{CV} dV_{CV}$$

$$RSITRK = \int_{SC \in core} \Phi_{SC}^* \Phi_{SC} dV_{SC}$$

Additionally, if there is a gas space in the reactor (for example, fuel salt disappears because of fuel dump, etc.) then the last parameter may be used:

$$RGITRK = \int_{CV \in core} \Phi_{CV}^* \Phi_{CV} dV_{CV,atms}$$

An additional problem with using the formula for N , shown above, is the definition of the volume of solids, V_{SC} . The concentration of isotopes on SCs is defined in SPECTRA per unit surface area, $N_{s,SC}$ (atoms/m²). The total number of atoms of given isotope is therefore given as:

$$\sum_{SC \in core} N_{s,SC} \times A_{SC}$$

Here A_{SC} is the surface area of SC (m²). The adsorbed isotopes may be stored at the surface or diffuse inside the material. Calculations performed with MSRE model showed that in case of Xe-135 the diffusion depth is of order of centimeters.

SPECTRA Code Manuals - Volume 2: User's Guide

2.9.35 Examples of Isotope Transformation Input Data

Three examples are given below, to illustrate input for Isotope Transportation model.

Example 1. Simplified Xenon Chain

This example shows how to prepare input data for a certain isotope chain. The Xenon chain is chosen for this example input. It should be noted however that in practice there is no need to prepare data for the Xenon chain, since this chain is present in the built-in isotope transformation library (see section 2.9.36) and need only to be activated as shown in section 2.9.22

The example defines isotope data for the analysis of poison material - Xenon-135. ¹³⁵Xe has an extremely large absorption cross section, and therefore is important in reactor analyses. The example input provides data for a simplified ¹³⁵Xe chain. The simplified chain is shown in Figure 2-52. (For comparison, a full ¹³⁵Xe chain is shown in Figure 2-51).

The half-lives of ¹³⁵I and ¹³⁵Xe are equal to 6.58 hr and 9.17 hr respectively ([5], figure 15-1). That means: $\lambda_I = 2.93 \cdot 10^{-5} \text{ s}^{-1}$, and $\lambda_{Xe} = 2.01 \cdot 10^{-5} \text{ s}^{-1}$. The yield fractions from fission of ²³⁵U are: $\gamma_I = 6.32\%$, and $\gamma_{Xe} = 0.26\%$ [17]. The absorption cross-section for ¹³⁵Xe is $2.772 \cdot 10^6$ barn [17]. The fission cross-section of ²³⁵U is 505 barn [17]. The input defines six isotopes:

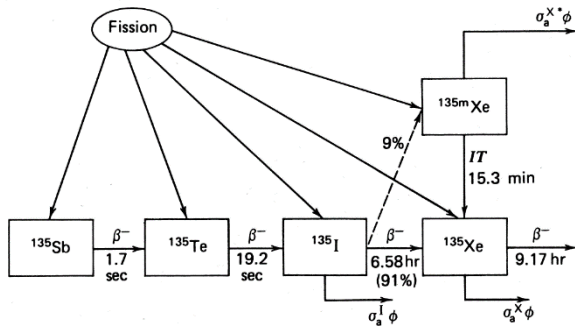


Figure 2-51 Full decay scheme for ¹³⁵Xe ([5], figure 15-1).

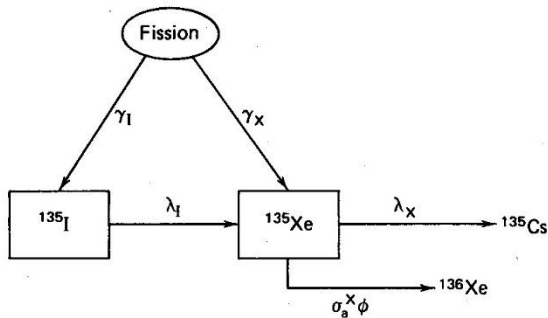


Figure 2-52 Simplified decay scheme for ¹³⁵Xe ([5], figure 15-2).

- 1.) ²³⁵U (note that at least one fissile isotope must be present),
- 2.) ²³⁸U,

SPECTRA Code Manuals - Volume 2: User's Guide

- 3.) ¹³⁵I,
- 4.) ¹³⁵Xe,
- 5.) ¹³⁵Cs,
- 6.) ¹³⁶Xe.

There is only one fissile nuclide - ²³⁵U. The fuel is assumed to be composed of ²³⁵U and ²³⁸U, with enrichment of $e = 2\%$. This means the ratio of ²³⁸U to ²³⁵U is equal to:

$$\frac{N_{U-238}}{N_{U-235}} = \frac{1-e}{e} = \frac{1-0.02}{0.02} = 49.0$$

The isotopes ²³⁸U, ¹³⁵Cs, ¹³⁶Xe, are included here only to make the example input more instructive. In the present example these isotopes neither absorb neutrons ($\sigma_c=0.0$), nor decay ($\lambda=0.0$). Therefore they have no effect on reactivity or decay heat production, and they could as well be skipped. In such case no yield fractions from decay of ¹³⁵Xe, and from neutron absorption in ¹³⁵Xe, would be specified. That means record 741004 would contain only two words, and record number 742004 would contain only one word.

```

=====
*          ISOTOPES DATA
=====
*
*      Isotope names
I05001 U-235      * Isotope No. 1
I05002 U-238      * Isotope No. 2
I05003 I-135      * Isotope No. 3
I05004 Xe-135     * Isotope No. 4
I05005 Cs-135     * Isotope No. 5
I05006 Xe-136     * Isotope No. 6
*
*      Decay data
*
*      Decay      Decay      Yield fractions
*      constant   heat
*      (1/s)      (W)      Isotope Yield
741003 2.93E-5    0.0    4      1.0    * I-135 -> Xe-135
741004 2.107E-5  0.0    5      1.0    * Xe-135 -> Cs-135
*
*      Absorption data
*
*      Absorption      Yield fractions
*      cross section
*      (barn)          Isotope Yield
742004 2.722E6        6      1.0    * Xe-135 -> Xe-136
*
*      Fission data
*
*      Fission      Yield fractions
*      cross section (1)      (2)
*      (barn)      Isotope Yield      Isotope Yield
743001 505.0      3      0.0632  4      0.0026  * U-235
*
*      Initial core composition - Uranium, enrichment: e = 2%
746001 1.0      * mass fraction of U-235 = 100% (no other fissionable nuclides)
740002 49.0 1 * U-238/U-235 = (1 - e)/e = (1 - 0.02)/0.02 = 49
*

```

Example 2. Continuous Fuel Reload

In example 2 the built-in isotope library is used (see section 2.9.36). The initial enrichment (at the start of the calculations) of the fuel is assumed to be equal to $e_{core} = 4.7\%$. This means the ratio of ^{238}U and ^{235}U concentrations in the fuel present in the core is equal to:

$$\left[\frac{N_{U-238}}{N_{U-235}} \right]_{core} = \frac{1-e}{e} = \frac{1-0.047}{0.047} = 20.3$$

Fuel is continuously reloaded. Fresh fuel, which is being loaded into the core, has the enrichment of $e_{fresh} = 8.1\%$. This means the ratio of ^{235}U concentration in the fresh fuel to the ^{235}U concentration in the fuel present in the core is equal to:

$$\frac{[N_{U-235}]_{fresh}}{[N_{U-235}]_{core}} = \frac{e_{fresh}}{e_{core}} = \frac{0.081}{0.047} = 1.723$$

The ratio of ^{238}U and ^{235}U concentrations in the fresh fuel is equal to:

$$\left[\frac{N_{U-238}}{N_{U-235}} \right]_{fresh} = \frac{1-e_{fresh}}{e_{fresh}} = \frac{1-0.081}{0.081} = 11.3$$

Fuel is being loaded to and removed from the core with the same rate - use is made of a Control Function, in this example it is CF-029. This CF is built to control the fuel reloading rate in order to keep constant power. Volume 3 shows examples how to build such a function.

Suppose further that only fuel that has reached a specified burn-up is being removed from the core (such procedure is applied in PBMR reactors). In the present example, which is based on PBMR plant specification, the reactor target burn-up is: $B = 80,000 \text{ MWd/t}$. The corresponding enrichment of the spent fuel is, according to the specification, equal to about 1.3%. If the neutron flux is known, then this value may be also estimated from the following simple calculation. For the reactor fission power of $Q_f = 252 \text{ MW}$, and the heavy metal mass of $M = 2.97 \text{ t}$, the time needed to reach the target burn-up is equal to: $t = BM/Q_f = 80,000 \cdot 2.970 / 252 = 943 \text{ days} = 8.15 \cdot 10^7 \text{ s}$. The concentration of U-235 in this fuel is estimated from the formula:

$$\frac{dN_{U-235}}{dt} = -\sigma_f N_{U-235} \Phi$$

Solution of this differential equation gives:

$$N/N_0 = \exp(-\sigma_f \Phi t) = \exp(-505 \cdot 10^{-28} \cdot 4.5 \cdot 10^{17} \cdot 8.15 \cdot 10^7) = 0.157.$$

where Φ is the neutron flux. The concentration of U-235 in the fuel which reached the target burn-up is therefore equal to the initial concentration times 0.157. This is approximately equal to the enrichment ratio, so the enrichment of the spent fuel is $0.157 \cdot 8.1\% \approx 1.3\%$, in agreement with the plant specification.

SPECTRA Code Manuals - Volume 2: User's Guide

Finally, the ratio of U-235 concentration in the spent fuel to the concentration of the fuel initially present in the core is equal to:

$$\frac{[N_{U-235}]_{spent}}{[N_{U-235}]_{core}} = \frac{e_{spent}}{e_{core}} = \frac{0.013}{0.047} = 0.277$$

```
*=====
*      ISOTOPE DATA
*=====
*
740000  0  111111 *  Request all built-in isotope data
*
*      Initial fuel composition, average enrichment:
*      Fresh fuel      : e=8.1%
*      Discarded fuel  : e=1.3%
*      Average fuel    : e=(8.1+1.3)/2 = 4.7%
*      Mass Fraction
746108   1.0   *   U-235,
740201  20.3  8 *   U-238/U-235 = (1-e)/e = (1-0.047)/0.047 = 20.3
*
*      Reload data
*
*      RR   RF(1)
747000 -29 -29 *   Use CF-029 for both removal and loading
*
*      Reload fuel composition, enrichment e=8.1%
721108  1.723 *   (Fresh U-235)/U-235 = 8.1/4.7 = 1.723
731201  11.3 108 *   (Fresh U-238/U-235) = (1-e)/e = (1-0.081)/0.081 = 11.3
*
*      Multipliers for removed fuel elements
720108  0.277 *   (Discarded U-235)/U-235 = 1.3/4.7 = 0.277
*
```

2.9.36 Built-In Isotope Transformation Data

The built-in isotope chains are described subsequently below. The built-in data is requested in record 740000 (section 2.9.22). The following built-in data is available in the code:

- Isotope chain for ^{233}U / ^{235}U fuel (8 isotopes).
- Isotope chain for ^{239}U / ^{239}Pu / ^{241}Pu fuel (8 isotopes).
- Isotope chain for ^{135}Xe poison (3 isotopes).
- Isotope chain for ^{149}Sm poison (3 isotopes).
- Isotope chain for ^{157}Gd poison (2 isotopes).
- 11 groups of main isotopes responsible for the decay heat generation.

- **Isotope chain for $^{233}\text{U} / ^{235}\text{U}$ fuel (isotopes 101 ÷ 108)**

The isotope chain for $^{233}\text{U} / ^{235}\text{U}$ fuel is shown in Figure 2-53 (reproduced from [8]). The chain implemented in the SPECTRA built-in isotope library is somewhat simplified - the isotopes beyond ^{235}U are not taken into account. The isotope chain for $^{233}\text{U} / ^{235}\text{U}$ fuel, as implemented in SPECTRA, is shown in Figure 2-54. The decay constants were taken from [8]. The decay constant for ^{234}Pa was taken from reference [6]. Decay heats were taken from [13]. One-group cross-sections are used; the fission and the capture cross-sections were obtained from [17].

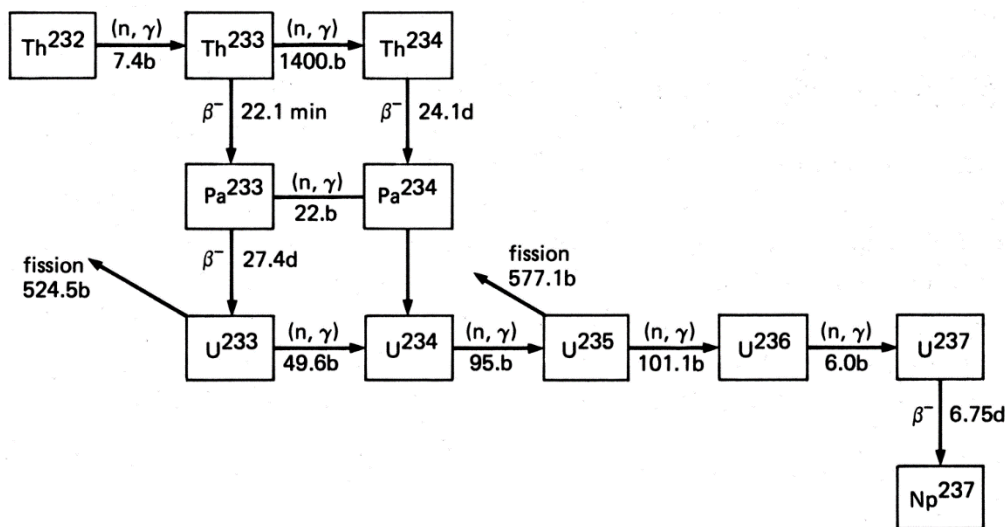


Figure 2-53 The isotope chain for $^{233}\text{U} / ^{235}\text{U}$ fuel ([8], figure 6.2).

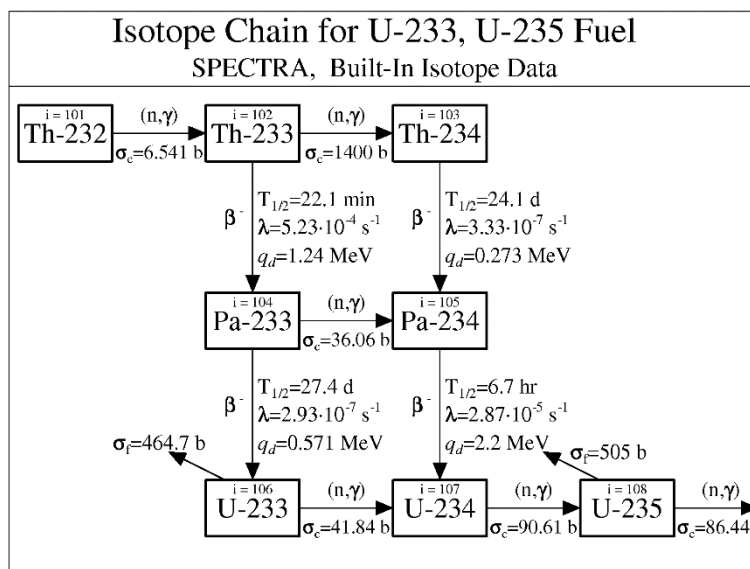


Figure 2-54 The isotope chain for $^{233}\text{U} / ^{235}\text{U}$ fuel, as implemented in SPECTRA.

- Isotope chain for $^{239}\text{U} / ^{239}\text{Pu} / ^{241}\text{Pu}$ fuel (isotopes 201 ÷ 208)

The isotope chain for $^{239}\text{U} / ^{239}\text{Pu} / ^{241}\text{Pu}$ fuel is shown in Figure 2-55 (reproduced from [8]). The chain implemented in the SPECTRA built-in isotope library is somewhat simplified - the isotopes beyond ^{241}Pu are not taken into account. The isotope chain for $^{239}\text{U} / ^{239}\text{Pu} / ^{241}\text{Pu}$ fuel, as implemented in SPECTRA, is shown in Figure 2-56. Decay data were taken from [8] and [13]. One-group cross-sections are used; the fission and the capture cross-sections were obtained from [17].

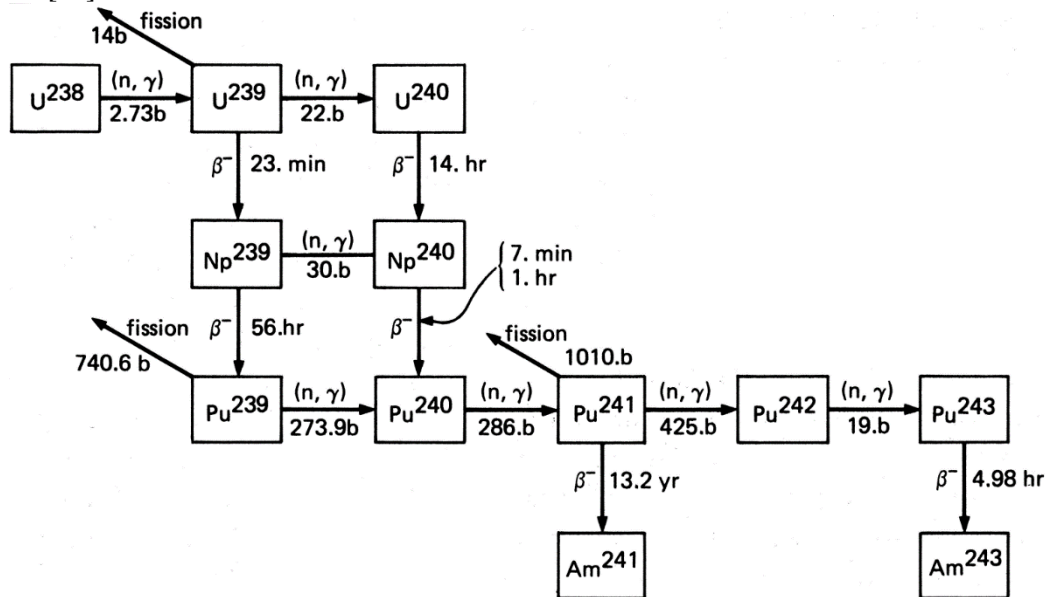


Figure 2-55 The isotope chain for $^{239}\text{U} / ^{239}\text{Pu} / ^{241}\text{Pu}$ fuel ([8], figure 6.1).

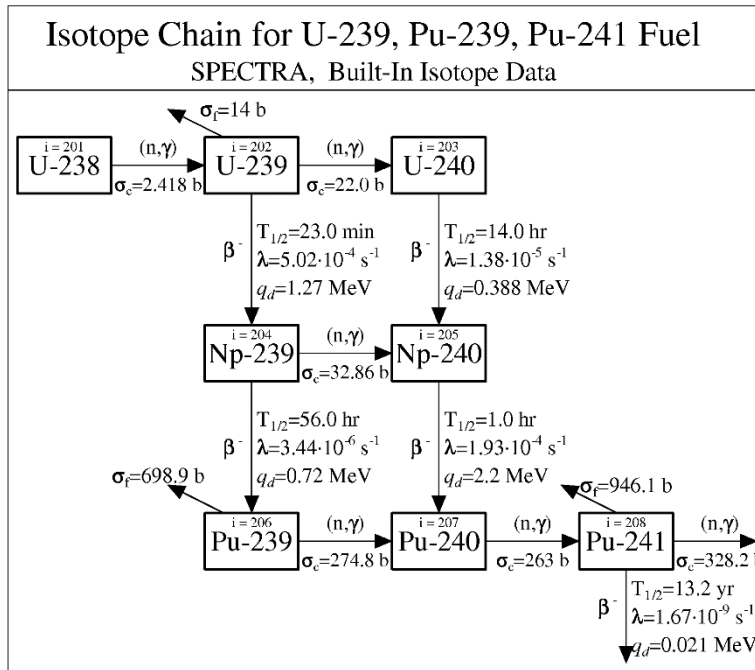


Figure 2-56 The isotope chain for $^{239}\text{U} / ^{239}\text{Pu} / ^{241}\text{Pu}$ fuel, as implemented in SPECTRA.

SPECTRA Code Manuals - Volume 2: User's Guide

Correction for resonance capture by ^{232}Th and ^{238}U

In case of ^{232}Th and ^{238}U there is a significant neutron capture in resonances. To take that into account, the neutron capture cross sections for those two nuclides are modified. The "effective" cross sections are calculated from (compare [11], equation 7.119):

$$\sigma_{c,i} = \sigma_{c,i}^{true} \left(1 + (1 - p_i) \varepsilon \nu P_{FNL} \frac{\sum_j \sigma_{f,j} N_j}{\sigma_{c,i}^{true} N_i} \right)$$

where:

- $\sigma_{c,i}$ - effective cross section for isotope i , $i=1$ (^{232}Th) or $=9$ (^{238}U),
- p_i - probability of escaping resonance absorption in isotope i ,
- ε - fast fission factor,
- ν - number of neutrons generated per fission,
- P_{FNL} - fast non-leakage probability,
- $\sigma_{f,j}$ - fission cross section for isotope j , (barn),
- N_i, N_j - concentrations of isotopes i, j , (1/m3).

In the above equation the true capture cross section is given with the superscript "true", and the sum is taken over all fissile isotopes. The resonance escape probability is given by ([11], equation 6.119):

$$p_i = \exp(-c_i I_i N_i)$$

where I_i is the resonance integral for isotope i and c is certain constant, the value of which varies for different reactors. The resonance integral is given by ([11], equation 6.120): $I_i = A_i + C_i/(r\rho)^{1/2}$, where r is rod diameter (cm), ρ is fuel density (kg/cm³), and A_i, C_i are constants, equal to ([11], table 6.5):

- $i = ^{238}\text{U}$ (metal)	$A_i = 2.8$	$C_i = 38.3,$
- $i = ^{238}\text{UO}_2$	$A_i = 3.0$	$C_i = 39.6,$
- $i = ^{232}\text{Th}$ (metal)	$A_i = 3.9$	$C_i = 20.9,$
- $i = ^{232}\text{ThO}_2$	$A_i = 3.4$	$C_i = 24.5.$

It is assumed that resonance absorption occurs only in ^{232}Th and ^{238}U . Therefore the individual resonance escape probabilities, p_i , are related to the overall resonance escape probability, p , by: $p_1 p_9 = p$. The value of p is a user input (see section 2.9.1). After easy transformations one obtains the following expressions for p_1, p_9 :

$$p_1 = \exp\left(\ln(p) \frac{I_1 N_1}{I_1 N_1 + I_9 N_9}\right) \quad p_9 = \exp\left(\ln(p) \frac{I_9 N_9}{I_1 N_1 + I_9 N_9}\right)$$

The following values are assumed for calculations: $r=1.0$, $\rho=19.1$, A_i , C_i for dioxides. These gives $I_1 = 9.0$, $I_9 = 12.1$. The effective cross sections are calculated based on initial concentrations, and are not modified during the transient. It must be remembered that the effective cross sections are calculated as described above only if the built-in library is being used (IDITRK \geq 3, section 2.9.22), and if the capture cross sections for ^{232}Th , ^{238}U are not modified in the input data. Thus, the user can calculate his own resonance integrals, and enter the effective capture cross sections in the input data, overwriting the default values.

- *Isotope chain for ^{135}Xe poison (isotopes 301 ÷ 303)*

The isotope chain for ^{135}Xe fission product poison is shown in Figure 2-57. A simplified chain is used, and the short life isotopes, ^{135}Sb , ^{135}Te , are neglected. The yield fraction of ^{135}I is taken as a sum of the yield fractions for ^{135}Sb , ^{135}Te , and ^{135}I . The decay constants were taken from reference [5] (figure 15-1). The decay heats were taken from [13]. The fission product yields were taken from reference [17] (table 8). One-group cross-sections are used; the fission and the capture cross-sections were obtained from [17].

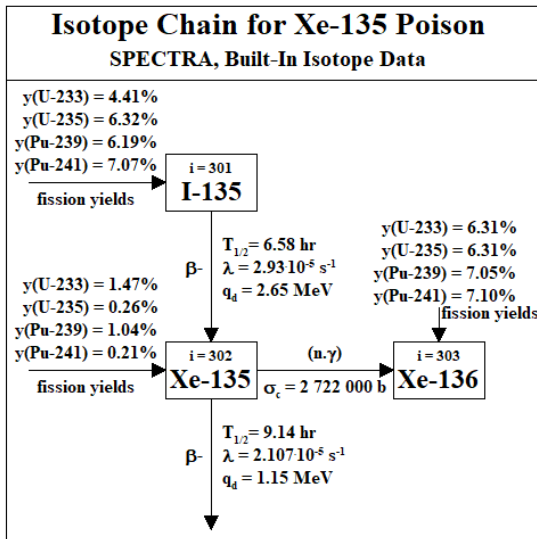


Figure 2-57 The isotope chain for ^{135}Xe fission product poison, as implemented in SPECTRA.

- *Isotope chain for ^{149}Sm poison (isotopes 401 ÷ 403)*

The isotope chain for ^{149}Sm fission product poison is shown in Figure 2-58. The decay constants were taken from reference [8] (figure 6.3). The decay heats were taken from [13]. The fission product yields were taken from reference [17] (table 8). One-group cross-sections are used; the fission and the capture cross-sections were obtained from [17].

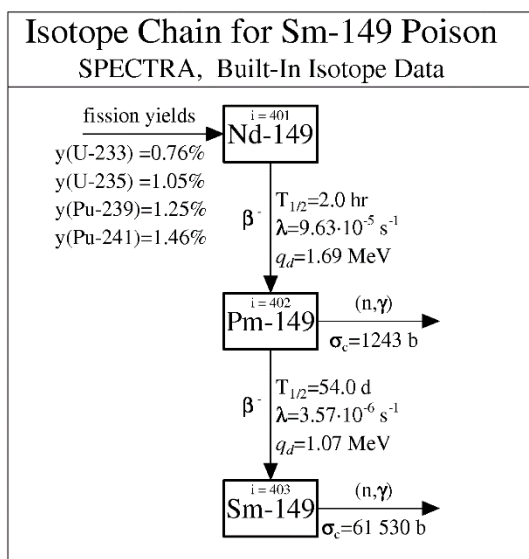


Figure 2-58 The isotope chain for ^{149}Sm fission product poison, as implemented in SPECTRA.

- *Isotope chain for ^{157}Gd poison (isotopes 501 ÷ 502)*

The isotope chain for ^{157}Gd fission product poison is shown in Figure 2-59. The decay constants were taken from reference [17] (table 6). The decay heats were taken from [13]. The fission product yields were taken from reference [17] (table 8). One-group cross-sections are used; the fission and the capture cross-sections were obtained from [17].

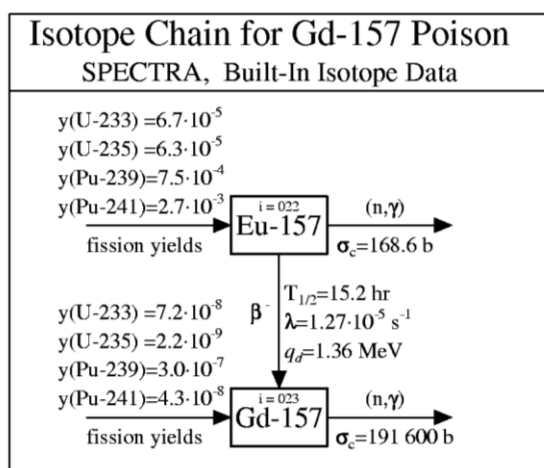


Figure 2-59 The isotope chain for ^{157}Gd fission product poison, as implemented in SPECTRA.

- Isotope groups of main decay heat producers (isotopes 601 ÷ 611)

The decay heat producers are represented by 11 groups of "isotopes", similarly as in [15]. The decay constants and fission yields of these groups were established based on data from [15] and comparisons with ANS standard [2]. Detailed description and comparisons with ANS standard are presented in Volumes 1 and 3.

For all decay heat groups the values of the decay constant, λ_i , and the decay heat, $q_{d,i}$ are positive. The neutron absorption is neglected, thus the neutron capture cross section, $\sigma_{c,i}$, as well as fission cross section, $\sigma_{f,i}$, are equal to zero. Therefore, for the decay heat groups, the general isotope balance equation (see Volume 1) reduces to:

$$-\frac{dN_i}{dt} = -\lambda_i N_i + \sum_j \lambda_j N_j \gamma_{d,j \rightarrow i} + \sum_j \sigma_j N_j \Phi \gamma_{f,j \rightarrow i}$$

where:

- N_i - concentration of nuclides from group i , ($1/m^3$),
- λ_i - decay constant of group i , ($1/s$),
- $\gamma_{d,j \rightarrow i}$ - decay yield fractions (probability that a decay of nuclide from group j will result in creation of nuclide in group i),
- $\gamma_{f,j \rightarrow i}$ - fission yield fractions (probability that a fission of nuclide from a fissile group j will result in creation of nuclide in group i),
- Φ - neutron flux, ($1/m^2/s$).

The value of decay heat of each group is calculated as:

$$Q_{d,i} = \lambda_i N_i q_{d,i}$$

where:

- $Q_{d,i}$ - decay heat density, group i , (W/m^3),
- $q_{d,i}$ - heat release per decay, group i , ($W/decay$).

The values of the decay constants, λ_i , the fission yield fractions, $\gamma_{f,k \rightarrow i}$, the decay yield fractions, $\gamma_{d,j \rightarrow i}$, as well as the energy per decay, $q_{d,i}$, are shown in Table 2-36 and Figure 2-60. Detailed description of how these values were derived is presented in Volume 1.

Table 2-36 Decay heat group constants.

Group No.	Isotope <i>i</i>	Decay constant, λ_i , (1/s)	Decay yields $y_{d, i \rightarrow i+1}$, (-)	U fission yields $y_{f, U \rightarrow i}$, (-)	Pu fission yields $y_{f, Pu \rightarrow i}$, (-)
1	601	1.77	1.000	0.2392	0.1600
2	602	0.577	1.000	0.4208	0.3000
3	603	6.74×10^{-2}	1.000	0.5800	0.5800
4	604	6.21×10^{-3}	0.602	0.3080	0.3080
5	605	4.74×10^{-4}	0.554	0.0000	0.0000
6	606	4.81×10^{-5}	0.358	0.0000	0.0000
7	607	5.34×10^{-6}	0.710	0.0000	0.0000
8	608	5.73×10^{-7}	0.700	0.0000	0.0000
9	609	1.04×10^{-7}	0.506	0.0000	0.0000
10	610	2.96×10^{-8}	1.000	0.0000	0.0000
11	611	7.59×10^{-10}		0.0000	0.0000

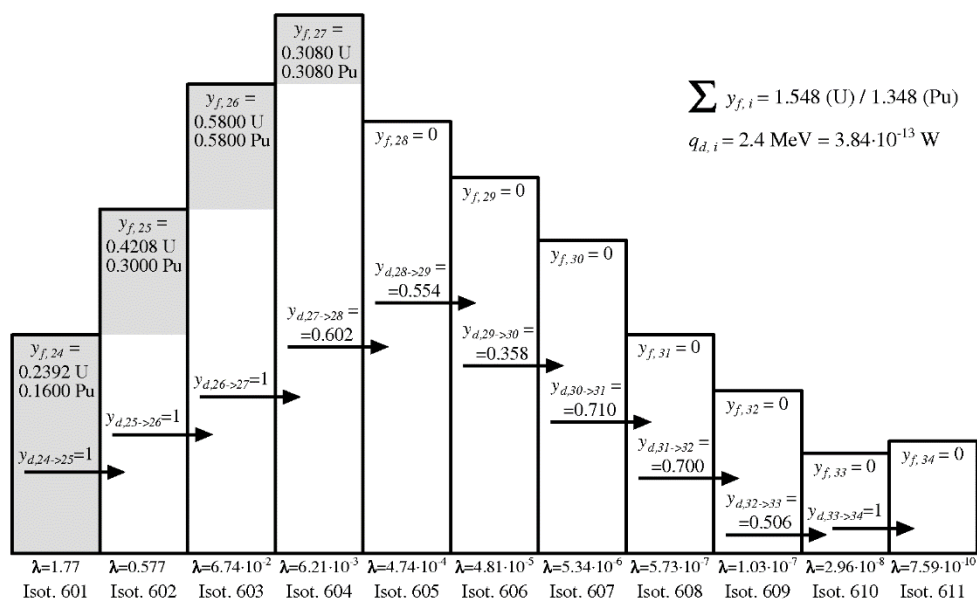


Figure 2-60 Decay heat group constants.

2.10.3 Records: 803XXX, Specific Heat Data

XXX is the material reference number. The material reference numbers need not be consecutive. The maximum number of materials is 100. Specific heat is assumed to be a function of temperature and is defined by pairs, giving the temperature and the specific heat for that temperature. Each record contains one or several data pairs. Records are read sequentially - the first record in the input is interpreted as containing the first set of data pairs. Total number of data pairs for a material may not exceed 100. To re-define the data, enter a record with a single entry of zero, followed by the new data table (see example in section 2.10.8).

- W-1 (R) : CPSMDX Temperature, (K).
Acceptable range: Temperature values must increase. Thus the value must be greater than the value of CPSMDX for the previous point.
Default value: none.
- W-2 (R) : CPSMDY Specific heat, (J/kg/K).
Acceptable range: $0.0 < \text{CPSMDY} \leq 10^{10}$.
Default value: none.

2.10.4 Records: 804XXX, Diffusion Coefficients for Fission Product Vapors

XXX is the material reference number. The material reference numbers need not be consecutive. The maximum number of materials is 100. The diffusion coefficients are used only if sorption of fission products is calculated. In such case they are used to calculate diffusion of the sorbed fission products into the SC or TC materials. The diffusion coefficient is calculated from:

$$D_{CS} = D_0 \cdot \exp\left(-\frac{A_D}{T}\right)$$

Limits are applied:

$$D_{\min} \leq D_{CS} \leq D_{\max}$$

- W-1 (R) : IVAP Fission product vapor class number.
Acceptable range: must be one of the existing fission product vapor classes.
Default value: none.
- W-2 (R) : DCS0MP Coefficient D_0 , (m^2/s), in the correlation for D_{CS} of the fission product vapor class IVAP in the solid material XXX. If zero or no value is entered for this material, the diffusion will not be calculated.
Acceptable range: $0.0 \leq \text{DCS0MP} \leq 1.0 \times 10^{+6}$
Default value: 0.0

SPECTRA Code Manuals - Volume 2: User's Guide

- W-3 (R) : ADCSMP Coefficient A_D , (K), in the correlation for D_{CS} of the fission product vapor class IVAP in the solid material XXX.
Acceptable range: $0.0 \leq \text{ADCSMP} \leq 1.0 \times 10^{10}$
Default value: 0.0
- W-4 (R) : DMINMP Lower limit, D_{\min} , (m^2/s), in the correlation for D_{CS} of the fission product vapor class IVAP in the solid material XXX.
Acceptable range: $0.0 \leq \text{DMINMP} \leq 1.0 \times 10^{-6}$
Default value: 0.0
- W-5 (R) : DMAXMP Upper limit, D_{\max} , (m^2/s), in the correlation for D_{CS} of the fission product vapor class IVAP in the solid material XXX.
Acceptable range: $\text{DMINMP} \leq \text{DMAXMP} \leq 1.0 \times 10^{-6}$
Default value: 1.0×10^{-6}

2.10.5 Records: 805XXX, Material Name

XXX is the material reference number. The material reference numbers need not be consecutive. The maximum number of materials is 100.

- W-1 (A) : NAMESM User defined name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.
Acceptable range: any string of up to 50 characters.
Default value: 50 "underline" characters: "_ _" .

2.10.6 Records: 806XXX, Materials Composed of Different Materials

XXX is the material reference number. The material reference numbers need not be consecutive. The maximum number of materials is 100.

Using this record, the user may specify a material that is composed from several (up to 10) different materials. The average thermophysical properties of such material are obtained from:

$$\overline{\rho \cdot c_p} = \sum_i x_i \cdot \rho_i \cdot c_{p,i} \quad \bar{k} = \sum_i x_i \cdot k_i \quad \text{or} \quad \overline{1/k} = \sum_i x_i / k_i$$

x_i = volumetric fraction of the material i in the mixture, (-)

ρ_i = density of the material i , (kg/m^3)

$c_{p,i}$ = specific heat of the material i , ($\text{J}/\text{kg}\cdot\text{K}$)

k_i = conductivity of the material i , ($\text{W}/\text{m}^2\cdot\text{K}$)

An example of the situation where this record is useful, is the fuel of high temperature reactor, consisting of graphite and TRISO particles, which in turn consist of fuel kernel and several coating layers.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-1 (R) : CCOMMP Option to calculate average thermal conductivity, (see Figure 2-61):
 |CCOMMP| = 1.0: use average thermal conductivity: $k = \sum(x_i k_i)$
 |CCOMMP| = 2.0: use average thermal resistance: $1/k = \sum(x_i/k_i)$
 $1.0 < |CCOMMP| < 2.0$: interpolate between the first and the second formula:
 $k = (2 - |CCOMMP|) \times \sum x_i k_i + (|CCOMMP| - 1) \times \sum x_i / k_i$
 Furthermore, this entry determines if the composition is defined by volume fractions or by mass fractions:
 CCOMMP > 0.0: XCOMMP are interpreted as volume fractions
 CCOMMP < 0.0: |XCOMMP| are interpreted as mass fractions
 Acceptable range: $1.0 < |CCOMMP| < 2.0$
 Default value: 2.0 (conservative: gives the lowest conductivity)
- W-2 (I) : ICOMMP Material number of the first material in the composition.
 (1) Acceptable range: This must be a single material, i.e. it cannot be a another composed material.
 Default value: none.
- W-3 (R) : XCOMMP Volumetric fraction (mass fraction if CCOMMP < 0.0) of the first material in the composition.
 (1) Acceptable range: $0.0 \leq XCOMMP \leq 1.0$
 Default value: none.
- W-4 (I) : ICOMMP Material number of the second material in the composition.
 (2) Acceptable range: This must be a single material, i.e. it cannot be a another composed material.
 Default value: none.
- W-5 (R) : XCOMMP Volumetric fraction (mass fraction if CCOMMP < 0.0) of the second material in the composition.
 Acceptable range: $0.0 \leq XCOMMP \leq 1.0$
 Default value: none.

... etc. until all materials are defined. The maximum number of materials is 10.

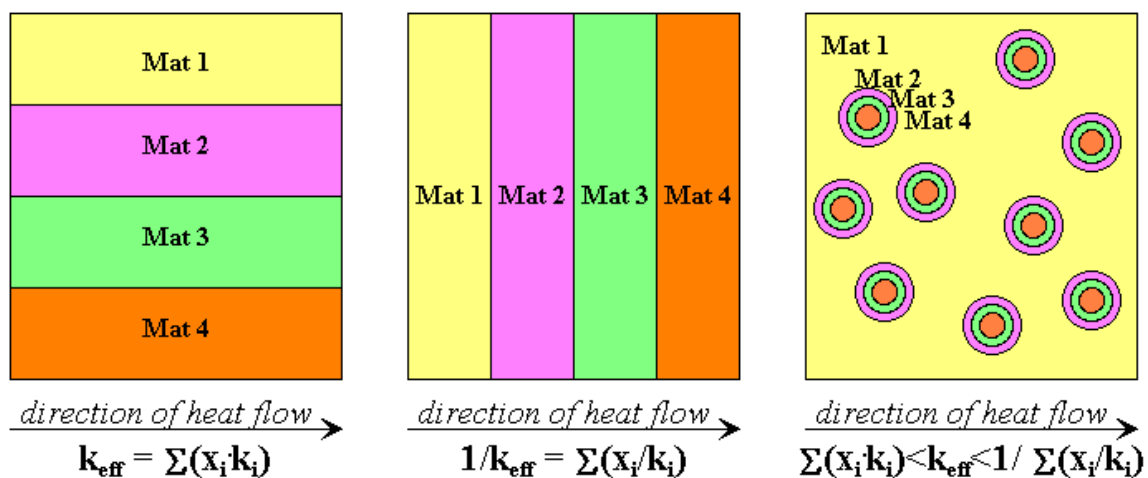


Figure 2-61 Examples of materials being a composition of different materials

2.10.7 Records: 800XXX, Constant Multipliers on the Material Properties

XXX is the material reference number. The material reference numbers need not be consecutive. The maximum number of materials is 100.

W-1 (R) : TCMLMP Multiplier on the thermal conductivity data, TCSMDY (defined in 801XXX).

Acceptable range: $0.01 < \text{TCMLMP} \leq 100.0$

Default value: 1.00

W-2 (R) : RHMLMP Multiplier on the density data, RHSMDY (defined in 802XXX).

Acceptable range: $0.01 < \text{RHMLMP} \leq 100.0$

Default value: 1.00

W-3 (R) : CPMLMP Multiplier on the specific heat data, CPSMDY (defined in 803XXX).

Acceptable range: $0.01 < \text{CPMLMP} \leq 100.0$

Default value: 1.00

2.10.8 Examples of Material Property Input Data

The input shown below defines material property for concrete (Stone 1-2-4 mix), stainless steel SS 304 and carbon steel SA533B1. The values for concrete are based on [9] (table A-3) and are valid for temperature of 20 °C. The values for stainless steel and carbon steel are based on graphs shown in [16] and define material properties valid for the temperature ranges:

- for stainless steel: from 300 K to 1300 K,
- for carbon steel: from 300 K to 1000 K.

```

* -----
*      Definition of material No. 001; Concrete
*      =====
805001 Concrete
*      Temperature      Thermal conductivity
*      (K)              (W/m/K)
801001      293.0        1.37      *
*      Temperature      Density
*      (K)              (kg/m3)
802001      293.0        2300.0    *
*      Temperature      Specific heat
*      (K)              (J/kg/K)
803001      293.0        880.0     *
*
* -----
*      Definition of material No. 002;  SS-304
*      =====
805002 Stainless steel,  SS-304
*      Temperature      Thermal conductivity
*      (K)              (W/m/K)
801002      300.0        13.5     *
801002      800.0        23.0     *
801002      1300.0       32.0     *
*      Temperature      Density
*      (K)              (kg/m3)
802002      300.0        7800.0   *
802002      800.0        7600.0   *
802002      1300.0       7350.0   *
*      Temperature      Specific heat
*      (K)              (J/kg/K)
803002      300.0        410.0   *
803002      500.0        450.0   *
803002      800.0        500.0   *
803002      1300.0       550.0   *
*
* -----
*      Definition of material No. 003;  SA533B1
*      =====
805003 Carbon steel,  SA533B1
*      Temperature      Thermal conductivity
*      (K)              (W/m/K)
801003      300.0        52.0     *
801003      600.0        44.0     *
801003      800.0        38.0     *
801003      1000.0       30.0     *
*      Temperature      Density
*      (K)              (kg/m3)
802003      300.0        7850.0   *
802003      500.0        7790.0   *
802003      700.0        7720.0   *
*      Temperature      Specific heat
*      (K)              (J/kg/K)
803003      300.0        450.0   *
803003      600.0        600.0   *
803003      800.0        700.0   *
803003      1000.0       950.0   *

```

SPECTRA Code Manuals - Volume 2: User's Guide

* -----

The same input may be defined by specifying multiple data pairs in a single data record:

```

*
805001 Concrete
*      T (K)  Value
801001  293.0  1.37  * Thermal conductivity (W/m/K)
802001  293.0 2300.0 * Density (kg/m3)
803001  293.0  880.0 * Specific heat (J/kg/K)
*
*
805002 Stainless steel, SS-304
*      T (K)  Value  T (K)  Value  T (K)  Value  T (K)  Value  *
801002  300.0  13.5  800.0  23.0  1300.0  32.0  * Thermal conductivity
802002  300.0 7800.0  800.0 7600.0  1300.0 7350.0 * Density
803002  300.0  410.0  500.0  450.0  800.0  500.0  1300.0  550.0 * Specific heat
*
*
805003 Carbon steel, SA533B1
*      T (K)  Value  T (K)  Value  T (K)  Value  T (K)  Value  *
801003  300.0  52.0  600.0  44.0  800.0  38.0  1000.0  30.0 * Thermal conductivity
802003  300.0 7850.0  500.0 7790.0  700.0 7720.0 * Density
803003  300.0  450.0  600.0  600.0  800.0  700.0  1000.0  950.0 * Specific heat

```

The following records illustrates how to re-define material property data:

```

*      T (K)      k (W/m/K)
801002  300.0      13.5  * old data point 1
801002  800.0      23.0  * old data point 2
801002      0          * start re-defining the k data
801002  273.0      125.0 * new data point 1
801002  973.0      225.0 * new data point 2

```

The following records illustrates how to define a material composed of several materials. The example defines TRISO particles in graphite matrix with packing factor of 0.25 (volumetric fraction of TRISO particles is 25%): It is assumed that the properties of graphite and TRISO particles are defined as:

- Material 502 - graphite
- Material 111 - fuel kernel
- Material 122 - PyC (buffer)
- Material 123 - iPyC
- Material 121 - SiC
- Material 124 - oPyC

Volume fractions of the fuel and coatings in a single TRISO particle were calculated assuming the following dimensions: fuel kernel diameter 500 μm , buffer 95 μm , iPyC 40 μm , SiC 35 μm , oPyC 40 μm . The input deck defining such material is shown below.

```

805572 Graphite-Fuel
*      Graphite      Fuel      buffer      iPyC      SiC      oPyC
*      k  Mat. Vol.fr.  Mat. Vol.fr.  Mat. Vol.fr.  Mat. Vol.fr.  Mat. Vol.fr.  Mat. Vol.fr.
806572 0  502  0.7500  111  0.04013  122  0.06534  123  0.04110  121  0.04372  124  0.05971

```

2.11 User-Defined Gas Data

The SPECTRA code contains six built-in gases:

- H₂ hydrogen
- He helium
- H₂O steam
- N₂ nitrogen
- O₂ oxygen
- CO₂ carbon dioxide

These gases are treated as real gases. For all the gases except for the steam, the virial equation of state is used. The properties are tabulated versus temperature and pressure - see Volume 1.

On top of the built-in gases, user-defined gases are available. The total number of gases (built-in + user-defined) is 20. The user-defined gases are treated as semi-perfect gases. The perfect gas equation of state is used. The specific heat, the viscosity, and the thermal conductivity, are assumed to be functions of temperature.

The user has to define the following parameters:

- Molar weight, M_w , (kg/kmol)
- Molecular diffusion volume, Σ , (-)
- Specific heat, $c_p(T)$, (J/kg-K)
- Viscosity, $\eta(T)$, (kg/m-s)
- Thermal conductivity, $k(T)$, (W/m-K)

2.11.1 Record: G05XXX, Name of the User-Defined Gas

XXX is the user-defined gas number. The gas numbers must start at 007 (because there are six built-in gases) and be consecutive. The maximum number of gases is equal to: $NGMXFL = 20$.

W-1 (A) : GASNFL User-defined gas name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.

Note that in some places in the output file only the first 3 characters are printed. Therefore the user is advised to use a 3-character abbreviation, followed by a comma and a full name, for example:

Kr , Krypton

Acceptable range: any string of up to 50 characters.

Default value: 50 "underline" characters: "_ _" .

2.11.2 Record: 830XXX, Molar Weight, Diffusion Volume, Reference Energy

XXX is the user-defined gas number. The gas numbers must start at 007 (because there are six built-in gases) and be consecutive. The maximum number of gases is equal to: NGMXFL = 20.

W-1 (R) : WMOLFL Molar weight, M_w (kg/kmol), of the user-defined gas XXX. Used to calculate the individual gas constant, R , (needed for the perfect gas equation of state):

$$R = \frac{R_u}{M_w}$$

R_u universal gas constant (=8314.51), (J/kmol-K)

R individual gas constant, (J/kg-K)

M_w gas molar weight, (kg/kmol)

The molar weights of some elements and compounds are given in Table 2-37.

Acceptable range: $10^{-1} < \text{WMOLFL} < 10^3$

Default value: none

W-2 (R) : DVGSFL Molecular diffusion volume, Σ , of the user-defined gas XXX. Used to calculate the diffusion coefficients for a gas mixture.

The molecular diffusion volume of some elements and compounds are given in Table 2-37.

Table 2-37 Molar weights [39] (page 1-7) and molecular diffusion volumes, [43] (table 11-1).

Element	M_w	Σ	Compound	M_w	Σ
C	12.01	15.90	H ₂	2.02	6.12
H	1.01	2.31	D ₂	4.03	6.84
O	16.00	6.11	N ₂	28.00	18.50
N	14.00	5.43	O ₂	32.00	16.30
F	19.00	14.70	Air	28.01	19.70
Cl	35.45	21.00	CO	28.80	18.0
Br	79.90	21.90	CO ₂	44.01	26.90
I	126.90	29.80	N ₂ O	44.00	35.90
S	32.06	22.90	NH ₃	16.02	20.70
He	4.00	2.67	H ₂ O	18.02	13.10
Ne	20.18	5.98	SF ₄	108.06	71.30
Ar	39.95	16.20	Cl ₂	70.91	38.40
Kr	83.80	24.50	Br ₄	159.80	69.00
Xe	131.30	32.70	SO ₂	64.06	41.80

For other materials the value may be estimated from the following correlations:

elements: $\Sigma \sim 1.3 \cdot M_w^{0.66}$

compounds: $\Sigma \sim 2.5 \cdot M_w^{0.66}$

Results obtained with the above correlations are shown in Figure 2-62.

Acceptable range: $0.0 < DVGSFL < 10^3$

a warning message is issued if the value is outside the range: $1.3 \cdot M_w^{0.66} \times 0.5 \div 2.5 \cdot M_w^{0.66} \times 2.0$

Default value: none

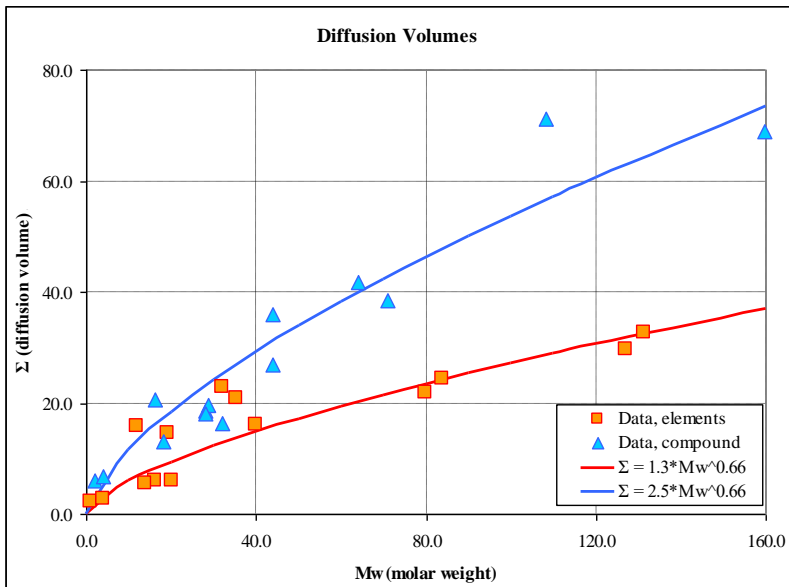


Figure 2-62 Diffusion volumes - data and correlations: $\Sigma = 1.3 \cdot M_w^{0.66}$, $\Sigma = 2.5 \cdot M_w^{0.66}$.

W-3(R) : UREFFL Value of the internal energy, u_{ref} (J/kg), at the reference point, T_0 . The reference point is assumed to be the first point in the specific heat data table (the first value of XCPGFL in the record 831XXX). The internal energy of gas XXX at this temperature will be equal to UREFFL. For other temperatures the internal energy is calculated by integrating the specific heat data provided by the user in the record 831XXX, as:

$$u(T) = u_{ref} + \int_{T_0}^T [c_p(T') - R] dT'$$

Here R is the gas constant.

Acceptable range: UREFFL \geq 0.0

Default value: 0.0

2.11.3 Record: 831XXX, Specific Heat

XXX is the user-defined gas number. The gas numbers must start at 007 (because there are six built-in gases) and be consecutive. The maximum number of gases is equal to: $NGMXFL = 20$. Specific heat is assumed to be a function of temperature and is defined by pairs, giving the temperature and the specific heat for that temperature. Each record contains one or several data pairs. Records are read sequentially - the first record in the input is interpreted as containing the first set of data pairs. The total number of data pairs for a single gas may not exceed 100. To re-define the data, enter a record with a single entry of zero, followed by the new data table (see example in section 2.11.6).

- W-1 (R) : XCPGFL Temperature, T (K).
Acceptable range: $0.0 < T < 10^4$. Temperature values must increase. Thus the value must be greater than the value of T for the previous point. The first value is set as a reference temperature, T_{ref} , and cannot be larger than 270 K. The recommended value is 0.0.
Default value: none.
- W-2 (R) : YCPGFL Specific heat at the temperature T , $c_p(T)$ (J/kg-K).
Acceptable range: $2 \times R < YCPGFL < 10^5$ (R is the gas constant)
Default value: none

2.11.4 Record: 832XXX, Dynamic Viscosity

XXX is the user-defined gas number. The gas numbers must start at 007 (because there are six built-in gases) and be consecutive. The maximum number of gases is equal to: $NGMXFL = 20$. Viscosity is assumed to be a function of temperature and is defined by pairs, giving the temperature and the viscosity for that temperature. Each record contains one or several data pairs. Records are read sequentially - the first record in the input is interpreted as containing the first set of data pairs. The total number of data pairs for a single gas may not exceed 100. To re-define the data, enter a record with a single entry of zero, followed by the new data table (see example in section 2.11.6).

- W-1 (R) : XVSGFL Temperature, T (K).
Acceptable range: $0.0 < T < 10^4$. Temperature values must increase. Thus the value must be greater than the value of T for the previous point.
Default value: none.
- W-2 (R) : YVSGFL Viscosity at the temperature T , $\eta(T)$ (kg/m-s).
Acceptable range: $10^{-10} < YVSGFL < 10^{+1}$
Default value: none

SPECTRA Code Manuals - Volume 2: User's Guide

2.11.6 Examples of the User-Defined Gas Data

The input below defines carbon monoxide, argon, and neon, as user-defined gases number 7, 8, 9.

```
*
*
= User-defined gas data, Data for CO, Ar, Ne
*
*
*   Ref.:
*   (Lide, 1992) - D.R. Lide, et al., "CRC Handbook of Chemistry and Physics,
*   A Ready-Reference Book of Chemical and Physical Data",
*   72-nd edition, ISBN-0-8493-0472-5, CRC Press Inc., 1991-1992.
*
*
G05007 CO , Carbon monoxide
*
*   Molar      Diffusion   U-ref
*   weight     volume      (J/kg)
830007  28.8      18.0      0.0
*
*   T      Value      T      Value      T      Value      T      Value
831007  0.0  1030.7      T      Value      T      Value      T      Value      * Cp (J/kg-K) ((Lide, 1992), p. 8-50)
832007  300.0  1.78E-5      400.0  2.21E-5      500.0  2.58E-5      600.0  2.91E-5 * Visc, (kg/m-s) ((Lide, 1992), p. 6-154)
833007  300.0  0.0250      400.0  0.0323      500.0  0.0392      600.0  0.0457 * k, (W/m-K) ((Lide, 1992), p. 6-162)
*
*
G05008 Ar , Argon
*
*   Molar      Diffusion   U-ref
*   weight     volume      (J/kg)
830008  39.95      16.2      0.0
*
*   T      Value      T      Value      T      Value      T      Value
831008  0.0  520.0      T      Value      T      Value      T      Value      * Cp (J/kg-K) ((Lide, 1992), p. 6-68)
832008  300.0  2.29E-5      400.0  2.88E-5      500.0  3.42E-5      600.0  3.90E-5 * Visc, (kg/m-s) ((Lide, 1992), p. 6-154)
833008  300.0  0.0179      400.0  0.0226      500.0  0.0268      600.0  0.0306 * k, (W/m-K) ((Lide, 1992), p. 6-162)
*
*
G05009 Ne , Neon
*
*   Molar      Diffusion   U-ref
*   weight     volume      (J/kg)
830009  20.18      5.98      0.0
*
*   T      Value      T      Value      T      Value      T      Value
831009  0.0  1030.0      T      Value      T      Value      T      Value      * Cp (J/kg-K) ((Lide, 1992), p. 5-68)
832009  300.0  3.21E-5      400.0  3.89E-5      500.0  4.50E-5      600.0  5.08E-5 * Visc, (kg/m-s) ((Lide, 1992), p. 6-154)
833009  300.0  0.0498      400.0  0.0603      500.0  0.0699      600.0  0.0787 * k, (W/m-K) ((Lide, 1992), p. 6-162)
*
*
```

The following records illustrates how to re-define the gas property data:

```
831008  0.0  520.0      * Cp (J/kg-K) ((Lide, 1992), p. 6-68)
832008  300.0  2.29E-5      400.0  2.88E-5      500.0  3.42E-5      600.0  3.90E-5 * Visc, (kg/m-s) ((Lide, 1992), p. 6-154)
833008  300.0  0.0179      400.0  0.0226      500.0  0.0268      600.0  0.0306 * k, (W/m-K) ((Lide, 1992), p. 6-162)

833008  0 * start re-defining the k data
833008  300.0  0.179      400.0  0.226      500.0  0.268      600.0  0.306 * k values increased x 10 for sensitivity
```


W-2 (R) : DTSBFL Minimum subcooling for alternative fluid. Used only if IFLDFL > 1. In order to avoid saturated and subcooled boiling of the alternative fluids, calculations are stopped when the subcooling in any CV is below the value of DTSBFL: $T > T_{sat}(p) - DTSBFL$.
Acceptable range: $0.1 \leq DTSBFL \leq 10.0$
Default value: 1.0

2.12.2 Record: A05000, Name of the Alternative Fluid

W-1 (A) : NAMEFL User-defined name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.
Acceptable range: any string of up to 50 characters.
Default value: 50 "underline" characters: "_" .

2.12.3 Records: 841000, Thermodynamic Properties of the Alternative Fluid

Each record defines data for one temperature point. The record is repeated as many times as needed to define the fluid properties for the desired temperature range. The temperature values must be in ascending order. The maximum number of data points is 1000.

W-1 (R) : TTABFL Temperature for the thermodynamic property data tables, T_i , (K or °C). The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then all tables of the thermodynamic properties are filled using the built-in steam-water property data (in other words, all data that may follow in this record is ignored).
Acceptable range: $0 \leq T_i \leq 10^9$
 $T_{i-1} < T_i < T_{i-1} \times 10$
Default value: none

W-2 (R) : PTABFL Saturation pressure at the temperature T_i , $p_{sat}(T_i)$, (Pa). The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 < p_{sat}(T_i) \leq 10^9$
 $p_{sat}(T_{i-1}) < p_{sat}(T_i) < 10 \times p_{sat}(T_{i-1})$
Default value: none

W-3 (R) : HFTBFL Saturated liquid enthalpy at the temperature T_i , $h_f(T_i)$, (J/kg). The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq h_f(T_i) \leq 10^9$
 $h_f(T_{i-1}) < h_f(T_i) < 10 \times h_f(T_{i-1})$
Default value: none

SPECTRA Code Manuals - Volume 2: User's Guide

- W-4 (R) : HGTBFL Saturated vapor enthalpy at the temperature T_i , $h_g(T_i)$, (J/kg).
 The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq h_g(T_i) \leq 10^9$,
 $h_g(T_{i-1}) / 10 < h_g(T_i) < 10 \times h_g(T_{i-1})$
Default value: none
- W-5 (R) : RFTBFL Saturated liquid density at the temperature T_i , $\rho_f(T_i)$, (kg/m³).
 The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq \rho_f(T_i) \leq 10^9$,
 $\rho_f(T_{i-1}) / 10 < \rho_f(T_i) < \rho_f(T_{i-1})$
Default value: none
- W-6 (R) : RGTBFL Saturated vapor density at the temperature T_i , $\rho_g(T_i)$, (kg/m³).
 The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq \rho_g(T_i) \leq 10^9$,
 $\rho_g(T_{i-1}) < \rho_g(T_i) < \rho_g(T_{i-1}) \times 10$
Default value: none
- W-7 (R) : SFTBFL Saturated liquid entropy at the temperature T_i , $s_f(T_i)$, (J/kg·K).
 The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq s_f(T_i) \leq 10^9$
 $s_f(T_{i-1}) < s_f(T_i) < 10 \times s_f(T_{i-1})$
Default value: none
- W-8 (R) : SGTBFL Saturated vapor entropy at the temperature T_i , $s_g(T_i)$, (J/kg·K).
 The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq s_g(T_i) \leq 10^9$,
 $s_g(T_{i-1}) / 10 < s_g(T_i) < s_g(T_{i-1}) \times 10$
Default value: none
- W-9 (I) : I Data point number. If no value, or zero is entered, then the data are read sequentially - the first record in the input is interpreted as containing the first data set (lowest temperature, I=1), then I=2, etc.
Acceptable range: $0 < I \leq 1000$
Default value: none.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-6 (R) : PFTBFL Saturated liquid Prandtl number at temperature T_i , $Pr_f(T_i)$, (-).
 The entered values must be positive for all data points or zero for all data points.
Acceptable range: $0 \leq Pr_f(T_i) \leq 10^9$,
 $Pr_f(T_{i-1}) / 10 < Pr_f(T_i) < Pr_f(T_{i-1}) \times 10$
Default value: $Pr_f = c_{pf} \times \eta_f / k_f$
 where: η_f = viscosity value: VFTBFL
 k_f = thermal conductivity value: TFTBFL
 c_{pf} = specific heat = dh_f/dT , with h_f = HFTBFL
 A warning message is issued if the entered value is more than 1% different from the default value.
- W-7 (R) : PGTBFL Saturated vapor Prandtl number at temperature T_i , $Pr_g(T_i)$, (-).
 The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq Pr_g(T_i) \leq 10^9$,
 $Pr_g(T_{i-1}) / 10 < Pr_g(T_i) < Pr_g(T_{i-1}) \times 10$
Default value: none
- W-8 (R) : STTBFL Surface tension at temperature T_i , σ_{fg} , (N/m).
 The entered values must be positive for all data points or zero for all data points. If zeroes are entered, then this table is filled using the built-in steam-water property data.
Acceptable range: $0 \leq \sigma_{fg}(T_i) \leq 10^9$,
 $\sigma_{fg}(T_{i-1}) / 10 < \sigma_{fg}(T_i) < \sigma_{fg}(T_{i-1}) \times 10$
Default value: none
- W-9 (I) : I Data point number. If no value, or zero is entered, then the data are read sequentially - the first record in the input is interpreted as containing the first data set (lowest temperature, I=1), then I=2, etc.
Acceptable range: $0 < I \leq 1000$
Default value: none

2.12.5 Record: 843000, Heat Transfer Option

- W-1 (R) : IHTCFL Heat transfer option:
 =1: use only the forced convection correlations, defined in the records 843XXX, below.
 =2: use the forced convection correlations, defined in the records 843XXX below, as well as the natural convection correlations, the same as in case of the standard fluid.
Acceptable range: 1 or 2
Default value: 1

SPECTRA Code Manuals - Volume 2: User's Guide

- W-5 (R) : A2HCFL A_2 in the user-defined correlation.
Acceptable range: $-10^{10} \leq A2HCFL \leq 10^{10}$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-6 (R) : B2HCFL B_2 in the user-defined correlation.
Acceptable range: $-100.0 \leq B2HCFL \leq 100.0$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-7 (R) : C2HCFL C_2 in the user-defined correlation.
Acceptable range: $-100.0 \leq C2HCFL \leq 100.0$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-8 (R) : D2HCFL D_2 in the user-defined correlation.
Acceptable range: $-100.0 \leq D2HCFL \leq 100.0$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-9 (R) : A3HCFL A_3 in the user-defined correlation.
Acceptable range: $-10^{10} \leq A3HCFL \leq 10^{10}$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-10 (R) : B3HCFL B_3 in the user-defined correlation.
Acceptable range: $-100.0 \leq B3HCFL \leq 100.0$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-11 (R) : C3HCFL C_3 in the user-defined correlation.
Acceptable range: $-100.0 \leq C3HCFL \leq 100.0$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-12 (R) : D3HCFL D_3 in the user-defined correlation.
Acceptable range: $-100.0 \leq D3HCFL \leq 100.0$
Default value: 0.0 for XXX=1, value from XXX-1 for XXX>1
- W-13 (R) : XVISFL Power in viscosity ratio. If a non-zero value is specified, the correlation is multiplied by a viscosity ratio to the power of XVISFL:

$$\left(\frac{\mu_f}{\mu_w} \right)^x$$

Here μ_f is the fluid viscosity obtained at the bulk fluid temperature, while μ_w is the fluid viscosity obtained at the wall surface temperature. The power x is the input parameter XVISFL.

Acceptable range: $-100.0 \leq XVISFL \leq 100.0$
Default value: 0.0

2.12.7 Record: 843YYY, Heat Transfer Correlation Sets for Alternative Fluid

YYY is the correlation set number. The correlation sets starts at 101 and must be consecutive. The maximum number of correlation sets is 99: $101 \leq YYY \leq 199$.

If a single heat transfer correlation is needed, then it may be defined using the records 843XXX. Such correlation is valid for the entire range of Reynolds numbers. If multiple correlations are needed, then a set of correlations may be defined in the present record. Up to ten correlations may be used in a single set. All correlations must be defined in the records 843XXX.

Correlation 1

- W-1 (I) : ICORFL(1) Correlation 1.
Acceptable range: must be one of the correlations defined in the records 843XXX
Default value: none
- W-2 (R) : RELFL(1) Lower limit of the Reynolds number to apply Correlation 1. Typically this should be zero. If a positive value is used, the value of heat transfer correlation for Re smaller than the minimum value, will be constant and equal to the value for $Re = RELFL(1)$.
Acceptable range: $RELFL(1) \geq 0.0$.
Default value: 0.0
- W-3 (R) : REULFL(1) Upper limit of the Reynolds number to apply Correlation 1.
Acceptable range: $REULFL(1) > 0.0$
Default value: none

Correlation 2

- W-4 (I) : ICORFL(2) Correlation 2.
Acceptable range: must be one of the correlations defined in the records 843XXX
Default value: none
- W-5 (R) : RELFL(2) Lower limit of the Reynolds number to apply Correlation 2. Linear interpolation is performed in the range between the upper limit for Correlation 1 and the lower limit for Correlation 2.
Acceptable range: $RELFL(2) > REULFL(1) \times 1.1$
Default value: none
- W-6 (R) : REULFL(2) Upper limit of the Reynolds number to apply Correlation 2.
Acceptable range: $REULFL(2) > RELFL(2) \times 1.1$
Default value: none

(...) until all correlations are defined. Maximum number of correlations is 10.

SPECTRA Code Manuals - Volume 2: User's Guide

2.12.8 Example of the Alternative Fluid Data - Data for Liquid Lead

The input below defines liquid lead as the alternative fluid. The recommended heat transfer correlations are used (see Volume 1). The data fields for the spherical geometry are left empty; therefore the cylindrical geometry correlation will be used for the spherical geometry.

```
*
*
= Alternative Fluid Property Data - Liquid Lead
*
* =====
*
ATTACH LEAD-K.ATT * PROPERTIES OF LEAD
*
HEAT TRANSFER CORRELATION
*
*
* A0 A1 B1 C1 A2 B2 C2 D2 A3 B3 C3 D3 * RECTANGULAR GEOMETRY
843001 5.60 0.019 0.775 0.775 *
843002 3.66 0.62 0.5 0.333 3.923E-4 0.625 0.00 0.80 0.543 0.00 -0.667 -0.250 * CYLINDRICAL GEOMETRY
843003 * SPERICAL GEOMETRY
*
```

The file LEAD-K.ATT contains properties of liquid lead tabulated versus temperature in Kelvins. The method to create such file is discussed in Volume 3. Below some parts of this file are listed

```
*
* PROPERTIES OF LIQUID LEAD
*
A05000 LIQUID LEAD
*
840000 2 * DATA TABLES IN KELVINS
*
* 1.) THERMODYNAMIC DATA OF THE LEAD
*
* T (K) P (Pa) Hf (J/kg) Hg (J/kg) Rf (kg/m3) Rg (kg/m3) Sf (J/kg-K) Sg (J/kg-K)
*
841000 6.00000E+02 5.38066E-07 6.45682E+04 0.00000E+00 1.06496E+04 0.00000E+00 0.00000E+00 0.00000E+00
841000 6.10000E+02 9.52207E-07 6.60983E+04 0.00000E+00 1.06384E+04 0.00000E+00 0.00000E+00 0.00000E+00
841000 6.20000E+02 1.71474E-06 6.77231E+04 0.00000E+00 1.06265E+04 0.00000E+00 0.00000E+00 0.00000E+00
841000 6.30000E+02 3.03078E-06 6.93449E+04 0.00000E+00 1.06145E+04 0.00000E+00 0.00000E+00 0.00000E+00
841000 6.40000E+02 5.26237E-06 7.09638E+04 0.00000E+00 1.06026E+04 0.00000E+00 0.00000E+00 0.00000E+00
. . .
841000 1.98000E+03 8.66948E+04 2.67839E+05 0.00000E+00 9.00209E+03 0.00000E+00 0.00000E+00 0.00000E+00
841000 1.99000E+03 9.17306E+04 2.69210E+05 0.00000E+00 8.99014E+03 0.00000E+00 0.00000E+00 0.00000E+00
841000 2.00000E+03 9.70040E+04 2.70579E+05 0.00000E+00 8.97820E+03 0.00000E+00 0.00000E+00 0.00000E+00
841000 2.01000E+03 1.02524E+05 2.71949E+05 0.00000E+00 8.96626E+03 0.00000E+00 0.00000E+00 0.00000E+00
841000 2.02000E+03 1.05957E+05 2.72770E+05 0.00000E+00 8.95909E+03 0.00000E+00 0.00000E+00 0.00000E+00
*
* 2.) THERMO-PHYSICAL DATA OF THE LEAD
*
* T (K) Vf (kg/m-s) Vg (kg/m-s) Tf (W/m-K) Tg (W/m-K) Prf (-) Prg (-) ST (N/m)
*
842000 6.00000E+02 2.69778E-03 0.00000E+00 1.58066E+01 0.00000E+00 2.52231E-02 0.00000E+00 4.51132E-01
842000 6.10000E+02 2.62479E-03 0.00000E+00 1.59100E+01 0.00000E+00 2.43592E-02 0.00000E+00 4.50070E-01
842000 6.20000E+02 2.55164E-03 0.00000E+00 1.60200E+01 0.00000E+00 2.34947E-02 0.00000E+00 4.48940E-01
842000 6.30000E+02 2.48275E-03 0.00000E+00 1.61300E+01 0.00000E+00 2.26818E-02 0.00000E+00 4.47810E-01
842000 6.40000E+02 2.41779E-03 0.00000E+00 1.62400E+01 0.00000E+00 2.19163E-02 0.00000E+00 4.46680E-01
. . .
842000 1.98000E+03 7.80704E-04 0.00000E+00 3.09800E+01 0.00000E+00 3.47789E-03 0.00000E+00 2.95260E-01
842000 1.99000E+03 7.78589E-04 0.00000E+00 3.10900E+01 0.00000E+00 3.45739E-03 0.00000E+00 2.94130E-01
842000 2.00000E+03 7.76501E-04 0.00000E+00 3.12000E+01 0.00000E+00 3.43718E-03 0.00000E+00 2.93000E-01
842000 2.01000E+03 7.74438E-04 0.00000E+00 3.13100E+01 0.00000E+00 3.41726E-03 0.00000E+00 2.91870E-01
842000 2.02000E+03 7.73214E-04 0.00000E+00 3.13760E+01 0.00000E+00 3.40544E-03 0.00000E+00 2.91192E-01
```

2.13 Heat Transfer Model Coefficients

The heat transfer model coefficients are applied for all 1-D and 2-D Solid Heat Conductors.

2.13.1 Records: 810010, CHF Model Data

Typically the CHF increases with decreasing diameter. The dependency is well represented by:

$$CHF \sim \left(\frac{D}{D_0} \right)^n$$

where D_0 is a reference diameter (equal to 0.008 m) and n is between $-1/3$ and $-1/2$. This relation holds for diameters larger than a certain critical diameter, D_{crit} . Below the critical diameter, CHF decreases with decreasing diameter. Measurement data indicate that the critical diameter depends on subcooling. For large subcooling (55 K) the critical diameter is smaller than 0.3 mm [46]. For subcooling of about 20 K it is about 1 - 2 mm [47]. For saturated liquid it is as large as 7 mm [48]. This data is approximated in SPECTRA by the following correlation:

$$D_{crit} = D_c \cdot \exp[-A_c X]$$

Here X is quality and D_c and A_c are constants. The data points are shown in Figure 2-63. The following constants are selected: $D_c = 0.007$ m and $A_c = 30.0$. The line obtained with the correlation is shown in Figure 2-63. The coefficients D_c and A_c may be redefined in this record.

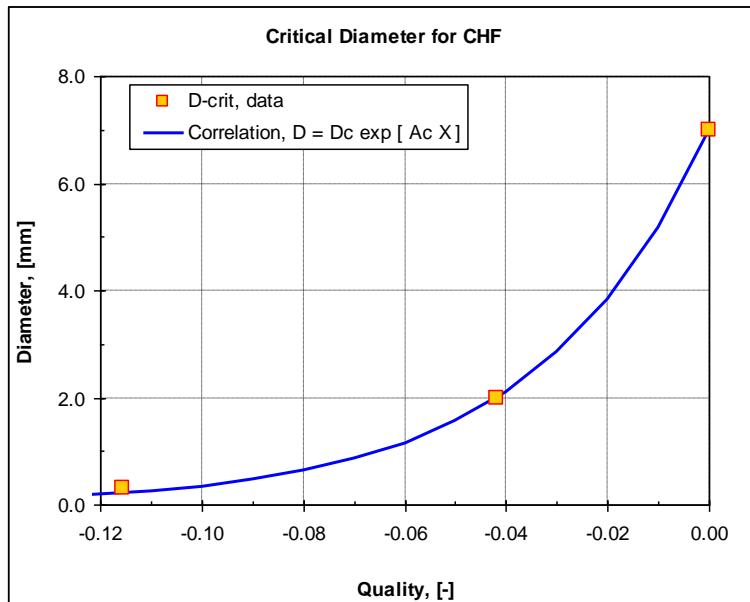


Figure 2-63 Critical diameter for CHF

2.13.2 Records: 810020, Heat and Mass Transfer Model Data

This record allows to modify the heat and mass transfer correlations used for condensation or evaporation from pool surface, droplet surface, and bubble surface.

- Heat transfer
The heat transfer coefficient, h (W/m²-K), at gas-liquid interfaces is obtained from the Nusselt number (see Volume 1, Heat and Mass Transfer Correlations):

$$h = Nu \cdot \frac{k}{d}$$

Here k is the thermal conductivity and d is the characteristic dimension. The Nusselt number is obtained from appropriate correlations as shown in Volume 1. Using this record, the user may modify the Nusselt number obtained from the correlations by defining a constant multiplier on the Nusselt number, X_{Nu} :

$$h = X_{Nu} \cdot Nu \cdot \frac{k}{d}$$

- Mass transfer
The mass transfer coefficient, K_M , (kg/m²-s), at gas-liquid interfaces is obtained using the Sherwood number (see Volume 1, Heat and Mass Transfer Correlations):

$$K_M = Sh \cdot \frac{D_C}{d}$$

Here D_C is the diffusion coefficient and d is the characteristic dimension. The Sherwood number is obtained from appropriate correlations as shown in Volume 1. Using this record, the user may modify the Sherwood number obtained from the correlations by defining a constant multiplier on the Sherwood number, X_{Sh} :

$$K_m = X_{Sh} \cdot Sh \cdot \frac{D_C}{d}$$

- | | | |
|-----------|--------|---|
| W-1 (R) : | XNUPHT | Nusselt number multiplier, X_{Nu} , heat transfer on the pool surface.
<i>Acceptable range:</i> $0.0 \leq XNUPHT \leq 100.0$
<i>Default value:</i> 1.0 (a small number, $<10^{-50}$, sets the value to 0.0) |
| W-2 (R) : | XNUDHT | Nusselt number multiplier, X_{Nu} , heat transfer on the droplet surface.
<i>Acceptable range:</i> $0.0 \leq XNUDHT \leq 100.0$
<i>Default value:</i> 1.0 (a small number, $<10^{-50}$, sets the value to 0.0) |
| W-3 (R) : | XNUBHT | Nusselt number multiplier, X_{Nu} , heat transfer on the bubble surface.
<i>Acceptable range:</i> $0.0 \leq XNUBHT \leq 100.0$
<i>Default value:</i> 1.0 (a small number, $<10^{-50}$, sets the value to 0.0) |

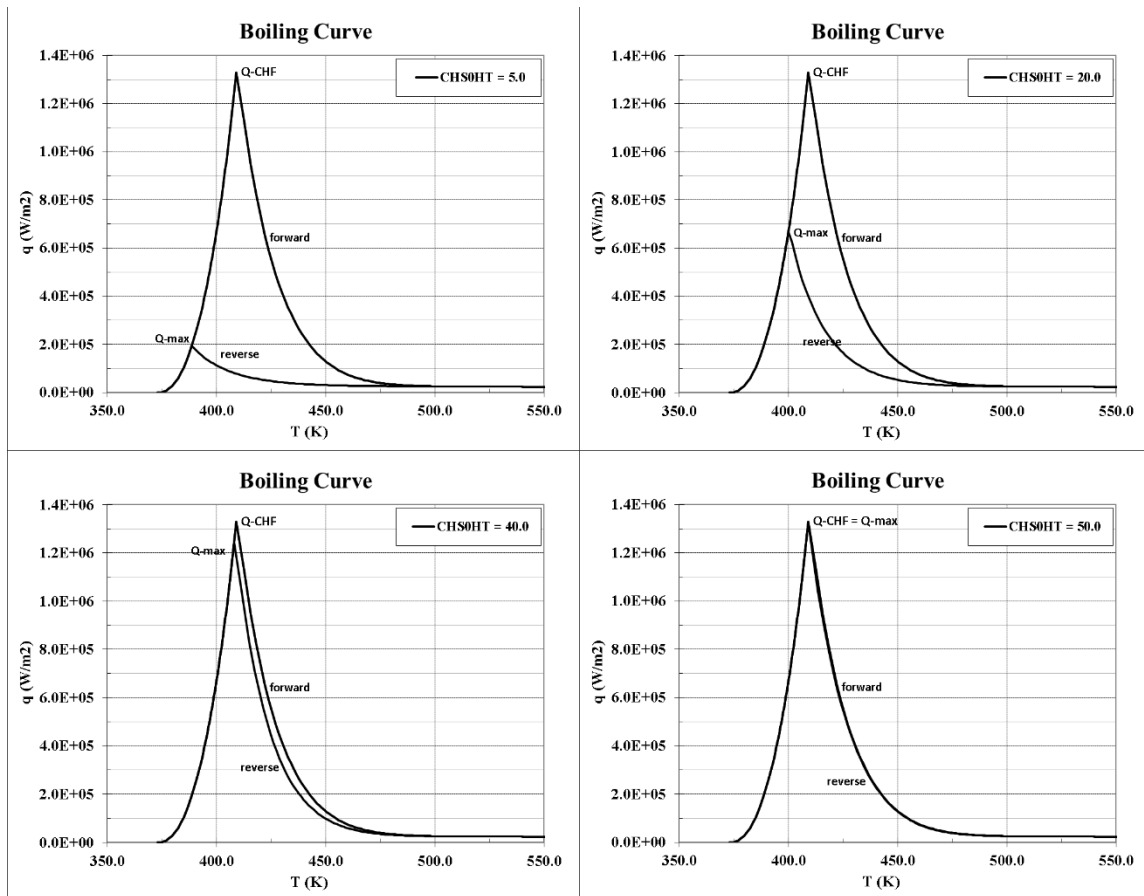


Figure 2-64 Boiling hysteresis, effect of C_{hyst} (CBHOHT)

- W-3 (R) : CBHOHT Boiling curve, hysteresis coefficient, C_{hyst} , (-), vertical surfaces.
Acceptable range: $1.0 \leq CBHOHT \leq 1.0 \times 10^{10}$
Default value: 5.0
- W-4 (R) : CBH1HT Boiling curve, hysteresis coefficient, C_{hyst} , (-), horizontal surfaces, facing down.
Acceptable range: $1.0 \leq CBH1HT \leq 1.0 \times 10^{10}$
Default value: CBHOHT
- W-5 (R) : CBH2HT Boiling curve, hysteresis coefficient, C_{hyst} , (-), horizontal surfaces, facing up.
Acceptable range: $1.0 \leq CBH2HT \leq 1.0 \times 10^{10}$
Default value: CBHOHT

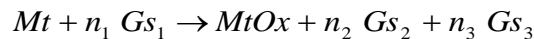
2.14 Material Oxidation Data

Material oxidation is activated for each 1-D or 2-D Solid Heat Conductor in records 381XXX, 382XXX, and 480XXX. Several oxidation models are built-in - see Volume 1. The user may define his own oxidation model using the data specified in these records.

2.14.1 Records: 8500XX, Oxidation Reaction Definition

XX is the number of the user-defined oxidation model. The maximum number of user-defined oxidation models is 10. The oxidation models must be numbered consecutively, XX=01, 02, 03, ...

The oxidation reaction is assumed to have the following general form:



<i>Mt</i>	oxidized material
<i>MtOx</i>	material oxide
<i>Gs₁</i>	gas 1 (oxidizing gas, for example steam, oxygen)
<i>Gs₂</i>	gas 2 (product of reaction, for example hydrogen)
<i>Gs₃</i>	gas 3 (optional second product of reaction)
<i>n₁</i>	reaction ratio 1 - moles of gas <i>Gs₁</i> per one mole of oxidized material
<i>n₂</i>	reaction ratio 2 - moles of gas <i>Gs₂</i> per one mole of oxidized material
<i>n₃</i>	reaction ratio 3 - moles of gas <i>Gs₃</i> per one mole of oxidized material

The reaction kinetics is assumed to have the following general form:

$$\frac{dm^x}{dt} = \left(\frac{1}{K_T(T) \cdot C_T(T, p_i)} + \frac{1}{K_v(v, T)} \right)^{-1} \cdot K_p(p_1) \cdot M(B, \dots)$$

<i>m</i>	mass of reacted material per unit surface area (kg/m ²),
<i>x</i>	exponent, (-) (<i>x</i> =2 for a parabolic oxidation rate)
<i>t</i>	time (s),
<i>K</i>	reaction rate ((kg/m ²) ^{<i>x</i>} /s),
<i>T</i>	temperature, (K),
<i>v</i>	velocity of the oxidizing gas, (m/s),
<i>p_i</i>	partial pressure of the gas <i>i</i> , (Pa),
<i>p₁</i>	partial pressure of the oxidizing gas, (Pa),
<i>K_T</i>	temperature-dependent term (defined in record 8510XX)
<i>C_T</i>	correction to the temperature-dependent term (defined in record 8511XX)
<i>K_v</i>	velocity-dependent term (defined in record 8520XX)
<i>K_p</i>	temperature-dependent term (defined in record 8530XX)
<i>M(B, ...)</i>	multiplier to account for the effect of burn-off

SPECTRA Code Manuals - Volume 2: User's Guide

W-1 (I) :	IGS1OX	Identifier of gas 1, G_{S1} . (1= H ₂ , 2=He, 3=H ₂ O, 4=N ₂ , 5=O ₂ , 6=CO ₂ , >6=user defined gas). <i>Acceptable range:</i> must be one of the gases in SPECTRA fluid property data base. <i>Default value:</i> none.
W-2 (I) :	IGS2OX	Identifier of gas 2, G_{S2} . (1= H ₂ , 2=He, 3=H ₂ O, 4=N ₂ , 5=O ₂ , 6=CO ₂ , >6=user defined gas). <i>Acceptable range:</i> must be one of the gases in SPECTRA fluid property data base. <i>Default value:</i> none.
W-3 (R) :	RRT1OX	Reaction ratio 1, n_1 - number of moles of gas 1 per one mole of oxidized material <i>Acceptable range:</i> $0.01 \leq RRT1OX \leq 100.0$. <i>Default value:</i> none.
W-4 (R) :	RRT2OX	Reaction ratio 2, n_2 - number of moles of gas 2 per one mole of oxidized material <i>Acceptable range:</i> $0.0 \leq RRT2OX \leq 100.0$. <i>Default value:</i> 0.0.
W-5 (R) :	XOX	Exponent in the reaction rate, x , ($x=2.0$ for parabolic reaction). <i>Acceptable range:</i> $0.1 \leq XOX \leq 10.0$. <i>Default value:</i> 2.0.
W-6 (R) :	QOXIOX	Reaction heat per unit mass of oxidized material, Q_{ox} , (J/kg). <i>Acceptable range:</i> $-10^{10} \leq QOXIOX \leq 10^{10}$. <i>Default value:</i> none.
W-7 (R) :	OEXPOX	Volumetric growth ratio, σ_{ox} . Ratio of the material oxide volume, $V(MtO_n)$, to the volume of the material only $V(Mt)$. In other words, this is a ratio of the thickness of a fully oxidized material to the original thickness of an un-oxidized material. <i>Acceptable range:</i> $10^{-10} \leq OEXPOX \leq 100.0$. <i>Default value:</i> none.
W-8 (R) :	RHMTOX	Density ρ_{Mt} , of the material being oxidized, Mt , (kg/m ³). <i>Acceptable range:</i> $10.0 \leq RHMTOX \leq 50,000.0$. <i>Default value:</i> none.
W-9 (R) :	WMMTOX	Molecular weight, M_{Mt} , of the material being oxidized, Mt , (kg/kmole). <i>Acceptable range:</i> $1.0 \leq WMMTOX \leq 1000.0$. <i>Default value:</i> none.

2.14.3 Records: 8510XX, Temperature-Dependent Reaction Rate

XX is the number of the user-defined oxidation model. The maximum number of user-defined oxidation models is 10. The oxidation models must be numbered consecutively, XX=01, 02, 03, ...

The temperature-dependent oxidation rate is assumed to have the following general form:

$$K_T(T) = \begin{cases} A_1 \exp[-B_1/T] & \text{for: } T < T_1 \\ A_2 \exp[-B_2/T] & \text{for: } T > T_2 \end{cases}$$

K_T	temperature-dependent reaction rate, ((kg/m ²) ^x /s),
A_1	coefficient determining the reaction rate at low temperatures, ((kg/m ²) ^x /s),
B_1	coefficient determining the reaction rate at low temperatures, (K),
T_1	maximum temperature limit to apply the low temperature kinetics, (K),
A_2	coefficient determining the reaction rate at high temperatures, ((kg/m ²) ^x /s),
B_2	coefficient determining the reaction rate at high temperatures, (K),
T_2	minimum temperature limit to apply the high temperature kinetics, (K),
T	current temperature, (K).

W-1 (R) :	A1OX	First coefficient in the low temperature kinetics equation, A_1 , ((kg/m ²) ^x /s). <i>Acceptable range:</i> $10^{-50} \leq A1OX \leq 10^{50}$. <i>Default value:</i> none.
W-2 (R) :	B1OX	Second coefficient in the low temperature kinetics equation, B_1 , (K). <i>Acceptable range:</i> $0.0 \leq B1OX \leq 10^{10}$. <i>Default value:</i> none.
W-3 (R) :	T1OX	Upper temperature limit to apply the low temperature kinetics equation, T_1 (K). <i>Acceptable range:</i> $273.0 \leq T1OX \leq 10,000$ <i>Default value:</i> 9999.0
W-4 (R) :	A2OX	First coefficient in the high temperature kinetics equation, A_2 , ((kg/m ²) ^x /s). <i>Acceptable range:</i> $0.0 \leq A2OX \leq 10^{50}$. <i>Default value:</i> 0.0
W-5 (R) :	B2OX	Second coefficient in the high temperature kinetics equation, B_2 , (K). <i>Acceptable range:</i> $0.0 \leq B2OX \leq 10^{10}$. <i>Default value:</i> 0.0
W-6 (R) :	T2OX	Lower temperature limit to apply the high temperature kinetics equation, T_2 (K). <i>Acceptable range:</i> $T1OX + 1.0 \leq T2OX \leq 10,000$ <i>Default value:</i> 10,000.0
W-7 (R) :	TMINOX	Minimum temperature for oxidation, T_{min} , (K). Oxidation rate is set to zero for $T < T_{min}$. A linear interpolation from zero to a full value is performed between T_{min} and $T_{min} + 10.0$ K.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $273.0 \leq \text{TMINOX} \leq 1000.0$.
Default value: 600.0.

W-8 (R) : TMAXOX Maximum temperature for oxidation, T_{\max} , (K). For temperatures higher than T_{\max} , the oxidation rate is calculated using $T=T_{\max}$.
Acceptable range: $2000.0 \leq \text{TMAXOX} \leq 10,000.0$.
Default value: 10,000.0.

Post-breakaway reaction

The following input defines additional reaction coefficients for a post-breakaway reaction. The breakaway reaction is observed in case of air oxidation of Zircaloy, for example in case of loss of water in Spent Fuel Pool. In absence of other factors, $C_T, K_v, K_p, M(B, \dots)$, the reaction rate is calculated from:

$$\frac{dm^y}{dt} = K_T(T)$$

$$K_T(T) = \begin{cases} A_3 \exp[-B_3/T] & \text{for: } T < T_3 \\ A_4 \exp[-B_4/T] & \text{for: } T > T_4 \end{cases}$$

W-9 (R) : YOX Exponent in the reaction rate, y , applied in the post-breakaway regime.
Acceptable range: $0.1 \leq \text{YOX} \leq 10.0$.
Default value: none

W-10 (R) : A3OX First coefficient in the low temperature post-breakaway kinetics equation, A_3 , ((kg/m²)^y/s).
Acceptable range: $0.0 \leq \text{A3OX} \leq 10^{50}$.
Default value: 0.0

W-11 (R) : B3OX Second coefficient in the low temperature post-breakaway kinetics equation, B_3 , (K).
Acceptable range: $0.0 \leq \text{B1OX} \leq 10^{10}$.
Default value: 0.0

W-12 (R) : T3OX Upper temperature limit to apply the low temperature kinetics equation, T_3 (K).
Acceptable range: $273.0 \leq \text{T3OX} \leq 10,000$
Default value: 9999.0

W-13 (R) : A4OX First coefficient in the high temperature post-breakaway kinetics equation, A_4 , ((kg/m²)^y/s).
Acceptable range: $0.0 \leq \text{A4OX} \leq 10^{50}$.
Default value: 0.0

SPECTRA Code Manuals - Volume 2: User's Guide

- W-14 (R) : B4OX Second coefficient in the high temperature post-breakaway kinetics equation, B_4 , (K).
Acceptable range: $0.0 \leq B4OX \leq 10^{10}$.
Default value: 0.0
- W-15 (R) : T4OX Lower temperature limit to apply the high temperature kinetics equation, T_4 (K).
Acceptable range: $T3OX + 1.0 \leq T4OX \leq 10,000$
Default value: 10,000.0

The point of breakaway is calculated in one of two ways, using a critical time to breakaway or a critical oxidation depth at breakaway, both temperature-dependent.

- Option 1: critical time to breakaway:
 A time to breakaway function is tabulated versus temperature, $\tau(T)$. For a transient conditions a cumulative damage approach is used:

$$CD = \int_0^t \frac{dt'}{\tau(T)}$$

Breakaway occurs when $CD = 1.0$. For $CD < 1.0$ pre-breakaway reaction coefficients are used. For $CD > 1.0 + BINTOX$ (default=0.5), post-breakaway reaction coefficients are used. For $1.0 < CD < 1.0 + BINTOX$, a linear interpolation is performed between the pre- and the post-breakaway reaction kinetics.

- Option 2: critical oxidation depth at breakaway:
 A critical oxidation depth at breakaway is tabulated versus temperature, $\delta_1(T)$. This is the upper limit of the pre-breakaway reaction. For $\delta < \delta_1(T)$ pre-breakaway reaction coefficients are used. For $\delta > \delta_1(T) \times (1.0 + BINTOX)$, post-breakaway reaction coefficients are used. For $\delta_1(T) < \delta < \delta_1(T) \times (1.0 + BINTOX)$, a linear interpolation is performed between the pre- and the post-breakaway reaction kinetics.

- W-16 (I) : I1OX Pointer to a Tabular Function defining time to breakaway function is tabulated versus temperature, $\tau(T)$ or the critical oxidation depth function, $\delta_1(T)$ (m).
 Data is interpreted as $\tau(T)$ if all tabulated points are within the range $0.0 \div 1.0$. An error message is issued if not all values of the table fulfill this condition.
 Data is interpreted as $\delta_1(T)$ if all tabulated points are within the range $100 \div 10^{20}$. An error message is issued if not all values of the table fulfill this condition.
Acceptable range: reference to a Tabular Function. If the catalyst model is present (ICATOX>0), then the Option 1, cumulative damage function, should be used.
Default value: none.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-17 (R) : BINTOX Interpolation zone for breakaway reaction. Interpolation between pre-breakaway and post-breakaway reaction is performed in the range:
 Option 1 (cumulative damage) $1.0 < CD < 1.0 + \text{BINTOX}$
 Option 2 (critical depth): $\delta_i(T) < \delta < \delta_i(T) \times (1.0 + \text{BINTOX})$
 Acceptable range: $0.1 \leq \text{BINTOX} \leq 10.0$
 Default value: 0.5
- W-18 (I) : ICATOX Indicator for catalyst needed for breakaway.
 =0: no catalyst is needed
 > 0: catalyst is needed for breakaway. The catalyst is a gas number ICATOX. The critical time to breakaway (cumulative damage) is calculated only if the concentration of the gas ICATOX exceeds the minimum limit of XCATOX.
- Acceptable range: 0 or a gas number
 Default value: 0
- W-19 (R) : XCATOX Minimum concentration of catalyst gas needed for breakaway (used if ICATOX>0). Breakaway will only be possible when the volume fraction of gas ICATOX exceeds the value of XCATOX.
 Acceptable range: $0.0 \leq \text{XCATOX} \leq 1.0$
 Default value: 0.0

2.14.4 Records: 8511XX, Corrector for Temperature-Dependent Reaction Rate

XX is the number of the user-defined oxidation model. The maximum number of user-defined oxidation models is 10. The oxidation models must be numbered consecutively, XX=01, 02, 03, ...

The corrector to the temperature-dependent oxidation rate is assumed to have the following general form:

$$C_T(T, p_i) = \frac{1}{1 + A_C \exp[B_C / T] \cdot p_1^{X_1} \cdot p_2^{X_2} \cdot p_3^{X_3}}$$

- C_T correction to the temperature-dependent reaction rate, (-),
- A_C first coefficient, (-),
- B_C second coefficient, (K),
- p_1 partial pressure of the gas G_{S1} (oxidizing gas), (Pa),
- p_2 partial pressure of the gas G_{S2} (first reaction product), (Pa),
- p_3 partial pressure of the gas G_{S3} (second reaction product), (Pa),
- X_1 exponent for the gas G_{S1}
- X_2 exponent for the gas G_{S2}
- X_3 exponent for the gas G_{S3}

- W-1 (R) : ACOX First coefficient, A_C , (-).
 Acceptable range: $0.0 \leq \text{AC3OX} \leq 10^{50}$
 Default value: 0.0
- W-2 (R) : BCOX Second coefficient, B_C , (K).
 Acceptable range: $-10.0 \leq \text{BCOX} \leq 10^{10}$

		<i>Default value:</i>	0.0
W-3 (R) :	X1OX	First exponent, X_1 , (-).	
		<i>Acceptable range:</i>	$-10.0 \leq X1OX \leq 10.0$
		<i>Default value:</i>	0.0
W-4 (R) :	X2OX	Second exponent, X_2 , (-).	
		<i>Acceptable range:</i>	$-10.0 \leq X2OX \leq 10.0$
		<i>Default value:</i>	0.0
W-5 (R) :	X3OX	Second exponent, X_3 , (-).	
		<i>Acceptable range:</i>	$-10.0 \leq X3OX \leq 10.0$
		<i>Default value:</i>	0.0

2.14.5 Records: 8520XX, Velocity-Dependent Reaction Rate

XX is the number of the user-defined oxidation model. The maximum number of user-defined oxidation models is 10. The oxidation models must be numbered consecutively, XX=01, 02, 03, ...

The velocity-dependent reaction rate is defined by:

$$K_v(v, T) = C \cdot v^D \cdot T^E$$

K_v	velocity-dependent term, ((kg/m ²) ^x /s),
v	gas velocity, (m/s)
T	temperature, (K)
C	coefficient determining the reaction rate, (kg ^x m ^{-2x-D} s ^{-1+D} K ^E)
D	first exponent, (-)
E	second exponent, (-)

W-1 (R) :	CKVOX	Coefficient, C , (kg ^x m ^{-2x-D} s ^{-1+D} K ^E). If the value is zero or not entered, then the velocity-dependent term is not used.	
		<i>Acceptable range:</i>	$0.0 \leq CKVOX \leq 10^{10}$.
		<i>Default value:</i>	none.
W-2 (R) :	DKVOX	First exponent in the velocity-dependent term, D , (-).	
		<i>Acceptable range:</i>	$0.0 \leq DKVOX \leq 10.0$.
		<i>Default value:</i>	none.
W-3 (R) :	EKVOX	Second exponent in the velocity-dependent term, E , (-).	
		<i>Acceptable range:</i>	$0.0 \leq EKVOX \leq 10.0$.
		<i>Default value:</i>	none.
W-4 (R) :	VMINOX	Minimum velocity, v_{min} , (m/s). For velocities lower than v_{min} the oxidation rate is calculated using $v=v_{min}$.	
		<i>Acceptable range:</i>	$0.001 \leq VMINOX \leq 999.0$
		<i>Default value:</i>	0.01.

SPECTRA Code Manuals - Volume 2: User's Guide

W-5 (R) : VMAXOX Maximum velocity, v_{\max} , (m/s). For velocities higher than v_{\max} the oxidation rate is calculated using $v=v_{\max}$.
Acceptable range: $V_{\text{MINOX}}+1.0 \leq V_{\text{MAXOX}} \leq 1000.0$.
Default value: 1000.0.

2.14.6 Records: 8530XX, Pressure-Dependent Reaction Rate

XX is the number of the user-defined oxidation model. The maximum number of user-defined oxidation models is 10. The oxidation models must be numbered consecutively, XX=01, 02, 03, ...

The pressure-dependent coefficient is defined by:

$$K_p(p) = \left(\frac{p}{p_{\text{ref}}} \right)^F$$

p partial pressure of the oxidizing gas (G_{S1} - see section 2.14.1), (Pa)
 p_{ref} reference pressure, (Pa)
 F exponent, (-)

W-1 (R) : FKPOX Exponent, F , (-). If the value is zero or not entered, then the pressure-dependent term is not used.
Acceptable range: $0.0 \leq \text{FKPOX} \leq 10.0$.
Default value: none.

W-2 (R) : PREFOX Reference pressure, p_{ref} , (Pa).
Acceptable range: $1.0 \leq \text{PREFOX} \leq 1.0 \times 10^7$.
Default value: 1.0

W-3 (R) : PMINOX Minimum pressure, p_{min} , (Pa). Oxidation rate is set to zero for $p < p_{\text{min}}$. A linear interpolation from zero to a full value is performed between p_{min} and $p_{\text{min}} \times 2.0$.
Acceptable range: $1.0 \leq \text{PMINOX} \leq 1.0 \times 10^3$.
Default value: 1.0.

W-4 (R) : PMAXOX Maximum pressure, p_{max} , (Pa). For pressures higher than p_{max} the oxidation rate is calculated using $p=p_{\text{max}}$.
Acceptable range: $1.0 \times 10^4 \leq \text{PMAXOX} \leq 1.0 \times 10^7$.
Default value: 1.0×10^7 .

2.14.7 Records: 8540XX, Burn-off Factor

XX is the number of the user-defined oxidation model. The maximum number of user-defined oxidation models is 10. The oxidation models must be numbered consecutively, XX=01, 02, 03, ...

W-1 (I) : IBOFOX Pointer to a Tabular or Control Function that defines the burn-off factor, $M(B, \dots)$.

001 ≤ IBOFOX ≤ 999: $M(B, \dots)$ will be defined by a Tabular Function with the reference number: IBOFOX. The argument to this TF is always the depth of oxidized material: $M(B, \dots) = TF(d_{ox})$.

001 ≤ -IBOFOX ≤ 999: $M(B, \dots)$ will be defined by a Control Function with the reference number: |IBOFOX|. The value obtained from Tabular or Control Function will be restricted to the limit given by BMINOX, BMAXOX, defined below.

IBOFOX = 1001: $M(B, \dots)$ will be calculated from the built-in correlation, defined below. The value obtained from the correlation will be restricted to the limit given by BMINOX, BMAXOX, defined below.

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

W-2 (R) : BMINOX Minimum value of $M(B, \dots)$.
Acceptable range: $10^{-10} \leq \text{BMINOX} \leq 2.0$
Default value: 10^{-2}

W-3 (R) : BMAXOX Maximum value of $M(B, \dots)$.
Acceptable range: $\text{BMINOX} \leq \text{BMAXOX} \leq 10^{10}$
Default value: 10^{+2}

Built-in correlation

The built-in correlation, developed within the ARCHER project, has the following form (see Volume 3, 3.11.9, Graphite Oxidation by Steam - Validation Calculations):

$$M(B, P) = f_B(B) \cdot [f_{P,\infty}(P) - f_{P,0}(P)] + f_{P,0}(P)$$

where:

$$f_B(B) = \begin{cases} 1 - \left(\frac{B}{B_\infty} - 1 \right)^2 & \text{if } B < B_\infty \\ 1 & \text{if } B > B_\infty \end{cases}$$

$$f_{P,0}(P) = A_0 \cdot \exp(B_0 P)$$

$$f_{P,\infty}(P) = A_1 \cdot \exp(B_1 P)$$

$B_\infty = 0.3 \times 10^{-3}$ m. The pressure range for the correlations is limited to $P < 55 \times 10^5$ Pa.

W-4 (R) : A0FPOX Coefficient A_0 in the built-in correlation for burn-off factor.
Acceptable range: $10^{-3} \leq \text{A0FPOX} \leq 10^3$
Default value: 0.35

W-5 (R) : B0FPOX Coefficient B_0 in the built-in correlation for burn-off factor.
Acceptable range: $-10^{-6} \leq \text{B0FPOX} \leq 10^{-6}$
Default value: -7.0×10^{-8}

W-6 (R) : A1FPOX Coefficient A_1 in the built-in correlation for burn-off factor.
Acceptable range: $10^{-3} \leq \text{A1FPOX} \leq 10^3$
Default value: 1.7

SPECTRA Code Manuals - Volume 2: User's Guide

- W-7 (R) : B1FPOX Coefficient B_1 in the built-in correlation for burn-off factor.
Acceptable range: $-10^{-6} \leq \text{B1FPOX} \leq 10^{-6}$
Default value: -1.8×10^{-7}
- W-8 (R) : BINFOX Coefficient B_∞ in the built-in correlation for burn-off factor.
Acceptable range: $10^{-6} \leq \text{BINFOX} \leq 10^{-2}$
Default value: 0.3×10^{-3}
- W-9 (R) : PMNBOX Minimum pressure to be applied in the correlation for $f_{P,0}$ and $f_{P,\infty}$.
Acceptable range: $0.0 \leq \text{PMNBOX} \leq 10^{10}$
Default value: 0.0 Pa
- W-10 (R) : PMXBOX Maximum pressure to be applied in the correlation for $f_{P,0}$ and $f_{P,\infty}$.
Acceptable range: $0.0 \leq \text{PMXBOX} \leq 10^{10}$
Default value: 5.5×10^6 Pa

2.14.8 Records: 855000, Options for Insufficient Oxidant

In case there is not enough oxidant available for the reaction, the oxidation reaction rate is decreased. This decrease is referred to here as the oxidant starvation limit. The parameters determining how the reaction rate decreases with decreasing oxidant fraction are defined in this record.

- W-1 (R) : C1OX Critical concentration, c_1 . If the concentration (volume fraction) of the oxidizing gas is above this limit, there is no restriction for oxidation rate and the reaction proceeds according to the defined reaction kinetics. If the concentration is below c_1 , the reaction rate is interpolated to reach zero at the concentration value of c_0 . The value of c_0 is constant and set to $c_0 = 0.1 \times c_1$. Figure 2-66 illustrates the interpolation and the values of c_0 and c_1 .
Acceptable range: $10^{-6} \leq \text{C1OX} \leq 10^{-2}$
Default value: 10^{-4}
- W-2 (I) : INTPOX Type of interpolation.
= 1: linear interpolation: $x_1 = (c - c_0) / (c_1 - c_0)$
= 2: third order interpolation: $x_2 = (3 - 2x_1) x_1^2$
= 3: sixth order interpolation: $x_3 = x_2^2 = ((3 - 2x_1) x_1^2)^2$
The three interpolation types are shown in Figure 2-66. The interpolation is important in case of very intensive oxidation, when the oxidizing gas is consumed as soon as it enters the Control Volume. This may lead to numerical instabilities and time step reductions. Test calculations showed that the best results are obtained with sixth order interpolation. Therefore this option is set as default.
Acceptable range: 1, 2, 3
Default value: 3

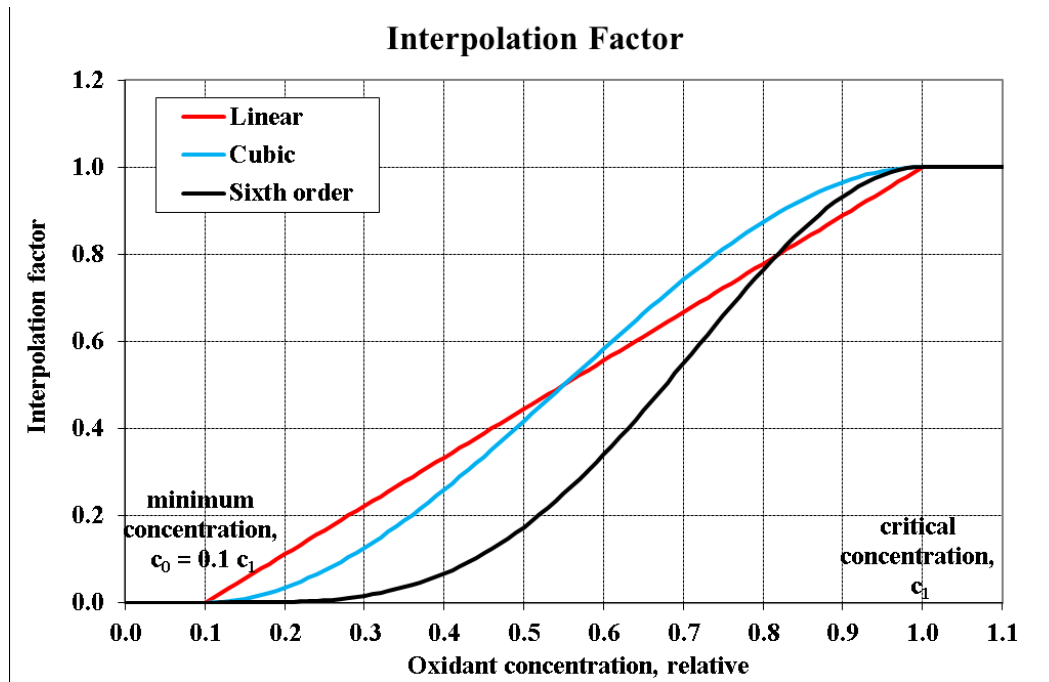


Figure 2-66 Interpolation performed in case of oxidant starvation

2.14.9 Built-in Oxidation Models

Data for three steam oxidation reactions is built into the code, as the reactions number -01, -02, and -03. These are:

- -01 Zr oxidation by steam, Cathcart + Urbanic-Heidrich model.
- -02 Zr oxidation by steam, Urbanic-Heidrich model.
- -03 Steel oxidation by steam, White model.

The data for these reactions is shown in Table 2-38.

Data for two O₂ oxidation reactions is built into the code, as the reactions number -04 and -05. These are:

- -04 Zr oxidation by O₂, Benjamin et al. model.
- -05 Graphite oxidation by O₂, Roes model.

The data for these reactions is shown in Table 2-39.

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-38 Built-in oxidation reaction data for steam oxidation.

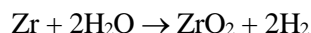
Coefficient	Reaction		
	Zr+2H ₂ O→ZrO ₂ +2H ₂ , Cathcart (low T), Urbanic-Hedrich (high T)	Zr+2H ₂ O→ZrO ₂ +2H ₂ , Urbanic-Hedrich	Fe+H ₂ O→FeO+H ₂ , 2Cr+3H ₂ O→Cr ₂ O ₃ +3H ₂ , White
<i>n</i> ₁	2.0	2.0	1.1
<i>n</i> ₂	2.0	2.0	1.1
<i>x</i>	2.0	2.0	2.0
<i>Q</i> _{ox}	6.45×10 ⁶	6.45×10 ⁶	0.477×10 ⁶
<i>σ</i> _{ox}	1.5	1.5	3.92
<i>ρ</i> _{ox}	<i>ρ</i> (Zr) = 6490.0	<i>ρ</i> (Zr) = 6490.0	<i>ρ</i> (Fe) = 8020.0
<i>M</i> _{ox}	<i>M</i> (Zr) = 91.22	<i>M</i> (Zr) = 91.22	<i>M</i> (St) = 51.70
<i>A</i> ₁	2×16.8×(<i>M</i> _{Zr} / <i>M</i> _{O₂}) ² = 273.0	29.6	2.51×10 ⁹
<i>B</i> ₁	20,060.0	16,820.0	42,428.0
<i>T</i> ₁	1783.0	1783.0	full temperature range
<i>A</i> ₂	2×5.41×(<i>M</i> _{Zr} / <i>M</i> _{O₂}) ² = 87.9	87.9	-
<i>B</i> ₂	16,610.0	16,610.0	
<i>T</i> ₂	1853.0	1853.0	
<i>C</i>	0.0	0.0	0.0
<i>D</i>	-	-	-
<i>E</i>	-	-	-
<i>F</i>	0.0	0.0	0.0
<i>p</i> _{pref}	-	-	-
<i>T</i> _{min} / <i>T</i> _{max}	600.0 / 10,000.0	600.0 / 10,000.0	600.0 / 10,000.0

Table 2-39 Built-in oxidation reaction data for oxidation by O₂.

Coefficient	Reaction	
	Zr+O ₂ →ZrO ₂ , Benjamin et al.	C+O ₂ →CO ₂ , Roes
<i>n</i> ₁	1.0	1.0
<i>n</i> ₂	0.0	1.0
<i>x</i>	2.0	1.0
<i>Q</i> _{ox}	12.1×10 ⁶	32.8×10 ⁶
<i>σ</i> _{ox}	1.5	0.01
<i>ρ</i> _{ox}	<i>ρ</i> (Zr) = 6490.0	<i>ρ</i> (C) = 2250.0
<i>M</i> _{ox}	<i>M</i> (Zr) = 91.22	<i>M</i> (C) = 12.01
<i>A</i> ₁	50.4	7.5×10 ³
<i>B</i> ₁	14,630.0	16,140.0
<i>T</i> ₁	full temperature range	full temperature range
<i>A</i> ₂	-	-
<i>B</i> ₂		
<i>T</i> ₂		
<i>C</i>	0.0	8.03×10 ⁻⁴
<i>D</i>	-	0.65
<i>E</i>	-	0.34
<i>F</i>	0.0	1.0
<i>p</i> _{pref}	-	1.0×10 ⁵
<i>T</i> _{min} / <i>T</i> _{max}	600.0 / 10,000.0	600.0 / 10,000.0
<i>v</i> _{min} / <i>v</i> _{max}	-	0.01 / 1000.0
<i>p</i> _{min} / <i>p</i> _{max}	-	1.0×10 ¹ / 1.0×10 ⁷

2.14.10 Examples of the User-Defined Oxidation Models

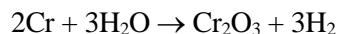
The inputs shown below define four oxidation models. The first model is exactly the same as the built-in Cathcart model for the steam-Zr oxidation, i.e. the reaction:



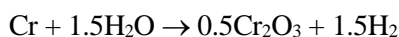
```

*
005001 Steam-Zr Reaction, Cathcart Model
*      Gs1 Gs2  n1   n2   x   Q       V   RHO   MW
850001  3   1  2.0  2.0   2.0 6.45E6  1.5  6490.0  91.22
*
*      T coefficients:
*      A1   B1     T1     A2   B2     T2   T-min  T-max
851001 273.0 20060.0 1783.0  87.9 16610.0 1853.0  600.0 10000.0
*
    
```

The second model defines chromium oxidation by steam:



or:



using only one (lower) set of coefficients. The reaction kinetics coefficients and the reaction heat are taken from reference [35].

```

*
005002 Steam-Cr Reaction
*      Gs1 Gs2  n1   n2   x   Q       V   RHO   MW
850002  3   1  1.5  1.5   2.0 2.442E6  1.5  2000.0  26.98
*
*      T coefficients:
*      A1   B1     T1     A2   B2     T2   T-min  T-max
851002 2.42E9 42400.0 9998.0   1.0   1.0  9999.0  600.0 10000.0
*
    
```

The third model defines steel oxidation by O₂. It is assumed that only Fe is oxidized, therefore the reaction considered is:



The reaction kinetics is based on data from Nanni et al. [37]. The data is correlated by:

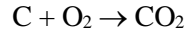
$$\frac{dm^2}{dt} = K_T(T) = 2.34 \times 10^{10} \exp[-45,350.0/T]$$

The reaction heat, 4.9×10^6 (W/kg), is obtained from [39]. Other parameters are assumed to be the same as for steam oxidation. Listing of the oxidation model is shown below (listing of a full input deck for a test case involving this oxidation reaction is shown in Volume 3).

```

*
005003 Steel-Oxygen reaction, Nanni et al. data
*      Gs1 Gs2  n1   n2   x   Q       V   RHO   MW
850003  5   1  0.5  0.0   2.0 4.9E6   3.92 8020.0  51.7
*
*      T coefficients:
*      A1   B1     T1     A2   B2     T2   T-min  T-max
851003 2.34E10 45350.0 9998.0   1.0   1.0  9999.0  600.0 10000.0
*
    
```


The fourth model is exactly the same as the built-in model for the graphite oxidation by O₂, i.e.:

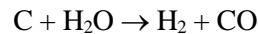


```

*
005004 Graphite-Oxygen reaction, Roes Model
*      Gs1 Gs2 n1  n2   x   Q       V   RHO   MW
850004 5    6  1.0  1.0   1.0 32.8E6 0.01 2250.0 12.01
*
*      T coefficients:
*      A1    B1      T1      A2    B2      T2    T-min  T-max
851004 7.5E3 16140.0 9998.0   1.0   1.0   9999.0 600.0 10000.0
*
*      v coefficients:
*      C      D      E      v-min  v-max
852004 8.03E-4 0.65  0.34  0.01   1000.0
*
*      p-coefficients
*      F      p-ref  p-min  p-max
853004 1.0    1.0E5  1.0   1.0E+7
*

```

The fifth model defines graphite oxidation by steam. The reaction is:



The reaction kinetics is defined following by Kubaschewski-Heinrich [38]:

$$\frac{dm}{dt} = \frac{6.4 \cdot 10^{11} \cdot \exp\left[-\frac{256,000}{8.315 \cdot T}\right] \cdot P_{H_2O}^{0.44}}{1 + 7.5 \cdot 10^{-5} \cdot \exp\left[\frac{121,000}{8.315 \cdot T}\right] \cdot P_{H_2}^{0.9} \cdot P_{H_2O}^{-0.4}}$$

Here pressure is in (bar), and reaction rate in (mg/cm²-hr). First, the formula is converted to SI units:

$$\frac{dm}{dt} = \frac{1.78 \cdot 10^6 \cdot \exp\left[-\frac{256,000}{8.315 \cdot T}\right] \cdot \left(\frac{P_{H_2O}}{10^5}\right)^{0.44}}{1 + 7.5 \cdot 10^{-5} \cdot \exp\left[\frac{121,000}{8.315 \cdot T}\right] \cdot \left(\frac{P_{H_2}}{10^5}\right)^{0.9} \cdot \left(\frac{P_{H_2O}}{10^5}\right)^{-0.4}}$$

Here pressure is in (Pa), reaction rate in (kg/m²-s) and temperature in (K). Furthermore, the formula is rearranged as follows:

$$\frac{dm}{dt} = \frac{1.12 \cdot 10^4 \cdot \exp\left[-\frac{30788}{T}\right] \cdot (P_{H_2O})^{0.44}}{1 + 2.37 \cdot 10^{-7} \cdot \exp\left[\frac{14552}{T}\right] \cdot (P_{H_2})^{0.9} \cdot (P_{H_2O})^{-0.4}}$$

SPECTRA Code Manuals - Volume 2: User's Guide

The reaction rate is defined using the temperature-dependent factor $K_T(T)$, the correction to the temperature-dependent factor $C_T(T, p_i)$, and the pressure-dependent factor, $K_p(p_i)$:

$$\frac{dm}{dt} = K_T(T) \cdot C_T(T, p_i) \cdot K_p(p_{H_2O})$$

- Temperature-dependent factor, $K_T(T)$:

$$K_T = 1.12 \cdot 10^4 \cdot \exp\left[-\frac{30788}{T}\right]$$

- Correction to temperature-dependent factor, $C_T(T, p_i)$:

$$C_T = \frac{1}{1 + 2.37 \cdot 10^{-7} \cdot \exp\left[\frac{14552}{T}\right] \cdot (p_{H_2})^{0.9} \cdot (p_{H_2O})^{-0.4}}$$

- Pressure-dependent factor, $K_p(p_i)$

$$K_p = (p_{H_2O})^{0.44}$$

The reaction heat, $131.3 \text{ kJ/mol} = 131.3 \times 10^6 \text{ (J/kmol)} = 10.9 \times 10^6 \text{ (J/kgC)}$. Input defining this reaction is shown below.

```

*
005005 Graphite-steam reaction, Kubaschewski-Heinrich
*      Gs1 Gs2 n1  n2   x   Q       V   RHO   MW   XW   Gs3  n3
850005  3   1  1.0  1.0   1.0 10.9E6 0.01 2250.0 12.01  0   7   1.0
*
*      K-T coefficients:
*      A1      B1      T1      A2      B2      T2      T-min  T-max
851005 1.12E+4 30788.0 9998.0   1.0     1.0 9999.0  600.0 10000.0
*
*      C-T coefficients:
*      A3      B3      X1      X2      X3
851105 2.37E-7 14552.0 -0.4   0.9   0.0
*
*      K-p coefficients
*      F      p-ref  p-min  p-max
853005  0.44  0.0     1.0   1.0E+7

```

SPECTRA Code Manuals - Volume 2: User's Guide

The sixth model defines graphite oxidation by steam using the correlation of Kubaschewski-Heinrich and the best estimate multiplier $M_{BE}(B,P)$, described in detail in Volume 3. The correlation of Kubaschewski-Heinrich is already shown above. Here the multiplier is shown. The simplest way to activate the best estimate multiplier is to use default values of Words 4 through 10 on record 8540XX. Below an alternative way is shown, where the multiplier is defined as a general 2-D Tabular Function. The applied function will give the same results as setting IBOFOX=1001 in the record 8540XX. The tabulated data is shown below.

Best estimate multiplier $M_{BE}(B,P)$ (see Volume 3)

B [m]:	0.00E+00	6.00E-05	1.20E-04	1.80E-04	2.40E-04	3.00E-04	
B/B [∞] [-]:	0.00	0.20	0.40	0.60	0.80	1.00	
f(B/B [∞]) [-]:	0.00	0.36	0.64	0.84	0.96	1.00	
P [Pa]	1.00E+05	0.35	0.82	1.19	1.46	1.62	1.67
	5.00E+05	0.34	0.78	1.12	1.36	1.51	1.55
	1.00E+06	0.33	0.72	1.03	1.24	1.38	1.42
	1.50E+06	0.32	0.67	0.94	1.14	1.26	1.30
	2.00E+06	0.30	0.62	0.87	1.04	1.15	1.19
	2.50E+06	0.29	0.58	0.80	0.96	1.05	1.08
	3.00E+06	0.28	0.54	0.74	0.88	0.96	0.99
	3.50E+06	0.27	0.50	0.68	0.80	0.88	0.91
	4.00E+06	0.26	0.47	0.62	0.74	0.80	0.83
	4.50E+06	0.26	0.44	0.58	0.68	0.74	0.76
	5.00E+06	0.25	0.41	0.53	0.62	0.67	0.69
5.50E+06	0.24	0.38	0.49	0.57	0.62	0.63	

The input deck defining this 2-D table is:

```

705901 M(B,P) Best Estimate
* Group Number Fact. Const.
700901 1 5 1.0 0.0 * Type : General TF
* y1 y2 y3 y4 y5 y6
708901 0.0E+00 6.0E-5 1.2E-4 1.8E-4 2.4E-4 3.0E-4 * y-coordinate data points (B)
* Arguments
* Pointers: (1) (2) (3) (4) Fact. Const.
710901 1 102 13 1 1.0 0.0 * x-argument: CV-102, total pressure
710901 6 901 1 0 1.0 0.0 * uses TF-901 for y = y1 (B = 0.0E+0)
710901 6 902 1 0 1.0 0.0 * uses TF-902 for y = y2 (B = 6.0E-5)
710901 6 903 1 0 1.0 0.0 * uses TF-903 for y = y3 (B = 1.2E-4)
710901 6 904 1 0 1.0 0.0 * uses TF-904 for y = y4 (B = 1.8E-4)
710901 6 905 1 0 1.0 0.0 * uses TF-905 for y = y5 (B = 2.4E-4)
710901 6 906 1 0 1.0 0.0 * uses TF-906 for y = y6 (B = 3.0E-4)
710901 3 102 30 1 -1.0 0.001 * y-argument: SC-102, oxidized depth
*
*
605901 f(P) for B = 0.0
* P (Pa) f(P)
600901 1.00E+05 0.35
600901 5.00E+05 0.34
600901 1.00E+06 0.33
600901 1.50E+06 0.32
600901 2.00E+06 0.30
600901 2.50E+06 0.29
600901 3.00E+06 0.28
600901 3.50E+06 0.27
600901 4.00E+06 0.26
600901 4.50E+06 0.26
600901 5.00E+06 0.25
600901 5.50E+06 0.24
*
605902 f(P) for B = 6.0E-5)
* P (Pa) f(P)
600902 1.00E+05 0.82
600902 5.00E+05 0.78

```

SPECTRA Code Manuals - Volume 2: User's Guide

600902	1.00E+06	0.72
600902	1.50E+06	0.67
600902	2.00E+06	0.62
600902	2.50E+06	0.58
600902	3.00E+06	0.54
600902	3.50E+06	0.50
600902	4.00E+06	0.47
600902	4.50E+06	0.44
600902	5.00E+06	0.41
600902	5.50E+06	0.38
*		
605903	f(P) for	B = 1.2E-4
*	P (Pa)	f(P)
600903	1.00E+05	1.19
600903	5.00E+05	1.12
600903	1.00E+06	1.03
600903	1.50E+06	0.94
600903	2.00E+06	0.87
600903	2.50E+06	0.80
600903	3.00E+06	0.74
600903	3.50E+06	0.68
600903	4.00E+06	0.62
600903	4.50E+06	0.58
600903	5.00E+06	0.53
600903	5.50E+06	0.49
*		
605904	f(P) for	B = 1.8E-4
*	P (Pa)	f(P)
600904	1.00E+05	1.46
600904	5.00E+05	1.36
600904	1.00E+06	1.24
600904	1.50E+06	1.14
600904	2.00E+06	1.04
600904	2.50E+06	0.96
600904	3.00E+06	0.88
600904	3.50E+06	0.80
600904	4.00E+06	0.74
600904	4.50E+06	0.68
600904	5.00E+06	0.62
600904	5.50E+06	0.57
*		
605905	f(P) for	B = 2.4E-4
*	P (Pa)	f(P)
600905	1.00E+05	1.62
600905	5.00E+05	1.51
600905	1.00E+06	1.38
600905	1.50E+06	1.26
600905	2.00E+06	1.15
600905	2.50E+06	1.05
600905	3.00E+06	0.96
600905	3.50E+06	0.88
600905	4.00E+06	0.80
600905	4.50E+06	0.74
600905	5.00E+06	0.67
600905	5.50E+06	0.62
*		
605906	f(P) for	B = 3.0E-4
*	P (Pa)	f(P)
600906	1.00E+05	1.67
600906	5.00E+05	1.55
600906	1.00E+06	1.42
600906	1.50E+06	1.30
600906	2.00E+06	1.19
600906	2.50E+06	1.08
600906	3.00E+06	0.99
600906	3.50E+06	0.91
600906	4.00E+06	0.83
600906	4.50E+06	0.76
600906	5.00E+06	0.69
600906	5.50E+06	0.63
*		

2.15 Radioactive Particle Transport Data

2.15.1 Record: 860000, RT Package Global Activators, Main Aerosol Data

- W-1 (I) : MGACRT Global activator of the Radioactive Particle Transport (RT) Package.
=0: the RT calculations are by default inactive in all Control Volumes, Junctions, 1-D Solid Heat Conductors, and 2-D Solid Heat Conductors. Individual Control Volumes, Junctions and Heat Conductors can be included in the RT calculations, using the records 170XXX, 270XXX, 370XXX, 470XXX.
=1: the RT calculations are by default active in all Control Volumes, Junctions, 1-D Solid Heat Conductors, and 2-D Solid Heat Conductors. Individual Control Volumes, Junctions and Heat Conductors can be excluded from the RT calculations, using the records 170XXX, 270XXX, 370XXX, 470XXX.
=2: the RT calculations are by default active in all Control Volumes and Junctions.
=3: the RT calculations are by default active in all Control Volumes.
Acceptable range: 0, 1, 2, 3.
Default value: 0.
- W-2 (I) : IJNART Global activator of the Solid Heat Conductors (SC/TC) and JN associations (for details see records 371XXX, 471XXX).
=-1: The global activator is off. The associations may be specified individually for each SC and TC in the records 371XXX, 471XXX.
= 1: Each boundary surface of a SC and TC is associated with this junction connected to the boundary Control Volume, which has the largest flow area. These associations may be changed individually for each SC and TC in the records 371XXX, 471XXX.
= 2: Each boundary surface of a SC and TC is associated with this junction connected to the boundary Control Volume, which has the smallest flow area. These associations may be changed individually for each SC and TC in the records 371XXX, 471XXX.
= 11 or 12: Same as 1 and 2 above, but additionally the junction area reduction calculation is automatically activated for all junctions. The default width is equal to the square root of the junction flow area, and may be redefined using the records 371XXX, 471XXX.
Acceptable range: -1, 1, 2, 11, 12.
Default value: -1.
- W-3 (I) : IGRVRT Global selection of the gravity factors GRV1RT, GRV2RT.
=-1: the global activator is off. All gravity factors are equal to zero, unless specified otherwise in the records 372XXX, 472XXX. Setting IGRVRT to -1 is an easy way to globally deactivate the gravitational deposition on all surfaces.
=+1: Rectangular geometry: the default value of the gravity factors is: +1 for horizontal, up-facing surfaces, -1 for horizontal, down-facing surfaces, and 0.0 for vertical surfaces. Cylindrical and spherical geometry: one half of the theoretical value for the upper half of a

cylinder or sphere (see discussion of GRV1RT, GRV2RT in sections 2.15.14, 2.15.15). The values are:

horizontal cylinders: $1/\pi = 0.3183$.

spheres: $\pi/8 = 0.3927$.

=+2: Rectangular geometry: as above, i.e. +1 for horizontal, up-facing surfaces, -1 for horizontal, down-facing surfaces, and 0.0 for vertical surfaces. Cylindrical and spherical geometry: zero (therefore there is no gravitational deposition on these surfaces). The gravity factors are entered individually for each SC and TC in the records 372XXX, 472XXX.

Acceptable range: 1, 2.

Default value: 1.

- W-4 (R) : DENART Density of aerosol particles, ρ_p , (kg/m³).
Acceptable range: $0.01 \leq \text{DENART} \leq 22,600.0$ (density of iridium)
Default value: 1000.0.
- W-5 (R) : TCONRT Thermal conductivity of aerosol particles, k_p , (W/m/K).
Acceptable range: $0.01 \leq \text{TCONRT} \leq 500.0$.
Default value: 10.0.
- W-6 (R) : PORSRT Porosity of the deposited layer, ε_{dep} , (-). The thickness, t_{dep} , and the effective thermal conductivity of the deposited aerosol layer, k_{dep} are calculated as:
- $$t_{dep} = \frac{m_{dep}}{A\rho_{dep}(1 - \varepsilon_{dep})} \quad k_{dep} = k_p \cdot (1 - \varepsilon_{dep})$$
- where m_{dep} is the deposited mass (kg) and A is the deposition area (m²).
Acceptable range: $0.0 \leq \text{PORSRT} \leq 0.9$.
Default value: 0.5.
- W-7 (R) : FJNMRT Minimum area fraction for junctions blocked by the deposited aerosols (see records 370XXX, 470XXX), (-). The junction open fraction will never be smaller than this value:
- $$A_{jN}(t) \geq \text{FJNMRT} \cdot A_0$$
- where A_0 is the total flow area of the junction.
Acceptable range: $0.0 \leq \text{FJNMRT} \leq 1.0$.
Default value: 0.01.
- W-8 (I) : IRMGRT Global activator of a resuspension model on all surfaces of Solid Heat Conductors (SC/TC).
 = 0: The global activator is off. The resuspension models may be specified individually for each SC and TC in the records 377XXX, 477XXX.
 ≠ 0: The resuspension model number IRMGRT is activated globally for all SC/TC surfaces. The resuspension model may be changed individually for each SC and TC in the records 377XXX, 477XXX.
Acceptable range: 0 or a number of an existing resuspension model

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 0

W-9 (R) : VFMXRT Maximum volumetric fraction of aerosols in a Control Volume. Calculations are stopped and an error message is printed if the volume of aerosols divided by the total volume of a control volume exceeds this number.
Acceptable range: 0.001 ≤ VFMXRT ≤ 1.0
Default value: 0.1

W-10 (R) : DTMXRT Maximum deposited layer thickness, (m), on a Solid Heat Conductor surface. Calculations are stopped and an error message is printed if the deposited layer thickness exceeds this number.
Acceptable range: 10⁻³ ≤ DTMXRT ≤ 10³
Default value: 1.0

W-11 (R) : VMINRT Minimum velocity for transport of aerosol particles or fission product isotopes through a junction. If the calculated velocity is smaller than this value, it is set to zero. This prevents transport of extremely small quantities of particles or fission product isotopes, which could lead to numerical problems.
Acceptable range: 10⁻⁷ ≤ VMINRT ≤ 10⁻³
Default value: 10⁻⁵

W-12 (I) : ILBORT Option for Langmuir-Blodgett correlation (see Volume 1).
 = 1: Use the unmodified L-B correlation:

$$\eta = \eta_{\max} \cdot \frac{Stk^2}{(Stk + C_{LB})^2}$$

= 2: Use the modified L-B correlation:

$$\eta = \eta_{\max} \cdot \begin{cases} \frac{0.25}{C_{LB}} \cdot Stk & \text{for } Stk < C_{LB} \\ \frac{Stk^2}{(Stk + C_{LB})^2} & \text{for } Stk > C_{LB} \end{cases}$$

Acceptable range: 1 or 2

Default value: 2

2.15.2 Records: 170XXX, Control Volume Activators

XXX is the Control Volume reference number, 001 ≤ XXX ≤ 999.

W-1 (I) : MICVRT Individual activator of the RT Package in a Control Volume.
 <0: the RT package is inactive in the Control Volume XXX.
 >1: the RT package is active in the Control Volume XXX.
 =0: the RT package is inactive when the global activator MGACRT is equal to 0 (record 860000), or active when MGACRT=1, 2, 3.
Acceptable range: if two Control Volumes are connected by a junction, then the RT package must be either active or inactive in both Control Volumes.

Default value: 0.

2.15.3 Records: 270XXX, Junction Activators

XXX is the Junction reference number, $001 \leq XXX \leq 999$.

W-1 (I) : MIJNRT Individual activator of the RT Package in a Junction.
<0: the RT package is inactive in the Junction XXX.
>0: the RT package is active in the Junction XXX.
=0: the RT package is inactive when the global activator MGACRT is equal to 0 (record 860000), or active when MGACRT=1, 2.
Acceptable range: if the RT package is active in a Junction, then it must also be active in both Control Volumes it connects.
Default value: 0.

2.15.4 Records: 370XXX, 1-D Solid Heat Conductor Activators

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : MISCRT Individual activator of the RT Package in a 1-D Solid Heat Conductor.
<0: the RT package is inactive in the 1-D Solid Heat Conductor XXX.
>1: the RT package is active in the 1-D Solid Heat Conductor XXX.
=0: the RT package is inactive when the global activator MGACRT is equal to 0 (record 860000), or active when MGACRT=1.
Acceptable range: if any of the boundary surfaces of the heat conductor is transferring heat to a Control Volume with an active RT package, then a warning message is produced if the RT package is inactive in the heat conductor.
Default value: 0.

2.15.5 Records: 470XXX, 2-D Solid Heat Conductor Activators

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : MITCRT Individual activator of the RT Package in a 2-D Solid Heat Conductor.
<0: the RT package is inactive in the 2-D Solid Heat Conductor XXX.
>1: the RT package is active in the 2-D Solid Heat Conductor XXX.
=0: the RT package is inactive when the global activator MGACRT is equal to 0 (record 860000), or active when MGACRT=1.
Acceptable range: if any of the boundary cells of the heat conductor is transferring heat to a Control Volume with an active RT package, then a warning message is produced if the RT package is inactive in the heat conductor.
Default value: 0.

2.15.6 Records: 171000, Control Volume – Pool Related Data

Using this record one may specify the parameters described in record 171XXX for all Control Volumes in the model - see description of record 171XXX below.

2.15.7 Records: 171XXX, Control Volume – Pool Related Data

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$.

W-1 (R) : FRFCRT Friction factor for turbulent deposition calculation on the pool surface. If zero or no value is entered, then the turbulent deposition will not be calculated for the pool surface. If a positive value is entered, then the turbulent deposition will be calculated for the pool surface assuming the friction factor is equal to FRFCRT.
Acceptable range: $0.001 \leq \text{FRFCRT} \leq 1.0$.
Default value: 0.1.

W-2 (R) : CRAPRT Critical ratio for aerosol to pool mass, to start resuspending deposited aerosols. When a water pool is evaporated, the aerosols deposited in the pool will be resuspended. The model is set up in such a way that the resuspension is gradual, to avoid sudden resuspension of all mass when the pool becomes empty. The resuspension starts when the aerosol mass exceeds the pool mass multiplied by CRAPRT.
Acceptable range: $0.001 \leq \text{CRAPRT} \leq 0.1$.
Default value: 0.01.

W-3 (R) : VINPRT(1) vertical velocity (m/s) of a size 1 particle in stagnant pool, v_∞ . Positive velocity means the particles will flow up, towards the pool surface.
 $|\text{VINPRT}| \leq 100$: use constant velocity, equal to VINPRT
 VINPRT > 100: use the correlation:

$$v_\infty = \left(\frac{4/3 \cdot Dg(\rho_f - \rho_p)}{C_D \cdot \rho_f} \right)^{1/2}$$

g gravity constant, = 9.81 (m/s²)
 ρ_p particle density, (kg/m³)
 ρ_f fluid density, (kg/m³)
 D particle diameter, (m)
 C_D drag coefficient
 VINPRT<1000: drag coefficient: $C_{D,Re \rightarrow \infty} = \text{VINPRT} - 100$
 VINPRT>1000: constant drag coeff.: $C_D = \text{const.} = \text{VINPRT} - 1000$
 The velocity will be positive (upwards) if the particle density ($\rho_p = \text{DENART}$) is smaller than the fluid density ($\rho_f = \text{current pool density}$).
Acceptable range: $-100.0 \leq \text{VINPRT}(1) \leq +100.0$, or
 $+100.0 < \text{VINPRT}(1) \leq +200.0$ ($0.0 < C_{D,Re \rightarrow \infty} \leq 100.0$)
 $+1000.0 < \text{VINPRT}(1) \leq +1100.0$ ($0.0 < C_D \leq 100.0$)
Default value: = 0.0 for size section 1

= VINPRT(1) for size sections > 1

W-4 (R) : VINPRT(2) vertical velocity (m/s) of a size 2 particle in stagnant pool

(...) until VINPRT is defined for all size sections

NOTE!

- If the aerosol particle field is used to represent very light particles (for example gas bubbles), which can be transported to the pool surface (VINPRT>0) then the deposition mechanism should be disabled. This is done by setting IDEPRT(1) to -1, record 865002. Otherwise the light particles may be transported back to the liquid phase due to gravitational settling, turbulent impaction, etc.
- The option ISVBCV may be needed to prevent the transport to pool surface (in favor of transport to the volume above) when CV is full of liquid - Figure 2-3.
- If the correlation is used (VINPRT > 100), then the correlation for small particles may be activated using C_{small} (CSMLCV, record 161000). The correlation for small particles is:

$$v_{\infty} = \frac{1}{18} \cdot \frac{D_p^2 g (\rho_f - \rho_p)}{\eta_f} \cdot C_{small}$$

2.15.8 Records: 172000, Option for Pool-Gas Transport of Particles – Global

Using this record one may specify the parameter described in record 172XXX for all Control Volumes in the model - see description of record 172XXX below.

2.15.9 Records: 172XXX, Option for Pool-Gas Transport of Particles – Individual

XXX is the Control Volume reference number, 001 ≤ XXX ≤ 999.

- W-1 (I) : KPATRT Pool-gas transport of aerosol particles.
 =1 : transport occurs on the pool-atmosphere surface
 =2 : transport occurs on the bubble-pool surface.
 =3 : transport occurs on droplet-atmosphere surface.
 NOTE: with option 2, fission products are transported from one CV to another with bubble flow. With option 3, fission products are not transported with droplets from one CV to another. Therefore the droplet to and from CV is automatically disabled: IDFAJN is set to 1.
 Acceptable range: KPATRT = 1, 2, 3
 Default value: 1
- W-2 (R) : YPATRT Multiplier for the pool-gas transport of aerosol particles. The pool-gas transport calculated by the model described in record 171XXX, is multiplied by this value. This parameter is used for any transport defined by KPATRT. It may be used for example to model sticking fraction in case of pool-bubble transport.
 Acceptable range: 0.0 ≤ YPATRT ≤ 10.0
 Default value: 1.0 (a small number, <10⁻⁵⁰, sets the value to 0.0).

W-3 (I) : KSVBCV Indicator for aerosol transport from pool to atmosphere. The meaning is the same as in case of bubble transport: ISVBCV - see Figure 2-3.
Acceptable range: $0 \leq \text{KSVBRT} \leq 100$
Default value: ISVBCV

2.15.10 Records: 271000, Aerosol Transport Through Junctions

Using this record one may specify the parameters described in record 271XXX for all Junctions in the model - see description of record 271XXX below.

2.15.11 Records: 271XXX, Aerosol Transport Through Junctions

XXX is the Junction reference number, $001 \leq \text{XXX} \leq 999$. NOTE: if XXX = 000, then the parameters defined in this record are applied to all Junctions.

W-1 (R) : SLFART Slip factor, S_A , for aerosols size section 1 flow with the atmosphere.
 (1) The slip factor is defined as the ratio of the aerosol particle velocity to that of the carrier gas. The particle transport through a junction is calculated using the particle velocity, v_p , defined as:

$$v_p = S_A \cdot v_g - J_{JN} \cdot v_{d,grav}$$

where:

- S_A - slip factor, SLFART(1), (-)
- v_g - gas velocity, (m/s)
- $v_{d,grav}$ - deposition velocity due to gravitational settling, (m/s)
- J_{JN} - junction direction indicator (IVERJN, record 200XXX):
 = -1: if the positive flow direction is down
 = 0: if the junction flow is horizontal
 = +1: if the positive flow direction is up

If -1.0 is entered, then the slip factor is calculated using the diffusiophoretic theory, as:

$$S_A = \sqrt{\frac{M_1}{M_2}} = \sqrt{\frac{R_2}{R_1}}$$

where:

- M_1 - molecular weight of gas in the upstream CV, (kg/kmole)
- M_2 - molecular weight of gas in the downstream CV,
- R_1 - gas constant in the upstream CV, (J/kg/K)
- R_2 - gas constant in the downstream CV

Acceptable range: $0.0 \leq \text{SLFART}(1) \leq 10.0$, or $\text{SLFART}(1) \leq -1.0$.
 (a small number, $<10^{-50}$, sets the value to 0.0).

Default value: 1.0.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-2 (I) : SLFPRT Slip factor, S_A , for aerosols size section 1 flow with the pool.
 (1) The slip factor is defined as the ratio of the aerosol particle velocity to that of the carrier liquid. The particle transport through a junction is calculated using the particle velocity, v_p , defined as:

$$v_p = S_p \cdot v_l + J_{JN} \cdot v_\infty$$

where:

- S_p - slip factor, SLFPRT(1), (-)
 v_l - liquid velocity, (m/s)
 J_{JN} - junction direction indicator, described above
 v_∞ - vertical velocity (m/s) of a single particle in stagnant pool

Acceptable range: $0.0 \leq \text{SLFPRT}(1) \leq 10.0$.
 (a small number, $<10^{-50}$, sets the value to 0.0).

Default value: 1.0.

- W-3 (I) : VINFRT(1) vertical velocity (m/s) of a size 1 particle in stagnant pool, v_∞ . Positive velocity means the particles will flow vertically up.
 $|\text{VINFRT}| \leq 100$: use constant velocity, equal to VINFRT
 $\text{VINFRT} > 100$: use the correlation:

$$v_\infty = \left(\frac{4/3 \cdot Dg(\rho_f - \rho_p)}{C_D \cdot \rho_f} \right)^{1/2}$$

- g gravity constant, = 9.81 (m/s²)
 ρ_p particle density, (kg/m³)
 ρ_f fluid density, (kg/m³)
 D particle diameter, (m)
 C_D drag coefficient

VINFRT<1000: drag coefficient: $C_{D,Re \rightarrow \infty} = \text{VINFRT} - 100$
 VINFRT>1000: constant drag coeff.: $C_D = \text{const.} = \text{VINFRT} - 1000$
 The velocity will be positive (upwards) if the particle density ($\rho_p = \text{DENART}$) is smaller than the fluid density ($\rho_f = \text{current pool density}$).

Acceptable range: $-100.0 \leq \text{VINFRT}(1) \leq +100.0$, or
 $+100.0 < \text{VINFRT}(1) \leq +200.0$ ($0.0 < C_{D,Re \rightarrow \infty} \leq 100.0$)
 $+1000.0 < \text{VINFRT}(1) \leq +1100.0$ ($0.0 < C_D \leq 100.0$)

Default value: = 0.0 for size section 1
 = VINFRT(1) for size sections > 1

The three words described above are repeated for all size sections (defined in record 861000). Thus the number of entries in this record should be $3 \times N$, where N is the number of aerosol size sections.

Note that if the correlation is used ($\text{VINFRT} > 100$), then the correlation for small particles may be activated using C_{small} (CSMLCV, record 161000). The correlation for small particles is:

$$v_\infty = \frac{1}{18} \cdot \frac{D_p^2 g(\rho_f - \rho_p)}{\eta_f} \cdot C_{small}$$

2.15.12 Records: 371XXX, 1-D Solid Heat Conductors - Junctions Associations

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : IJN1RT Reference number of a junction associated with the SC left surface.
 (1) = 0: No association with junction. Turbulent deposition is calculated using the gas velocity at the SC left surface, multiplied by XVT1RT(1) (Word 3).
 > 0: Left surface of this SC is associated with the junction number IJN1RT(1). Turbulent deposition is calculated using either the junction velocity, or the gas velocity at the SC left surface, depending on the indicator IVTDRT (word 15 in the record 865000). The velocity is multiplied by XVT1RT(1) (Word 3).
 Acceptable range: the junction must be connected to the Control Volume that is a boundary volume for the left surface of the SC.
 Default value: The default value depends on the global activator IJNART (record 860000):
 if IJNART ≤ 0: 0
 if IJNART = 1 or 11: JN with the smallest flow area
 if IJNART = 2 or 12: JN with the largest flow area.

W-2 (R) : WJN1RT Representative width, W , of the junction defined by IJN1RT(1), above.
 (1) If -1.0 is entered then the deposition on the left surface of the SC will not affect the flow area of the junction IJN1RT(1). If a positive value is entered, then the deposition on the surface of the SC will reduce the junction flow area as (see Figure 2-67):

$$A(t) = A_0 - W D(t)$$

A_0 junction total flow area, (m²)
 W junction width, (m)
 $D(t)$ thickness of the deposited layer, (m)
 $A(t)$ current open area of the junction (m²)

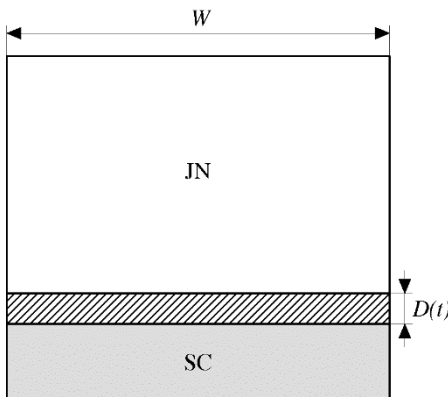


Figure 2-67 Junction area reduction in case of deposition on a 1-D conductor.

SPECTRA Code Manuals - Volume 2: User's Guide

Note that if the SC has a multiplicity not equal to 1.0 (for example, it represents multiple plates), then the deposit thickness, $D(t)$, will be multiplied by the SC multiplicity. Therefore the width entered here should represent in such case the width of a single plate. Several SC-s can be associated with a single junction. In this case the total area reduction of the junction will be given by:

$$A(t) = A_0 - \sum_{SC} W_{SC} D_{SC}(t)$$

The total reduction of the flow area is internally limited by the code, so the junction area will never be smaller than $FJNMRT \times A_0$, where $FJNMRT$ is the minimum area fraction, entered in the record 860000. If the user does not want to have junction area reduction, but at the same time wants to calculate the turbulent deposition, then the junction number should be specified using $IJN1RT(1)$, while the area reduction should be deactivated by setting $WJN1RT(1)$ to -1.0 .

Acceptable range: $0.01 \leq WJN1RT(1) \leq 10.0$, or $WJN1RT(1) \leq -1.0$.
Area reduction due to deposition cannot be calculated for a valve junction. The default value depends on the global activator $IJNART=0$ (record 860000):

Default value: if $IJNART < 10$: 0.0
if $IJNART > 10$: $A_0^{1/2}$ (A_0 is the junction total flow area).

- W-3 (I) : XVT1RT Gas velocity multiplier for turbulent deposition calculation on the left
 (1) surface (see description of $IJN1RT$ - word 1 above).
Acceptable range: $0.0 < XVT1RT \leq 1000.0$.
Default value: 1.0.
- W-4 (I) : IJN1RT Reference number of a junction associated with the SC right surface.
 (2) = 0: No association with junction. Turbulent deposition is calculated
 using the gas velocity at the SC right surface, multiplied by $XVT1RT(2)$
 (Word 6).
 > 0: Right surface of this SC is associated with the junction number
 $IJN1RT(2)$. Turbulent deposition is calculated using either the junction
 velocity, or the gas velocity at the SC right surface, depending on the
 indicator $IVTDRT$ (word 15 in the record 865000). The velocity is
 multiplied by $XVT1RT(2)$ (Word 6).
Acceptable range: the junction must be connected to CV that is a
 boundary volume for the right surface of the SC.
Default value: The default value depends on the global activator
 $IJNART$ (record 860000):
 if $IJNART \leq 0$: 0
 if $IJNART = 1$ or 11: JN with the smallest flow area
 if $IJNART = 2$ or 12: JN with the largest flow area.
- W-5 (R) : WJN1RT Representative width, W , of the junction defined by $IJN1RT(2)$, above.
 (2) Meaning, as described above, at $WJN1RT(1)$ description, but in relation
 to the right surface of the SC.
Acceptable range: $0.01 \leq WJN1RT(2) \leq 10.0$, or $WJN1RT(2) \leq -1.0$.

SPECTRA Code Manuals - Volume 2: User's Guide

Area reduction due to deposition cannot be calculated for a valve junction. The default value depends on the global activator IJNART=0 (record 860000):

Default value: if IJNART<10: 0.0
if IJNART>10: $A_0^{1/2}$ (A_0 is the junction flow area).

W-6 (I) : XVT1RT Gas velocity multiplier for turbulent deposition calculation on the
(2) right surface (see description of IJN1RT(2) - word 4 above).
Acceptable range: $0.0 < XVTDR(2) \leq 1000.0$.
Default value: 1.0.

2.15.13 Records: 471XXX, 2-D Solid Heat Conductors – Junctions Associations

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : I1 Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for association with junction. The junction association, defined by Word 3, will be applied for the boundary cells I, $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number.
Default value: none.

W-2 (I) : I2 Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for association with junction. The junction association, defined by Word 3, will be applied for the boundary cells I, $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number. $I2 \geq I1$.
Default value: none.

W-3 (I) : IJN2RT Reference number of a junction associated with the boundary cells, I:
(I) $I = I1$ through $I2$.
= 0: No association with junction. Turbulent deposition is calculated using the gas velocity at the cell I surface, multiplied by XVT2RT(I) (Word 4).
> 0: Cell I surface of this TC is associated with the junction number IJN2RT(I). Turbulent deposition is calculated using either the junction velocity, or the gas velocity at the cell I surface, depending on the indicator IVTDRT (word 15 in the record 865000). The velocity is multiplied by XVT2RT(2) (Word 4).
Acceptable range: the junction must be connected to CV that is a boundary volume for the right surface of the SC.
Default value: The default value depends on the global activator IJNART (record 860000):
if IJNART≤0: 0
if IJNART=1 or 11: JN with the smallest flow area
if IJNART=2 or 12: JN with the largest flow area.

W-4 (R) : WJN2RT Representative width, W, of the junction defined by IJN2RT(I), above.
(I) If zero or no value is entered then the deposition on cell I of the TC will not affect the flow area of the junction IJN2RT(I). If a positive value is

entered, then the deposition on cell IBC of the TC will reduce the junction flow area by: $W_k \times D_k(t)$. The total area reduction of the junction will be equal to the sum of reductions due to deposit on individual cell (see Figure 2-68):

$$A(t) = A_0 - \sum_k W_k D_k(t)$$

- A_0 junction total flow area, (m²)
- W_k width related to cell k , (m)
- $D_k(t)$ thickness of the deposited layer on the cell k , (m)
- $A(t)$ current open area of the junction, (m²)

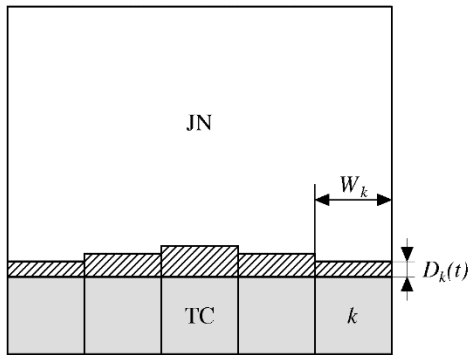


Figure 2-68 Junction area reduction in case of deposition on 2-D conductor.

Note that if the TC has a multiplicity not equal to 1.0 (for example, it represents multiple plates), then the deposit thickness, $D_k(t)$, will be multiplied by the TC multiplicity. Therefore the width entered here should represent in such case the width of a single plate. Several TC-s (and SC-s) can be associated with a single junction. In this case the total area reduction of the junction will be given by:

$$A(t) = A_0 - \sum_{SC} W_{SC} D_{SC}(t) - \sum_{TC} \sum_k W_{TC,k} D_{TC,k}$$

The total reduction of the flow area is internally limited by the code, so the junction area will never be smaller than $FJNMRT \times A_0$, where $FJNMRT$ is the minimum area fraction, entered in the record 860000. If the user does not want to have junction area reduction, but at the same time wants to calculate the turbulent deposition, then the junction number should be specified using $IJN2RT(I)$, while the area reduction should be deactivated by setting $WJN2RT(I)$ to -1.0 .

Acceptable range: $0.01 \leq WJN2RT(I) \leq 10.0$, or $WJN2RT(I) \leq -1.0$.
 Area reduction due to deposition cannot be calculated for a valve junction. The default value depends on the global activator $IJNART=0$ (record 860000):

Default value: if $IJNART < 10$: 0.0

if IJNART>10: $A_0^{1/2}$ (A_0 is the junction flow area).

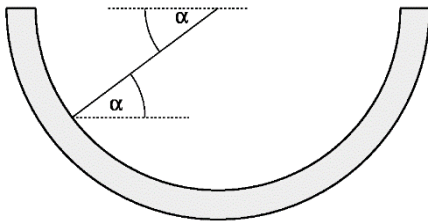
W-5 (I) : XVT2RT Gas velocity multiplier for turbulent deposition calculation on the
(I) boundary surface I (see description of IJN2RT(I) - word 1 above).
Acceptable range: $0.0 < XVT2RT(I) \leq 1000.0$.
Default value: 1.0.

The data set consisting of the five words described above is repeated until the junctions are defined for all desired boundary cells. The data may be entered in several records with the same number. The number of entries in a single record must be always a multiple of 5.

2.15.14 Records: 372XXX, 1-D Solid Heat Conductors Gravity Factors

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (R) : GRV1RT SC left surface orientation related to the gravity vector.
(1) =-1.0: horizontal surface, facing down
= 0.0: vertical surface
=+1.0: horizontal surface, facing up
Other values: $GRV1RT(1) = \sin(\alpha)$, where α is the angle between the normal to the surface and the horizontal direction.
The gravitational deposition velocity is multiplied by GRV1RT. In case of vertical surfaces the gravitational deposition does not contribute to the total deposition. In case of horizontal surfaces facing up the gravitational deposition has a positive effect (i.e. the gravitational deposition is added to the other velocities to obtain the total deposition velocity). In case of horizontal surfaces facing down the gravitational deposition has a negative effect (i.e. the gravitational deposition is subtracted from the other velocities to obtain the total deposition velocity).
For rectangular structures the default values are based on the SC vertical orientation parameter (IVERSC). For cylindrical and spherical structures the default values depend on the global activator IGRVRT (see record 860000). If the user models a horizontal pipe, then the best way is to divide it into two parts, the lower half and the upper half (each half can be modelled for example using cylindrical SC with a multiplicity factor of 0.5).
The gravity indicator should then be specified as, for example: +1.0 for the SC representing the lower half of the pipe and -1.0 for the SC representing the upper half of the pipe.
Strictly speaking, the gravity indicator on the surface of the half-pipe should be equal to the average $\sin(\alpha)$ of the surface angle. This is obtained as:



$$GRV1RT(1) = \frac{\int_0^{\pi/2} \sin(\alpha) r d\alpha}{\int_0^{\pi/2} r d\alpha} = \frac{1.0}{\pi/2} = 0.637$$

Therefore, for the SC representing the lower half of the pipe GRV1RT(1) will be equal to 0.637, while for the SC representing the upper half of the pipe GRV1RT(1) will be equal to -0.637. Similarly the average gravity factors can be calculated for the lower (and the upper) half of a sphere:

$$GRV1RT(1) = \frac{\int_0^{\pi/2} 2\pi r \sin^2(\alpha) d\alpha}{\int_0^{\pi/2} 2\pi r \sin(\alpha) d\alpha} = \frac{\pi/4}{1.0} = 0.785$$

Acceptable range: $-1.0 \leq GRV1RT(1) \leq +1.0$
 (a small number, $<10^{-50}$, sets the value to 0.0).

Default value: rectangular geometry (IGEOSC=1):
 equal to the natural convection indicator, INCLSC:
 - vertical (IVERSC=0): 0.0,
 - horizontal down (IVERSC=-1): -1.0,
 - horizontal up (IVERSC=+1): +1.0,
 cylindrical and spherical geometry: if the global selector, IGRVRT (section 2.15.1), is equal to 2, then GRV1RT is 0.0 (no gravitational deposition). If the global selector equal to 1, then GRV1RT is set to one half of the theoretical value for the upper half of the structure. This means $1/\pi = 0.3183$ for horizontal cylinders, and $\pi/8 = 0.3927$ for the spheres.
 If fins/spines are present, then the default value is 0.0 if IGRVRT=2 or the upwards area fraction if IGRVRT=1. The upwards area fraction is:
 $1.0/A_f$ for horizontal walls (vertical fins),
 $0.5 \times (1.0 - 1.0/A_f)$ for vertical walls (horizontal fins),
 $0.3183/A_f$ for horizontal cylinders (vertical fins).
 (A_f is the surface area increase ratio due to fins).

W-2 (R) : GRV1RT SC right surface orientation related to the gravity vector.
 (2) =-1.0: horizontal surface, facing down
 = 0.0: vertical surface.
 =+1.0: horizontal surface, facing up.
 Other values: GRV1RT(2) = $\sin(\alpha)$, where α is the angle between the normal to the surface and the horizontal direction.

For a SC representing lower half of a pipe GRV1RT(2) will be equal to -0.637, while for a SC representing upper half of the pipe GRV1RT(2) will be equal to 0.637.

Acceptable range: $-1.0 \leq \text{GRV1RT}(2) \leq +1.0$.

(a small number, $<10^{-50}$, sets the value to 0).

Default value: rectangular geometry (IGEOSC=1):

equal to the natural convection indicator, INCRSC:

- vertical (IVERSC=0): 0.0,

- horizontal down (IVERSC=-1): +1.0,

- horizontal up (IVERSC=+1): -1.0,

cylindrical and spherical geometry: if the global selector, IGRVRT (section 2.15.1), is equal to 2, then GRV1RT is 0.0 (no gravitational deposition). If the global selector is equal to 1, then GRV1RT is set to one half of the theoretical value for the upper half of the structure. This means $1/\pi = 0.3183$ for horizontal cylinders, and $\pi/8 = 0.3927$ for the spheres.

If fins/spines are present, then the default value is 0.0 if IGRVRT=2 or the upwards area fraction if IGRVRT=1. The upwards area fraction is:

$1.0/A_f$ for horizontal walls (vertical fins),

$0.5 \times (1.0 - 1.0/A_f)$ for vertical walls (horizontal fins),

$0.3183/A_f$ for horizontal cylinders (vertical fins).

(A_f is the surface area increase ratio due to fins).

2.15.15 Records: 472XXX, 2-D Solid Heat Conductors Gravity Factors

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$.

W-1 (I) : I1 Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for gravity vector definition. The gravity vector, defined by Word 3, will be applied for the boundary cells I, $I1 \leq I \leq I2$.

Acceptable range: must be an existing boundary cell number.

Default value: none.

W-2 (I) : I2 Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for gravity vector definition. The gravity vector, defined by Word 3, will be applied for the boundary cells I, $I1 \leq I \leq I2$.

Acceptable range: must be an existing boundary cell number. $I2 \geq I1$.

Default value: none.

W-3 (R) : GRV2RT TC, boundary cell I, surface orientation related to the gravity vector.

(I) = -1.0: horizontal surface, facing down

= 0.0: vertical surface

= +1.0: horizontal surface, facing up

Other values: $\text{GRV2RT}(I) = \sin(\alpha)$, where α is the angle between the normal to the surface and the horizontal direction.

Acceptable range: $-1.0 \leq \text{GRV2RT}(I) \leq +1.0$.

Default value: (a small number, $<10^{-50}$, sets the value to 0).
rectangular geometry (IGEOSC=1): equal to the natural convection indicator, INCBTC.
cylindrical geometry: if the global selector, IGRVRT (section 2.15.1), is equal to 2, then GRV2RT is 0.0 (no gravitational deposition). If the global selector is equal to 1, then for the horizontal cylindrical walls GRV2RT is set to one half of the theoretical value for the upper half of the cylinder: $1/\pi = 0.3183$.

The data set consisting of the three words described above is repeated until the gravity factors are defined for all desired boundary cells. The data may be entered in several records with the same number. The number of entries in a single record must be always a multiple of 3.

2.15.16 Records: 361XXX, Electric Field Strength at 1-D Solid Heat Conductors

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$.

W-1 (R) : EFS1RT(1) Electric field strength towards the left surface of the 1-D Solid Heat Conductor, (V/m). Used to calculate the electrophoretic deposition.
Acceptable range: $-1.0 \times 10^{10} \leq \text{EFS1RT}(1) \leq 1.0 \times 10^{10}$
Default value: 0.0

W-2 (R) : EFS1RT(2) Electric field strength towards the right surface of the 1-D Solid Heat Conductor, (V/m). Used to calculate the electrophoretic deposition.
Acceptable range: $-1.0 \times 10^{10} \leq \text{EFS1RT}(2) \leq 1.0 \times 10^{10}$
Default value: 0.0

2.15.17 Records: 461XXX, Electric Field Strength at 2-D Solid Heat Conductors

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$.

W-1 (I) : I1 Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for the electric field strength definition. The electric field strength, defined by Word 3, will be applied for the boundary cells I, $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number.
Default value: none.

W-2 (I) : I2 Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for the electric field strength definition. The electric field strength, defined by Word 3, will be applied for the boundary cells I, $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number. $I2 \geq I1$.
Default value: none.

W-3 (R) : EFS2RT(I) Electric field strength towards the boundary surfaces I, $I1 \leq I \leq I2$ of the 2-D Solid Heat Conductor, (V/m). Used to calculate the electrophoretic deposition.
Acceptable range: $-1.0 \times 10^{10} \leq \text{EFS2RT}(I) \leq 1.0 \times 10^{10}$
Default value: 0.0

The data set consisting of the three words described above is repeated until the electric force strengths are defined for all desired boundary cells. The data may be entered in several records with the same number. The number of entries in a single record must be always a multiple of 3.

2.15.18 Record: 861000, Aerosol Size Sections

W-1 (R) : DASCRT Representative equivalent diameter of the aerosol size section 1, (m).
 (1) *Acceptable range:* $1.0 \times 10^{-8} \leq \text{DASCRT}(1) \leq 1.0 \times 10^{-2}$.
 Default value: 1.0×10^{-6} .

W-2 (R) : DASCRT Representative equivalent diameter of the aerosol size section 2, (m).
 (2) *Acceptable range:* $\text{DASCRT}(i-1) < \text{DASCRT}(i) \leq 1.0 \times 10^{-2}$. The diameter ratio, $\text{DASCRT}(i)/\text{DASCRT}(i-1)$, must be at least equal to 0.5 times the previous ratio $\text{DASCRT}(i-1)/\text{DASCRT}(i-2)$, for $i \geq 3$.
 Default value: 3.0×10^{-6} .

. . . , until all diameters are entered. The number of aerosol size sections, NSIZRT, will be equal to the number of input entries in this record. The maximum number of the aerosol size sections is 20.

The default aerosol size sections include 5 sections, with the following representative diameters:

Sec. number	1	2	3	4	5
Diameter, (m)	1.0×10^{-6}	3.0×10^{-6}	1.0×10^{-5}	3.0×10^{-5}	1.0×10^{-4}

It is recommended that for each the size sections $i > 1$ the diameter is at least 1.25 times the diameter of the previous section:

$$\text{DASCRT}(i) \geq 1.25 \times \text{DASCRT}(i-1)$$

This condition approximately corresponds to:

$$V_i \geq 2V_{i-1}$$

(the exact value that leads to $V_i = 2 V_{i-1}$ is $D_i = 1.2599 D_{i-1}$). The default size sections are set in such way that the ratios of the section volumes are approximately 30: $V_i \sim 30 V_{i-1}$.

2.15.19 Record: 861001, Aerosol Surface Areas

The surface area of aerosol particles is used for sorption calculations if the sorption model is activated (records 898001 through 898004). For the sorption model to work properly the surface area of aerosol

SPECTRA Code Manuals - Volume 2: User's Guide

... , until the initial masses are specified for all size sections. Several records with the same number may be entered, each record containing data for different boundary cells.

2.15.25 Records: 175XXX, External Sources of Aerosols

XXX is the Control Volume reference number, $001 \leq XXX \leq 999$.

- W-1 (R) : ZSRCRT Elevation of the source above bottom of the CV, (m).
Acceptable range: $0.0 \leq \text{ZSRCRT} \leq \text{HEIGCV}$ (CV height).
Default value: 0.0.
- W-2 (I) : ISRCRT Indicator defining the aerosol source for the size section 1 in the CV.
 (1) If the number is positive, then the source will be defined by a Tabular Function with the reference number: ISRCRT(1). If the number is negative, then the source will be defined by a Control Function with the reference number: $|\text{ISRCRT}(1)|$. The units obtained from the Tabular or Control Function are assumed to be (kg/s).
Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.
Default value: 0.
- W-3 (I) : ISRCRT Indicator defining the aerosol source for the size section 2 in the CV.
 (2) If the number is positive, then the source will be defined by a Tabular Function with the reference number: ISRCRT(2). If the number is negative, then the source will be defined by a Control Function with the reference number: $|\text{ISRCRT}(2)|$. The units obtained from the Tabular or Control Function are assumed to be (kg/s).
Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.
Default value: 0.

... , until the sources are specified for all size sections.

2.15.26 Records: 375XXX, External Sources of Aerosols Deposited on 1-D Surfaces

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

- W-1 (R) : IBC Surface indicator.
 =1: left surface,
 =2: right surface
Acceptable range: 1 or 2
Default value: none
- W-2 (I) : ISC1RT(1) Indicator defining the aerosol source for the size section 1, deposited on the surface IBC of the 1-D Solid Heat Conductor XXX. If the number is positive, then the source will be defined by a Tabular Function with the reference number: ISC1RT. If the number is negative, then the source will be defined by a Control Function with the reference number:

SPECTRA Code Manuals - Volume 2: User's Guide

| ISC1RT | . The units obtained from the Tabular or Control Function are assumed to be (kg/s).

Acceptable range: must be a valid reference number of a Tabular or a Control Function, if non-zero.

Default value: 0.

- W-3 (I) : ISC1RT(2) Indicator defining the aerosol source for the size section 2, deposited on the surface IBC of the 1-D Solid Heat Conductor XXX. If the number is positive, then the source will be defined by a Tabular Function with the reference number: ISC1RT. If the number is negative, then the source will be defined by a Control Function with the reference number: | ISC1RT | . The units obtained from the Tabular or Control Function are assumed to be (kg/s).
- Acceptable range:* must be a valid reference number of a Tabular or a Control Function, if non-zero.
- Default value:* 0.

. . . , until the sources are specified for all size sections.

2.15.27 Records: 475XXX, External Sources of Aerosols Deposited on 2-D Surfaces

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

- W-1 (R) : IBC Boundary cell number.
- Acceptable range:* $1 \leq IBC \leq NBCLTC$
- Default value:* none
- W-2 (I) : ISC2RT(1) Indicator defining the aerosol source for the size section 2, deposited on the surface IBC of the 2-D Solid Heat Conductor XXX. If the number is positive, then the source will be defined by a Tabular Function with the reference number: ISC2RT. If the number is negative, then the source will be defined by a Control Function with the reference number: | ISC2RT | . The units obtained from the Tabular or Control Function are assumed to be (kg/s).
- Acceptable range:* must be a valid reference number of a Tabular or a Control Function, if non-zero.
- Default value:* 0.
- W-3 (I) : ISC2RT(2) Indicator defining the aerosol source for the size section 2, deposited on the surface IBC of the 2-D Solid Heat Conductor XXX. If the number is positive, then the source will be defined by a Tabular Function with the reference number: ISC2RT. If the number is negative, then the source will be defined by a Control Function with the reference number: | ISC2RT | . The units obtained from the Tabular or Control Function are assumed to be (kg/s).
- Acceptable range:* must be a valid reference number of a Tabular or a Control Function, if non-zero.
- Default value:* 0.

. . . , until the sources are specified for all size sections.

2.15.28 Records: 275XXX, Aerosol Filter Model

XXX is the Junction reference number, $001 \leq XXX \leq 999$. The default values of parameters are appropriate for a glass fibre filter (reference [34], table 9.1).

W-1 (I) : IFLTRT Filter type.
 =0: No filter.
 =1: Filter type 1 – user defined efficiency.
 =2: Filter type 2 – glass fibre filter.
 Acceptable range: 0, 1, 2.
 Default value: 0.

FILTER TYPE 1 DATA

W-2 (R) : JFLTRT(1) Reference number of a Tabular or a Control Function that defines filter efficiency for the aerosol size section 1, (-).
 Acceptable range: must be a valid reference number of a Tabular or Control Function, if nonzero
 Default value: 0.0.

W-3 (R) : JFLTRT(2) Reference number of a Tabular or a Control Function that defines filter efficiency for the aerosol size section 2, (-).
 Acceptable range: must be a valid reference number of a Tabular or Control Function, if nonzero
 Default value: 0.0.

. . . , until the efficiencies are specified for all size sections.

FILTER TYPE 2 DATA

W-2 (R) : ALPFRT Packing density or solidity of the filter, α , (-). The packing density is equal to one minus the porosity, ε , of the filter:

$$\alpha = 1 - \varepsilon$$

Acceptable range: $0.01 \leq ALPFRT \leq 0.99$.
 Default value: 0.10 [34].

W-3 (R) : THCFRT Thickness of the filter, t_f , (m).
 Acceptable range: $1.0 \times 10^{-5} \leq ALPFRT \leq 1.0 \times 10^{-2}$.
 Default value: 2.3×10^{-4} [34].

W-4 (R) : DPNFRT Pressure drop at the velocity of 0.27 m/s for a new filter, Δp , (Pa). If no value or zero is entered, then the pressure drop is calculated using the fiber diameter, d_f (m) (Word 5 below), from ([34], Chapter 9):

$$\Delta p = \frac{\eta t_f U_0 f(\alpha)}{d_f^2}$$

where:

- η - gas viscosity (equal to the air viscosity: 1.8×10^{-5} kg/m/s),
 - T - gas temperature (equal to 300 K),
 - U_0 - face velocity (equal to 2.7×10^{-1} m/s),
- and:

$$f(\alpha) = 64\alpha^{1.5} (1 + 56\alpha^3) \quad \text{for } 0.006 < \alpha < 0.3$$

Note! The forward and reverse loss coefficients, FLCFJN and FLCRJN, entered in the record 210XXX, are checked for consistency with the filter data. The minimum loss factor is calculated from:

$$K_{\min} = \frac{2\Delta p}{\rho v^2} = \frac{2\Delta p}{1.2 \cdot 0.27^2}$$

where 1.2 is the air density at normal conditions. If the value of the loss coefficient is smaller than K_{\min} , then a warning message is printed and the loss coefficient is re-set to the value of K_{\min} .

Acceptable range: $1.0 \times 10^2 \leq \text{DPNFRT} \leq 1.0 \times 10^5$, if non-zero.

Default value: 2.0×10^3 [34].

W-5 (R) : DSFFRT Diameter of a single fiber, d_f (m). If no value or zero is entered, then the fiber diameter is calculated using the pressure drop Δp , (Pa) (Word 4 above):

$$d_f = \sqrt{\frac{\eta t_f U_0 f(\alpha)}{\Delta p}}$$

Acceptable range: $1.0 \times 10^{-8} \leq \text{DFSFRT} \leq 1.0 \times 10^{-4}$, if non-zero.

Default value: 1.0×10^{-6} (the range 0.1 – 4 μm is given in [34]).

2.15.29 Records: 276XXX, Pool Scrubbing Model

XXX is the Junction reference number, $001 \leq \text{XXX} \leq 999$. When a stream of gas enters a pool region of the receiving Control Volume, then it forms bubbles in the pool. The gas is assumed to quickly reach equilibrium at the entrance to the pool (the equilibrium conditions are calculated by the Bubble Collapse Model). At the end of the bubble collapse the mass flow of gas entering the pool, W_B , is divided into the mass flow of gas, W_G , and condensed liquid, W_L . The flow W_G forms bubbles in the pool, while W_L remains in the pool. The aerosols entering the pool with the stream of gas are divided as follows:

- The part W_L/W_B remains in the pool.
- The part W_G/W_B is transported partly to the atmosphere and partly remains in the pool, depending on the pool scrubbing efficiency.

Therefore the division of aerosol particles is:

SPECTRA Code Manuals - Volume 2: User's Guide

- Fraction remaining in the pool: $\frac{W_G}{W_B} E_{PS} + \frac{W_L}{W_B}$
- Fraction reaching the atmosphere: $\frac{W_G}{W_B} (1 - E_{PS})$

In the above formulae E_{PS} is the pool scrubbing efficiency, defined in this record.

W-1 (I) : IPLSRT Pool scrubbing model.
 =1: Model 1 – user defined scrubbing efficiency.
 =2: Model 2 - theoretical model.
 Acceptable range: 1, 2.
 Default value: 1.

MODEL 1 DATA

W-2 (R) : JPLSRT(1) Reference number of a Tabular or a Control Function that defines pool scrubbing efficiency, E_{PS} , for the aerosol size section 1, (-).
 Acceptable range: must be a valid reference number of a Tabular or Control Function, if nonzero
 Default value: 0.1.

W-3 (R) : JPLSRT(2) Reference number of a Tabular or a Control Function that defines pool scrubbing efficiency, E_{PS} , for the aerosol size section 2, (-).
 Acceptable range: must be a valid reference number of a Tabular or Control Function, if nonzero
 Default value: 0.1.

... , until the efficiencies are specified for all size sections.

MODEL 2 DATA

A correlation is available in to calculate the pool scrubbing efficiency. The correlation is:

$$E_{PS} = A \cdot (1 - \exp[-B \cdot D_p])$$

W-2 (R) : APLSRT Coefficient A in the pool scrubbing correlation, (-). Default value provides a conservative (too low) estimation for the pool scrubbing efficiency. The best-estimate value is close to 1.0 (see Volume 1)
 Acceptable range: $0.0 \leq \text{APLSRT} \leq 1.0$
 Default value: 0.5.

W-3 (R) : BPLSRT Coefficient B in the pool scrubbing correlation, (-).
 Acceptable range: $0.0 \leq \text{BPLSRT} \leq 1.0 \times 10^{10}$
 Default value: 0.5×10^6

2.15.30 Record: 376XXX, Inertial Impaction Model for 1-D Solid Heat Conductors

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$.

- W-1 (I) : MII1RT(1) Inertial impaction model on the left surface of the 1-D Solid Heat Conductor number XXX.
 = 0: no model
 < 0: collection efficiency is defined by a Control Function [MII1RT]. The values obtained from the Control Function are limited to the range between 0.0 and 1.0.
 0 < MII1RT < 1000: collection efficiency is calculated from a general correlation as a function of Stokes number, *Stk*:

$$\eta = f(Stk)$$

The function *f* is defined using a Tabular Function number MII1RT. The independent variable for the function is the Stokes number.
 = 1001: collection efficiency is calculated from the Ciemat correlation [41], appropriate for tube bundle:

$$\eta = \frac{\eta_{\max}}{1 + c_1 \cdot \exp(-c_2 \cdot Stk^{c_3})}$$

Here η_{\max} , c_1 , c_2 , c_3 are user defined coefficients with the default values of 0.75, 29.31, 3.85, and 0.5 respectively. The values are defined in the record 865000. *Stk* is the Stokes number, defined as:

$$Stk = \frac{C_m \cdot \rho_p \cdot d_p^2 \cdot v_g}{18 \cdot \mu_g \cdot D_i}$$

- C_m Cunningham correction factor, (-)
- ρ_p particle density, (kg/m³)
- d_p particle diameter, (m)
- v_g gas velocity at the vicinity of the impactor, (m/s)
- μ_g gas viscosity, (kg/m/s)
- D_i impactor dimension, (m)

= 1002: collection efficiency is calculated from the correlation appropriate for a tube bend [42]:

$$\eta = \eta_{\max} \cdot (1 - 10^{-c_1 \cdot Stk})$$

Here η_{\max} , c_1 , are user defined coefficients with the default values of 1.0 and 0.963 respectively. The values are defined in the record 865000.

Acceptable range: 1001, 1002, or a valid reference to a TF or a CF.

Default value: 0

- W-2 (I) : JII1RT(1) Junction association for the inertial impaction on the left surface. This word determines whether the gas velocity is taken from the CV next to the SC surface or from a junction.

SPECTRA Code Manuals - Volume 2: User's Guide

= 0: no junction association, the gas velocity, v_{g0} (needed to compute the velocity v_g that is used to calculate the Stokes number), is equal to the gas velocity in the Control Volume next to the SC.

< 0: use junction association defined in the record 371XXX. The gas velocity, v_{g0} (needed to compute the velocity v_g that is used to calculate the Stokes number) is taken from the associated junction. If no association is specified in the records 371XXX, the local gas velocity at the SC surface is used.

> 0: reference number of the associated junction. The gas velocity, v_{g0} is taken from the associated junction.

Acceptable range: ≤ 0 or a valid reference to a JN

Default value: 0

W-3 (R) : FJI1RT(1) Jet energy dissipation factor, F_{jet} . Used to calculate the gas velocity at the impactor surface. The gas velocity is equal to:

$$v_g = v_{g0} \cdot F_{jet}$$

The jet dissipation factor may be used to account for the decrease of the gas velocity when the impactor is located in some distance from the source.

Acceptable range: $0.0 < \text{FJI1RT}(1) \leq 10.0$

Default value: 1.0

W-4 (R) : DII1RT(1) Impactor dimension, D_i , (m). The value of D_i is used to calculate the Stokes number, Stk .

Acceptable range: $\text{DII1RT}(1) > 0.0$

Default value: rectangular: square root of the surface area
other: diameter

W-5 (R) : FRI1RT(1) Fraction of the total inertial impaction deposition caused by the jet coming from the associated junction that is deposited on the left surface of the 1-D Solid Heat Conductor, $F_{R,i}$. This input entry allows the user to associate multiple surfaces with the same junction and distribute the total impaction among them. The sum of fractions for a given junction must be not larger than 1.0.

Acceptable range: $0.0 < \text{FRI1RT}(1) \leq 1.0$

Default value: 1.0

W-6 (I) : MII1RT(2) Inertial impaction model on the right surface of the 1-D Solid Heat Conductor number XXX. See the description of MII1RT(1) above.

Acceptable range: 1001, 1002, or a valid reference to a TF or a CF.

Default value: 0

W-7 (I) : JII1RT(2) Junction association for the inertial impaction on the right surface. See the description of JII1RT(1) above.

Acceptable range: ≤ 0 or a valid reference to a JN

Default value: 0

W-8 (R) : FII1RT(2) Jet energy dissipation factor, F_{jet} . See the description of FJI1RT(1) above.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 < FJI1RT(2) \leq 10.0$

Default value: 1.0

W-9 (R) : FRI1RT(2) Fraction of the total inertial impaction deposition caused by the jet coming from the associated junction that is deposited on the right surface of the 1-D Solid Heat Conductor, $F_{R,i}$. See the description of FRI1RT(1) above.

Acceptable range: $0.0 < FRI1RT(1) \leq 1.0$

Default value: 1.0

W-9 (R) : DII1RT(2) Impactor dimension, D_i , (m). See the description of DII1RT(1) above.

Acceptable range: $DII1RT(1) > 0.0$

Default value: rectangular: square root of the surface area
other: diameter

2.15.31 Record: 476XXX, Inertial Impaction Model for 2-D Solid Heat Conductors

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : I1 Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for the inertial impaction model. The inertial impaction data, defined by Words 3 through 7, will be applied for the boundary cells I, $I1 \leq I \leq I2$.

Acceptable range: must be an existing boundary cell number.

Default value: none.

W-2 (I) : I2 Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for the inertial impaction model. The inertial impaction data, defined by Words 3 through 6, will be applied for the boundary cells I, $I1 \leq I \leq I2$.

Acceptable range: must be an existing boundary cell number. $I2 \geq I1$.

Default value: none.

W-3 (I) : MII2RT(I) Inertial impaction model on the boundary surface I of the 2-D Solid Heat Conductor number XXX. See description of MII1RT(1) in the records 376XXX.

Acceptable range: 1001, 1002, or a valid reference to a TF or a CF.

Default value: 0

W-4 (I) : JII2RT(I) Junction association for the inertial impaction on the boundary surface I of the 2-D Solid Heat Conductor. See description of JII1RT(1) in the records 376XXX.

Acceptable range: ≤ 0 or a valid reference to a JN

Default value: 0

W-5 (R) : FJI2RT(I) Jet energy dissipation factor, F_{jet} . See the description of FJI1RT(1) in the records 376XXX.

Acceptable range: $0.0 < FJI2RT(I) \leq 10.0$

Default value: 1.0

- W-6 (R) : DII2RT(I) Impactor dimension, D_i , (m). See the description of DII1RT(1) in the records 376XXX.
 Acceptable range: DII2RT(I) > 0.0
 Default value: smaller of the cell dimensions
- W-7 (R) : FRI2RT(I) Fraction of the total inertial impaction deposition caused by the jet coming from the associated junction that is deposited on the boundary surface I of the 2-D Solid Heat Conductor, $F_{R,i}$. See the description of FRI1RT(1) in the records 376XXX.
 Acceptable range: 0.0 < FRI2RT(I) ≤ 1.0
 Default value: 1.0

2.15.32 Record: 862000, Agglomeration Shape Factors

- W-1 (R) : YSHFRT Agglomeration shape factor, γ , for aerosols section 1, (-).
 (1) *Acceptable range:* 1.0 ≤ YSHFRT(1) ≤ 100.0.
 Default value: 1.0.
- W-2 (R) : YSHFRT Agglomeration shape factor, γ , for aerosols section 2, (-).
 (2) *Acceptable range:* 1.0 ≤ YSHFRT(2) ≤ 100.0.
 Default value: 1.0.

... , until the agglomeration shape factors are specified for all size sections.

2.15.33 Record: 863000, Dynamic Shape Factors

- W-1 (R) : XSHFRT Dynamic shape factor, χ , for aerosols section 1, (-).
 (1) *Acceptable range:* 1.0 ≤ XSHFRT(1) ≤ 100.0.
 Default value: 1.0.
- W-2 (R) : XSHFRT Dynamic shape factor, χ , for aerosols section 2, (-).
 (2) *Acceptable range:* 1.0 ≤ XSHFRT(2) ≤ 100.0.
 Default value: 1.0.

... , until the dynamic shape factors are specified for all size sections.

2.15.34 Record: 864000, Cunningham Slip Correction Factor Model Data

This record defines the coefficients in the Cunningham slip correction factor correlation:

$$C_m = 1 + Kn \cdot [A_1 + A_2 \exp(-A_3 / Kn)]$$

where Kn is the Knudsen number.

- W-1 (R) : A1CMRT Coefficient A_1 in the Cunningham slip correction factor:

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq A1CMRT \leq 2.0$.
Default value: 1.257.

W-2 (R) : A2CMRT Coefficient A_2 in the Cunningham slip correction factor:
Acceptable range: $0.0 \leq A2CMRT \leq 1.0$.
Default value: 0.4.

W-3 (R) : A3CMRT Coefficient A_3 in the Cunningham slip correction factor:
Acceptable range: $0.0 \leq A3CMRT \leq 2.0$.
Default value: 1.1.

2.15.35 Record: 865000, Deposition Model Data

W-1 (I) : ITMSRT Thermophoresis model selection:
=1: use Brock correlation.
=2: use Ha and Ahmadi correlation.
=3: use Brock correlation for $Kn \leq 0.1$, Ha and Ahmadi for $Kn \geq 0.2$
(linear interpolation is performed for $0.1 < Kn < 0.2$).
=4: do not use the thermophoretic deposition model.
Acceptable range: 1, 2, 3, or 4
Default value: 3

W-2 (I) : IBLDRT Model selection for the diffusion boundary layer calculation:
=-1: use input value TBLDRT (Word 3 below)
=+1: use the model based on Sherwood number, Sh , correlation. Sh is related to δ_{BL} by:

$$\delta_{BL} = \frac{D_{hyd}}{Sh}$$

where:

D_{hyd} - characteristic dimension (assumed equal to the hydraulic diameter, i.e. the forced convection characteristic dimension, D_{FC} – see sections 2.3.11 word DFCLSC, section 2.3.12 word DFCRSC, and section 2.4.13 word DFCBTC).

The Sherwood number is calculated using the heat and mass transfer analogy ($Nu \rightarrow Sh, Pr \rightarrow Sc$), from the laminar and the turbulent flow correlations:

$$Sh = \begin{cases} C_{lam} & (laminar) \\ C_{tur} Re^a Sc^b & (turbulent) \end{cases}$$

where Re, Sc, Sh are Reynolds number, particle Schmidt number, and Sherwood number respectively. The constants, C_{lam}, C_{tur}, a, b , are defined by the words 9, 10, 11, 12, below.

The formula for δ_{BL} comes from an assumption that the deposition velocity equals the mass transfer coefficient, $v=K_m$, (m/s), calculated for the particle Schmidt number:

$$K_m = \frac{Sh \cdot D_C}{D_{hyd}}$$

where D_C is the diffusion coefficient (m²/s). Therefore:

$$v = K_m = \frac{Sh \cdot D_C}{D_{hyd}} = \frac{D_C}{(D_{hyd} / Sh)}$$

The deposition velocity is equal to $v = D_C / \delta_{BL}$ (see for example [31], page 8) and therefore $\delta_{BL} = D_{hyd} / Sh$. The Reynolds number is taken from the Junction data (with a limit in the RT package the same as in the JN package: $Re_{min} = 100.0$), while the Sc number is calculated from:

$$Sc = \frac{3\pi \mu_g^2 D_p \chi}{k_B \rho_g T C_m}$$

where:

- μ_g gas viscosity, (kg/m/s)
- D_p particle diameter, (m)
- χ dynamic shape factor, (-)
- k_B Boltzman constant (=1.38×10⁻²³ (J/K))
- ρ_g gas density, (kg/m³)
- T gas temperature, (K)
- C_m Cunningham correction factor, (-)

The boundary layer thickness, calculated as described above, is limited to by a minimum value of 1.0×10⁻⁷ m, and a maximum value of 1.0×10⁻³ m.

Acceptable range: IBLDRT = -1 or 1. The value of 1 (correlation) is in effect only for those surfaces which are associated with junctions (see records 371XXX, 471XXX). For surfaces not associated with junctions TBLDRT will be used.

Default value: -1.

W-3 (R) : TBLDRT Diffusion boundary layer thickness, (m). Used if IBLDRT=-1.
Acceptable range: 1.0×10⁻⁷ ≤ TBLDRT ≤ 1.0×10⁻³.
Default value: 1.0×10⁻⁵.

W-4 (I) : IBLTRT Model selection for the thermophoretic boundary layer calculation:
 =-1: use input value TBLTRT (Word 5 below)
 =+1: use the model:

$$\delta_{BL} = \frac{k}{h}$$

where k is the gas thermal conductivity, and h is the heat transfer coefficient. The formula comes from the assumption that the convected

SPECTRA Code Manuals - Volume 2: User's Guide

heat, q , is transported through the boundary layer of thickness δ_{BL} , through gas conduction:

$$q = \frac{k}{\delta_{BL}} (T - T_{wall})$$

where T is the gas temperature and T_{wall} is the wall surface temperature. The convective heat flux is of course equal to:

$$q = h(T - T_{wall})$$

Therefore the boundary layer thickness is given by $\delta_{BL} = k/h$. The heat transfer coefficient is taken from the SC/TC data, with an internal limit imposed by the RT package: $h_{min}=1.0$ W/m²/K.

Acceptable range: IBLTRT = -1 or 1.

Default value: 1.

- | | | |
|------------|--------|---|
| W-5 (R) : | TBLTRT | Thermophoretic boundary layer thickness, (m). Used if IBLTRT=-1.
<i>Acceptable range:</i> $1.0 \times 10^{-4} \leq TBLDRT \leq 1.0 \times 10^{-2}$.
<i>Default value:</i> 2.0×10^{-3} . |
| W-6 (R) : | FSLPRT | Slip correction factor, F_{slip} , used by the thermophoresis model, Brock correlation.
<i>Acceptable range:</i> $0.0 \leq FSLPRT \leq 2.0$.
<i>Default value:</i> equal to the coefficient A_1 in the Cunningham slip correction factor (A1CMRT in the record 864000) |
| W-7 (R) : | CTCORT | Thermal accommodation coefficient, C_t , used by the thermophoresis model, Brock correlation.
<i>Acceptable range:</i> $1.0 \leq CTCORT \leq 5.0$.
<i>Default value:</i> 2.5. |
| W-8 (R) : | CSCORT | Thermal exchange coefficient, C_s , used by the thermophoresis model, Brock correlation.
<i>Acceptable range:</i> $0.0 \leq CSCORT \leq 5.0$.
<i>Default value:</i> 1.17. |
| W-9 (R) : | CSLBRT | Constant C_{lam} in the Sherwood number correlation used to calculate diffusion boundary layer thickness (used when IBLDRT=1).
<i>Acceptable range:</i> $10^{-3} \leq CSLBRT \leq 10^3$.
<i>Default value:</i> 3.656 [14]. |
| W-10 (R) : | CSTBRT | Constant C_{tur} in the Sherwood number correlation used to calculate diffusion boundary layer thickness (used when IBLDRT=1).
<i>Acceptable range:</i> $10^{-3} \leq CSTBRT \leq 10^3$.
<i>Default value:</i> 0.023 [30]. |
| W-11 (R) : | ASTBRT | Constant a in the Sherwood number correlation used to calculate diffusion boundary layer thickness (used when IBLDRT=1).
<i>Acceptable range:</i> $0.1 \leq ASTBRT \leq 2.0$. |

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 0.8 [30].

W-12 (R) : BSTBRT Constant b in the Sherwood number correlation used to calculate diffusion boundary layer thickness (used when IBLDRT=1).
Acceptable range: $0.1 \leq \text{BSTBRT} \leq 2.0$.
Default value: 0.4 [30].

W-13 (I) : IDMSRT Diffusiophoresis model selection:
 =1: use differential molecular impact effect in both evaporation and condensation.
 =2: use differential molecular effect only in case of condensation (MELCOR model, see [35] RN Reference Manual, section 2.4.2.2).
 =3: do not use the diffusiophoretic deposition model.
Acceptable range: 1, 2, or 3.
Default value: 1.

W-14 (R) : ATDVRT Constant A in the correlation for the turbulent deposition velocity (see Volume 1):

$$v_{D,2}^+ = A \cdot (\tau_p^+)^2$$

Acceptable range: $0.0 \leq \text{ATDVRT} \leq 1.0 \times 10^{-3}$.
 (a small number, $< 10^{-50}$, sets the value to 0).
Default value: 4.5×10^{-4} .

W-15 (I) : IVTDRT Gas velocity calculation for turbulent deposition.
 =1: Use the gas velocity at the surface of 1-D or 2-D Solid Heat Conductor. The obtained gas velocity is multiplied by the factor XVT1RT (SC - see records 371XXX) or XVT2RT (TC - see records 471XXX).
 =2: Use gas velocity in a junction associated with the surface of 1-D or 2-D Solid Heat Conductor if such association exists (see records 371XXX, 471XXX), otherwise use the gas velocity at the surface of 1-D or 2-D Solid Heat Conductor (same as 1). The obtained gas velocity is multiplied by the factor XVT1RT (SC - see records 371XXX) or XVT2RT (TC - see records 471XXX).
Acceptable range: 1, 2.
Default value: 1.

W-16 (R) : EMCIRT Constant η_{\max} in the tube bundle (CIEMAT) correlation for the inertial impaction. The inertial impaction model is selected in the records 376XXX and 476XXX. The correlation is:

$$\eta = \frac{\eta_{\max}}{1 + c_1 \cdot \exp(-c_2 \cdot Stk^{c_3})}$$

Acceptable range: $0.0 < \text{EMCIRT} \leq 1.0$
Default value: 0.75

W-17 (R) : C1CIRT Constant c_1 in the tube bundle (CIEMAT) correlation for the inertial impaction.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 < C1CIRT \leq 1000.0$
Default value: 29.31

W-18 (R) : C2CIRT Constant c_2 in the tube bundle (CIEMAT) correlation for the inertial impaction.
Acceptable range: $0.0 < C2CIRT \leq 100.0$
Default value: 3.85

W-19 (R) : C3CIRT Constant c_3 in the tube bundle (CIEMAT) correlation for the inertial impaction.
Acceptable range: $0.0 < C3CIRT \leq 10.0$
Default value: 0.5

W-20 (R) : EBIIRT Constant η_{\max} in the pipe bend correlation for the inertial impaction. The inertial impaction model is selected in the records 376XXX and 476XXX. The correlation is:

$$\eta = \eta_{\max} \cdot (1 - 10^{-c_1 \cdot St^k})$$

Acceptable range: $0.0 < EBIIRT \leq 1.0$
Default value: 1.0

W-21 (R) : C1BIRT Constant c_1 in the pipe bend correlation for the inertial impaction.
Acceptable range: $0.0 < C1CIRT \leq 100.0$
Default value: 0.963

W-22 (R) : SFIIRT(1) Slip factor, S , for aerosol size section 1. Used for the inertial impaction. Used only if there is no association with junction. The associations are specified for each deposition surface in the records 376XX, 476XX (JI1RT, JI2RT). The slip factor is used to calculate the deposition velocity (see Volume 1):

$$v_D = \eta \cdot S \cdot v_g$$

where:

S slip factor SFIIRT(1), (-)
 v_g gas velocity, (m/s)
 η collection efficiency for the inertial impaction
 v_D deposition velocity for the inertial impaction:
Acceptable range: $0.0 \leq SFIIRT(1) \leq 10.0$
Default value: 1.0

W-23 (R) : SFIIRT(2) Slip factor, S , for aerosol size section 2. Used for the inertial impaction. See the description above.
Acceptable range: $0.0 \leq SFIIRT(2) \leq 10.0$
Default value: 1.0

...
 until the slip factors are defined for all aerosol size sections.

2.15.36 Record: 865001, Electrophoretic Deposition - Particle Charge

W-1 (R) : CQEDRT(1) Constant C_q in the formula for the electric charge, q , of the particle size section 1. The electric charge is calculated from:

$$q = C_q \cdot (D_p \times 10^6)^{x_q}$$

Here D_p is the particle diameter (m).
An equilibrium (minimum) charge may be approximated by (see Volume 1):

$$q = 3.8 \times 10^{-19} \cdot \sqrt{D_p \times 10^6}$$

This is achieved by setting CQEDRT = 3.8×10^{-19} , XQEDRT = 0.5.
An maximum charge may be approximated by (see Volume 1):

$$q = 4.5 \times 10^{-14} \cdot (D_p \times 10^6)^2$$

This is achieved by setting CQEDRT = 4.5×10^{-14} , XQEDRT = 2.0.
Acceptable range: $0.0 \leq \text{CQEDRT}(1) \leq 1.0 \times 10^6$
Default value: 0.0

W-2 (R) : XQEDRT(1) Constant x_q in the formula for the electric charge, q , of the particle size section 1.

Acceptable range: $0.0 \leq \text{XQEDRT}(1) \leq 10.0$
Default value: 0.0

W-3 (R) : CQEDRT(2) Constant C_q in the formula for the electric charge, q , of the particle size section 2.

Acceptable range: $0.0 \leq \text{CQEDRT}(2) \leq 1.0 \times 10^6$
Default value: 0.0

W-4 (R) : XQEDRT(2) Constant x_q in the formula for the electric charge, q , of the particle size section 2.

Acceptable range: $0.0 \leq \text{XQEDRT}(2) \leq 10.0$
Default value: 0.0

...
until the data is defined for all aerosol size sections.

2.15.37 Record: 865002, Global Activators of Deposition Processes

The aerosol deposition may be deactivated in this record.

W-1 (I) : IDEPRT(1) Activator of the aerosol deposition models on the pool surface in all Control Volumes.
= -1: Model inactive. No deposition is allowed on the pool in any CV

= +1: Model active. Deposition is allowed on the pool in every CV.

Acceptable range: -1, +1

Default value: +1

W-2 (I) : IDEPRT(2) Activator of the aerosol deposition models on the surface in all 1-D Solid Heat Conductors.

= -1: Model inactive. No deposition is allowed on any SC.

= +1: Model active. Deposition is allowed on every SC.

Acceptable range: -1, +1

Default value: +1

W-3 (I) : IDEPRT(3) Activator of the aerosol deposition models on the surface in all 2-D Solid Heat Conductors.

= -1: Model inactive. No deposition is allowed on any TC.

= +1: Model active. Deposition is allowed on every TC.

Acceptable range: -1, +1

Default value: +1

2.15.38 Record: 866000, Coagulation Model Data

W-1 (I) : ICEMRT Collision efficiency model selection:

=1: use Fuchs model, approximate formula ([32], section 4.3).

=2: use Fuchs model, exact formula ([32], section 4.3).

=3: use Pruppacher and Klett model ([32], section 4.3).

Acceptable range: 1, 2, or 3.

Default value: 1.

W-2 (I) : ICBMRT Brownian coagulation model selection:

=1: use diffusion model ([32], section 4.2.1). The diffusion model is valid for large particles and is therefore not recommended.

=2: use slip flow model ([32], section 4.2.3).

=3: use Fuchs model ([32], section 4.2.4).

Acceptable range: 1, 2, or 3.

Default value: 2.

W-3 (R) : ETDRRT Turbulence dissipation rate, applied in the turbulent flow range, ε_{TT} . The value is used by the turbulent coagulation model. The actual turbulence dissipation rate is calculated from:

- Laminar flow, $Re < Re_{lam}$

$$\varepsilon_T = 0.0$$

- Turbulent flow, $Re > Re_{tur}$

$$\varepsilon_T = \varepsilon_{TT}$$

- Transition flow, $Re_{lam} < Re < Re_{tur}$

$$\varepsilon_T = \varepsilon_{TT} \left(3 - 2 \frac{Re - Re_{lam}}{Re_{tur} - Re_{lam}} \right) \cdot \left(\frac{Re - Re_{lam}}{Re_{tur} - Re_{lam}} \right)^2$$

In the transition region the value is calculated using a smooth, third order interpolation. The limiting Reynolds numbers are defined by words 4 and 5 below.

Acceptable range: $0.0 \leq \text{ETDRRT} \leq 1.0$.

Default value: 0.001.

- W-4 (R) : RELART Limiting Reynolds number for laminar flow, Re_{lam} . If a negative number is entered, then the turbulence dissipation rate, ε_T , will be constant, and equal to ETDRRT (ε_{TT}) independently of the Reynolds number (as it is in the MELCOR code). The value is used also for the multiplier on the turbulent deposition velocity correlation.
Acceptable range: $100.0 \leq \text{RELART} \leq 10,000.0$ if positive.
Default value: 2200.0 ([14], page 7-27).
- W-5 (R) : RETURT Limiting Reynolds number for turbulent flow, Re_{tur} . The value is used for the turbulence dissipation rate and the turbulent deposition velocity calculation.
Acceptable range: $2.0 \times \text{RELART} \leq \text{RETURT} \leq 50,000.0$.
Default value: 10,000.0 ([14], page 7-27).
- W-6 (R) : CSTCRT Particle sticking coefficient. The coagulation kernel, as calculated by the correlations, is multiplied by this value. The value of CSTCRT may be set to zero by entering a negative number. CSTCRT of zero will disable the coagulation model.
Acceptable range: $0.0 \leq \text{CSTCRT} \leq 10.0$, or $\text{CSTCRT} < 0.0$.
Default value: 1.0.
- W-7 (I) : ICD1RT Model selection for coagulation of particles deposited on 1-D Solid Heat Conductor surfaces (this coagulation is important in case of resuspension).
=1: no coagulation of deposited particles.
=2: coagulation of deposited particles is estimated using the deposited layer thickness and the input parameter XCD1RT (see below).
Acceptable range: 1 or 2.
Default value: 2.
- W-8 (R) : XCD1RT If coagulation of particles deposited on 1-D Solid Heat Conductor surfaces is selected (ICD1RT=2), then the deposited particles whose size is smaller than the product of the deposited layer thickness and this parameter are transferred to the first size section whose size is larger than this product. The meaning of XCD1RT is illustrated in Figure 2-69. Coagulation into the size section i is initiated when the deposited layer thickness, t , is larger than $XCD1RT \times d_i$:

$$t \geq d_i \times XCD1RT$$

Here d_i is the diameter of the section i . Coagulation then proceeds with the user-defined rate, R_c (word RCD1RT, below).

Acceptable range: $0.1 \leq \text{XCD1RT} \leq 100.0$.

Default value: 1.0.

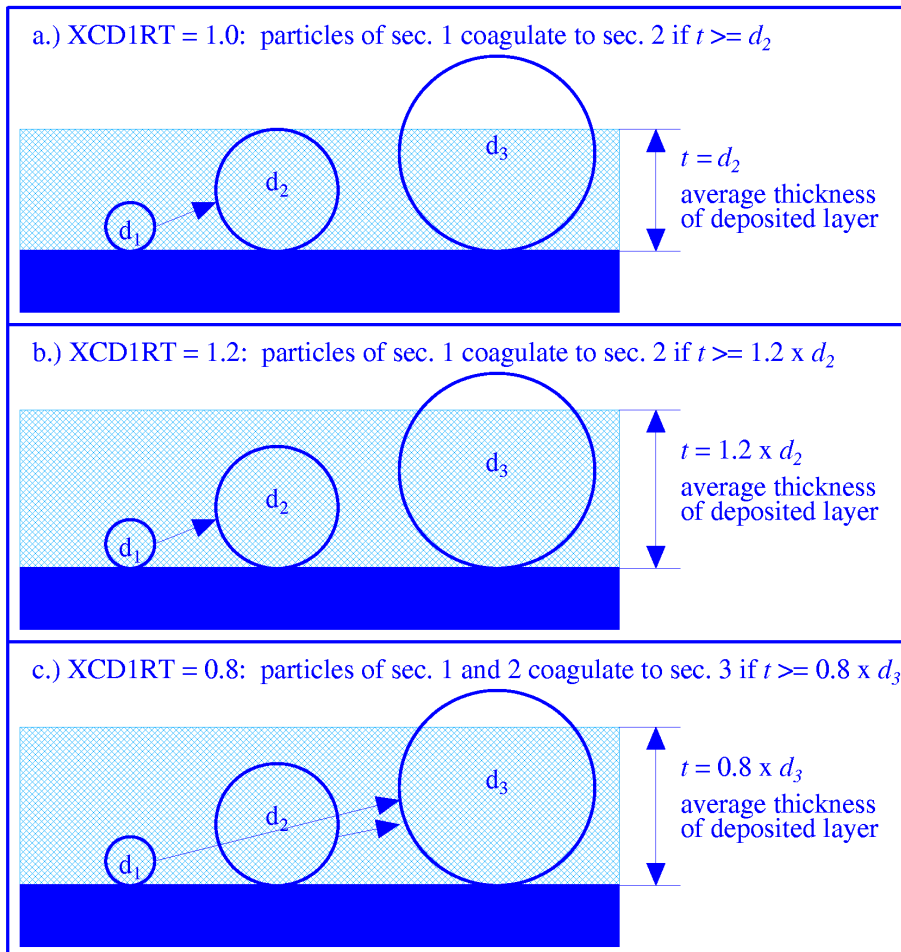


Figure 2-69 Coagulation of deposited aerosol particles.

W-9 (R) : RCD1RT Coagulation rate of particles deposited on 1-D Solid Heat Conductor surfaces, R_c (1/s). If the condition determined by XCD1RT is fulfilled, the transfer rate from a given size section i due to coagulation is calculated from:

$$\frac{dm_i}{dt} = -R_c m_i$$

Acceptable range: $1.0 \times 10^{-10} \leq \text{RCD1RT} \leq 1.0$, and
 $R_c \Delta t \leq 100.0$ where Δt is the maximum time step

Default value: 1.0×10^{-3} .

SPECTRA Code Manuals - Volume 2: User's Guide

- W-10 (I) : ICD2RT Model selection for coagulation of particles deposited on 2-D Solid Heat Conductor surfaces (this coagulation is important in case of resuspension).
1: no coagulation of deposited particles.
2: coagulation of deposited particles is estimated using the deposited layer thickness and the input parameter XCD2RT (see below).
Acceptable range: 1 or 2.
Default value: 2.
- W-11 (R) : XCD2RT If coagulation of particles deposited on 2-D Solid Heat Conductor surfaces is selected (ICD2RT=2), then all deposited particles whose size is smaller than the product of the deposited layer thickness and this parameter are transferred to the first size section whose size is larger than this product (see description of XCD1RT, above).
Acceptable range: $0.1 \leq XCD2RT \leq 100.0$.
Default value: 1.0.
- W-12 (R) : RCD2RT Coagulation rate of particles deposited on 2-D Solid Heat Conductor surfaces, R_c (1/s) (see description of RCD1RT, above).
Acceptable range: $1.0 \times 10^{-10} \leq RCD1RT \leq 1.0$, and $R_c \Delta t \leq 100.0$ where Δt is the maximum time step
Default value: 1.0×10^{-3} .

2.15.39 Records: 377XXX, 1-D Solid Heat Conductors Resuspension Model Selection

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

- W-1 (R) : IRM1RT SC left surface resuspension model.
(1) =-2: no resuspension model applied on the left surface.
 =-1: parametric resuspension model (defined in the records 867000, 868XXX, and 868XXX) is applied on the left surface.
 > 0: mechanistic model number IRM1RT(1) (defined in the records 8700XX through 8793XX) is applied on the left surface.
Acceptable range: $-2 \leq IRM1RT(1) \leq +10$.
Default value: IRMGRT (global activator of the resuspension model, record 860000)
- W-2 (R) : IRM1RT SC right surface resuspension model.
(2) =-2: no resuspension model applied on the right surface.
 =-1: parametric resuspension model (defined in the records 867000, 868XXX, and 868XXX) is applied on the right surface.
 > 0: mechanistic model number IRM1RT(2) (defined in the records 8700XX through 8793XX) is applied on the right surface.
Acceptable range: $-2 \leq IRM1RT(2) \leq +10$.
Default value: IRMGRT (global activator of the resuspension model, record 860000)

2.15.41 Record: 867000, Parametric Resuspension Model - Main Data

The parametric resuspension model with user-defined coefficients is selected in this record. The resuspension model is selected for each surface of a 1-D Solid Heat Conductor, and each boundary cell of a 2-D Solid Heat Conductor in the records 377XXX and 477XXX respectively. The model coefficients are defined in the records 868XXX and 869XXX, below.

The resuspension can be calculated as a result of:

- Large velocity of the gas flowing along the surface with deposited aerosols.
- Fast depressurization.
- A combination of both gas velocity and depressurization rate.

The resuspension rate is calculated for each process from a linear and power function.

- Velocity-dependent resuspension:

$$R_v(t) = C_1(v - v_0) + C_2(v - v_0)^x$$

- Depressurization-dependent resuspension:

$$R_p(t) = C_1 \left(\frac{dp}{dt} - \left(\frac{dp}{dt} \right)_0 \right) + C_2 \left(\frac{dp}{dt} - \left(\frac{dp}{dt} \right)_0 \right)^x$$

where: R_i - resuspension rate due to process i , (1/s). $R_i = (1/m)(dm/dt)$, where m is the deposited mass (kg).
 v - fluid velocity parallel to the deposition surface, (m/s).
 v_0 - minimum fluid velocity for resuspension, (m/s).
 dp/dt - depressurization rate, (Pa/s) (positive when pressure decreases).
 $(dp/dt)_0$ - minimum depressurization rate for resuspension, (Pa/s).
 C_i - model coefficients, an internal limit is imposed:
 $0.0 \leq C_i \leq 1.0$ in case of velocity-dependent resuspension,
 $0.0 \leq C_i \leq 1.0 \times 10^{-3}$ in case of depressurization-dependent resuspension,
 x - exponent, ($0.1 < x < 10.0$), (-).

The total resuspension rate is obtained from:

$$R(t) = [1.0 - (1.0 - R_v(t)) \cdot (1.0 - R_p(t))] \cdot f(\Delta t, B)$$

The term: $f(\Delta t, B)$ gives decay of the resuspension rate with time, and is approximately proportional to $\sim R_0 \exp(-Bt)$. The model coefficients can be defined for all size sections, or separately for each aerosol size section, as described in the records 868XXX, 869XXX below.

W-1 (I) : IRSMRT Resuspension model selection.
 =0: No resuspension is calculated
 =1: Resuspension is calculated based on gas velocities.
 =2: Resuspension model is calculated based on depressurization rates.

SPECTRA Code Manuals - Volume 2: User's Guide

- =3: Resuspension model is calculated based on both velocities and depressurization rates.
Acceptable range: 0, 1, 2, 3.
Default value: 0.
- W-2 (I) : IVELRT Gas velocity calculation for resuspension.
 =1: Use the fluid velocity at the surface of 1-D or 2-D Solid Heat Conductor. The obtained fluid velocity is multiplied by the factor XVELRT (next word).
 =2: Use gas velocity in a junction associated with the surface of 1-D or 2-D Solid Heat Conductor if such association exists (see records 371XXX, 471XXX), otherwise use the fluid velocity at the surface of 1-D or 2-D Solid Heat Conductor (same as 1). The obtained fluid velocity is multiplied by the factor XVELRT (next word).
Acceptable range: 1, 2.
Default value: 1.
- W-3 (I) : XVELRT Multiplier for the gas velocity.
Acceptable range: $0.0 < XVELRT \leq 1000.0$.
Default value: 1.0.
- W-4 (I) : IHUMRT Option to calculate the relative humidity for resuspension calculation.
 =1: Use current gas relative humidity at the surface.
 =2: Use RHUMRT (word 3 below).
 =3: Use the maximum relative humidity recorded over the calculated time period.
 =4: Use maximum value of RHUMRT and the maximum relative humidity recorded over the calculated time period.
 =5: Use time averaged relative humidity over the calculated time period.
 =6: Use maximum value of RHUMRT and the time averaged relative humidity over the calculated time period.
Acceptable range: 1, 2, 3, 4, 5, 6.
Default value: 5.
- W-5 (R) : RHUMRT Relative humidity for resuspension calculation. The use of this word depends on the option specified by IHUMRT, above.
Acceptable range: $0.0 \leq RHUMRT \leq 1.0$.
Default value: 0.0.
- W-6 (I) : IRMTRT Indicator for calculating decay of the resuspension rate with time. If the gas velocity (or depressurization rate) is constant over a certain period of time, t , then the velocity-induced resuspension rate changes as:
 $R \sim R_0 \exp(-Bt)$
-1: No model, $R = R_0$.
+1: Model 1, $R \leq R_0$ (see Figure 2-70)
+2: Model 2, $R \leq R_0$; $R = R_0$ for increasing R_0 (see Figure 2-71)
Acceptable range: -1, +1 or +2.
Default value: +1.

SPECTRA Code Manuals - Volume 2: User's Guide

Note that the re-defining records 868XXX must be placed in the input file below the record 868000. (The data entered in 868000 is immediately assigned to all size sections, so if any previous data for individual size sections were entered, they would be overwritten by the data in the record 868000.)

The minimum velocity for resuspension and the coefficients are obtained as follows:

$$\begin{aligned}v_0 &= v_{00} + v_{0h}H + v_{0n}n + v_{0T}T \\C_1 &= C_{10} + C_{1h}H + C_{1n}n + C_{1T}T \\C_2 &= C_{20} + C_{2h}H + C_{2n}n + C_{2T}T\end{aligned}$$

where: H - relative humidity, (-)
 n - concentration of airborne particles, (1/m³)
 T - temperature, (K)

The resuspension coefficients as well as the limiting velocity depend on the relative humidity gas pressure and temperature. The influence of humidity was observed in resuspension experiments [33]. Mono-layer particles subject to air currents can be resuspended by impaction of other particles [34]. Therefore the influence of airborne particles concentration, n , is present. The resuspension measurements indicate temperature dependency [34], T , which is therefore included. The resuspension behaviour depends on a long term humidity rather than an instantaneous humidity at the moment of resuspension. The user can choose the humidity definition in the record 867000.

- W-1 (R) : VV00RT v_{00} , (m/s) in the formula for the minimum velocity, v_0 .
Acceptable range: $0.0 \leq \text{VV00RT} \leq 1000.0$.
Default value: 0.0.
- W-2 (R) : VV0HRT v_{0h} , (m/s) in the formula for the minimum velocity, v_0 .
Acceptable range: $0.0 \leq \text{VV0HRT} \leq 1000.0$.
Default value: 0.0.
- W-3 (R) : VV0NRT v_{0n} , (m⁴/s) in the formula for the minimum velocity, v_0 .
Acceptable range: $-1.0 \times 10^{-3} \leq \text{VV0NRT} \leq 0.0$.
Default value: 0.0.
- W-4 (R) : VV0TRT v_{0T} , ((m/s)/K) in the formula for the minimum velocity, v_0 .
Acceptable range: $-1.0 \leq \text{VV0TRT} \leq 1.0$.
Default value: 0.0.
- W-5 (R) : CV10RT C_{10} , ((1/s)/(m/s))=(m⁻¹), in the formula for the coefficient C_1 .
Acceptable range: $0.0 \leq \text{CV10RT} \leq 1.0 \times 10^{-1}$.
Default value: 0.0.
- W-6 (R) : CV1HRT C_{1h} , ((1/s)/(m/s))=(m⁻¹), in the formula for the coefficient C_1 .
Acceptable range: $-1.0 \times 10^{-1} \leq \text{CV1HRT} \leq 0.0$.
Default value: 0.0.
- W-7 (R) : CV1NRT C_{1n} , ((m³/s)/(m/s))=(m²), in the formula for the coefficient C_1 .
Acceptable range: $0.0 \leq \text{CV1NRT} \leq 1.0 \times 10^{-7}$.
Default value: 0.0.

SPECTRA Code Manuals - Volume 2: User's Guide

W-8 (R) :	CV1TRT	C_{1T} , $((1/s \text{ K})/(m/s))=(m^{-1} \text{ K}^{-1})$, in the formula for the coefficient C_1 . <i>Acceptable range:</i> $-1.0 \times 10^{-4} \leq CV1TRT \leq 1.0 \times 10^{-4}$. <i>Default value:</i> 0.0.
W-9 (R) :	CV20RT	C_{20} , $((1/s)/(m/s)^x)$ in the formula for the coefficient C_2 . <i>Acceptable range:</i> $0.0 \leq CV20RT \leq (1.0 \times 10^{-1})^x$. <i>Default value:</i> 0.0.
W-10 (R) :	CV2HRT	C_{2h} , $((1/s)/(m/s)^x)$ in the formula for the coefficient C_2 . <i>Acceptable range:</i> $-(1.0 \times 10^{-1})^x \leq CV2HRT \leq 0.0$. <i>Default value:</i> 0.0.
W-11 (R) :	CV2NRT	C_{2n} , $((m^3/s)/(m/s)^x)$ in the formula for the coefficient C_2 . <i>Acceptable range:</i> $0.0 \leq CV2NRT \leq 1.0 \times 10^{-6} \times (1.0 \times 10^{-1})^x$. <i>Default value:</i> 0.0.
W-12 (R) :	CV2TRT	C_{2T} , $((1/s \text{ K})/(m/s)^x)$ in the formula for the coefficient C_2 . <i>Acceptable range:</i> $-10^{-3} \times (10^{-1})^x \leq CV2TRT \leq 10^{-3} \times (10^{-1})^x$. <i>Default value:</i> 0.0.
W-13 (R) :	XV00RT	x , exponent in the formula for resuspension. <i>Acceptable range:</i> $0.001 \leq XV00RT \leq 10.0$. <i>Default value:</i> 3.0.

2.15.43 Records: 869XXX, Parametric Resuspension Model - P-Coefficients

The model coefficients for the depressurization-dependent resuspension are entered in these records. XXX is the aerosol size section number. If $XXX > 000$, then the set of coefficients defined below is valid for the size section XXX. If $XXX = 000$, then the set of coefficients defined below is valid for all size sections. The user can define first the set of coefficients for all size sections using the record 869000, and then re-define the coefficients for selected size sections using records 869XXX, with $XXX > 000$. Note that the re-defining records 869XXX must be placed in the input file below the record 869000.

The minimum depressurization rate for resuspension and the coefficients are obtained as follows:

$$\left(\frac{dp}{dt}\right)_0 = \left(\frac{dp}{dt}\right)_{00} + \left(\frac{dp}{dt}\right)_{0h} H + \left(\frac{dp}{dt}\right)_{0n} n + \left(\frac{dp}{dt}\right)_{0T} T$$

$$C_1 = C_{10} + C_{1h}H + C_{1n}n + C_{1T}T$$

$$C_2 = C_{20} + C_{2h}H + C_{2n}n + C_{2T}T$$

where: H - relative humidity, (-)
 n - concentration of airborne particles, $(1/m^3)$
 T - temperature, (K)

The resuspension coefficients as well as the limiting depressurization rate depend on the relative humidity gas pressure and temperature. The influence of humidity was observed in resuspension

SPECTRA Code Manuals - Volume 2: User's Guide

experiments [33]. Mono-layer particles subject to air currents can be resuspended by impaction of other particles [34]. Therefore the influence of airborne particles concentration, n , is present. The resuspension measurements indicate temperature dependency [34], T , which is therefore included. The resuspension behavior depends on a long term humidity rather than an instantaneous humidity at the moment of resuspension. The user can choose the humidity definition in the record 867000.

W-1 (R) :	DP00RT	$(dp/dt)_{00}$, (Pa/s) in the formula for the minimum depressurization rate, $(dp/dt)_0$. <i>Acceptable range:</i> $0.0 \leq DP00RT \leq 1.0 \times 10^6$. <i>Default value:</i> 0.0.
W-2 (R) :	DP0HRT	$(dp/dt)_{0h}$, (Pa/s) in the formula for the minimum depressurization rate, $(dp/dt)_0$. <i>Acceptable range:</i> $0.0 \leq DP0HRT \leq 1.0 \times 10^6$. <i>Default value:</i> 0.0.
W-3 (R) :	DP0NRT	$(dp/dt)_{0p}$, ((Pa/s)·m ³) in the formula for the minimum depressurization rate, $(dp/dt)_0$. <i>Acceptable range:</i> $-1.0 \leq DP0NRT \leq 0.0$. <i>Default value:</i> 0.0.
W-4 (R) :	DP0TRT	$(dp/dt)_{0T}$, ((Pa/s)/K), in the formula for the minimum depressurization rate, $(dp/dt)_0$. <i>Acceptable range:</i> $-1.0 \times 10^3 \leq DP0TRT \leq 1.0 \times 10^3$. <i>Default value:</i> 0.0.
W-5 (R) :	CP10RT	C_{10} , ((1/s)/(Pa/s))=(Pa ⁻¹), in the formula for the coefficient C_1 . <i>Acceptable range:</i> $0.0 \leq CP10RT \leq 1.0 \times 10^{-3}$. <i>Default value:</i> 0.0.
W-6 (R) :	CP1HRT	C_{1h} , ((1/s)/(Pa/s))=(Pa ⁻¹), in the formula for the coefficient C_1 . <i>Acceptable range:</i> $-1.0 \times 10^{-3} \leq CP1HRT \leq 0.0$. <i>Default value:</i> 0.0.
W-7 (R) :	CP1NRT	C_{1n} , ((m ³ /s)/(Pa/s))=(m ³ /Pa), in the formula for the coefficient C_1 . <i>Acceptable range:</i> $0.0 \leq CP1NRT \leq 1.0 \times 10^{-9}$. <i>Default value:</i> 0.0.
W-8 (R) :	CP1TRT	C_{1T} , ((1/s K)/(Pa/s))=(Pa ⁻¹ K ⁻¹), in the formula for the coefficient C_1 . <i>Acceptable range:</i> $-1.0 \times 10^{-6} \leq CP1TRT \leq 1.0 \times 10^{-6}$. <i>Default value:</i> 0.0.
W-9 (R) :	CP20RT	C_{20} , ((1/s)/(Pa/s) ^x) in the formula for the coefficient C_2 . <i>Acceptable range:</i> $0.0 \leq CP20RT \leq (1.0 \times 10^{-3})^x$. <i>Default value:</i> 0.0.
W-10 (R) :	CP2HRT	C_{2h} , ((1/s)/(Pa/s) ^x) in the formula for the coefficient C_2 . <i>Acceptable range:</i> $-(1.0 \times 10^{-3})^x \leq CP2HRT \leq 0.0$. <i>Default value:</i> 0.0.
W-11 (R) :	CP2NRT	C_{2n} , ((m ³ /s)/(Pa/s) ^x) in the formula for the coefficient C_2 .

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq \text{CP2NRT} \leq 10^{-6} \times (1.0 \times 10^{-3})^x$.
Default value: 0.0.

W-12 (R) : CP2TRT C_{2T} , $((1/\text{s K})/(\text{Pa/s})^x)$ in the formula for the coefficient C_2 .
Acceptable range: $-10^{-3} \times (10^{-3})^x \leq \text{CP2TRT} \leq 10^{-3} \times (10^{-3})^x$.
Default value: 0.0.

W-13 (R) : XP00RT x , exponent in the formula for resuspension.
Acceptable range: $0.001 < \text{XP00RT} < 10.0$.
Default value: 3.0.

2.15.44 Records: 8700XX, Mechanistic Resuspension - Main Data

The mechanistic resuspension model data is specified in these records. XX is the model number. Up to 20 models may be used. The model numbers, XX, must be consecutive (starting with 01). The resuspension model is selected for each surface of a 1-D Solid Heat Conductor, and each boundary cell of a 2-D Solid Heat Conductor in the records 377XXX and 477XXX respectively.

W-1 (R) : CF0RRT Coefficient C_{f0} , (-), in the formula for the frequency of vibration, f_0 :

$$f_0 = C_{f0} \frac{f \rho_g V_g^2}{8 \mu_g}$$

If a negative value of C_{f0} is entered, then f_0 will be constant and equal to:

$$f_0 = |C_{f0}| \quad \text{if } C_{f0} < 0.0$$

Acceptable range: $1.0 \times 10^{-6} \leq \text{CF0RRT} \leq 1.0 \times 10^1$ if $\text{CF0RRT} > 0.0$
 $1.0 \times 10^{-3} \leq -\text{CF0RRT} \leq 1.0 \times 10^3$ if $\text{CF0RRT} < 0.0$
Default value: 3.33×10^{-3} .

W-2 (R) : XFRRT Power x_F , (-), in the formula for the resuspension rate, $R_m(t)$:

$$R_m(t) = f_0 \exp \left[- \left(\frac{F_{a\tau}}{F_d} \right)^{x_F} \right]$$

Acceptable range: $0.1 \leq \text{CF0RRT} \leq 100.0$.
Default value: 1.33.

W-3 (R) : CHIRRT Constant C_χ , (-), in the formula for the equivalent spring stiffness χ :

$$\chi = C_\chi \cdot K^{2/3} \cdot D_{eff,0}^{1/3} \cdot F_a^{1/3}$$

Acceptable range: $0.1 \leq \text{CHIRRT} \leq 10.0$.
Default value: 1.13.

SPECTRA Code Manuals - Volume 2: User's Guide

W-4 (R) : VIPRRT Poisson's ratio for the particles ν_p , (-). Used to calculate K :

$$K = \frac{4}{3} \left(\frac{1 - \nu_p^2}{E_p} + \frac{1 - \nu_s^2}{E_s} \right)^{-1}$$

Acceptable range: $0.1 \leq \text{VIPRRT} \leq 1.0$.

Default value: 0.3.

W-5 (R) : EYPRRT Young modulus for the particles E_p , (Pa). Used to calculate K :

Acceptable range: $1.0 \times 10^5 \leq \text{EYPRRT} \leq 1.0 \times 10^{18}$.

Default value: 1.0×10^{11} .

W-6 (R) : VISRRT Poisson's ratio for the surface ν_s , (-). Used to calculate K :

Acceptable range: $0.1 \leq \text{VISRRT} \leq 1.0$.

Default value: 0.3.

W-7 (R) : EYSRRT Young modulus for the surface E_s , (Pa). Used to calculate K :

Acceptable range: $1.0 \times 10^5 \leq \text{EYSRRT} \leq 1.0 \times 10^{18}$.

Default value: 1.0×10^{11} .

W-8 (R) : CFARRT Constant C_{Fa} , (-), in the formula for the tangential pull-off force, $F_{a\tau}$:

$$F_{a\tau} = C_{Fa} \cdot \frac{F_a^{3/2}}{D_{eff,0}^{1/2} \cdot \chi^{1/2}}$$

The formula is used if a positive value of C_{Fa} is entered. In such case the ratio between the $F_{a\tau}$ and the adhesion force, F_a , is further limited by the input parameters TMNRRT, TMXRRT (records 8791XX), so that:

$$\text{TMNRRT} \leq \left(\frac{F_{a\tau}}{F_a} \right) \leq \text{TMXRRT}$$

If a negative value of C_{Fa} is entered, then a scaled adhesion force, F_a , will be used with the scaling factor equal to the absolute value of C_{Fa} :

$$F_{a\tau} = |C_{Fa}| \cdot F_a \quad \text{if } C_{Fa} < 0.0$$

Acceptable range: $0.1 \leq \text{CFARRT} \leq 10.0$ if $\text{CFARRT} > 0.0$

$1.0 \times 10^{-5} \leq -\text{CFARRT} \leq 10.0$ if $\text{CFARRT} < 0.0$

Default value: 2.0.

W-9 (I) : IVELRT Gas velocity calculation for resuspension.

=1: Use the fluid velocity at the surface of 1-D or 2-D Solid Heat Conductor. The obtained fluid velocity is multiplied by the factor XVELRT (next word).

=2: Use gas velocity in a junction associated with the surface of 1-D or 2-D Solid Heat Conductor if such association exists (see records 371XXX, 471XXX), otherwise use the fluid velocity at the surface of

SPECTRA Code Manuals - Volume 2: User's Guide

1-D or 2-D Solid Heat Conductor (same as 1). The obtained fluid velocity is multiplied by the factor XVELRT (next word).

Acceptable range: 1, 2.

Default value: 1.

- W-10 (I) : XVELRT Multiplier for the gas velocity.
Acceptable range: $0.0 < XVELRT \leq 1000.0$.
Default value: 1.0.
- W-11 (I) : IAFRRT Adhesion force or surface asperity distribution selection.
1: Adhesion force distribution, $\varphi(F_a)$, is specified in the records 87YYXX.
2: Surface asperity distribution, $\varphi_{as}(r_{as})$, is specified in the records 87YYXX.
Acceptable range: 1 or 2.
Default value: 1.
- W-12 (I) : IDTRRT Adhesion force distribution type.
1: Lognormal distribution
2: Tabular distribution
Acceptable range: 1 or 2.
Default value: 1.
- W-13 (I) : IDORRT Adhesion force distribution option.
1: Particle balance separately for each F_a -section. Adhesion force distribution is used only during deposition, to distribute the newly deposited particles in the appropriate F_a -sections. During resuspension a balance of particles is considered for each F_a -section, so the resuspension from a given F_a -section stops when there are no particles left in this section.
2: The same distribution is kept constant throughout the transient. This option is not recommended for general application. It is included mainly for test calculations for comparisons with analytical solutions obtained assuming a fixed adhesion force distribution.
Acceptable range: 1 or 2.
Default value: 1.
- W-14 (I) : NSCRRT Number of F_a -sections (if IAFRRT=1), or r_{as} -sections (if IAFRRT=2), N_{sec} (see Figure 2-72).
Acceptable range: $1 \leq NSCRRT \leq 99$.
The total number of integration points, equal to $NSCRRT \times NJSRRT + 1$, must be not smaller than 3 and not larger than 500.
Default value: 51 if the adhesive spread, $\text{Max}(\text{SAMRRT})$, is ≤ 10 .
99 if the adhesive spread, $\text{Max}(\text{SAMRRT})$, is > 10 .
Note: an uneven number of sections has the advantage of having a middle section with the F_a (or r_{as}) equal to the mean value.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-15 (I) : NJSRRT Number of integration intervals per single F_a -section or r_{as} -section, N_j , (see Figure 2-72).
Acceptable range: $1 \leq NJSRRT \leq 5$.
 The total number of integration points, equal to $NSCRRT \times NJSRRT + 1$, must be not smaller than 3 and not larger than 500.
Default value: 1.
- W-16 (R) : CUTRRT Cut-off limit for high negative exponents (low resuspension rates). The resuspension rates are proportional to $R \sim \exp(-Y)$, where Y is equal to $(F_{av}/F_d)^X$. CUTRRT is the maximum value of Y that is considered in the resuspension calculations. The resuspension rates is set to 0.0 for those F_a -sections for which $Y > CUTRRT$. The value of 20 means practically no cut-off (only the terms $R < \exp(-20) \sim 10^{-10}$ s are eliminated). The value of 10 means that the terms $R < \exp(-10) \sim 10^{-5}$ s are eliminated. Those terms give resuspension times of $\sim 10^5$ s. According to experimental observations such slow resuspension rates are not realistic. CUTRRT is a convenient parameter that can filter out the slow resuspension rates. A discussion of this parameter is found in Volume 3.
Acceptable range: $10.0 \leq CUTRRT \leq 20.0$.
Default value: 15.0.

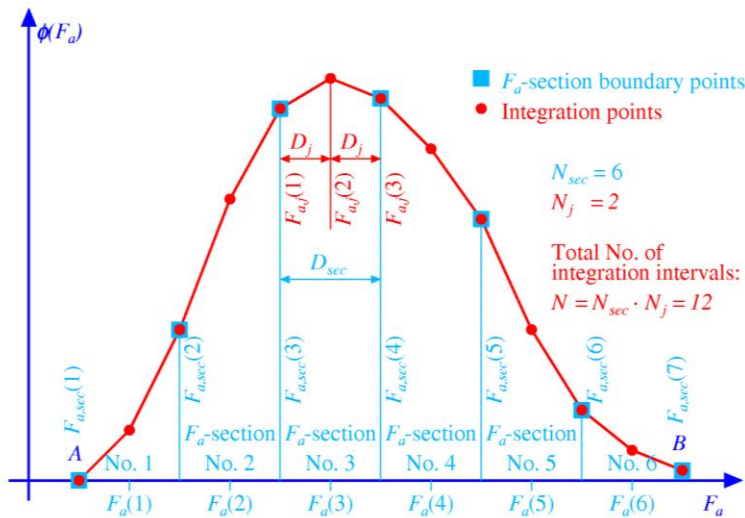


Figure 2-72 Lognormal distribution of adhesion forces.

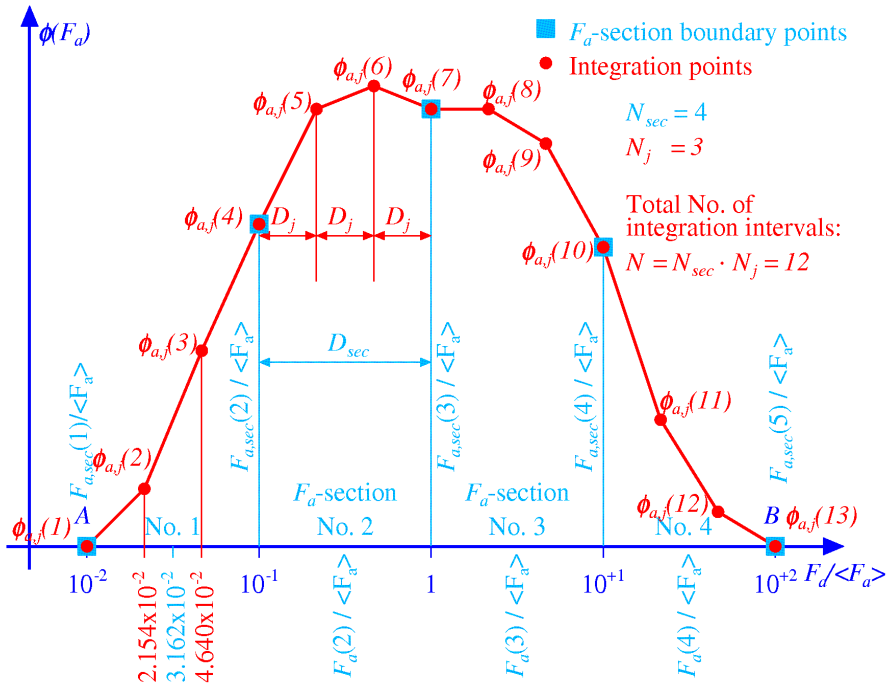


Figure 2-73 Tabulated distribution of adhesion forces.

Section boundaries:

$$F_{a,sec}(i+1) = F_{a,sec}(i) \cdot D_{sec} = A \cdot D_{sec}^i$$

Representative forces:

$$F_a(i) = \sqrt{F_{a,sec}(i) \cdot F_{a,sec}(i+1)}$$

Integration interval:

$$D_j = \exp\left(\frac{\ln(B/A)}{N_{sec} \cdot N_j}\right)$$

Integration points:

$$F_{a,j}(j+1) = F_{a,j}(j) \cdot D_j = F_{a,sec}(i) \cdot D_j^j$$

For example, if $\sigma_a = 4.64$, then $\sigma_a^3 = 100.0$ and $A = \langle F_a \rangle \times 10^{-2}$, $B = \langle F_a \rangle \times 10^{+2}$. If the number of F_a -sections is assumed as 4, $N_{sec} = 4$, then:

- The relative section boundaries, $F_{a,sec}(i)/\langle F_a \rangle$, will be equal to: 10^{-2} , 10^{-1} , 1.0 , 10^{+1} , 10^{+2} .
- The section representative forces, $F_a(i)/\langle F_a \rangle$: 3.162×10^{-2} , 3.162×10^{-1} , 3.162 , $3.162 \times 10^{+1}$.

If the number of integration intervals per F_a -section is assumed as 3, then:

- The integration point interval “length”, D_j , is equal to 2.154. The integration points, $F_{a,j}(i)/\langle F_a \rangle$, are: 10^{-2} , 2.154×10^{-2} , 4.640×10^{-2} , 10^{-1} , 2.154×10^{-1} , ..., etc.

Such distribution is illustrated in Figure 2-73. Values of the distribution function, ϕ , must be specified in these points as the table FASRRRT. The total number of points must be equal to

SPECTRA Code Manuals - Volume 2: User's Guide

Section boundaries: $r_{as,sec}(i+1) = r_{as,sec}(i) \cdot D_{sec}$

Representative values of $r_{as}(i)$: $r_{as}(i) = \sqrt{r_{as,sec}(i) \cdot r_{as,sec}(i+1)}$

If RASRRT < 0.0, then r_{as} a single value is used for all F_a -sections:
 $r_{as}(i) = |RASRRT|$.

Acceptable range: $|RASRRT| \leq 1.0 \times 10^{-4}$.

use a small value ($\leq 10^{-50}$) to set RASRRT to zero.

Default value: $1. \times 10^{-7}$ (based on Reeks and Hall, $f' = 0.027$, $D_p = 10 \mu\text{m}$, $f' \times D_p = 0.027 \times 10 \times 10^{-6} / 2 \text{ m}$).

W-2 (R) : SASRRT Spread factor for the asperity radius distribution, σ_{as} . Used only if the mean adhesion force distribution, $\varphi_a(F_a)$, is selected (IAFRRT=1, record 8700XX) and if the mean asperity radius, RASRRT (Word 6 above), is positive value.

Acceptable range: $1.1 \leq SASRRT \leq 20.0$.

Default value: 4.0.

W-3 (R) : XPORRT Constant $x_{p,0}$ in the formula for the effective diameter, $D_{eff,0}$, (note that $D_{eff,0}$, is used to calculate the “spring” stiffness and finally the tangential pull-off force - see record 8700XX, W-8: CFARRT):

$$D_{eff,0} = \frac{1}{\frac{1}{x_{p,0} D_p} + \frac{1}{x_{as,0} 2r_{as}}}$$

Acceptable range: $0.1 \leq XPORRT \leq 1.0 \times 10^{10}$.

Default value: 1.0.

W-4 (R) : XAORRT Constant $x_{as,1}$ in the formula for the effective diameter, $D_{eff,0}$.

Acceptable range: $0.1 \leq XAORRT \leq 1.0 \times 10^{10}$.

Default value: 3.0 (a particle typically rests on three asperities)

W-5 (R) : TMNRRT Minimum ratio of the tangential pull-off force, F_{at} , and the adhesion force, F_a . Used only if the tangential pull-off force is obtained from the Vainshtein’s expression (CFARRT>0.0 - records 8700XX). The ratio of F_{at} to F_a , depends on the effective “spring” stiffness, therefore the user must be very careful changing the parameters (CHIRRT, XPORRT, XAORRT). The minimum limit is set to avoid unreasonable values of the pull-off force for some combination of these input parameters. The ratio of the tangential pull-off force and the adhesion force is limited by:

$$TMNRRT \leq \left(\frac{F_{at}}{F_a} \right) \leq TMXRRT$$

Acceptable range: $1.0 \times 10^{-5} \leq TMNRRT \leq 5.0$.

Default value: 1.0×10^{-3} .

W-6 (R) : TMXRRT Maximum ratio of the tangential pull-off force, F_{at} , and the adhesion force, F_a .

Acceptable range: $2.0 \times \text{TMNRRT} \leq \text{TMXRRT} \leq 10.0$.
Default value: 1.0.

2.15.47 Records: 8792XX, Mechanistic Resuspension - Adhesion Force Calculation

The mechanistic resuspension model data is specified in these records. XX is the model number. Up to 20 models may be used. The model numbers, XX, must be consecutive (starting with 01). The data specified in this record is used to calculate the mean adhesion forces for each particle size section if they are not given by the user in the record 87YYXX (FAMRRT \leq 0.0)

W-1 (R) : A1ARRT Constant A_1 in the formula for the adhesion force, $F_{a,1}$:

$$F_{a,1} = \frac{A_1}{R^{x_1}} D_{eff,1}$$

Note that the value of A_1 that gives the same adhesion force as the Vainshtein model for a smooth surface is a function of the parameter $\Delta\gamma$ (adhesive surface energy, J/m²):

$$A_1 = \frac{3}{4} \pi \cdot 10^{-9} \cdot \Delta\gamma = 2.356 \times 10^{-9} \cdot \Delta\gamma$$

Reference [33] gives values of $\Delta\gamma = 0.15$ for graphite particles and 0.56 for alumina particles. The corresponding values of A_1 are 3.53×10^{-10} and 1.32×10^{-9} respectively.

Acceptable range: $0.0 \leq \text{A1ARRT} \leq 1.0 \times 10^{10}$.

If a negative value is entered, A1ARRT is set to zero.

Default value: 5.0×10^{-10} .

W-2 (R) : X1ARRT Constant x_1 in the formula for the adhesion force, $F_{a,1}$.

Acceptable range: $0.0 \leq \text{X1ARRT} \leq 10.0$.

If a negative value is entered, X1ARRT is set to 0.

Default value: 1.0.

W-3 (R) : RGHRRT Surface roughness, R , in the formula for the adhesion force, $F_{a,1}$.

Acceptable range: $\text{RGHRRT} \leq 1.0 \times 10^{-4}$.

If $\text{RGHRRT} \leq 10^{-10}$, then RGHRRT is set to zero (smooth). Smooth surface is recommended if the asperity distribution option is used (IAFRRT = 2, record 8700XX)

Default value: 10^{-5} if IAFRRT=1 (adhesion force correlations)
 0.0 if IAFRRT=2 (asperity distribution)

W-4 (R) : XP1RRT Constant $x_{p,1}$ in the formula for the effective diameter, $D_{eff,1}$, in the formula for the adhesion force, $F_{a,1}$:

$$D_{eff,1} = \frac{1}{\frac{1}{x_{p,1} D_p} + \frac{1}{x_{as,1} 2r_{as}}}$$

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.1 \leq \text{XP1RRT} \leq 1.0 \times 10^{10}$.
Default value: 1.0 if IAFRRT=1 (adhesion force correlations)
 10^{10} if IAFRRT=2 (asperity distribution)

W-5 (R) : XA1RRT Constant $x_{as,1}$ in the formula for the effective diameter, $D_{eff,1}$, in the formula for the adhesion force, $F_{a,1}$.
Acceptable range: $0.1 \leq \text{XA1RRT} \leq 1.0 \times 10^{10}$.
Default value: 10^{10} if IAFRRT=1 (adhesion force correlations)
 1.0 if IAFRRT=2 (asperity distribution)

W-6 (R) : A2ARRT Constant A_2 in the formula for the adhesion force, $F_{a,2}$:

$$F_{a,2} = A_2 \cdot f(H) \cdot \sigma \cdot D_{eff,2}$$

Acceptable range: $0.0 \leq \text{A2ARRT} \leq 100.0$ if IAFRRT=1
 $\text{A2ARRT} = 0$ if IAFRRT=2
 If a negative value is entered, A2ARRT is set to 0.
Default value: 6.28 if IAFRRT=1 (adhesion force correlations)
 0.0 if IAFRRT=2 (asperity distribution)

W-7 (R) : RHUMRT Relative humidity, H , in the formula for the adhesion force, $F_{a,2}$.
Acceptable range: $0.0 \leq \text{RHUMRT} \leq 1.0$.
Default value: 0.0.

W-8 (R) : SIGRRT Surface tension, σ , in the formula for the adhesion force, $F_{a,2}$.
Acceptable range: $0.0 \leq \text{SIGRRT} \leq 1.0$.
Default value: 6.0×10^{-2} .

W-9 (R) : XP2RRT Constant $x_{p,2}$ in the formula for the effective diameter, $D_{eff,2}$, in the formula for the adhesion force, $F_{a,2}$:

$$D_{eff,2} = \frac{1}{\frac{1}{x_{p,2} D_p} + \frac{1}{x_{as,2} 2r_{as}}}$$

Acceptable range: $0.1 \leq \text{XP2RRT} \leq 1.0 \times 10^{10}$.
Default value: 1.0.

W-10 (R) : XA2RRT Constant $x_{as,2}$ in the formula for the effective diameter, $D_{eff,2}$, in the formula for the adhesion force, $F_{a,2}$.
Acceptable range: $0.1 \leq \text{XA2RRT} \leq 1.0 \times 10^{10}$.
Default value: 1.0.
Default value: 1.0

2.15.48 Records: 8793XX, Mechanistic Resuspension - Drag Force Calculation

The mechanistic resuspension model data is specified in these records. XX is the model number. Up to 20 models may be used. The model numbers, XX, must be consecutive (starting with 01).

W-1 (R) : XDRRT Multiplier X_d , (-), in the formula for the drag force, F_d :

$$F_d = X_d \cdot F'_d = X_d \cdot 8.0 \cdot \frac{\mu_g^2}{\rho_g} \cdot (D_p^+)^2$$

Acceptable range: 0.0 < XDRRT ≤ 1000.0.

Default value: 0.3.

W-2 (R) : XLRRT Multiplier X_L , (-), in the formula for the lift force, F_L . Note that the lift force is not used in the Vainshtein model. In the present resuspension model the lift force may be used if it is activated by the option IDRRT (Word 3 below).

$$F_L = X_L \cdot \begin{cases} F'_{L,Soltani} = 0.975 \cdot \frac{\mu_g^2}{\rho_g} \cdot (D_p^+)^{3.0} & \text{if } D_p^+ < 8.34 \\ F'_{L,Hall} = 4.215 \cdot \frac{\mu_g^2}{\rho_g} \cdot (D_p^+)^{2.31} & \text{if } D_p^+ > 8.34 \end{cases}$$

Acceptable range: 0.0 < XLRRT ≤ 1000.0.

Default value: 1.0.

W-3 (I) : IDRRT Option for calculation of F_d in the resuspension model:
=1: Use the drag force, F_d (calculated with the multiplier XDRRT)

$$R_m(t) = f_0 \exp \left[- \left(\frac{F_{a\tau}}{F_d} \right)^{x_F} \right] = f_0 \exp \left[- \left(\frac{F_{a\tau}}{(X_d F'_d)} \right)^{x_F} \right]$$

=2: Use the lift force, F_L (calculated with the multiplier XLRRT)

$$R_m(t) = f_0 \exp \left[- \left(\frac{F_{a\tau}}{F_L} \right)^{x_F} \right] = f_0 \exp \left[- \left(\frac{F_{a\tau}}{(X_L F'_L)} \right)^{x_F} \right]$$

=3: Use the sum of F_d and F_L :

$$R_m(t) = f_0 \exp \left[- \left(\frac{F_{a\tau}}{F_d + F_L} \right)^{x_F} \right] = f_0 \exp \left[- \left(\frac{F_{a\tau}}{(X_d F'_d) + (X_L F'_L)} \right)^{x_F} \right]$$

Acceptable range: 1 < IDRRT ≤ 3.

Default value: 1.

2.15.49 Records: 8794XX, Mechanistic Resuspension, C_1 and C_2 , All Sections

The mechanistic resuspension model data is specified in these records. XX is the model number. Up to 20 models may be used. The model numbers, XX, must be consecutive (starting with 01). This record defines constants C_1 and C_2 for all size sections. These constants may be defined section-by-section in records 8795XX and 8796XX.

W-1 (R) : C1ERRT Constant C_1 , (-), in the extended resuspension model:

$$R_m = f_0 \exp \left[-C_1 \left(\frac{F_{ar} - C_2 F_d}{F_d} \right)^{x_f} \right]$$

A limit is imposed on the difference, such that it never becomes negative ($F_{ar} - C_2 F_d \geq 0.0$). Therefore if $C_2 F_d \geq F_{ar}$ the result is independent on the forces and is always equal to: $f_0 \exp(0) = f_0$

Acceptable range: $1.0 \times 10^{-6} < C1ERRT \leq 1.0 \times 10^6$.

Default value: 1.0.

W-2 (R) : C2ERRT Constant C_2 , (-), in the extended resuspension model.

Acceptable range: $0.0 < C2ERRT \leq 1.0 \times 10^6$.

Default value: 0.0.

2.15.50 Records: 8795XX, Mechanistic Resuspension, C_1 Per Size Section

The mechanistic resuspension model data is specified in these records. XX is the model number. Up to 20 models may be used. The model numbers, XX, must be consecutive (starting with 01). This record defines constants C_1 section-by-section.

W-1 (R) : C1ERRT(1) Constant C_1 , (-), in the extended resuspension model. Valid for size section 1.

Acceptable range: $1.0 \times 10^{-6} < C1ERRT(1) \leq 1.0 \times 10^6$.

Default value: 1.0.

W-2 (R) : C1ERRT(2) Constant C_1 , (-), in the extended resuspension model. Valid for size section 2.

Acceptable range: $1.0 \times 10^{-6} < C1ERRT(2) \leq 1.0 \times 10^6$.

Default value: C1ERRT(1)

...

until C1ERRT is defined for all size sections. The default value for all size sections > 1 is the value for the size section 1: C1ERRT(1).

2.15.51 Records: 8796XX, Mechanistic Resuspension, C₂ Per Size Section

The mechanistic resuspension model data is specified in these records. XX is the model number. Up to 20 models may be used. The model numbers, XX, must be consecutive (starting with 01). This record defines constants C₂ section-by-section.

W-1 (R) : C2ERRT(1)Constant C₂, (-), in the extended resuspension model. Valid for size section 1.

Acceptable range: 0.0 < C2ERRT(1) ≤ 1.0×10⁶.

Default value: 0.0.

W-2 (R) : C2ERRT(2)Constant C₂, (-), in the extended resuspension model. Valid for size section 2.

Acceptable range: 0.0 < C2ERRT(2) ≤ 1.0×10⁶.

Default value: C2ERRT(1)

...
until C2ERRT is defined for all size sections. The default value for all size sections > 1 is the value for the size section 1: C2ERRT(1).

An example input for the resuspension model with tabulates distribution is shown below. The adhesive force distribution corresponds to the one shown in Figure 2-73, with 4 F_a-sections and 3 integration intervals per section. The mean value for each of the 5 particle size sections is calculated internally by the code. The adhesive spread factor is 4.64 for each size section.

```

*
*      MECHANISTIC RESUSPENSION MODEL No. 01
*
*      Distribution
*      Cf0  XF  Chi  Vp  Ep  Vs  Es  CFa  Ivel  Fa  Log  Opt  Nsec  Nj
870001  0  0  0  0  0  0  0  0  0  1  2  1  4  3  *
*
*      Adhesion force distribution
*      Table
*      <Fa> sigma  1  2  3  4  5  6  7  8  9  10  11  12  13
870101  0.0  4.64  0.0  1.0  5.0  10.0  15.0  17.0  15.0  15.0  13.0  9.0  4.0  2.0  0.0  * size section 1
870201  0.0  4.64  0.0  1.0  5.0  10.0  15.0  17.0  15.0  15.0  13.0  9.0  4.0  2.0  0.0  * size section 2
870301  0.0  4.64  0.0  1.0  5.0  10.0  15.0  17.0  15.0  15.0  13.0  9.0  4.0  2.0  0.0  * size section 3
870401  0.0  4.64  0.0  1.0  5.0  10.0  15.0  17.0  15.0  15.0  13.0  9.0  4.0  2.0  0.0  * size section 4
870501  0.0  4.64  0.0  1.0  5.0  10.0  15.0  17.0  15.0  15.0  13.0  9.0  4.0  2.0  0.0  * size section 5
*
*      <Ras> sigma          xp0  xa0          Tmn  Tmx
879101  0.0  4.64          0.0  0.0          0.0  0.0
*
*      Adhesion force mean value <Fa> calculation - model constants
*      van der Waals          Adsorbed liquid          Electrostatic          Gravity
*      A1  x1  R  xp1  xa1          A2  H  sig  xp2  xa2          A3  xE3  Cq3  Xq3          Dgrav
879201  5.0E-10  0.0  1.0E-6  0.0  0.0          0.0  0.0  0.0  0.0  0.0          9.0E9  0.5  3.8E-16  0.5          0.0
*
*      Drag force calculation
*      Xd  XL  ID
879301  0.3  1.0  1
*
*****

```

Further examples of resuspension models, including the Rock'n Roll Model, the quasi static on/off models (NRG3, NRG4) are discussed in Volume 3.

2.15.52 Record: 880000, Fission Product Main Data

The fission product chains considered by the Radioactive Particle Transport (RT) Package are very similar to the isotope chains, used by the Reactor Kinetics (RK) Package. In some cases the fission product chains may duplicate the chains from the RK package (for example the Xe-135 chain). In general, the RK chains include only those isotopes which are important for the reactivity (Xe-135, Sm-149, etc.), while the fission product chains include those isotopes which may be released from the core and thus pose a radioactive threat to the environment. In short, the difference between the isotopes which are used by the RK package and the RT package is that the former are never released from the core, while the latter do not affect the reactivity.

It was decided to adopt this modelling approach, and treat the fission product isotopes separately from the isotopes present within the RK Package for the following reason. The isotopes from the RK Package need to be solved all at once (large matrix), since they are all interconnected through the fission product yields. Only few isotopes are important for the reactivity, therefore the total size of the matrix remains relatively small. The RT package on the other hand considers large amount of short chains, with only the members of one particular chain interacting through the decay process. Therefore each short chain can be solved separately using a small matrix. If those chains were put into the common matrix together with the isotopes affecting the reactivity, a very large matrix would be created.

- W-1 (I) : IMFPRT Indicator for the initial mass of fission products in the core.
 =1 : Initial masses are calculated outside SPECTRA (for example by the ORIGEN code) and defined in records 880XXY.
 =2 : Initial masses are calculated internally by the code, using a user-defined fuel burn-up (Word 6 below).
 Acceptable range: 1 or 2.
 Default value: 2.
- W-2 (I) : IBFPRT Request for built-in isotope data (see section 2.15.111). The entry has ten-digit format: *jihgfedcba*. For each digit 0 means don't use data.
 a≠0 : use built-in data for the 131 isotope chain, (6 isotopes),
 b≠0 : use built-in data for the 132 isotope chain (3 isotopes),
 c≠0 : use built-in data for the 133/134 isotope chain (9 isotopes),
 d≠0 : use built-in data for the 134 isotope chain (3 isotopes),
 e≠0 : use built-in data for the 135/136 isotope chain (5 isotopes),
 f≠0 : use built-in data for the 137 isotope chain (4 isotopes),
 g≠0 : use built-in data for the 138 isotope chain (2 isotopes),
 h≠0 : use built-in data for the 85 isotope chain (5 isotopes),
 i≠0 : use built-in data for the 90 isotope chain (6 isotopes),
 j≠0 : use built-in data for the 106 isotope chain (3 isotopes),
 For example, to use all built in data enter 1111111111; to use all data except for the 132 chain, enter 1111111101.
 Acceptable range: IDITRK ≥ 0.
 Default value: 000000000
 (10 decay chains are used, NDCHRT=10)
- W-3 (R) : TICMRT Indicator for the transient calculation of the in-core fission product masses.

>0.0 : The in-core isotope masses are constant, and equal to the initial masses specified in records 880XXY until the time of scram. The value of TICMRT specifies the time of scram in seconds. After scram ($t > \text{TICMRT}$), the isotope decay is calculated, according to the decay chain data, specified in the records 881XXY. Use of this option means that the reactor is assumed to operate at the full power for $t < \text{TICMRT}$ (in-core isotopes are at their equilibrium) and is instantaneously shut-down at $t = \text{TICMRT}$ (the isotope production and capture ceases at that time, and only the decay mechanism remains). This option is always available, independently whether the reactor kinetics model is used or not.

≤0.0 : The in-core isotope masses are calculated according to the (variable) reactor fission power, obtained from the reactor kinetics model. The source from fission, the radioactive decay, and the neutron capture are taken into account in solving the mass balance. The source from fission is obtained from the Reactor Kinetics Package. This option is available only if the reactor kinetics model is used.

Acceptable range: all real numbers if the reactor kinetics is used.
Positive numbers if the reactor kinetics is not used.

Default value: 0.0 if the reactor kinetics model is used. 10^{10} if the reactor kinetics model is not used.

W-4 (I) : NDFPRT Indicator for normalization of decay yield fractions (see section 2.15.55). If the sum of the decay yield fractions is larger than 1.0, then the fractions will always be normalized, to give the sum of 1.0. If the sum of yield fractions is smaller than 1.0, then the fractions will, or will not be normalized to 1.0, depending on the value of this word.

1 = do not normalize fractions if sum is smaller than 1.0,
2 = normalize fractions if sum is smaller than 1.0.

Acceptable range: 1, 2.

Default value: 1 .

W-5 (I) : NCFPRT Indicator for normalization of neutron capture yield fractions (see section 2.15.56). If the sum of the yield fractions is larger than 1.0, then the fractions will always be normalized, to give the sum of 1.0. If the sum of yield fractions is smaller than 1.0, then the fractions will, or will not be normalized to 1.0, depending on the value of this word.

1 = do not normalize fractions if sum is smaller than 1.0,
2 = normalize fractions if sum is smaller than 1.0.

Acceptable range: 1, 2.

Default value: 1 .

W-6 (R) : BNUPRT Fuel burn-up, B , (MWd/kg). Used if the initial masses of the fission products need to be calculated by the code (IMFPRT=2 – see Word 1 above). The initial masses of fission product masses are calculated by integrating the isotope balance equation over the burn-up time, t_B , equal to:

$$t_B = \frac{m_{fuel}}{e} \frac{B \cdot 8.64 \times 10^{10}}{Q_R}$$

SPECTRA Code Manuals - Volume 2: User's Guide

Q_R	reactor fission power, (W) (PINIRK, see record 751000, section 2.9.5).
e	fuel enrichment, (-) (ENRFRT - Word 6 below)
m_{fuel}	total mass of fuel (fissile isotopes) in the core, (kg), calculated based on the data from the RK Package, equal to:

$$m_{fuel} = \frac{V_R M_{wf}}{A_v} \cdot \sum_{i \in fis} (N_{f,i})$$

V_R	reactor volume, (m ³) (RVOLRK, see record 751000, section 2.9.5)
$M_{w,f}$	average molar weight of the fuel (AMWFRT -Word 7)
A_v	Avogadro number (=6.022×10 ²⁶), (1/kmol)
$\sigma_{f,j}$	fission cross section for fissile material j (from the RK Package), (barn)
$N_{f,i}$	concentration of fissile material i (from the RK Package), (m ⁻³)

Acceptable range: 0.0 ≤ BNUPRT ≤ 155.0 [56]

Default value: 80.0.

Note: there is an internal limit on $t_B = 1.0$ s. Therefore reducing BNUPRT below the values corresponding to $t_B = 1.0$ s will not have any effect on the results. The value of t_B is printed in the SPECTRA output file below the value of BNUPRT, as BTIMRT:

```
AVERAGE FUEL BURN-UP          BNUPRT = 1.00000E-06 [Mwd/kg]
CORRESPONDING BURN-UP TIME    BTIMRT = 9.56688E-01 [s]
```

Reducing the value of BNUPRT further will not have any effect, because with the current value of BNUPRT, BTIMRT is already smaller than 1.0 s.

W-7 (R) : ENRFRT Fuel enrichment, e , (-). Used if the initial masses of the fission products need to be calculated by the code (see Words 1 and 6 above).
Acceptable range: 0.01 ≤ ENRFRT ≤ 0.99.
Default value: 0.05.

W-8 (R) : AMWFRT Average molar weight of fuel, M_f , (-). Used if the initial masses of the fission products need to be calculated by the code (see Words 1 and 6 above).
Acceptable range: 200.0 ≤ AMWFRT ≤ 250.0.
Default value: 235.0.

W-9 (I) : ISRGRT Global activator of a sorption model on all surfaces of Solid Heat Conductors (SC/TC).
 = 0: The global activator is off. The sorption sorption model may be specified individually for each SC and TC in the records 395XXX, 495XXX.
 ≠ 0: The sorption set number ISRGRT is activated globally for all SC/TC surfaces. The sorption model may be changed individually for each SC and TC in the records 395XXX, 495XXX.
Acceptable range: 0 or a number of an existing sorption set
Default value: 0

SPECTRA Code Manuals - Volume 2: User's Guide

- W-10 (I) : IMEART Acceptance of mass error for Solid Heat Conductors (SC/TC).
 = 1: Mass error not accepted. Time step reduction is performed.
 = 2: Mass error is accepted. No time step reduction.
 Acceptable range: 1 or 2
 Default value: 1
- W-11 (R) : AMFPRT End-of-time-step error correction for fission product masses.
 ≤ 0.0 : End-of-time-step error correction is not performed.
 > 0.0 : End-of-time-step error correction is performed. If at the end of
 time step the relative mass error of fission products is smaller than
 AMFPRT, then all masses are rescaled to eliminate the mass error made
 during time step. If the mass error is larger than AMFPRT, an error
 message is printed and calculations are stopped.
 Note: mass conservation is possible only if:
 (1) fission products cannot flow to/from time-dependent CVs
 (2) there is no sorption on surfaces linked to time-dependent CVs
 (3) all daughter products of radioactive decay are tracked
 (full radioactive chains)
 If (1), (2), or (3) is not fulfilled, AMFPRT should be set to ≤ 0.0 .
 Acceptable range: AMFPRT ≤ 1.0
 Default value: 0.0 if (1), (2), or (3) is not fulfilled
 10^{-2} otherwise
- W-12 (I) : IDESRT Indicator on desorption calculations on gas-covered surfaces.
 = 1: Full calculations. Desorbed masses are taken into account in the
 fluid flow solution.
 = 2: Desorbed masses are not taken into account in the fluid flow
 solution. When large time steps are used, desorption may cause
 numerical problems. This option may be useful in obtaining fast results
 if desorption is small and can be neglected.
 Acceptable range: 1 or 2
 Default value: 1

2.15.53 Records: F05XXY, Fission Product Data - Isotope Names

XX is the isotope chain reference number, $01 \leq XX \leq 99$. The chain numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK >0), then the user-defined chains must have higher numbers than the mapped chains. The recommended numbers are $XX > 20$. The maximum number of chains is 24. Y is the isotope number within the chain XX. The isotope numbers must be consecutive (starting with 01).

- W-1 (A) : NMPRT User defined name, length up to 7 characters. The name is read as a 7-
 character string, starting from the first non-blank character after the
 record identifier. There must be at least one blank character, separating
 the name from the record identifier. Examples of the isotope names are:
 I-131, Xe-131m.
 Acceptable range: any string of up to 7 characters.
 Default value: 7 "underline" characters: " _ " .

2.15.54 Records: 880XXY, Fission Product Data – Initial Masses, Molar Weights, etc.

XX is the isotope chain reference number, $01 \leq XX \leq 99$. The chain numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK>0), then the user-defined chains must have higher numbers than the mapped chains. The recommended numbers are $XX > 20$. The maximum number of chains is 24. Y is the isotope number within the chain XX. The isotope numbers must be consecutive (starting with 01).

- W-1 (R) : XMPRT Initial mass of the isotope XXY, (kg) in the core. Used if the initial masses are not calculated by the code, i.e. IMFPRT = 1 (see record 880000).
Acceptable range: XMPRT \geq 0.0.
Default value: 0.0.
- W-2 (R) : WMPRT Molar weight of the isotope XXY, (kg/kmol).
Acceptable range: $1.0 \leq$ WMPRT \leq 250.0.
Default value: available if the built-in isotope data is requested (see Figure 2-83 through Figure 2-91).
- W-3 (R) : EBFRT Fraction of the decay energy carried by the beta particle, E_β , (-).
Acceptable range: $0.0 \leq$ EBFRT \leq 1.0.
Default value: $1.0 -$ EGFRT, where EGFRT is the fraction of energy carried by the gamma radiation, defined below.
- W-4 (R) : EGFRT Fraction of the decay energy carried by the gamma radiation, E_γ , (-).
Acceptable range: $0.0 \leq$ EGFRT \leq 1.0.
Default value: available if the built-in isotope data is requested (see Figure 2-83 through Figure 2-91). Each of the built-in isotopes has its default energy fractions. In case of beta decay (β^-) both beta and gamma fractions are assumed to be 0.5, following [35]. In case of Isomeric Transition (IT) the gamma fraction is of course equal to 1.0. If more than one decay mode is possible (for example Te-131m - Figure 2-83), then the average energy fraction is calculated using the decay yields as weighting factors. For example, Te-131m experiences β^- decay with the yield of $\gamma_d = 77.8\%$, and Isomeric Transition, with the yield of $\gamma_d = 22.2\%$ (Figure 2-83). The average energy fraction is obtained from: $E_\gamma = 0.778 \times 0.5 + 0.222 \times 1.0 = 0.611$.
- W-5 (R) : YFFRT Average yield of the isotope XXY from fission, γ_f , (-). The fission yields are not used if the initial masses of isotopes are specified from external calculations (IMFPRT = 1 – see section 2.15.52).
Acceptable range: $0.0 \leq$ YFFRT \leq 2.0.
Default value: available if the built-in isotope data is requested (see Figure 2-83 through Figure 2-91). The built-in fission yields are those for fission of U-235.

SPECTRA Code Manuals - Volume 2: User's Guide

Example:

The following input defines one average yield, appropriate for U-235 (3.513%):

```
F05371 Kr-88
*      M-core MW beta gamma fission yield
880371 0 88 0.159 0.841 3.513E-02
```

Using the following inputs, the user may define individual yield fractions, specific to all fissile isotopes in the problem. If the input entries are present, there must be exactly the same values as the number of fissile isotopes (isotopes with positive fission cross section, SFITRK>0.0) present in the RK Package. Zeroes may be entered; in such case the value will be set to the average yield, YFFPRT.

W-6 (R) : YIFPRT(1) Individual yield of the isotope XXY from the first fissile isotope in the Reactor Kinetics Package.
Acceptable range: $0.0 \leq YIFPRT(1) \leq 1.0$.
Default value: YFFPRT

W-7 (R) : YIFPRT(2) Individual yield of the isotope XXY from the second fissile isotope in the Reactor Kinetics Package.
Acceptable range: $0.0 \leq YIFPRT(2) \leq 1.0$.
Default value: YFFPRT

[. . .] until the yields are defined for all fissile isotopes.

Example:

In the example below, the fission yields of Kr-88 are defined. The yields of Kr-88 are equal to:

- U-235: 3.513%
- Pu-239: 1.272%
- Pu-241: 0.9765%

Assuming that all default fuel chains are present, the fissile isotopes are:

- U-233, U-235, U-239, Pu-239, Pu-241.

The following input defines individual yields for the Pu fuels.

```
F05371 Kr-88
*
*      M-core MW beta gamma fission yield individual fission yields
*      U-233 U-235 U-239 Pu-239 Pu-241
880371 0 88 0.159 0.841 3.513E-02 0 0 0 1.272E-02 9.765E-3
```

In this case the fission yields for all Uranium isotopes is 3.513E-2. The actual fission yield will be determined based on the current fuel composition, using the values of YIFPRT. The value of YFFPRT is serving only as a definition of the default value. The correctness of input may be checked in the *.OUT file, where it is printed in the following block:

```
=RT= INDIVIDUAL FISSION YIELDS FOR 5 DECAY CHAINS

GLOBAL INDIVIDUAL FOR FISSION ISOTOPES, YIFPRT:
YFFPRT U-233 U-235 U-239 Pu-239 Pu-241
-----
371 Kr-88 3.51300E-02 3.51300E-02 3.51300E-02 3.51300E-02 1.27200E-02 9.76500E-03
```


the sum of 1.0. If the sum of all yield fractions is smaller than 1.0, then the yield fractions will not be normalized, unless the normalization is requested by the user, through word 4 in record 880000 (section 2.15.52).

Note!

No individual fission yields are defined for the built-in isotopes, shown in section 2.15.111. However, if mapping from the RK chains (section 2.9.36) to the RT Package is requested (IMAPRK>0), and the first two chains (the $^{233}\text{U} / ^{235}\text{U}$ fuel chain and the $^{239}\text{U} / ^{239}\text{Pu} / ^{241}\text{Pu}$ fuel chain) are mapped, then the individual yields are defined for the next three chains: ^{135}Xe , ^{149}Sm , and ^{157}Gd chains, if they are mapped. The individual yields for those three chains are shown in section 2.9.36.

2.15.56 Records: 882XXY, Fission Product Data – Neutron Capture Data

XX is the isotope chain reference number, $01 \leq \text{XX} \leq 99$. The chain numbers need not be consecutive, however, if the mapping from RK package is requested (IMAPRK>0), then the user-defined chains must have higher numbers than the mapped chains. The recommended numbers are $\text{XX} > 20$. The maximum number of chains is 24. Y is the isotope number within the chain XX. The isotope numbers must be consecutive (starting with 01). Neutron capture data is not used if the initial masses of isotopes are specified from external calculations (IMFPRT = 1 – see section 2.15.52).

- W-1 (R) : SCFPRT Microscopic cross section for neutron capture, σ_c , (barn), for the isotope XXY.
Acceptable range: SCFPRT \geq 0.0.
Default value: available if the built-in isotope data is requested (see Figure 2-83 through Figure 2-91).
- W-2 (I) : J1 Reference number of the capture product.
Acceptable range: must be one of the isotopes in the chain XX.
Default value: none.
- W-3 (R) : YCFPRT Yield fraction of the isotope J1 from neutron capture in XXY, (-).
 (J1) This number is interpreted as a probability of the fact that a neutron capture by a nuclide of the isotope Y from the chain XX will result in production of a nuclide of the isotope J1 from the same chain.
Acceptable range: YCFPRT \geq 0.0 .
Default value: available if the built-in isotope data is requested (see Figure 2-83 through Figure 2-91). A small number, $< 10^{-50}$, sets the built-in value to 0.0.
- W-4 (I) : J2 Reference number of the capture product.
Acceptable range: must be one of the isotopes in the chain XX.
Default value: none.
- W-5 (R) : YCFPRT Yield fraction of the isotope J2 from neutron capture in XXY, (-).
 (J2) This number is interpreted as a probability of the fact that a neutron capture by a nuclide of the isotope Y from the chain XX will result in production of a nuclide of the isotope J2 from the same chain.
Acceptable range: YCFPRT \geq 0.0 .

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: available if the built-in isotope data is requested (see Figure 2-83 through Figure 2-91). A small number, $<10^{-50}$, sets the built-in value to 0.0.

... until all decay products are defined.

Note!

If the sum of all yield fractions is larger than 1.0, then the yield fractions will be normalized, to give the sum of 1.0. If the sum of all yield fractions is smaller than 1.0, then the yield fractions will not be normalized, unless the normalization is requested by the user, through word 5 in record 880000 (section 2.15.52).

2.15.57 Record: 883000, Definition of Fuel Regions for FP Release

The maximum number of fuel regions is $NLOMRT = 200$. The total mass of fission products, as specified in the records 880XXY, or calculated internally by the code, is assumed to be located within solid structures – 1-D or 2-D Solid Heat Conductors, representing the fuel. The properties of the fuel regions as well as the distribution (mass fraction) of fission products is specified in this record. This record must be specified if the reactor kinetics is not used. If the reactor kinetics is used and this record is not present, then the mass fractions are assumed to be the same as the fuel temperature weighting factors, defined in the record 791XXX (section 2.9.18).

- W-1 (I) : L1FPRT Fuel region indicator 1.
 =1: this fuel region is represented by a 1-D Solid Heat Conductor,
 =2: this fuel region is represented by a 2-D Solid Heat Conductor.
Acceptable range: 1 or 2 .
Default value: if the reactor kinetics model is used, the default values are equal to the regions indicators ITF1RK, specified for the fuel temperature weighting factor in record 791XXX. In this case the region indicator ITF1RK must refer to a 1-D or 2-D Heat Conductor (=1 or 2).
- W-2 (I) : L2FPRT Fuel region indicator 2. Equal to:
 Reference number of a 1-D Solid Heat Conductor, if L1FPRT = 1,
 Reference number of a 2-D Solid Heat Conductor, if L1FPRT = 2.
Acceptable range: Must be a valid reference number of a 1-D or a 2-D Solid Heat Conductor.
Default value: if the reactor kinetics model is used, the default values are equal to the regions indicators ITF2RK, specified for the fuel temperature weighting factor in record 791XXX.
- W-3 (R) : FRFPRT Fraction of total mass of fission products present in the region defined by L1FPRT and L2FPRT.
Acceptable range: $0.0 \leq FRFPRT \leq 1.0$.
Default value: if the reactor kinetics model is used, the default values are equal to the fuel temperature weighting factors, WTFRRK, specified in record 791XXX. In

SPECTRA Code Manuals - Volume 2: User's Guide

this case the region indicator ITF1RK must refer to a 1-D or 2-D Heat Conductor (=1 or 2).

- W-4 (R) : SOVFRT Value of the surface to volume ratio (S/V) for release calculation. The release rates calculated by the CORSOR-M or ARSAP model are multiplied by this value, and divided by the CORSOR-M reference value (see record 890000) or ARSAP reference value (see record 891000). A negative value will disable the use of (S/V) for release calculation (i.e. the CORSOR-M and ARSAP model will be used).
Acceptable range: $10.0 \leq \text{SOVFRT} \leq 10000.0$, or $\text{SOVFRT} < 0.0$.
Default value: $2.0/R_f$ for rectangular and cylindrical geometry.
 $3.0/R_f$ for spherical geometry, where R_f is the fuel radius, obtained as the outer radius of the cell:
 NGFRSC-1, if the gap model is present, or
 NCELSC-1, if no gap model is present
- W-5 (I) : N1FPRT Boundary cell indicator for cladding failure calculation (see record 883101). The cladding temperature for failure criterion will be taken from the cell N1FPRT of the SC with a reference number L2FPRT (if L1FPRT=1), or from the boundary cell number N1FPRT of the TC with a reference number L2FPRT (if L1FPRT=2).
Acceptable range: Must be a boundary cell of a 1-D or a 2-D Solid Heat Conductor. This means:
 =1 (left) or 2 (right), in case of SC
 =1 ÷ NBCLTC, in case of TC
Default value: =2, in case of SC (L2FPRT=1),
 =NBCLTC, in case of TC (L2FPRT=2).

The set of five words defined above is repeated until all fuel regions are described. The total number of entries in this record must be a multiple of 5. If the Reactor Kinetics Package is used, the total number of core regions must be the same as the number of the weighting factors in the Reactor Kinetics Package.

2.15.58 Record: 883101, Definition of Cladding Failure Criteria

This record defines the cladding failure criteria to be used for each fuel region, defined in the record 883000. If a cladding failure criterion is used for a given region, then the released fission products are kept within the fuel until the cladding fails. Afterwards they are released to the atmosphere of the Control Volume adjacent to the 1-D or 2-D Solid Heat Conductor representing this fuel region. If a cladding failure criterion is not used for a given region, then the released fission products are instantaneously released to the atmosphere of the Control Volume adjacent to the 1-D or 2-D Solid Heat Conductor representing this fuel region.

W-1 (I) : ICFCRT(1) Indicator defining the cladding failure criterion for the fuel region 1 (fuel regions are defined in the record 883000).
=0: no cladding failure criterion is used for this region
>0: cladding failure criterion is defined using a Tabular Function with the reference number equal to ICFCRT. The Tabular Function must be defined as to give a failure temperature (K), as a function of an oxidized cladding fraction (-). For example, the following TF:

Oxidized frac.(-)	Failure Temp. (K)
0.00	1300.0
0.50	1000.0
1.00	300.0

defines the failure temperature as equal to 1300 K for un-oxidized cladding, decreasing to 1000.0 K in case of 50% oxidation, and further to 300.0 K in case of full oxidation.

Acceptable range: Must be a valid reference number of a Tabular Function, if non-zero.

Default value: none.

W-2 (I) : ICFCRT(2) Indicator defining the cladding failure criterion for the fuel region 2.
Acceptable range: Must be a valid reference number of a Tabular Function, if non-zero.
Default value: none.

. . until the cladding failure criteria are defined for all fuel regions. (Fuel regions are defined in the record 883000.)

2.15.59 Record: 883102, Initial Cladding State

This record defines the initial cladding state for each fuel region, defined in the record 883000. If a cladding failure criterion is used for a given region, then the cladding may be initially intact or failed, depending on the data entered in this record. Typically the cladding is initially intact, however it may be initially failed for example in case of continuation of an earlier calculation (when the initial condition file, *.ICF, from a previous run is used, the initial cladding state is taken from this file).

W-1 (I) : ICFLRT(1) Cladding initial state for the fuel region 1 (fuel regions are defined in the record 883000).
=0: intact

SPECTRA Code Manuals - Volume 2: User's Guide

=1: failed
Acceptable range: 0 or 1.
Default value: 0.

W-2 (I) : ICFCRT(2) Cladding initial state for the fuel region 2.
Acceptable range: 0 or 1.
Default value: 0.

.. until the cladding initial state is defined for all fuel regions. (Fuel regions are defined in the record 883000.)

2.15.60 Record: 8832XX, Definition of Common Fuel Regions for Cladding Failure

XX is the common fuel region for cladding failure (single fuel rod). The region numbers must be consecutive (starting with 01). The common regions are introduced for the following reason. If a fuel rod is represented by several Solid Heat Conductors (there is an axial division of the fuel rods), then cladding failure in only one of these Solid Heat Conductors is needed to release the fission products present in the gap of all other Solid Heat Conductors. Therefore the common fuel regions must reflect the axial nodalization of the fuel rods.

If the SC gap model is used, and the SC fuel regions are defined in the record 340000, the common fuel regions for gap calculations in the SC Package (records 3402XX) must be consistent with the common fuel regions for cladding failure in the RT Package, defined in this record. The maximum number of fuel regions is NLOMRT = 200.

W-1 (I) : IICFRT(1) Fuel region number IICFRT(1) (defined in the record 883000) belongs to the common fuel region XX. Cladding failure in any of the regions belonging to the common region XX results in gap release from all fuel regions belonging to the common region XX.
Acceptable range: must be one of the core regions defined in records 883000.
Default value: XX.

W-2 (I) : IICFRT(2) Fuel region number IICFRT(2) (defined in the record 883000) belongs to the common fuel region XX. Cladding failure in any of the regions belonging to the common region XX results in gap release from all fuel regions belonging to the common region XX.
Acceptable range: must be one of the core regions defined in records 883000.
Default value: none.

W-3 (I) : IICFRT(3) Fuel region number IICFRT(3) (defined in the record 883000) belongs to the common fuel region XX. Cladding failure in any of the regions belonging to the common region XX results in gap release from all fuel regions belonging to the common region XX.
Acceptable range: must be one of the core regions defined in records 883000.
Default value: none.

. . . until all members of the common fuel regions are defined. The maximum number of fuel regions per a single common fuel region is NLOMRT = 200.

2.15.61 Record: 884XXY, Initial Fractions of Released (Gap) Fission Products

XX is the isotope chain reference number, $01 \leq XX \leq 99$. The chain numbers need not be consecutive. The maximum number of chains is 24. Y is the isotope number within the chain XX. The isotope numbers must be consecutive (starting with 01).

W-1 (R) : RFRAC(1) Mass fraction of the isotope XXY that is initially outside fuel (gap) in the fuel region 1.
Acceptable range: $0.0 \leq \text{RFRAC}(1) \leq 1.0$.
Default value: 0.0.

W-2 (R) : RFRAC(2) Mass fraction of the isotope XXY that is initially outside fuel (gap) in the fuel region 2.
Acceptable range: $0.0 \leq \text{RFRAC}(2) \leq 1.0$.
Default value: 0.0.

. . . until the released fractions for all fuel regions are defined. (Fuel regions are defined in the record 883000.)

2.15.62 Record: 885000, Release Model Indicator

W-1 (I) : MFPRRT Release model indicator.
= 0: do not apply any release model
= 1: CORSOR-M model (LWR reactors)
= 2: ARSAP model (LWR reactors)
= 3: HTR-FPR model (HTR reactors)
Acceptable range: 0, 1, 2, 3.
Default value: 0

W-2 (R) : CFPRRT Constant in the HTR-FPR model. Used only if MFPRRT = 3.
Acceptable range: $1.0 \leq \text{CFPRRT} \leq 5.0$
Default value: 3.0

2.15.63 Record: 885XXY, Release Classes

XX is the isotope chain reference number, $01 \leq XX \leq 99$. The chain numbers need not be consecutive. The maximum number of chains is 24. Y is the isotope number within the chain XX. The isotope numbers must be consecutive (starting with 01).

W-1 (I) : KFPRRT Release class indicator for the isotope XXY.
 =0: do not apply any release model for this isotope.
 >0: release class number. A built-in release model, defined in the record 885000 will be used, with the coefficient set applicable for the release class number KFPRRT.
 <0: use Control Function number |KFPRRT| to determine the release rate, R , (1/s). The release rate is defined as a fraction of the mass that is released per second:

$$R = \frac{1}{m} \frac{dm}{dt}$$

Acceptable range: must be a valid release class if positive, or a valid reference number of a Control Function if negative.
Default value: available if the built-in isotope data is requested (see Figure 2-83 through Figure 2-91).

2.15.64 Record: 886000, Fission Product Condensation

W-1 (I) : IFPCRT Fission product vapor condensation indicator.
 = -1 or 1: inactive.
 = 2: active. Condensation occurs when vapor pressure exceeds saturation pressure, defined for each vapor class in the records 886XXY.
Acceptable range: -1, 1, 2
Default value: 2

W-2 (I) : IASCRT Condensation of fission product vapors creates aerosols of the size section IASCRT.
Acceptable range: 1, 2, ..., NSIZRT (see record 861000)
Default value: NSIZRT

W-3 (I) : JASCRT Coagulation of aerosols created by condensation (section IASCRT).
 = -1 or 1: section IASCRT does not coagulate with other sections
 = 2: section IASCRT does coagulate with other sections
Acceptable range: -1, 1, 2
Default value: -1

W-4 (I) : ISATRT Saturation pressure calculation option.
 = 1: saturation pressure, as defined in records 8930XX, is used for every isotope of a given vapor class. For example, suppose the vapor class 4 consists of I-131 and Br-83. With this option the vapor pressure of each isotope may be as high as the saturation pressure for the vapor class 4. This is correct because I-131 and Br-83 are different chemical elements.

Since their properties are considered similar, they are grouped into the same vapor class, thus have the same saturation pressure, defined in 893004. However, the partial pressure of each of these elements is independent and may increase up to the saturation pressure.

= 2: saturation pressure, as defined in records 8930XX, is used for total vapor class. For example, suppose the vapor class 4 consists of I-131 and I-133. With this option the total vapor pressure of both isotopes may be as high as the saturation pressure for the vapor class 4. This is correct because I-131 and I-133 are both the same chemical element.

Acceptable range: 1, 2

Default value: 1

Note: clearly the saturation pressure treatment is not completely general. For example, neither option would be exactly correct if the vapor class 4 consisted of I-131, I-133, and Br-83. The default value was chosen to maximize the amount of vapor, which in general is more conservative. If the user wishes to have more appropriate treatment in such case, the best is to create a new vapor class, with properties such as saturation pressure and release coefficient, the same as the vapor class 4, and move Br-83 into this new class.

2.15.65 Record: 886XXY, Fission Product Vapor Pressure and Diffusion Volume

XX is the isotope chain reference number, $01 \leq XX \leq 99$. The chain numbers need not be consecutive. The maximum number of chains is 24. Y is the isotope number within the chain XX. The isotope numbers must be consecutive (starting with 01).

W-1 (I) : KFPVRT Indicator defining the vapor pressure for the isotope XXY.
=0: do not apply any vapor pressure model for this isotope. This isotope will form solid (or liquid) aerosols, but will never be evaporated to become gas.
>0: use vapor pressure coefficient set appropriate for the vapor class number KFPVRT, defined in the record 8930XX (XX=KFPVRT), see Table 2-40.

Acceptable range: must be a number of an existing release class, defined in the records 8930XX.

Default value: available if the built-in isotope data is requested.

W-2 (R) : SGFPRT Diffusion volume, Σ , of the isotope XXY. If a positive value is used, then the diffusion coefficient for fission product vapor diffusion in the atmosphere gas of a Control Volume is calculated from the general method, applicable for any gas mixture. If the diffusion volume for a particular element or compound is not available, then the following correlations are recommended to calculate the value of Σ (see Volume 1):

Elements: $\Sigma = 2.4 \cdot A^{0.66}$

Compounds: $\Sigma = 4.2 \cdot A^{0.66}$

A is the atomic number of the isotope XXY.

The diffusion volume is used to calculate diffusion coefficients, needed if the diffusion model is activated for junction flows (IDIFJN=2, record 256XXX).

Acceptable range: $0.0 \leq SGFPRT \leq 1000.0$

Default value: 0.0

2.15.66 Record: 8900XX, Fission Product Release Coefficients – CORSOR-M Model

XX is the release class number, $01 \leq XX \leq 20$. The class numbers, XX, must be consecutive. These records define coefficients for the CORSOR-M [35] fission product release model.

Each fission product, which can be released from the fuel and whose release is not determined by a user-defined Control Function, needs to be associated with one of the release class (the associations are specified in the records 883XXX), defined in these records (and 8910XX) as well as one of the fission product vapor class, defined in the records 8930XX. The release classes and the vapor classes are independent, and therefore the same isotope may be associated with a release class and a vapor class with different numbers. The fission product classes are shown in Table 2-40. The coefficients shown in Table 2-42 and Table 2-45 are specified based on reference [35]. For some classes the coefficients were modified, as described in Volume 1. The class numbering from reference [35] was preserved, therefore the release class and the vapor class for a given isotope have the same number. The CORSOR-M release rate given by:

$$R = A \cdot \exp\left(-\frac{B}{T}\right)$$

where: *R* - release rate, (1/s)
 A - fractional release rate coefficient, (1/s)
 B - release constant, (K)

Note that [35] uses somewhat different formulation and units:

$$R = k_0 \cdot \exp\left(-\frac{Q}{RT}\right)$$

where: *R* - release rate, (1/min)
 *k*₀ - fractional release rate coefficient, (1/min)
 Q - release constant, (kcal/mol)
 R - gas constant, equal to 1.987×10^{-3} (kcal/mol/K)

Conversion to the SI units (used by SPECTRA) is quite simple: $A = k_0 / 60.0$, $B = Q / R = Q / 1.987 \times 10^{-3}$. The release coefficients from [35] and the conversion to the SI units is shown in Table 2-41. The release rate equations, as applied in SPECTRA (SI units) for 12 release classes, defined following [35], are shown in Table 2-42.

W-1 (R) : AFPRRT Fractional release rate, *A*, (1/s), for the CORSOR-M model, release class XX.
 Acceptable range: $0.0 \leq \text{AFPRRT} < 1.0 \times 10^{10}$.
 Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default CORSOR-M model coefficients are shown in Table 2-41 and Table 2-42.

W-2 (R) : BFPRRT Release constant, *B*, (K), for the CORSOR-M model, release class XX.
 Acceptable range: $0.0 \leq \text{BFPRRT} < 1.0 \times 10^5$.
 Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default

Table 2-42 Release rate formulae, CORSOR-M model, SI units.

Class	A	B
1:	R = 3.333E+03	exp (- 32108.7 / T)
2:	R = 3.333E+03	exp (- 32108.7 / T)
3:	R = 1.583E+05	exp (- 50427.8 / T)
4:	R = 3.333E+03	exp (- 32108.7 / T)
5:	R = 3.333E+03	exp (- 32108.7 / T)
6:	R = 3.333E+08	exp (- 76899.8 / T)
7:	R = 5.000E+02	exp (- 32712.6 / T)
8:	R = 4.450E+06	exp (- 94715.7 / T)
9:	R = 2.433E+05	exp (- 72018.1 / T)
10:	R = 2.433E+05	exp (- 72018.1 / T)
11:	R = 1.317E+02	exp (- 30900.9 / T)
12:	R = 1.317E+03	exp (- 30900.9 / T)

2.15.67 Record: 890000, CORSOR-M Model Constants

W-1 (R): SOVCRT Reference value for surface to volume ratio $(S/V)_{\text{CORSOR-M}}$ for the CORSOR-M model. The release rates calculated by the CORSOR-M model are multiplied by the actual (S/V) (see record 883000), and divided by the reference value:

$$R = R_{\text{CORSOR-M}} \times (S/V) / (S/V)_{\text{CORSOR-M}}$$

Acceptable range: 10.0 ≤ SOVCRT ≤ 10000.0.

Default value: 422.5 [35].

W-2 (I): ITCCRT This word defines how the temperature T (needed for the CORSOR-M model release calculation) is obtained.
 =1: always use maximum cell temperature of the SC or TC of a given fuel region (SC/TC are assigned to fuel regions in record 883000).
 =2: always use cell average temperature of the SC or TC of a given fuel region (SC/TC are assigned to fuel regions in record 883000).

Acceptable range: 1 or 2.

Default value: 1.

2.15.68 Record: 8910XX, Fission Product Release Coefficients – ARSAP Model

XX is the release class number, $01 \leq XX \leq 20$. The class numbers, XX, must be consecutive. These records define coefficients for the ARSAP (Advanced Reactor Severe Accident Program) [36] fission product release model.

The ARSAP model is used [36], with the release rate given by:

$$R = \frac{C}{R_g} \cdot \exp\left(-\frac{c_1}{T}\right)$$

SPECTRA Code Manuals - Volume 2: User's Guide

where: R - release rate, (1/s)
 C, c_1 - coefficients
 R_g - grain size, (m) (RGARRT, record 891000)
 T - minimum of the current temperature the FCI temperature, (K)
 T_{FCI} - fuel-cladding interaction (FCI) temperature, (K) (TFCIRT, record 891000)

Note that [36] uses somewhat different formulation:

$$R = \frac{1}{R_g} \cdot \exp\left(-\frac{c_1}{T} + c_2\right)$$

In order to be consistent with the formulation of the CORSOR-M model, the above equation has been transformed in SPECTRA. The transformation is simple: $C = \exp(c_2)$. The release coefficients from [36] and the conversion to the SI units is shown in Table 2-43. The class numbering scheme from the CORSOR-M model (from [35]) was preserved here to avoid confusion. Therefore the elements shown in Table 2-43 are not in the same order as they are appearing in reference [36]. The release rate equations, as applied in SPECTRA for the 12 release classes, are shown in Table 2-44.

The principal differences between the ARSAP and CORSOR-M models are (apart from different values of coefficients): the use of grain size and the FCI temperature in ARSAP.

- W-1 (R) : CCARRT Coefficient C , (K), for the ARSAP model, release class XX.
Acceptable range: $0.0 \leq CCARRT < 1.0 \times 10^{15}$.
Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default ARSAP model coefficients are shown in Table 2-43 and Table 2-44.
- W-2 (R) : C1ARRT Coefficient c_1 , (K), for the ARSAP model, release class XX.
Acceptable range: $0.0 \leq C2ARRT < 1.0 \times 10^6$.
Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default ARSAP model coefficients are shown in Table 2-43 and Table 2-44.
- W-3 (R) : RMINRT Minimum release rate for the release class XX, R_{min} , (1/s).
Acceptable range: $0.0 \leq RMINRT \leq 1.0 \times 10^{-5}$.
Default value: 0.0.

SPECTRA Code Manuals - Volume 2: User's Guide

Table 2-43 Built-in release coefficients, ARSAP [36].

Release class	Elements, [36]	C, (s ⁻¹), (=exp(c ₂))	c ₁ , (K)
1	Krypton, Kr	exp(-1.49D+00) = 2.254E-01	37300.0
2	Cesium, Cs	exp(1.34D+00) = 3.819E+00	43000.0
3	Barium, Ba	exp(-2.20D+00) = 1.108E-01	45900.0
4	Iodine, I	exp(9.36D-01) = 2.550E+00	42100.0
5	Tellurium, Te	exp(1.19D+00) = 3.287E+00	44500.0
6	-	0.0	0.0
7	Molybdenum, Mo	exp(-4.94D+00) = 7.155E-03	34900.0
8	Cerium, Ce	exp(20.20D+00) = 5.926E+08	119000.0
9	Neodymium, Nd	exp(24.00D+00) = 2.649E+10	130000.0
10	-	0.0	0.0
11	Antimony, Sb	exp(-1.19D+00) = 3.042E-01	41500.0
12	-	0.0	0.0

Table 2-44 Release rate formulae, ARSAP model, $T = \text{Min}(T_{fuel}, T_{MCI})$.

Class	C	c1
1:	$R = (2.254E-01 / R_g) \exp(-37300.0 / T)$	
2:	$R = (3.819E+00 / R_g) \exp(-43000.0 / T)$	
3:	$R = (1.108E-01 / R_g) \exp(-45900.0 / T)$	
4:	$R = (2.550E+00 / R_g) \exp(-42100.0 / T)$	
5:	$R = (3.287E+00 / R_g) \exp(-44500.0 / T)$	
6:	$R = (0.000E+00 / R_g) \exp(-0.0 / T)$	
7:	$R = (7.155E-03 / R_g) \exp(-34900.0 / T)$	
8:	$R = (5.926E+08 / R_g) \exp(-119000.0 / T)$	
9:	$R = (2.649E+10 / R_g) \exp(-130000.0 / T)$	
10:	$R = (0.000E+00 / R_g) \exp(-0.0 / T)$	
11:	$R = (3.042E-01 / R_g) \exp(-41500.0 / T)$	
12:	$R = (0.000E+00 / R_g) \exp(-0.0 / T)$	

2.15.69 Record: 891000, ARSAP Model Constants

This record defines constants for the alternative fission product release correlation – ARSAP (Advanced Reactor Severe Accident Program) [36].

W-1 (R): SOVART Reference value for surface to volume ratio $(S/V)_{ARSAP}$ for the ARSAP model. The release rates calculated by the ARSAP model are multiplied by the actual (S/V) (see record 883000), and divided by the reference value:

$$R = R_{ARSAP} \times (S/V) / (S/V)_{ARSAP}$$

Acceptable range: $10.0 \leq \text{SOVART} \leq 10000.0$.

Default value: 422.5.

W-2 (R): RGARRT Equiaxed grain size R_g , (m), for the ARSAP model, all release classes.
Acceptable range: $1.0 \times 10^{-6} \leq \text{RGARRT} \leq 1.0 \times 10^{-3}$.

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: 3.0×10^{-5} based on VI and VECTORS tests (see Volume 3), [36] recommends 10^{-5} .

W-3 (R) : TFCIRT Fuel-cladding interaction (FCI) temperature, T_{FCI} , (K), for the ARSAP model, all release classes.
Acceptable range: $2000.0 \leq TFCIRT \leq 3000$.
Default value: 2500.0 based on VI and VECTORS tests (see Volume 3), [36] recommends 2000.0.

W-2 (I) : ITCART This word defines how the temperature T (needed for the ARSAP model release calculation) is obtained.
=1: always use maximum cell temperature of the SC or TC of a given fuel region (SC/TC are assigned to fuel regions in record 883000).
=2: always use cell average temperature of the SC or TC of a given fuel region (SC/TC are assigned to fuel regions in record 883000).
Acceptable range: 1 or 2.
Default value: 1.

2.15.70 Record: 892XXX, Fission Product Release Coefficients – HTR-FPR Model

XXX is the fuel region number, $001 \leq XXX \leq 200$. These records define coefficients for the HTR (High Temperature Reactor) fission product release model. The model is applicable to TRISO particles in graphite matrix, either in pebble bed, or in prismatic block reactors.

W-1 (R) : BTRIRT Relative burn-up, B , (-). $B=0.0$: fresh fuel, $B=1.0$: maximum burn-up, equal to 80,000 MWh/t.
Acceptable range: $0.0 \leq BTRIRT \leq 2.0$. A warning message is issued if the value is > 1.0 .
Default value: 0.0

W-2 (I) : ITRIRT Model determining the failed fraction of TRISO particles.
Acceptable range: 1 or a reference to a Control Function
Default value: 0.0
= 1 : use built-in correlation, which provides the failed fraction, F , as a function of temperature, T , and fuel burn-up, B (see Volume 1)
< 0 : Failed fraction is given by Control Function with the number $|ITRIRT|$. It must be a 2-D Tabular Function with the first arguments being the temperature (T) and the second argument being the the relative burnup (B). The values of T and B are those for the fuel region XXX, therefore the same CF may be used for multiple fuel regions. The actual arguments entered for the CF are not used for failed fraction calculation (they will only be used to calculate the value of CF printed in the CF block output).
The following limits are set internally on the value obtained from the Control Function: $0.0 \leq F(T,B) \leq 1.0$
Acceptable range: 1 or reference to a CF
Default value: 1

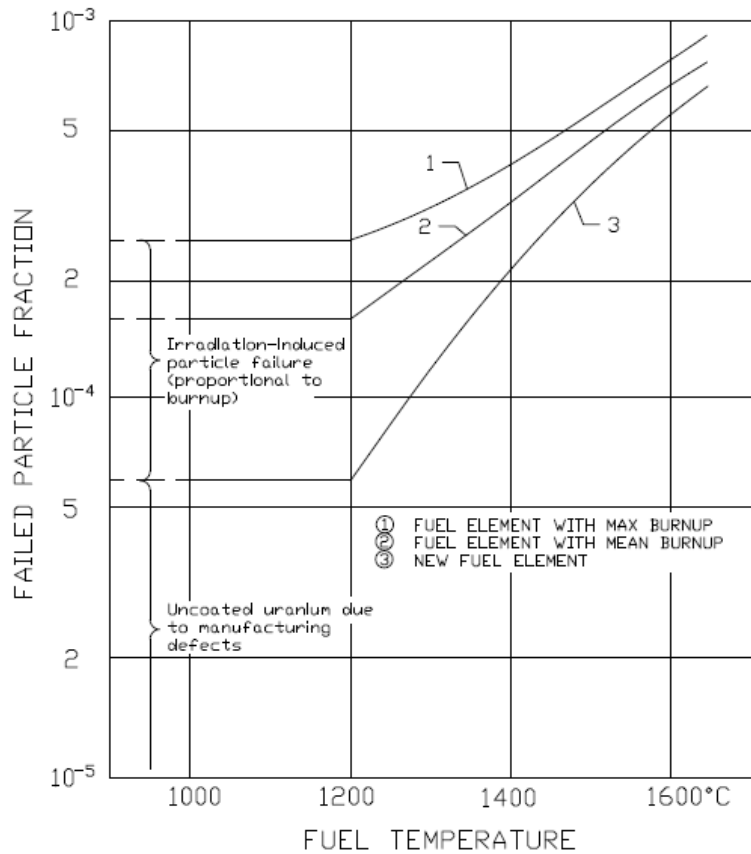
An example of the failure function is shown below.

SPECTRA Code Manuals - Volume 2: User's Guide

```

885000 3 * FP release model: HTR-FPR
*
*      BTRIRT ITRIRT
892001 1.0      -100 * Use CF-100 for the fuel region 1
*
*
705100 2-D Tabular Function Defining Failure fraction F(T,B)
*      Group Number Fact. Const.
700100 1      5      1.0  0.0 * Type : General TF
*      B=0.0 B=0.5 B=1.0
708100 0.0    0.5    1.0      * y-coordinate data points (relative burn-up)
* Arguments
* s : (1) (2) (3) (4) Fact. Const.
710100 9 000 1 0 1.0 0.0 * x-argument: dummy argument, for the F(T,B) calculation it
*      will be replaced by the temperature of the fuel region
710100 6 101 1 0 1.0 0.0 * uses TF-101 for y = 0.0
710100 6 102 1 0 1.0 0.0 * uses TF-102 for y = 0.5
710100 6 103 1 0 1.0 0.0 * uses TF-103 for y = 1.0
710100 9 000 1 0 1.0 0.0 * y-argument: dummy argument, for the F(T,B) calculation it
*      will be replaced by the relative burn-up in the fuel region
*
605101 FF(T,B=0.0)
*      T (C)      FF
600101 1171.6    2.62E-04
600101 1471.2    2.64E-04
600101 1500.4    2.77E-04
600101 1537.6    2.98E-04
600101 1569.1    3.19E-04
600101 1598.3    3.42E-04
600101 1626.6    3.69E-04
600101 1658.1    4.03E-04
600101 1695.3    4.48E-04
600101 1728.5    4.99E-04
600101 1761.6    5.51E-04
600101 1790.7    6.09E-04
600101 1819.8    6.72E-04
600101 1849.8    7.39E-04
600101 1878.9    8.17E-04
600101 1916.1    9.27E-04
*
605102 FF(T,B=0.5)
*      T (C)      FF
600102 1171.8    1.63E-04
600102 1473.1    1.64E-04
600102 1515.1    1.89E-04
600102 1559.6    2.22E-04
600102 1600.8    2.59E-04
600102 1648.5    3.07E-04
600102 1689.7    3.54E-04
600102 1733.4    4.19E-04
600102 1771.4    4.82E-04
600102 1813.4    5.65E-04
600102 1845.8    6.26E-04
600102 1884.6    7.08E-04
600102 1916.1    7.79E-04
*
605103 FF(T,B=1.0)
*      T (C)      FF
600103 1173.1    6.12E-05
600103 1472.7    6.12E-05
600103 1506.6    7.70E-05
600103 1531.6    9.13E-05
600103 1560.7    1.10E-04
600103 1588.1    1.33E-04
600103 1613.2    1.56E-04
600103 1645.5    1.88E-04
600103 1676.2    2.27E-04
600103 1701.2    2.59E-04
600103 1726.3    2.96E-04
600103 1753.7    3.39E-04
600103 1777.2    3.80E-04

```



SPECTRA Code Manuals - Volume 2: User's Guide

600103	1807.9	4.37E-04
600103	1838.6	4.98E-04
600103	1866.9	5.56E-04
600103	1891.1	6.14E-04
600103	1917.8	6.76E-04

*

If the following input parameters are not defined, no diffusion through the intact layer is calculated and the release will be only due to failure fraction. If they are defined, diffusion through the SiC layer will be calculated for the intact particles and will contribute to the total release. The release due to diffusion is calculated as follows:

$$\left(\frac{dM_{FP}}{dt}\right)_{diff} = -\frac{C_{FPR}}{R_{TRISO}} \cdot \frac{M_{FP}}{R_{diff}}$$

The diffusion resistance, R_{diff} , is given by:

$$R_{diff} = \frac{X_{ker}}{D_{ker}} + \frac{X_{SiC}}{D_{SiC}} + \frac{X_{PyC}}{D_{PyC}}$$

C_{FPR} constant, (=CFPRRT, record 885000)
 M_{FP} mass of fission product isotope in the kernel of all TRISO particles, (kg)
 R_{TRISO} radius of the kernel of a TRISO particle, (m)
 D_{ker} diffusion coefficient in the fuel kernel, (m²/s)
 X_{ker} effective thickness of the kernel, (m) (equal to 1/4 of the kernel radius RTRIRT)
 D_{SiC} diffusion coefficient in the SiC layer, (m²/s)
 X_{SiC} thickness of the SiC layer, (m), input parameter TTRIRT(1)
 D_{PyC} diffusion coefficient in the PyC layer, (m²/s)
 X_{PyC} thickness of the PyC layer, (m), input parameter TTRIRT(2)

W-3 (R) : RTRIRT Radius of the kernel of TRISO particle, R_{TRISO} (m).
Acceptable range: $0.0 < RTRIRT \leq 10^{-3}$ m
Default value: 250×10^{-6}

W-4 (I) : MTRIRT(0) Material number for the kernel.
Acceptable range: must be a reference to a material if non-zero
Default value: none

W-5 (R) : TTRIRT(1) Thickness of the SiC layer, X_{TRISO} , (m).
Acceptable range: $0.0 < RTRIRT(1) \leq 10^{-3}$ m
Default value: 35×10^{-6} (based on the GEMINI+ design)

W-6 (I) : MTRIRT(1) Material number for the SiC layer.
Acceptable range: must be a reference to a material if non-zero
Default value: none

W-7 (R) : TTRIRT(2) Thickness of the PyC layer, X_{PyC} , (m).
Acceptable range: $0.0 < RTRIRT(2) \leq 10^{-3}$ m
Default value: 175×10^{-6} (based on the GEMINI+ design)

W-8 (I) : MTRIRT(2) Material number for the PyC layer.
Acceptable range: must be a reference to a material if non-zero
Default value: none

2.15.71 Record: 8930XX, Fission Product Vapor Pressure Coefficients

XX is the vapor class number, $01 \leq XX \leq 40$. The class numbers, XX, must be consecutive. These records define coefficients for the fission product vapor model.

Each fission product, defined in records 880XXY, 881XXX, must be associated with one of the vapor class (the associations are specified in the records 884XXX), specified in these records and one of the fission product release class, specified in the records 8900XX. The vapor classes and the release classes are independent, and therefore the same isotope may be associated with a vapor class and a release class with different numbers. The default release classes and vapor classes, shown in Table 2-42 and Table 2-45, are specified based on reference [35]. The class numbering from reference [35] was preserved; therefore the release class and the vapor class for a given isotope have the same number.

The general formula used to compute the fission product vapor pressure is [35]:

$$\log_{10}(P) = -\frac{A}{T} + B + C \log_{10}(T)$$

P - saturation pressure, (Pa)
A, B, C coefficients,
T - temperature, (K)

Note that [35] uses pressure in mm Hg:

$$\log_{10}(P'[\text{mmHg}]) = -\frac{A'}{T} + B' + C' \log_{10}(T)$$

Conversion to the SI units is quite simple: $B = B' + \log_{10}(10^5/750) = B' + 2.125$ (*A* and *C* remain unchanged: $A=A'$, $C=C'$). The fission product vapor equations, as applied in SPECTRA (SI units) for 13 vapor classes (first 12 the same as the release classes – see record 8900XX, and the Class 13 - CsI), are shown in Table 2-45.

- W-1 (R) : AFPVRT Coefficient *A*, vapor class XX, coefficient set 1, applied for temperatures above the temperature limit specified by Word 4 below.
Acceptable range: $0.0 \leq \text{AFPVRT} < 1.0 \times 10^5$.
Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.
- W-2 (R) : BFPVRT Coefficient *B*, vapor class XX, coefficient set 1, applied for temperatures above the temperature limit specified by Word 4 below.
Acceptable range: $0.0 \leq \text{BFPVRT} < 1.0 \times 10^2$.
Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-3 (R) : CFPVRT Coefficient *C*, vapor class XX, coefficient set 1, applied for temperatures above the temperature limit specified by Word 4 below.
Acceptable range: $-10.0 < \text{CFPVRT} \leq 0.0$.
Default value: available if at least one chain from the built-in isotope data is requested ($\text{IBFPRT} \neq 0$). The default model coefficients are shown below.
- W-4 (R) : TFPVRT Temperature limit for the coefficient set given by the three preceding words. This is a lower limit. For the temperatures lower than this limit the coefficients of the previous set are used. For the temperatures below the lower limit of the first set the vapour pressure is equal to zero.
Acceptable range: $0.0 \leq \text{TFPVRT} < 10,000.0$.
Default value: available if at least one chain from the built-in isotope data is requested ($\text{IBFPRT} \neq 0$). The default model coefficients are shown below.

Up to three sets of coefficients may be entered. The number of entries in this record must be 4 (single set), 8 (two sets), or 12 (three sets). The temperature limit for a given set must be at least 50 K higher than the limit for the previous set.

Table 2-45 Fission product vapour pressures, SI units.

Class	A	B	C	T-lim
1: $\log(P) = -$	0.0 / T +	10.00 -	0.00 $\log(T)$,	T > 273.0
2: $\log(P) = -$	9400.0 / T +	23.71 -	3.75 $\log(T)$,	T > 390.0
	6870.8 / T +	10.12 -	0.00 $\log(T)$,	T > 1553.0
3: $\log(P) = -$	7836.0 / T +	8.57 -	0.00 $\log(T)$,	T > 422.0
4: $\log(P) = -$	3578.0 / T +	19.84 -	2.51 $\log(T)$,	T > 273.0
	3205.0 / T +	25.79 -	5.18 $\log(T)$,	T > 387.0
	2176.9 / T +	9.77 -	0.00 $\log(T)$,	T > 457.0
5: $\log(P) = -$	13940.0 / T +	25.63 -	3.52 $\log(T)$,	T > 534.0
6: $\log(P) = -$	33200.0 / T +	12.73 -	0.00 $\log(T)$,	T > 1460.0
7: $\log(P) = -$	32800.0 / T +	11.80 -	0.00 $\log(T)$,	T > 1504.0
8: $\log(P) = -$	21570.0 / T +	10.87 -	0.00 $\log(T)$,	T > 1032.0
9: $\log(P) = -$	21800.0 / T +	10.80 -	0.00 $\log(T)$,	T > 1046.0
10: $\log(P) = -$	32110.0 / T +	14.00 -	0.00 $\log(T)$,	T > 1338.0
11: $\log(P) = -$	13730.0 / T +	10.55 -	0.00 $\log(T)$,	T > 666.0
12: $\log(P) = -$	15400.0 / T +	10.28 -	0.00 $\log(T)$,	T > 758.0
13: $\log(P) = -$	10420.0 / T +	21.82 -	3.02 $\log(T)$,	T > 436.0
	9678.0 / T +	22.48 -	3.52 $\log(T)$,	T > 894.0
	7303.9 / T +	9.71 -	0.00 $\log(T)$,	T > 1553.0

2.15.72 Record: 8931XX, Minimum Half-Life for Vapor Class Isotopes

XX is the vapor class number, $01 \leq XX \leq 40$. The class numbers, XX, must be consecutive. These records define a minimum isotope half-life for a given vapor class.

W-1 (R) : T12MRT The absolute value T12MRT gives the minimum half-life, $T_{1/2,\min}$ (s), for vapor class XX. All isotopes that have a half-life shorter than $T_{1/2,\min}$ are excluded from this class. These isotopes are indicated in the code output as the class 0. The vapor models, such as adsorption/desorption, condensation, etc., do not apply to these isotopes. Only the radioactive decay takes place. If the value is negative then the stable isotopes are also eliminated from the vapor class XX and moved to the class 0.

Acceptable range: $-1.0 \times 10^{10} \leq T12MRT < 1.0 \times 10^{10}$ s

The maximum time step used for an analysis should not be larger than $|T12MRT|$ (the smallest value of all vapor classes)

Default value: 1.0×10^4 s

For example, let's consider the decay chain 133/134, shown in Figure 2-74. If the default value of T12MRT = 10^5 s (about 1.1 day) is used, then five isotopes are coming into the vapor classes :

- Xe-133m, Xe-133, Cs-133, Cs-134, Ba-134

If T12MRT is set to -10^5 s, then on top of the isotopes for which $T_{1/2,\min} < 10^5$ s, the stable isotopes, Cs-133 and Ba-134, are also eliminated. The following three isotopes are coming into the vapor classes:

- Xe-133m, Xe-133, Cs-134

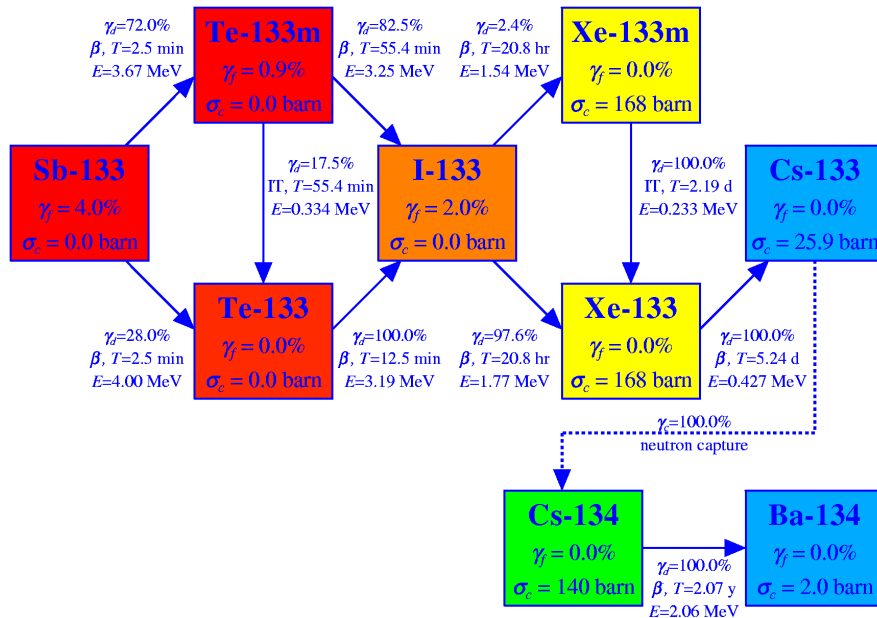


Figure 2-74 Decay chain 133/134

2.15.73 Record: 8932XX, Particle Size and Density of Vapor Class Isotopes

XX is the vapor class number, $01 \leq XX \leq 40$. The class numbers, XX, must be consecutive. By default, the fission product isotopes are transported in molecular form, until they are attached to aerosol particles (typical size of aerosol particles is $>10^{-6}$ m). With these records the user may define an alternative way of fission product transport, namely they will be transported as small particles (typical size $<10^{-6}$ m). The main difference is possibility of sedimentation of particles in the pool and different models for transport to bubbles and aerosol particles (use of Brownian force and inertial impaction rather than use of a Sherwood number correlation - see Volumes 1, 3).

W-1 (R) : DFPFRT Particle size of particles of the vapor class XX, (m)
Acceptable range: $1.0 \times 10^{-15} \leq \text{DFPFRT} < 1.0 \times 10^{-6}$, if non-zero
 DFPFRT and RHPFRT must be both zero or both positive.
Default value: 0.0 (transport in molecular form)

W-2 (R) : RHPFRT Density of particles of the vapor class XX, (kg/m³).
Acceptable range: $0.01 \leq \text{RHPFRT} < 22,600.0$, if non-zero
 DFPFRT and RHPFRT must be both zero or both positive.
Default value: 0.0

W-3 (I) : VIFPRT Vertical velocity (m/s) in a stagnant pool, v_∞ . Positive velocity means the particles will flow vertically up.
 | VIFPRT | \leq 100: use constant velocity, equal to VIFPRT
 VIFPRT > 100: use the correlation:

$$v_\infty = \left(\frac{4/3 \cdot Dg(\rho_f - \rho_p)}{C_D \rho_f} \right)^{1/2}$$

g gravity constant, = 9.81 (m/s²)
 ρ_p particle density, (kg/m³)
 ρ_f fluid density, (kg/m³)
 D particle diameter, (m) = DFPFRT
 C_D drag coefficient

VIFPRT < 1000: drag coefficient: $C_{D, Re \rightarrow \infty} = \text{VIFPRT} - 100$
 VIFPRT = 1000: constant drag coeff.: $C_D = \text{const.} = \text{VIFPRT} - 1000$
 The velocity will be positive (upwards) if the particle density ($\rho_p =$ RHPFRT) is smaller than the fluid density ($\rho_f =$ current pool density).
Acceptable range: $-100.0 \leq \text{VIFPRT}(1) \leq +100.0$, or
 $+100.0 < \text{VIFPRT}(1) \leq +200.0$ ($0.0 < C_{D, Re \rightarrow \infty} \leq 100.0$)
 $+1000.0 < \text{VIFPRT}(1) \leq +1100.0$ ($0.0 < C_D \leq 100.0$)
Default value: = 0.0

Note that if the correlation is used (VIFPRT > 100), then the correlation for small particles may be activated using C_{small} (CSMLCV, record 161000). The correlation for small particles is:

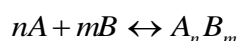
$$v_\infty = \frac{1}{18} \cdot \frac{D_p^2 g(\rho_f - \rho_p)}{\eta_f} \cdot C_{small}$$

2.15.74 Record: 8941XX, Chemical Reactions of Fission Product Vapors – Element A

Fission product chemistry is not implemented in the current code version. The equations shown below will be implemented in a future version.

XX is the vapor class number, $01 \leq XX \leq 40$. These records define combination of masses due to chemical reaction between elements during their release.

The chemical reaction is:



The elements *A* and *B* are reacting to form the compound $A_n B_m$. All isotopes of the element *A* and *B* should be taken into account in defining the reaction. This record defines the isotopes of the element *A*, as well as the number of moles *n*, for the reaction that gives source to the class XX.

W-1 (R) : XACVRT Number of moles of the element *A* per one mole of the compound, *n*, according to the reaction shown above.
Acceptable range: $0.1 \leq XACVRT \leq 10.0$.
Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.

W-2 (I) : IACVRT(1) Reference number of the first isotope of the element *A*, which upon release is to be combined with isotopes of the element *B* and enter the class XX.
Acceptable range: must be a valid reference number XXY, of an isotope, defined in records 880XXY through 884XXY.
Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.

W-3 (I) : IACVRT(2) Reference number of the second isotope of the element *A*, which upon release is to be combined with isotopes of the element *B* and enter the class XX.
Acceptable range: must be a valid reference number XXY, of an isotope, defined in records 880XXY through 884XXY.
Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.

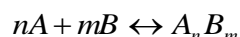
. . . , etc. until all isotopes of the element *A* are defined.

2.15.75 Record: 8942XX, Chemical Reaction of Fission Product Vapors – Element B

Fission product chemistry is not implemented in the current code version. The equations shown below will be implemented in a future version.

XX is the vapor class number, $01 \leq XX \leq 40$. These records define combination of masses due to chemical reaction between elements during their release.

The chemical reaction is:



The elements *A* and *B* are reacting to form the compound $A_n B_m$. All isotopes of the element *A* and *B* should be taken into account in defining the reaction. This record defines the isotopes of the element *B*, as well as the number of moles *m*, for the reaction that gives source to the class XX.

W-1 (R) : XBCVRT Number of moles of the element *B* per one mole of the compound, *m*, according to the reaction shown above.

Acceptable range: $0.1 \leq XBCVRT \leq 10.0$.

Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.

W-2 (I) : IBCVRT(1) Reference number of the first isotope of the element *B*, which upon release is to be combined with isotopes of the element *A* and enter the class XX.

Acceptable range: must be a valid reference number XXY, of an isotope, defined in records 880XXY through 884XXY.

Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.

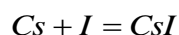
W-3 (I) : IBCVRT(2) Reference number of the second isotope of the element *B*, which upon release is to be combined with isotopes of the element *A* and enter the class XX.

Acceptable range: must be a valid reference number XXY, of an isotope, defined in records 880XXY through 884XXY.

Default value: available if at least one chain from the built-in isotope data is requested (IBFPRT \neq 0). The default model coefficients are shown below.

. . . , etc. until all isotopes of the element *B* are defined.

As an example the following chemical reaction is defined:



SPECTRA Code Manuals - Volume 2: User's Guide

The reaction is defined for all built-in isotopes of Cs and I:

- Cs : Cs-133, Cs-135, Cs-137
- I : I-131, I-132, I-133, I-134, I-135

The input data defining this reaction is shown in Table 2-46. The reference numbers for all built-in isotopes are listed in Table 2-47.

Table 2-46 Input defining class combination for CsI, for the built-in isotopes.

*						
* Class 13, element A:	n	Cs-131	Cs-133	Cs-135		
894113	1.0	037	054	072		
*						
* Class 13, element B:	m	I-131	I-132	I-133	I-134	I-135
894213	1.0	014	022	034	042	051

2.15.76 Record: 8943XX, Chemical Reaction Kinetics

Fission product chemistry is not implemented in the current code versions. The equations shown below will be implemented in the future version.

XX is the vapor class number, $01 \leq XX \leq 40$. The class numbers, XX, must be consecutive. These records define the kinetics of the chemical reaction, defined in the records 8941XX and 8942XX. The reaction kinetics is given by:

$$\frac{d[A_n B_m]}{dt} = R_{for}(T) \cdot [A] \cdot [B] - R_{rev}(T) \cdot [A_n B_m]$$

- (A) concentration of the element A, (kmol/m³)
 (B) concentration of the element B, (kmol/m³)
 (A_nB_m) concentration of the compound A_nB_m, (kmol/m³)
 R_{for} forward reaction rate, (m³/(kmol·s))
 R_{rev} reverse reaction rate, (1/s)

$$R_{for}(T) = R_{0,for} \cdot \exp\left(-\frac{A_{R,for}}{T}\right)$$

$$R_{rev}(T) = R_{0,rev} \cdot \exp\left(-\frac{A_{R,rev}}{T}\right)$$

- R_{0,for} forward reaction first coefficient, (m³/kmol-s)
 A_{R,for} forward reaction second coefficient, (K) (activation energy divided by the gas constant)
 R_{0,rev} reverse reaction first coefficient, (m³/kmol-s)
 A_{R,rev} reverse reaction second coefficient, (K) (activation energy divided by the gas constant)

SPECTRA Code Manuals - Volume 2: User's Guide

- W-1 (R) : R0FCRT Forward reaction first coefficient, $R_{0,for}$, ($\text{m}^3/\text{kmol}\cdot\text{s}$)
If a negative value is entered then the Tabular Function number |R0FCRT| is used instead of the analytical expression. The argument for the Tabular Function is the gas temperature.
Acceptable range: $0.0 \leq \text{R0FCRT} \leq 1.0 \times 10^{10}$ or a valid reference to a Tabular Function
Default value: none
- W-2 (R) : ARFCRT Forward reaction second coefficient, $A_{R,for}$, (K). Used only if R0FCRT > 0.0.
Acceptable range: $-1.0 \times 10^{10} \leq \text{ARFCRT} \leq 1.0 \times 10^{10}$
Default value: 0.0
- W-3 (R) : RMFCRT Lower limit on $R_{for}(T)$:

$$\text{RMFCRT} \leq R_{for}(T) \leq \text{RXFCRT}$$

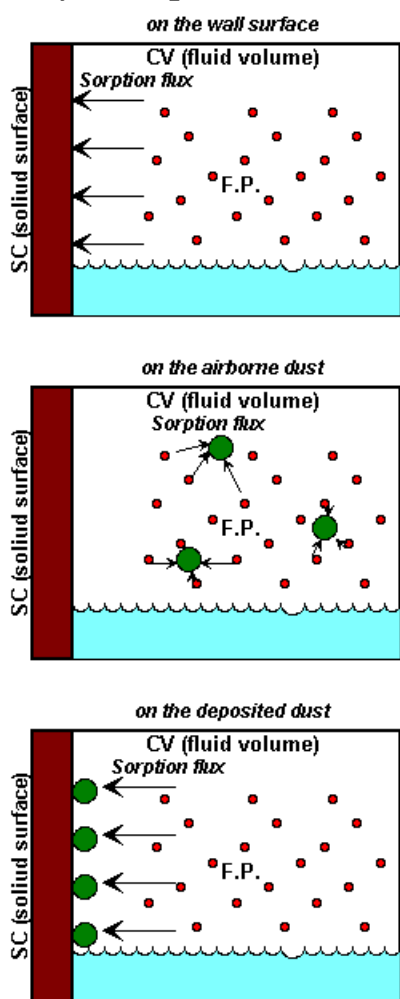
Acceptable range: $0.0 \leq \text{RMFCRT} \leq 10^{-1}$
Default value: 0.0
- W-4 (R) : RXFCRT Upper limit on $R_{for}(T)$.
Acceptable range: $\text{RMFCRT} \leq \text{RXFCRT} \leq 1.0$
Default value: 1.0
- W-5 (R) : R0RCRT Reverse reaction first coefficient, $R_{0,rev}$, (1/s)
If a negative value is entered then the Tabular Function number |R0RCRT| is used instead of the analytical expression. The argument for the Tabular Function is the gas temperature.
Acceptable range: $0.0 \leq \text{R0RCRT} \leq 1.0 \times 10^{10}$ or a valid reference to a Tabular Function
Default value: none
- W-6 (R) : ARRCRT Reverse reaction second coefficient, $A_{R,rev}$, (K). Used only if R0RCRT > 0.0.
Acceptable range: $-1.0 \times 10^{10} \leq \text{ARRCRT} \leq 1.0 \times 10^{10}$
Default value: 0.0
- W-7 (R) : RMRCRT Lower limit on $R_{rev}(T)$:

$$\text{RMRCRT} \leq R_{rev}(T) \leq \text{RXRCRT}$$

Acceptable range: $0.0 \leq \text{RMRCRT} \leq 10^{-1}$
Default value: 0.0
- W-8 (R) : RXRCRT Upper limit on $R_{rev}(T)$.
Acceptable range: $\text{RMRCRT} \leq \text{RXRCRT} \leq 1.0$
Default value: 1.0

W-2 (I) : ISRLRT Selection of sorption on liquid-covered surfaces - Figure 2-75.
 ISRLRT = 1: sorption only on gas-covered surface
 ISRLRT = 2: sorption only on liquid-covered surface
 Acceptable range: ISRLRT = 1, 2
 Default value: 1

ISRLRT = 1 (input record 895YXX)
Sorption on gas-covered surfaces



ISRLRT = 2 (input record 895YXX)
Sorption on liquid-covered surfaces

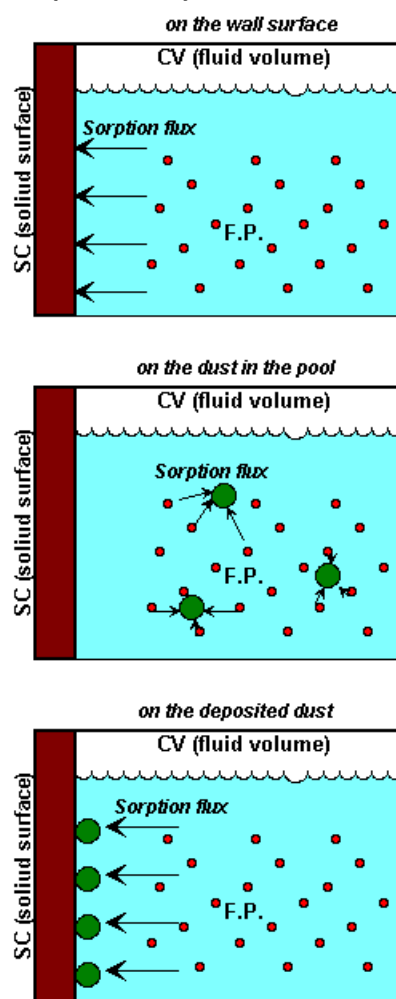


Figure 2-75 Selection of sorption process
 (1) sorption on gas-covered surfaces, applicable models: 0, 1, 2
 (2) sorption on liquid-covered surfaces, applicable models: 0, 1

ISORRT = 1: Sorption Model 1 (SPECTRA Model)

If ISORRT = 1 the words 2 - 25 define the model constants of the Sorption Model 1. The full equation is:

$$\left(\frac{dC_S}{dt}\right)_{total} = \begin{cases} A_S(T) \cdot C_V^{x_A} - B_S(T) \cdot C_d & \text{for } C_V \leq C_{sat}(T) \\ A_S(T) \cdot C_V^{x_{red}} \cdot \left(\frac{C_{sat}^{x_A}}{C_{sat}^{x_{red}}}\right) - B_S(T) \cdot C_d & \text{for } C_V > C_{sat}(T) \end{cases}$$

The adsorption coefficient, $A_S(T)$ and the desorption coefficient, $B_S(T)$, and $C_{sat}(T)$ are calculated from Tabular Functions or the following analytical expressions:

$$A_S(T) = A_0 \cdot \exp\left(-\frac{A_A}{T}\right)$$

$$B_S(T) = B_0 \cdot \exp\left(-\frac{A_B}{T}\right)$$

$$C_{sat}(T) = C_0 \cdot \exp\left(-\frac{A_C}{T}\right)$$

All coefficients for the Sorption Model 1 are defined by the Words 2 - 16 below. The model may be applied for either gas-covered or liquid-covered surfaces, depending on the selector ISRLRT, see W-17 below.

W-2 (R) : A0SRRT Constant A_0 in the expression for the adsorption coefficient, $A_S(T)$:

$$A_S(T) = A_0 \cdot \exp\left(-\frac{A_A}{T}\right)$$

If a negative value is entered then the Tabular Function number |A0SRRT| is used instead of the analytical expression. The argument for the Tabular Function is the wall temperature.

Acceptable range: $0.0 \leq A0SRRT \leq 1.0 \times 10^{20}$ or a valid reference to a Tabular Function

Default value: 0.0

W-3 (R) : AASRRT Constant A_A in the expression for the adsorption coefficient, $A_S(T)$. Used only if A0SRRT > 0.0.

Acceptable range: $-1.0 \times 10^{10} \leq AASRRT \leq 1.0 \times 10^{10}$

Default value: 0.0

W-4 (R) : XASRRT Constant x_A in the sorption model 1.

Acceptable range: $0.3 \leq XASRRT \leq 3.0$

Default value: 1.0

SPECTRA Code Manuals - Volume 2: User's Guide

W-5 (R) : AMSRRT Lower limit on $A_s(T)$:

$$AMSRRT \leq A_s(T) \leq AXSRRT$$

Acceptable range: $0.0 \leq AMSRRT \leq 10^{-1}$

Default value: 0.0

W-6 (R) : AXSRRT Upper limit on $A_s(T)$.

Acceptable range: $AMSRRT \leq AXSRRT \leq 1.0$

Default value: 1.0

W-7 (R) : B0SRRT Constant B_0 in the expression for the desorption coefficient, $B_s(T)$:

$$B_s(T) = B_0 \cdot \exp\left(-\frac{A_B}{T}\right)$$

If a negative value is entered then the Tabular Function number |B0SRRT| is used instead of the analytical expression. The argument for the Tabular Function is the wall temperature.

Acceptable range: $0.0 \leq B0SRRT \leq 1.0 \times 10^{20}$ or a valid reference to a Tabular Function

Default value: 0.0

W-8 (R) : ABSRRT Constant A_B in the expression for the desorption coefficient, $B_s(T)$.
Used only if B0SRRT > 0.0.

Acceptable range: $-1.0 \times 10^{10} \leq ABSRRT \leq 1.0 \times 10^{10}$

Default value: 0.0

W-9 (R) : BMSRRT Lower limit on $B_s(T)$:

$$BMSRRT \leq B_s(T) \leq BXSRRRT$$

Acceptable range: $0.0 \leq BMSRRT \leq 10^{-6}$

Default value: 0.0

W-10 (R) : BXSRRRT Upper limit on $B_s(T)$.

Acceptable range: $BMSRRT \leq BXSRRRT \leq 1.0$

Default value: 1.0

W-11 (I) : IDSRRT Indicator for negative sorption and C_d interpretation

|IDSRRT| = 1: negative sorption allowed, $dC_s/dt < 0.0$

|IDSRRT| = 2: negative sorption not allowed, $dC_s/dt \geq 0.0$

IDSRRT < 0: C_d = surface concentration (kg/m²)

IDSRRT > 0: C_d = volumetric concentration (kg/m³)

Acceptable range: IDSRRT = -2, -1, 1, 2

Default value: 1

SPECTRA Code Manuals - Volume 2: User's Guide

W-12 (R) : COSRRT Constant C_0 in the expression for $C_{sat}(T)$:

$$C_{sat}(T) = C_0 \cdot \exp\left(-\frac{A_C}{T}\right)$$

If a negative value is entered then the Tabular Function number |COSRRT| is used instead of the analytical expression. The argument for the Tabular Function is the wall temperature.

Acceptable range: $0.0 \leq \text{COSRRT} \leq 1.0 \times 10^{20}$ or a valid reference to a Tabular Function

Default value: 0.0

W-13 (R) : ACSRRT Constant A_C in the expression for the parameter $C_{sat}(T)$. Used only if COSRRT > 0.0.

Acceptable range: $-1.0 \times 10^{10} \leq \text{ACSRRT} \leq 1.0 \times 10^{10}$

Default value: 0.0

W-14 (R) : XRSRRT Reduced exponent, x_{red} , valid for high vapor concentrations, $C_V > C_{sat}(T)$. If zero is used then the adsorption term is independent on the vapor concentration, C_V , and equal to:

$$A_S(T_w) \cdot C_{sat}^{x_A}(T)$$

If a positive value is entered then the adsorption term increases with the vapor concentration, C_V , but the increase is slower. The adsorption term is given by:

$$A_S(T_w) \cdot C_V^{x_{red}} \cdot \left(\frac{C_{sat}^{x_A}(T)}{C_{sat}^{x_{red}}(T)} \right)$$

The term in brackets ensures continuity of the function at $C_V = C_{sat}(T)$

Acceptable range: $0.0 \leq \text{XRSRRT} < \text{XASRRT}$

Default value: 0.0

W-15 (R) : CMSRRT Lower limit on $C_{sat}(T)$:

$$\text{CMSRRT} \leq C_{sat}(T) \leq \text{CXSRRT}$$

Acceptable range: $0.0 \leq \text{CMSRRT} \leq 10^{-1}$

Default value: 0.0

W-16 (R) : CXSRRT Upper limit on $C_{sat}(T)$.

Acceptable range: $\text{CMSRRT} \leq \text{CXSRRT} \leq 1.0$

Default value: 1.0

W-17 (I) : ISRLRT Selection of sorption on liquid-covered surfaces - Figure 2-75.

ISRLRT = 1: sorption only on gas-covered surface

ISRLRT = 2: sorption only on liquid-covered surface

Acceptable range: ISRLRT = 1, 2

Default value: 1

W-18 (R) : DCSRRT Diffusion coefficient in liquid, D_C , (m²/s). Used only for sorption in liquids. i.e. if ISRLRT = 2. If no value or zero is entered, then the adsorption coefficient is obtained from the user-defined constants A_0 (A0SRRT), A_A (AASRRT) and the temperature-dependent formula: $A_S = A_0 \exp(-A_A/T)$.

If the diffusion coefficient, D_C , is defined, then the adsorption flux is computed using the heat and mass transfer analogy, where: $Nu \rightarrow Sh, Pr \rightarrow Sc$. The Sherwood number is: $Sh = A_S \times D_{FC}/D_C$, where D_{FC} is the characteristic dimension for forced convection (hydraulic diameter), D_C , is the diffusion coefficient, DCSRRT. The mass transfer correlation is defined by the following words, and has the form:

$$Sh = A_{Sh} + B_{Sh} \frac{Re^{C_{Sh}} Sc^{D_{Sh}}}{1 + E_{Sh} Re^{F_{Sh}} Sc^{G_{Sh}}}$$

For example, in case of internal forced convection, Dittus-Boelter correlation is:

$$Sh = 0.023 Re^{0.8} Sc^{0.4}$$

To apply this correlation, one needs to set $B_{Sh} = 0.023$, $C_{Sh} = 0.8$, $D_{Sh} = 0.4$, other coefficients being equal to zero.

If a positive value is entered, $D_C = DCSRRT$

If a negative value is entered, $D_C = TF \text{ number } |DCSRRT|$.

The argument for the TF is the fluid temperature.

Acceptable range: $0.0 \leq DCSRRT \leq 1.0$ or a valid reference to a Tabular Function

Default value: 0.0

W-19 (R) : ASSRRT A_{Sh} in the user-defined Sherwood number correlation:

Acceptable range: $-10^{10} \leq ASSRRT \leq 10^{10}$

Default value: 0.0

W-20 (R) : BSSRRT B_{Sh} in the Sherwood number correlation:

Acceptable range: $0.0 \leq BSSRRT \leq 10^{10}$

Default value: 0.0

W-21 (R) : CSSRRT C_{Sh} in the Sherwood number correlation:

Acceptable range: $0.0 \leq CSSRRT \leq 10.0$

Default value: 0.0

W-22 (R) : DSSRRT D_{Sh} in the Sherwood number correlation:

Acceptable range: $0.0 \leq DSSRRT \leq 10.0$

Default value: 0.0

W-23 (R) : ESSRRT E_{Sh} in the Sherwood number correlation:

Acceptable range: $0.0 \leq ESSRRT \leq 10^{10}$

Default value: 0.0

W-24 (R) : FSSRRT F_{Sh} in the Sherwood number correlation:

Acceptable range: $0.0 \leq FSSRRT \leq 10.0$

Default value: 0.0

W-25 (R) : GSSRRT G_{Sh} in the Sherwood number correlation:

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq \text{GSSRRT} \leq 10.0$
 Default value: 0.0

The next two words are used only if fission products are transported as particles (particle diameter $\text{DPFPRT} > 0.0$ and density $\text{RHPRT} > 0.0$) and transport on liquid-covered surfaces is active $\text{ISRLRT} = 2$. If that is the case, the Sh number correlation described above may be replaced by an alternative way of calculating the pool-gas transport (aerosol particles represent gas bubbles in this case), which uses Brownian diffusion and inertial impaction models on the surface of aerosol particles in the pool:

$$\mathcal{G}_{\text{pool-gas}} = v_{\text{Brown}} + v_{\text{inertial}}$$

where:

$$v_{\text{Brown}} = \frac{D_C}{\delta_{BL}}$$

$$v_{\text{inertial}} = v_{\infty} \cdot \eta \cdot A_{h,\text{bubb}} / A_{\text{bubb}} = v_{\infty} \cdot \eta / 4$$

- v_{Brown} Brownian deposition velocity, (m/s)
- v_{inertial} inertial impaction deposition velocity, (m/s)
- D_C diffusion coefficient, (m²/s)
- δ_{BL} diffusion boundary layer thickness, (m) (=10⁻⁵)
- $A_{h,\text{bubb}}$ horizontal cross section area of a "bubble", (m²), = $\pi \times D_{\text{bubb}}^2 / 4$
- A_{bubb} total surface area of a "bubble", (m²), = $\pi \times D_{\text{bubb}}^2$
- v_{∞} particle-to-"bubble" relative velocity, (m/s)
- η collection efficiency, calculated from one of three correlations, described below.

Langmuir and Blodgett (L-B) correlation - Figure 2-76

$$\eta = \eta_{\text{max}} \cdot \frac{\text{Stk}^2}{(\text{Stk} + C_{LB})^2}$$

- C_{LB} constant (=0.25, see [54], eq. 3)
- η_{max} maximum value of collection efficiency (=1.0)
- Stk Stokes number, (-), see Volume 1 for detailed description.

Modified Langmuir and Blodgett correlation - Figure 2-77

$$\eta = \eta_{\text{max}} \cdot \begin{cases} \frac{0.25}{C_{LB}} \cdot \text{Stk} & \text{for } \text{Stk} < C_{LB} \\ \frac{\text{Stk}^2}{(\text{Stk} + C_{LB})^2} & \text{for } \text{Stk} > C_{LB} \end{cases}$$

Correlation developed based on data of Yoon & Lutrell and Afruns & Kitchener - Figure 2-78

$$\eta = \text{Min} \left(\eta_{\text{max}}, A \cdot \frac{d_p^2}{D_b} \right)$$

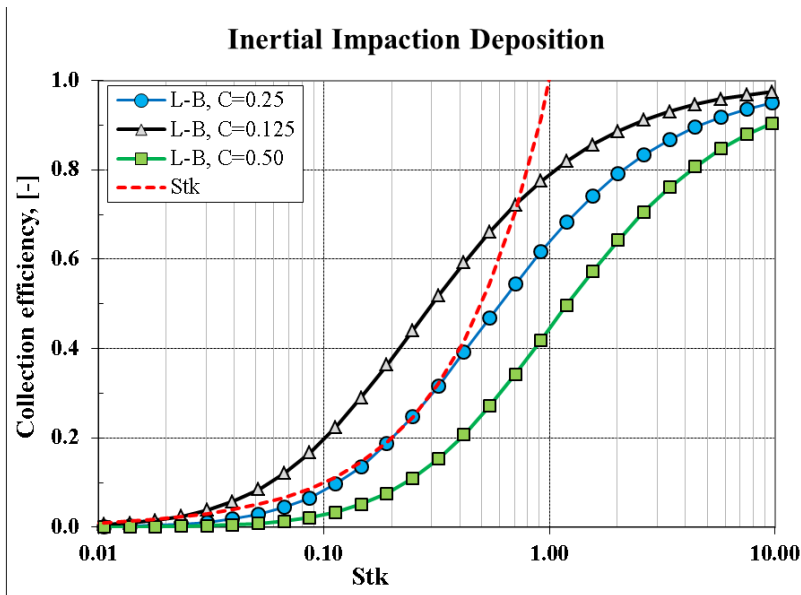


Figure 2-76 Langmuir and Blodgett correlation

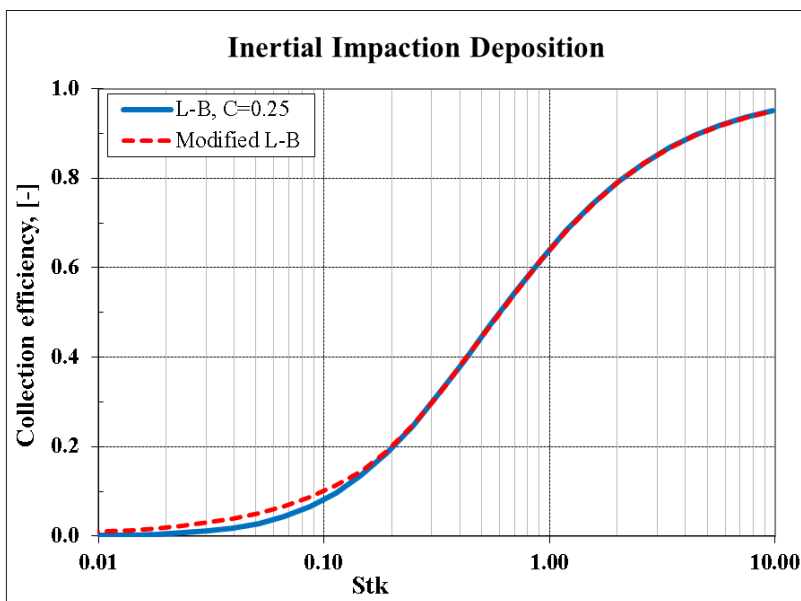


Figure 2-77 Modified versus original Langmuir and Blodgett correlation

In order to activate the model, non-zero values must be supplied for at least two out of the following three input entries:

W-26 (R) : TBL2RT Diffusion boundary layer thickness, δ_{BL} , (m).
 Acceptable range: $1.0 \times 10^{-7} \leq TBL2RT \leq 1.0 \times 10^{-3}$.
 Default value: none
 If the model is used, the recommended value is 5.0×10^{-5} .

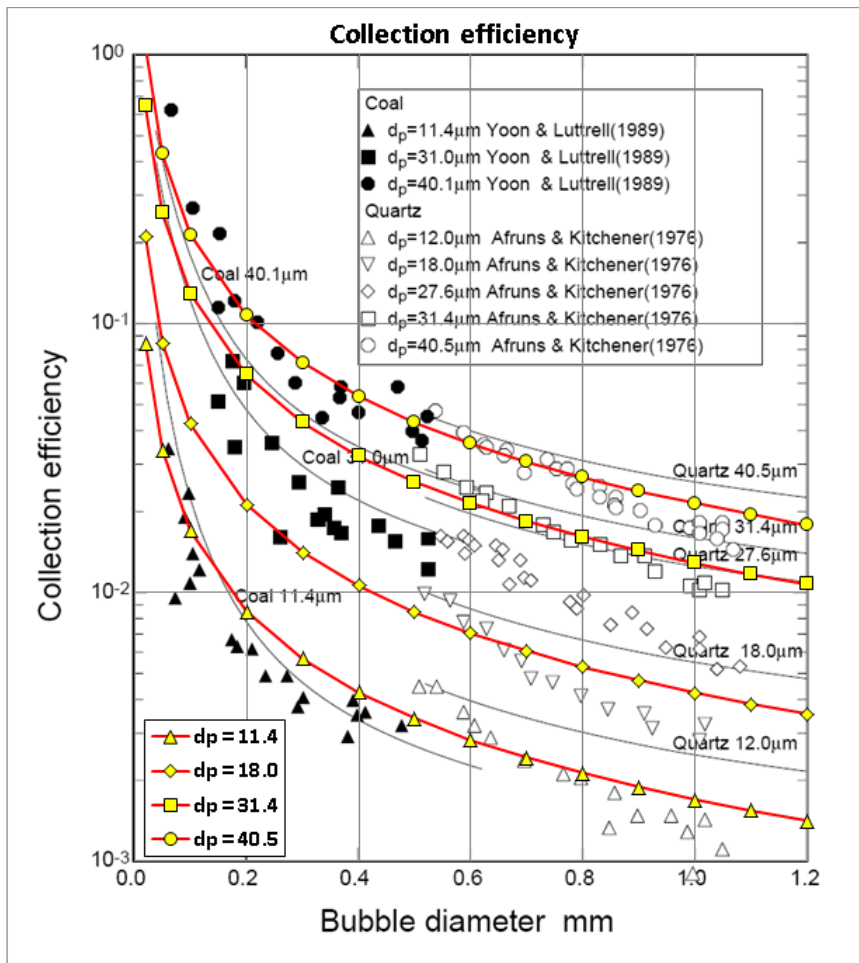


Figure 2-78 Data of Yoon & Luttrell and Afruns & Kitchener and correlation

- W-27 (R) : CLB2RT Constant in the correlation for inertial impaction.
 CLB2RT ≤ 10 : C_{LB} , in the L-B or modified L-B correlation (depending on ILBORT, record 860000)
 CLB2RT > 1000 : A in the correlation developed based on data of Yoon & Luttrell and Afruns & Kitchener
 Acceptable range: $10^{-2} \leq CLB2RT \leq 10^{+1}$ C_{LB} , in L-B, modified L-B
 $10^{+3} \leq CLB2RT \leq 10^{+5}$ A in YLAK correlation
 Default value: none
 For L-B and modified L-B, the recommended value is 0.25.
 For YLAK, the recommended values are 9,000 - 13,000.
- W-28 (R) : ELB2RT Maximum efficiency η_{max} , in the correlation for inertial impaction.
 Acceptable range: $10^{-3} \leq ELB2RT \leq 10^{+3}$
 Default value: 1.0 if the model is used
 (if TBL2RT >0.0 , CLB2RT >0.0)

ISORRT = 2: Sorption Model 2 (PATRAS/SPATRA model)

If ISORRT = 2 the words 2 - 29 define the model constants of the Sorption Model 2. The model is applicable for gas phase only. In case of liquid-covered surfaces, only desorption of the reversibly-bound particles is possible (when APSRRT > 0.0, see W-27 below). The equations are:

$$\left(\frac{dC_s}{dt}\right)_{total} = \alpha \cdot (1 - \theta) \cdot u \cdot C_\delta - \vartheta \cdot C_{rev} - \eta \cdot C_d$$

$$\left(\frac{dC_s}{dt}\right)_{diff} = \alpha \cdot (1 - \theta) \cdot u \cdot C_\delta \cdot (1 - \beta) - \eta \cdot C_d$$

- W-2 (R) : ALSRRT Sticking factor, α , (-).
Acceptable range: $0.0 \leq \text{ALSRRT} \leq 1.0$
Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0)
- W-3 (R) : CMSRRT Maximum number of adsorption sites per unit surface area, C_{max} , (m^{-2}).
 The value may be applied for each vapor individually or as a global value for all vapors, depending on the selector ICSRRT (Word 29 below). If a global value is used, then CMSRRT must be specified as the same for all vapors.
Acceptable range: $10^5 \leq \text{CMSRRT} \leq 10^{50}$
Default value: 1.0×10^{18}
- W-4 (R) : SGSRRT Diffusion volume, Σ , of the fission product class XX. If a positive value is used, then the diffusion coefficient for fission product vapor diffusion in the atmosphere gas of a Control Volume is calculated from the general method, applicable for any gas mixture. If the diffusion volume for a particular element or compound is not available, then the following correlations are recommended to calculate the value of Σ (see Volume 1):
 Elements: $\Sigma = 2.4 \cdot A^{0.66}$
 Compounds: $\Sigma = 4.2 \cdot A^{0.66}$
 A is the atomic number.
Acceptable range: $0.0 \leq \text{SGSRRT} \leq 1000.0$,
 either SGSRRT or ADSRRT must be positive
Default value: 0.0
- W-5 (R) : ADSRRT If the diffusion volume, Σ (SGSRRT), is equal to zero, then a Chapman-Enskog correlation is applied to calculate the diffusion coefficient:
- $$D_C = A_D \cdot \frac{T_g^{B_D}}{p}$$
- A_D user-defined coefficient
 B_D user-defined coefficient
 T_g gas temperature, (K)
 p gas pressure, (Pa)
 D_C diffusion coefficient, (m^2/s)

SPECTRA Code Manuals - Volume 2: User's Guide

ADSRRT is the coefficient A_D in this correlation. Note that this correlation is valid only for given gas and should not be applied when the gas composition may change during calculations, for example if helium is replaced by air.

Acceptable range: $0.0 \leq \text{ADSRRT} \leq 1.0 \times 10^3$
either SGSRRRT or ADSRRT must be positive

Default value: 0.0

W-6 (R) : BDSRRT Coefficient B_D in the Chapman-Enskog correlation. Used only if the diffusion volume, Σ (SGSRRT), is equal to zero.

Acceptable range: $0.0 \leq \text{BDSRRT} \leq 10.0$

Default value: 0.0

W-7 (R) : B0SRRT $(1-\beta_0)$ in the formula for the penetration factor, $(1-\beta)$:

$$1 - \beta = (1 - \beta_0) \cdot \exp\left(\frac{A_\beta}{T_w}\right)$$

Acceptable range: $0.0 \leq \text{B0SRRT} \leq 1.0$ for wall surfaces

B0SRRT = 0.0 for aerosol surfaces

Default value: 10^{-5} for wall surfaces, 0.0 for aerosol surfaces
(a small number, $< 10^{-50}$, sets the value to 0.0)

W-8 (R) : ABSRRT A_β in the formula for the penetration factor, $(1-\beta)$.

Acceptable range: $0.0 \leq \text{ABSRRT} \leq 1.0 \times 10^{10}$

Default value: 0.0

W-9 (R) : BMSRRT Lower limit on $(1-\beta)$, $(1-\beta)_{\min}$.

Acceptable range: $0.0 \leq \text{BMSRRT} \leq 1.0$

Default value: 0.0

W-10 (R) : BXRRT Upper limit on $(1-\beta)$, $(1-\beta)_{\max}$.

Acceptable range: $\text{BMSRRT} \leq \text{BXRRT} \leq 1.0$

Default value: 1.0

W-11 (R) : A0SRRT \mathcal{G}_0 in the formula for the desorption coefficient, \mathcal{G} :

$$\mathcal{G} = \mathcal{G}_0 \cdot \exp\left(-\frac{A_g}{T_w}\right)$$

Acceptable range: $0.0 \leq \text{A0SRRT} \leq 1.0 \times 10^{20}$

Default value: 0.0

W-12 (R) : AASRRT A_g in the formula for the desorption coefficient, \mathcal{G} .

Acceptable range: $0.0 \leq \text{AASRRT} \leq 1.0 \times 10^{10}$

Default value: 0.0

W-13 (R) : AMSRRT Lower limit on \mathcal{G} , \mathcal{G}_{\min} .

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq \text{AMSRRT} \leq 1.0$
Default value: 0.0

W-14 (R) : AXSRRT Upper limit on \mathcal{G} , \mathcal{G}_{\max} .
Acceptable range: $\text{AMSRRT} \leq \text{AXSRRT} \leq 1000.0$
Default value: 10.0

W-15 (R) : E0SRRT η_0 in the formula for the evaporation coefficient, η :

$$\eta = \eta_0 \cdot \exp\left(-\frac{A_g}{T_w}\right)$$

Acceptable range: $0.0 \leq \text{E0SRRT} \leq 1.0 \times 10^{20}$
Default value: 0.0

W-16 (R) : AESRRT A_η in the formula for the evaporation coefficient, η .
Acceptable range: $0.0 \leq \text{AESRRT} \leq 1.0 \times 10^{10}$
Default value: 0.0

W-17 (R) : EMSRRT Lower limit on η , η_{\min} .
Acceptable range: $0.0 \leq \text{EMSRRT} \leq 1.0$
Default value: 0.0

W-18 (R) : EXSRRT Upper limit on η , η_{\max} .
Acceptable range: $\text{EMSRRT} \leq \text{EXSRRT} \leq 1.0$
Default value: 1.0

W-19 (R) : ASSRRT A_{Sh} in the user-defined Sherwood number correlation:

$$Sh = A_{Sh} + B_{Sh} \frac{Re^{C_{Sh}} Sc^{D_{Sh}}}{1 + E_{Sh} Re^{F_{Sh}} Sc^{G_{Sh}}}$$

This correlation is used if $A_{Sh} > 0$ or $B_{Sh} > 0$ (Word 12 below). If A_{Sh} is negative, then the Gnielinski correlation is used:

$$Sh = \frac{r \cdot (Re - 1000) \cdot Sc}{1 + 12.7 \cdot \sqrt{r} \cdot (Sc^{2/3} - 1)} \cdot \left(1 + \left(\frac{d}{x}\right)^{2/3}\right) \cdot \left(\frac{T_{gas}}{T_{wall}}\right)^y$$

where:

$$r = (1/8) \cdot (1.82 \cdot \log_{10}(Re) - 1.64)^{-2}$$

T_{gas} , T_{wall} are the gas and wall temperature, d is the hydraulic diameter and x is the distance from tube entrance. The value of x is equal to the absolute value of ASSRRT: $x = |\text{ASSRRT}|$. The value of x may be specified individually for each SC/TC on the records 396XXX and 496XXX. The value of y is defined by YGNIRT, Word 28, below.

If both A_{Sh} and B_{Sh} are equal to zero, then the mass transfer coefficient is calculated from the heat and mass transfer analogy, using the same correlations as are being used for natural and forced convective heat transfer. For example, in case of internal flow forced convection this is Dittus-Boelter correlation, which is:

$$Sh = 0.023 Re^{0.8} Sc^{0.4}$$

Suppose the user wishes to apply this correlation in natural as well as forced convective regime. This may be done applying the user-defined Sherwood number correlation, with: $B_{Sh} = 0.023$, $C_{Sh} = 0.8$, $D_{Sh} = 0.4$, other coefficients being equal to zero.

Acceptable range: $-10^{10} \leq ASSRRT \leq 10^{10}$

Default value: 0.0

- | | | |
|------------|--------|---|
| W-20 (R) : | BSSRRT | <p>B_{Sh} in the Sherwood number correlation:
 <i>Acceptable range:</i> $0.0 \leq BSSRRT \leq 10^{10}$
 <i>Default value:</i> 0.0</p> |
| W-21 (R) : | CSSRRT | <p>C_{Sh} in the Sherwood number correlation:
 <i>Acceptable range:</i> $0.0 \leq CSSRRT \leq 10.0$
 <i>Default value:</i> 0.0</p> |
| W-22 (R) : | DSSRRT | <p>D_{Sh} in the Sherwood number correlation:
 <i>Acceptable range:</i> $0.0 \leq DSSRRT \leq 10.0$
 <i>Default value:</i> 0.0</p> |
| W-23 (R) : | ESSRRT | <p>E_{Sh} in the Sherwood number correlation:
 <i>Acceptable range:</i> $0.0 \leq ESSRRT \leq 10^{10}$
 <i>Default value:</i> 0.0</p> |
| W-24 (R) : | FSSRRT | <p>F_{Sh} in the Sherwood number correlation:
 <i>Acceptable range:</i> $0.0 \leq FSSRRT \leq 10.0$
 <i>Default value:</i> 0.0</p> |
| W-25 (R) : | GSSRRT | <p>G_{Sh} in the Sherwood number correlation:
 <i>Acceptable range:</i> $0.0 \leq GSSRRT \leq 10.0$
 <i>Default value:</i> 0.0</p> |
| W-26 (R) : | XLSRRT | <p>Limiting factor in the number of adsorption sites per unit surface area that may be taken by a single vapor during a time step, X_{lim}, (m^{-2}).
 <i>Acceptable range:</i> $0.90 \leq XLSRRT \leq 1.00$
 <i>Default value:</i> 0.99</p> |
| W-27 (R) : | APSRRT | <p>Desorption coefficient for pool-covered surfaces, \mathcal{G}_{pool}. On the pool-covered surfaces only desorption of the reversibly bound molecules (that had been adsorbed when the surface was uncovered) may occur. No adsorption, penetration, or evaporation is calculated during the period when the surface is covered by liquid. The mass transfer is:</p> |

$$\left(\frac{dC_{rev}}{dt} \right)_{total} = -g_{pool} \cdot C_{rev}$$

Acceptable range: $0.0 \leq \text{APSRRT} \leq 1.0$

Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0)

- W-28 (R) : YGNIRT The value of y in the Gnielinski correlation.
Acceptable range: $0.001 \text{ YGNIRT} \leq 1.00$
Default value: 0.015
- W-29 (R) : ICSRRT Method of calculation of CMSRRT (Word 3 above).
 ICSRRT = 1: CMSRRT is independent for each vapor
 ICSRRT = 2: CMSRRT is a global value for all vapors
Acceptable range: 1 or 2. ICSRRT must be entered consistently for all vapors within a sorption set (i.e. the same value must be applied for all vapors).
Default value: 1

2.15.78 Records: 395XXX, Selection of Sorption Processes on SC Surfaces

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$.

- W-1 (I) : IISRRT(1) Sorption set number (defined in records 895YXX) to be used on the left surface of the 1-D Solid Heat Conductor XXX. A negative number deactivates the sorption model.
Acceptable range: must be one of existing sorption sets, if positive
Default value: -1 if ISRGRT (global activator of the sorption model, record 880000) is 0, ISRGRT otherwise.
- W-2 (R) : YISRRT(1) Multiplier for the sorption model applied on the left surface of the 1-D Solid Heat Conductor XXX. The adsorption or desorption rate that is calculated by the sorption model selected by the previous word, is multiplied by this value when applied to the left surface of this SC.
Acceptable range: $0.0 \leq \text{YISRRT}(1) \leq 10.0$. For the sorption model 2 (see 895YXX) only 1.0 and 0.0 may be used.
Default value: 1.0.
- W-3 (I) : IISRRT(2) Sorption set number (defined in records 895YXX) to be used on the right surface of the 1-D Solid Heat Conductor XXX. A negative number deactivates the sorption model.
Acceptable range: must be one of existing sorption sets, if positive
Default value: -1 if ISRGRT (global activator of the sorption model, record 880000) is 0, ISRGRT otherwise.
- W-4 (R) : YISRRT(2) Multiplier for the sorption model applied on the right surface of the 1-D Solid Heat Conductor XXX. The adsorption or desorption rate that is calculated by the sorption model selected by the previous word, is multiplied by this value when applied to the right surface of this SC.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq Y1SRRT(2) \leq 10.0$. For the sorption model 2 (see 895YXX) only 1.0 and 0.0 may be used.

Default value: 1.0.

2.15.79 Records: 495XXX, Selection of Sorption Processes on TC Surfaces

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : I1 Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for sorption process definition. The sorption process, defined by Word 3, will be applied for the boundary cells I: $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number.
Default value: none.

W-2 (I) : I2 Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for sorption process definition. The sorption process, defined by Word 3, will be applied for the boundary cells I: $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number. $I2 \geq I1$.
Default value: none.

W-3 (I) : I2SRRT(I) Sorption set number (defined in records 895YXX) to be used on the boundary cell I, $I1 \leq I \leq I2$, of the 2-D Solid Heat Conductor XXX. A negative number deactivates the sorption model.
Acceptable range: must be one of existing sorption sets, if nonzero
Default value: -1 if ISRGRT (global activator of the sorption model, record 880000) is 0, ISRGRT otherwise.

W-4 (R) : Y2SRRT(I) Multiplier for the sorption model applied on the boundary cell I, $I1 \leq I \leq I2$, of the 2-D Solid Heat Conductor XXX. The adsorption or desorption rate that is calculated by the sorption model selected by the previous word, is multiplied by this value when applied to the boundary cell I of this TC.
Acceptable range: $0.0 \leq Y2SRRT(I) \leq 10.0$. For the sorption model 2 (see 895YXX) only 1.0 and 0.0 may be used.
Default value: 0.0.

The data set consisting of the four words described above is repeated until sorption reactions are defined for all desired boundary cells. The data sets may be entered in several records with the same number. The number of entries in a single record must be always a multiple of 4.

2.15.80 Records: 396XXX, Sorption Related Parameters for SC Surfaces

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : XGN1RT(1) Parameter x in the Gnielinsky correlation (see description of record 895YXX, Word 19, ASSRRT) to be used on the left surface of the 1-D Solid Heat Conductor XXX.

Acceptable range: $0.001 \leq XGN1RT(1) \leq 1000.0$

Default value: | ASSRRT |

W-2 (I) : XGN1RT(2) Parameter x in the Gnielinsky correlation (see description of record 895YXX, Word 19, ASSRRT) to be used on the right surface of the 1-D Solid Heat Conductor XXX.

Acceptable range: $0.001 \leq XGN1RT(2) \leq 1000.0$

Default value: | ASSRRT |

2.15.81 Records: 496XXX, Sorption Related Parameters for TC Surfaces

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

W-1 (I) : I1 Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for sorption process definition. The sorption process, defined by Word 3, will be applied for the boundary cells I: $I1 \leq I \leq I2$.

Acceptable range: must be an existing boundary cell number.

Default value: none.

W-2 (I) : I2 Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for sorption process definition. The sorption process, defined by Word 3, will be applied for the boundary cells I: $I1 \leq I \leq I2$.

Acceptable range: must be an existing boundary cell number. $I2 \geq I1$.

Default value: none.

W-3 (R) : XGN2RT(I) Parameter i in the Gnielinsky correlation (see description of record 895YXX, Word 19, ASSRRT) to be used on the boundary cell I, $I1 \leq I \leq I2$, of the 2-D Solid Heat Conductor XXX.

Acceptable range: $0.001 \leq XGN2RT(I) \leq 1000.0$

Default value: | ASSRRT |

The data set consisting of the four words described above is repeated until sorption reactions are defined for all desired boundary cells. The data sets may be entered in several records with the same number. The number of entries in a single record must be always a multiple of 3.

2.15.82 Records: 191XXX, Initial Masses of Isotopes in CV Atmosphere and Pool

XXX is the CV reference number, $001 \leq XXX \leq 999$.

- | | | |
|-----------|---------|---|
| W-1 (I) : | KKI | Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
<i>Acceptable range:</i> must be a valid reference number if nonzero
<i>Default value:</i> none. |
| W-2 (R) : | XMACRT | Initial mass of the isotope KKI in the atmosphere of the Control Volume XXX, (kg).
<i>Acceptable range:</i> $0.0 \leq XMACRT \leq 0.1 \times M_{atms}$
Here M_{atms} is the mass of atmosphere in CV
<i>Default value:</i> 0.0 |
| W-3 (R) : | X MPCRT | Initial mass of the isotope KKI in the pool of the Control Volume XXX, (kg).
<i>Acceptable range:</i> $0.0 \leq X MPCRT \leq 0.1 \times M_{pool}$
Here M_{pool} is the mass of pool in CV
<i>Default value:</i> 0.0 |

The data set consisting of the three words described above is repeated until initial masses of all desired isotopes are defined. The data sets may be entered in several records with the same number. The number of entries in a single record must be always a multiple of 2.

2.15.83 Records: 391XXX, Initial Masses of Isotopes in SC

This record defines initial masses of isotopes that have penetrated into 1-D solid structures due to the sorption processes. XXX is the SC reference number, $001 \leq XXX \leq 999$.

- | | | |
|-----------|--------|--|
| W-1 (I) : | KKI | Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
<i>Acceptable range:</i> must be a valid reference number if nonzero
<i>Default value:</i> none. |
| W-2 (R) : | XM1FRT | Initial mass of the isotope KKI in the 1-D Solid Heat Conductor XXX, (kg). This is a total mass in all cells of the SC. The cell-to-cell distribution may be specified for each vapor class in the records 392XXX. If the distribution is not specified in the record 392XXX, then the mass of XM1FRT is assumed to be uniformly distributed among the cells, i.e. with uniform material density (kg/m^3).
<i>Acceptable range:</i> $0.0 \leq XM1FRT \leq 0.001 \times M_{SC}$
Here M_{SC} is the mass of the SC material
<i>Default value:</i> 0.0 |

...

The set of two words is repeated until initial masses of all desired isotopes are defined. Several records with the same number may be used.

2.15.84 Records: 491XXX, Initial Masses of Isotopes in TC

This record defines initial masses of isotopes that have penetrated into 2-D solid structures due to the sorption processes. XXX is the TC reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.
- W-2 (R) : XM2FRT Initial mass of the isotope KKI in the 2-D Solid Heat Conductor XXX, (kg).
Acceptable range: $0.0 \leq XM2FRT \leq 0.001 \times M_{TC}$
Here M_{TC} is the mass of the TC material
Default value: 0.0

The set of two words is repeated until initial masses of all desired isotopes are defined. Several records with the same number may be used.

2.15.85 Records: 192XXX, External Sources of Isotopes

This record specifies any external sources of isotopes for a Control Volume. The term external sources is used to mean sources other than release from the core (calculated by one of the available release models - records 890000, 891000). XXX is the CV reference number, $001 \leq XXX \leq 999$.

- W-1 (R) : ZFSCRT Elevation of the source related to the bottom of CV. The value is also used as an indicator for a replacement of data - see the comment below the W-3 description.
Acceptable range: $0.0 \leq ZFSCRT \leq HEIGCV$ (see record 110XXX)
Default value: 0.0
- W-2 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.
- W-3 (I) : IFSCRT Pointer to a Tabular or Control Function that defines the source of the isotope KKI in the Control Volume XXX. If the number is positive, then the source will be defined by a Tabular Function with the reference number: IFSCRT. If the number is negative, then the source will be defined by a Control Function with the reference number: $|IFSCRT|$. If the current value of the Tabular or Control Function is smaller than 0.0, the source will be set to 0.0. If it is larger than 10^3 , the source will be set to 10^3 . The units are: (kg/s).
Acceptable range: must be a valid reference number of a Tabular or Control Function if nonzero
Default value: none

The data set consisting of the two words described above is repeated until all desired sources are defined. The data sets may be entered in several records with the same number and the same elevation of the source. If the elevation of the source is different than the elevation entered in previous record or records with the same number, then this record is treated as a replacement and replaces any previous data that has been entered in records 192XXX. The number of entries minus one in a single record must be always a multiple of 2.

2.15.86 Records: 392XXX, Initial Distribution of Vapors on the Surfaces of SC

This record defines initial distribution of the isotopes that are reversibly bound to the surface of 1-D solid structures. XXX is the SC reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : IVAP Vapor class number.
Acceptable range: must be a valid class number if nonzero
Default value: none.
- W-2 (R) : CR1FRT(1) Surface concentration of the reversibly bound molecules on the left surface of the 1-D Solid Heat Conductor XXX, (kg/m²). The total mass of the reversibly bound molecules on both left and right surface of SC cannot exceed the total mass that is initially present in the SC, determined in the record 391XXX. If the mass of the reversibly bound molecules on both left and right surfaces is smaller than the total mass in the SC, then the remaining part is assumed to be penetrated inside the SC. If the mass of the reversibly bound molecules on both left and right surfaces is larger than the total mass in the SC, then the reversibly bound masses are scaled to give the correct total mass. In such case there is no penetrated molecules.
Acceptable range: CR1FRT(1) ≥ 0.0
Default value: 0.0
- W-3 (R) : CR1FRT(2) Surface concentration of the reversibly bound molecules on the right surface of the 1-D Solid Heat Conductor XXX, (kg/m²).
Acceptable range: CR1FRT(2) ≥ 0.0
Default value: 0.0

2.15.87 Records: 492XXX, Initial Distribution of Vapors on the Surfaces of TC

This record defines initial distribution of the isotopes that are reversibly bound to the surface of 2-D solid structures. XXX is the TC reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : I1 Boundary cell number. Using I1 and I2 (below) the user specifies the cell range for the distribution of vapors on the boundary surfaces. The distribution defined by Words 3 and 4 will be applied for the boundary cells I: $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number.
Default value: none.
- W-2 (I) : I2 Boundary cell number. Using I2 and I1 (above) the user specifies the cell range for the distribution of vapors on the boundary surfaces. The distribution defined by Words 3 and 4 will be applied for the boundary cells I: $I1 \leq I \leq I2$.
Acceptable range: must be an existing boundary cell number. $I2 \geq I1$.
Default value: none.
- W-3 (I) : IVAP Vapor class number.
Acceptable range: must be a valid class number if nonzero
Default value: none.
- W-4 (R) : CR2FRT(I) Surface concentration of the reversibly bound molecules on the boundary cell I, $I1 \leq I \leq I2$, of the 2-D Solid Heat Conductor XXX, (kg/m^2). The total mass of the reversibly bound molecules on all surfaces of TC cannot exceed the total mass that is initially present in the SC, determined in the record 491XXX. If the mass of the reversibly bound molecules on all boundary surfaces is smaller than the total mass in the TC, then the remaining part is assumed to be penetrated inside the TC. If the mass of the reversibly bound molecules on all boundary surfaces is larger than the total mass in the TC, then the reversibly bound masses are scaled to give the correct total mass. In such case there is no penetrated molecules.
Acceptable range: CR2FRT(I) ≥ 0.0
Default value: 0.0

Several records with the same number may be used to define distributions of different fission product vapors.

2.15.88 Records: 393XXX, Initial Distribution of Vapor Classes Inside SC

This record defines initial distribution of the masses of isotopes that have penetrated into 1-D solid structures due to the sorption processes (the masses are defined in record 391XXX). XXX is the SC reference number, $001 \leq XXX \leq 999$.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-1 (I) : IVAP Vapor class number.
Acceptable range: must be a valid class number if nonzero
Default value: none.
- W-2 (R) : CD1FRT(1) Relative density, vapor class IVAP, in the cell number 1. The values are normalized and may therefore be scaled by any factor.
Acceptable range: CD1FRT(1) \geq 0.0
Default value: 0.0
- W-3 (R) : CD1FRT(2) Relative density, vapor class IVAP, in the cell number 2.
Acceptable range: CD1FRT(2) \geq 0.0
Default value: 0.0

. . . until all cells are defined

The last word is repeated until density in all cells are defined. Several records with the same number may be used to define distributions of different fission product vapors.

2.15.89 Records: 493XXX, Initial Distribution of Vapor Classes Inside TC

This record defines initial distribution of the masses of isotopes that have penetrated into 2-D solid structures due to the sorption processes (the masses are defined in record 391XXX). XXX is the TC reference number, $001 \leq \text{XXX} \leq 999$.

- W-1 (I) : IVAP Vapor class number.
Acceptable range: must be a valid class number if nonzero
Default value: none.
- W-2 (I) : L Row number in y-direction. The following data must specify NCLXTC values of internal power for all cells in the y-row number L.
Acceptable range: $1 \leq L \leq \text{NCLYTC}$.
Default value: none.
- W-3 (R) : CD2FRT Relative density, vapor class IVAP, cell (1,L), (x-row 1, y-row L), (-).
 (1,L) The values are normalized and may therefore be scaled by any factor. The values will be normalized during the input processing so that the total mass of the vapor class IVAP is always equal to the sum of the initial masses of all isotopes, specified in the record 491XXX, that belong to the class IVAP.
Acceptable range: CD2FRT(1,L) \geq 0.0
Default value: 0.0

The last word is repeated NCLXTC times density in all cells of row L are defined. Several records with the same number may be used to define distributions of different fission product vapors.

2.15.90 Records: 194XXX, Decay Heat Distribution Parameters for CV

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. This record, together with the records 394XXX and 494XXX, describes how the decay heat of the isotopes that are released from the core is distributed among the gas and liquid spaces of a Control Volume and solid structures. The default modelling is based on the following assumptions:

- β -radiation is absorbed by the gas in the atmosphere of a Control Volume.
- γ -radiation passes through the gas and is absorbed by solid structures and water pool.

Division of the decay heat of isotopes present in the atmosphere and pool of a Control Volume are discussed in this section.

W-1 (R): XATBRT Fraction of β -radiation absorbed in the gas space of the Control Volume XXX, $x_{atms, \beta}$, (-).
Acceptable range: $0.0 \leq \text{XATBRT} \leq 1.0$
Default value: 1.0

W-2 (R): XATGRT Fraction of γ -radiation absorbed in the gas space of the Control Volume XXX, $x_{atms, \gamma}$, (-).
Acceptable range: $0.0 \leq \text{XATGRT} \leq 1.0$
Default value: 0.0

2.15.91 Records: 394XXX, Decay Heat Distribution Parameters for SC

XXX is the 1-D Solid Heat Conductor reference number, $001 \leq \text{XXX} \leq 999$. This record, together with the records 194XXX and 494XXX, describes how the decay heat of the isotopes that are released from the core is distributed among the gas and liquid spaces of a Control Volume and solid structures. The default modelling is based on the following assumptions:

- β -radiation is completely absorbed by the solid structures.
- γ -radiation is completely absorbed by the solid structures.

Division of the decay heat of isotopes present in the 1-D Solid Heat Conductors are discussed in this section.

W-1 (R): XS1BRT Fraction of β -radiation absorbed in the solid material of the Heat Conductor XXX, $x_{solid, \beta}$, (-). Currently only default value is allowed.
Acceptable range: $1.0 \leq \text{XS1BRT} \leq 1.0$
Default value: 1.0

W-2 (R): XS1GRT Fraction of γ -radiation absorbed in the solid material of the Heat Conductor XXX, $x_{solid, \gamma}$, (-). Currently only default value is allowed.
Acceptable range: $1.0 \leq \text{XS1GRT} \leq 1.0$
Default value: 1.0

W-3 (R): WFSCRT Weighting factor, w_{sc} , (-), applied for the left surface in calculating the division of decay heat. The radiation emitted from the surface of an SC

is distributed among all surfaces present in a given enclosure based on the absorption fractions, defined as:

$$F_{abs,SC} = \frac{A_{SC} \cdot |w_{SC}|}{\sum_L A_L \cdot |w_L|}$$

A_{SC} - surface area of the solid heat conductor

w_{SC} - weighting factor of the surface SC

The summation is performed over all structures (1-D as well as 2-D) that are in contact with the boundary CV. Therefore the index L stands for any SC as well as TC in contact with the CV.

The values of $F_{abs,SC}$ are pre-computed during the input processing and are printed next to the weighting factors for CV related data of the RT Package, as a "CV enclosure data for decay heat calculations".

If w_{SC} is negative, the generating surface is not included in the distribution of the radiation emitted from its surface. Physically it means that the structure cannot radiate to itself. In such case the structure absorbs only half of the radiation generated at its surface. The other half is distributed among other structures of the enclosure, gas or pool. This means the fraction of the generated decay heat that the source structure receives is equal to:

$$\frac{1}{2}(\beta + \gamma)$$

If w_{SC} is positive, the generating surface is included in the distribution of the radiation emitted from its surface. Physically it means that the structure can radiate to itself. The total fraction of the generated decay heat that the source structure receives is equal to:

$$\frac{1}{2}(\beta + \gamma) + \frac{1}{2}[\beta(1 - x_{atms,\beta}) + \gamma(1 - x_{atms,\gamma})] \cdot (1 - X_{pool,SC} \cdot w_{pool,CV}) \cdot F_{abs,SC}$$

Acceptable range: $10^{-6} \leq |WFSCRT| \leq 10^6$

Default value: -1.0.

W-4 (R) : WFSCRT Weighting factor, w_i , (-), applied for the right surface in calculating the division of decay heat.

Acceptable range: $10^{-6} \leq |WFSCRT| \leq 10^6$

Default value: 1.0.

2.15.92 Records: 494XXX, Decay Heat Distribution Parameters for TC

XXX is the 2-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$. This record, together with the records 194XXX and 394XXX, describes how the decay heat of the isotopes that are released from the core is distributed among the gas and liquid spaces of a Control Volume and solid structures. The default modelling is based on the following assumptions:

- β -radiation is completely absorbed by the solid structures.
- γ -radiation is completely absorbed by the solid structures.

SPECTRA Code Manuals - Volume 2: User's Guide

Division of the decay heat of isotopes present in the 2-D Solid Heat Conductors are discussed in this section.

- W-1 (R) : XS2BRT Fraction of β -radiation absorbed in the solid material of the Heat Conductor XXX, $x_{solid, \beta}$, (-). Currently only default value is allowed.
Acceptable range: $1.0 \leq XS2BRT \leq 1.0$
Default value: 1.0
- W-2 (R) : XS2GRT Fraction of γ -radiation absorbed in the solid material of the Heat Conductor XXX, $x_{solid, \gamma}$, (-). Currently only default value is allowed.
Acceptable range: $1.0 \leq XS2GRT \leq 1.0$
Default value: 1.0
- W-3 (R) : WFTCRT Weighting factor, w_i , (-), applied for all boundary cells in calculating the division of decay heat.
Acceptable range: $10^{-3} \leq WFTCRT \leq 10^3$
Default value: 1.0.

2.15.93 Records: 295XXX, Vapor Filter Model

XXX is the Junction reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : IFLVRT Filter type:
 = -1: no filter.
 = 1: vapor filter, filter efficiency defined for each vapor class.
 = 2: isotope filter, filter efficiency defined for each isotope.
Acceptable range: -1, 1, 2
Default value: -1

If IFLVRT = 1

- W-2 (I) : JFLVRT(1) Reference number of a Tabular or a Control Function that defines filter efficiency for the vapor class 1.
Acceptable range: must be a valid reference number of a Tabular or Control Function, if nonzero
Default value: none
- W-3 (I) : JFLVRT(2) Reference number of a Tabular or a Control Function that defines filter efficiency for the vapor class 2.
Acceptable range: must be a valid reference number of a Tabular or Control Function, if nonzero
Default value: none

... , until the efficiencies are specified for all vapor classes.

If IFLVRT = 2

- W-2 (I) : I1 Isotope number

... , until the efficiencies are specified for all vapor classes.

2.15.95 Records: 195000, Pool-Gas Transport of FP Vapors - Global

This record contains global transport coefficient, $\mathcal{G}_{pool-atms}$, for the vapor classes (detailed description is provided in record 195XXX, containing individual activators).

W-1 (R) : DCPGRT(1) Global transport coefficient for the vapor class 1.
 Acceptable range: $0.0 \leq \text{DCPGRT}(1) \leq 10.0$
 Default value: 0.0

W-2 (R) : DCPGRT(2) Global transport coefficient for the vapor class 2.
 Acceptable range: $0.0 \leq \text{DCPGRT}(2) \leq 10.0$
 Default value: 0.0

... until coefficients are defined for all vapor classes.

2.15.96 Records: 195XXX, Pool-Gas Transport of FP Vapors - Individual

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. If fission product vapors are present in the pool, they may be transported to the pool-atmosphere (or pool-bubble) surface and enter the atmosphere of the Control Volume. The effect is calculated using a transport coefficient, defined below. the transfer process is calculated only if the pool-gas transport is activated in records 196000, 196XXX.

W-1 (R) : DCPART(1) Mass transfer coefficient (net velocity of FP molecules towards the pool surface or bubble surface) for the vapor class 1 isotopes present in the pool, $\mathcal{G}_{pool-gas}$, (m/s). The mass transfer rate is:

$$\frac{dm}{dt} = \mathcal{G}_{pool-gas} \cdot \rho_{pool} \cdot A_{pool} = \mathcal{G}_{pool-gas} \cdot \frac{M_{pool}}{V_{pool}} \cdot A_{pool}$$

- ρ_{pool} - density of the fission product in the pool, (kg/m³)
- A_{pool} - surface area (m²) (depending on IPATRT this may be pool-atmosphere, bubble-surface or both)
- V_{pool} - volume of the pool, (m³),
- M_{pool} - mass of the fission product in the pool, (kg)

SPECTRA Code Manuals - Volume 2: User's Guide

The rate of change of the fission product vapor mass in the pool is:

$$\left(\frac{dM_{pool}}{dt}\right) = \begin{cases} -\mathcal{G}_{pool-gas} \cdot \frac{M_{pool}}{V_{pool}} \cdot A_{pool} & \text{if } p_{atms} < p_{sat} \\ 0.0 & \text{if } p_{atms} > p_{sat} \end{cases}$$

If a negative number is entered, then the Sherwood number correlation is used, defined in the record 8960XX, where XX is the set number, equal to -DCPART

Acceptable range: $0 \leq \text{DCPART}(1) \leq 10$. or set number with minus sign

Default value: DCPGRT(1) - see record 195000

W-2 (R) : DCPART(2) Mass transfer coefficient for the vapor class 2 isotopes present in the pool, (m/s).

Acceptable range: $0 \leq \text{DCPART}(2) \leq 10$. or set number with minus sign

Default value: DCPGRT(2) - see record 195000

... until coefficients are defined for all vapor classes.

2.15.97 Records: 196000, Option for Pool-Gas Transport of FP Vapors – Global

Using this record one may specify the parameter described in record 196XXX for all Control Volumes in the model - see description of record 196XXX below.

2.15.98 Records: 196XXX, Option for Pool-Gas Transport of FP Vapors – Individual

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$. If fission product vapors are present in the pool, they may be transported to the pool-atmosphere (or pool-bubble) surface and enter the atmosphere of the Control Volume. This record defines where the transport is occurring.

W-1 (I) : IPATRT Pool-gas transport of fission products.

=0: no pool-gas transport of fission product occurs

=1 : transport occurs on the pool-atmosphere surface

=2 : transport occurs on the bubble-pool surface.

=3 : transport occurs on droplet-atmosphere surface.

NOTE: with option 2, fission products are transported from one CV to another with bubble flow. With option 3, fission products are not transported with droplets from one CV to another. Therefore the droplet to and from CV is automatically disabled: IDFAJN is set to 1.

Acceptable range: IPATRT = 0, 1, 2, 3

Default value: 0

W-2 (R) : XPATRT Multiplier for the pool-gas transport. The pool-gas transport calculated by the model described in record 8960XX, is multiplied by this value. This parameter is used for any transport defined by IPATRT. It may be used for example to model sticking fraction in case of pool-bubble transport.

Acceptable range: $0.0 \leq \text{XPATRT} \leq 10.0$

Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0).

W-3 (I) : ISVBRT Indicator for FP transport from pool to atmosphere. The meaning is the same as in case of bubble transport: ISVBCV - see Figure 2-3.
Acceptable range: $0 \leq \text{ISVBRT} \leq 100$
Default value: ISVBCV

2.15.99 Records: 8960XX, Pool-Gas Transport of FP Vapors Sh Correlation

XX is the set number. $01 \leq \text{XX} \leq 99$. The set number is selected for a given fission product vapor class in the records 195000 and 195XXX. If fission product vapors are present in the pool, they may be transported to the pool surface and/or bubble surface. The transport velocity is obtained using the Sherwood number correlation.

$$Sh = A_{Sh} + B_{Sh} \frac{Re^{C_{Sh}} Sc^{D_{Sh}}}{1 + E_{Sh} Re^{F_{Sh}} Sc^{G_{Sh}}}$$

Here Sh is the Sherwood number, Re is the Reynolds number, and Sc is the Schmidt number. The coefficients, A_{Sh} , B_{Sh} , C_{Sh} , D_{Sh} , E_{Sh} , F_{Sh} , G_{Sh} , are defined below. The mass transfer coefficient (net velocity of vapor flow towards the pool surface or bubble surface) is obtained from:

$$g_{pool-gas} = Sh \frac{D_C}{D_{hyd}}$$

Here D_{hyd} is the hydraulic diameter (m), and D_C is the diffusion coefficient (m^2/s).

W-1 (R) : DXPART Diffusion coefficient in liquid, D_C , (m^2/s).
 If a positive value is entered, $D_C = \text{DXPART}$
 If a negative value is entered, $D_C = \text{TF number} |\text{DXPART}|$.
 The argument for the TF is the liquid temperature.
Acceptable range: $0.0 < \text{DXPART} \leq 1.0$ or a valid reference to a Tabular Function
Default value: 0.0

W-2 (R) : ASPART A_{Sh} in the user-defined Sherwood number correlation:
Acceptable range: $-10^{10} \leq \text{ASPART} \leq 10^{10}$
Default value: 0.0

W-3 (R) : BSPART B_{Sh} in the Sherwood number correlation:
Acceptable range: $0.0 \leq \text{BSPART} \leq 10^{10}$
Default value: 0.0

W-4 (R) : CSPART C_{Sh} in the Sherwood number correlation:
Acceptable range: $0.0 \leq \text{CSPART} \leq 10.0$
Default value: 0.0

W-5 (R) : DSPART D_{Sh} in the Sherwood number correlation:
Acceptable range: $0.0 \leq \text{DSPART} \leq 10.0$
Default value: 0.0

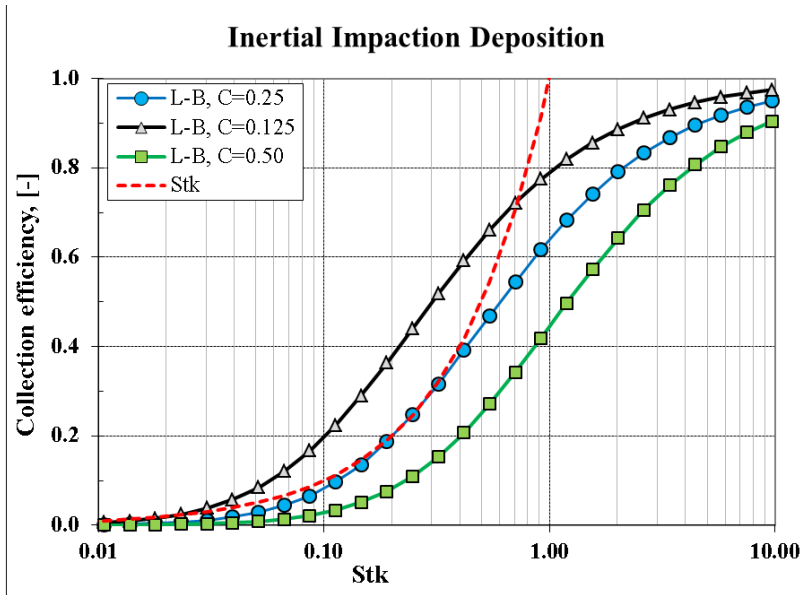


Figure 2-79 Langmuir and Blodgett correlation

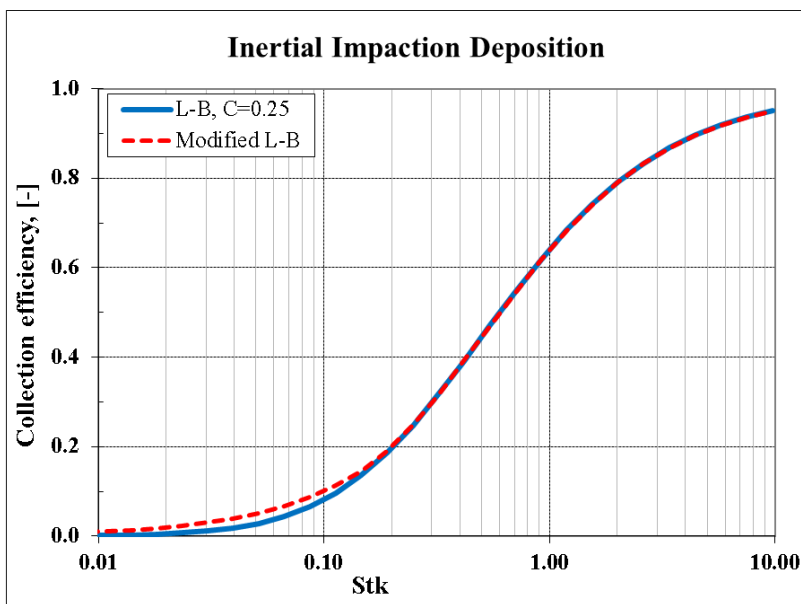


Figure 2-80 Modified versus original Langmuir and Blodgett correlation

Correlation developed based on data of Yoon & Lutrell and Afruns & Kitchener - Figure 2-81

$$\eta = \text{Min} \left(\eta_{\text{max}}, A \cdot \frac{d_p^2}{D_b} \right)$$

In order to activate the model, non-zero values must be supplied for at least two out of the following three input entries:

W-9 (R) : TBL1RT Diffusion boundary layer thickness, δ_{BL} , (m).

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $1.0 \times 10^{-7} \leq TBL1RT \leq 1.0 \times 10^{-3}$.

Default value: none

If the model is used, the recommended value is 5.0×10^{-5} .

W-10 (R) : CLB1RT Constant in the correlation for inertial impact, C_{LB} .
 CLB1RT ≤ 10 : C_{LB} , in the L-B or modified L-B correlation (depending on ILBORT, record 860000)
 CLB1RT > 1000 : A in the correlation developed based on data of Yoon & Luttrell and Afruns & Kitchener
 Acceptable range: $10^{-2} \leq CLB1RT \leq 10^{+1}$ C_{LB} , in L-B, modified L-B
 $10^{+3} \leq CLB1RT \leq 10^{+5}$ A in YLAK correlation
 Default value: none
 If the model is used, the recommended value is 0.25.

W-11 (R) : ELB1RT Maximum efficiency η_{max} , in the correlation for inertial impact
 Acceptable range: $10^{-3} \leq ELB1RT \leq 10^{+3}$
 Default value: 1.0 if the model is used
 (if TBL1RT > 0.0 , CLB1RT > 0.0)

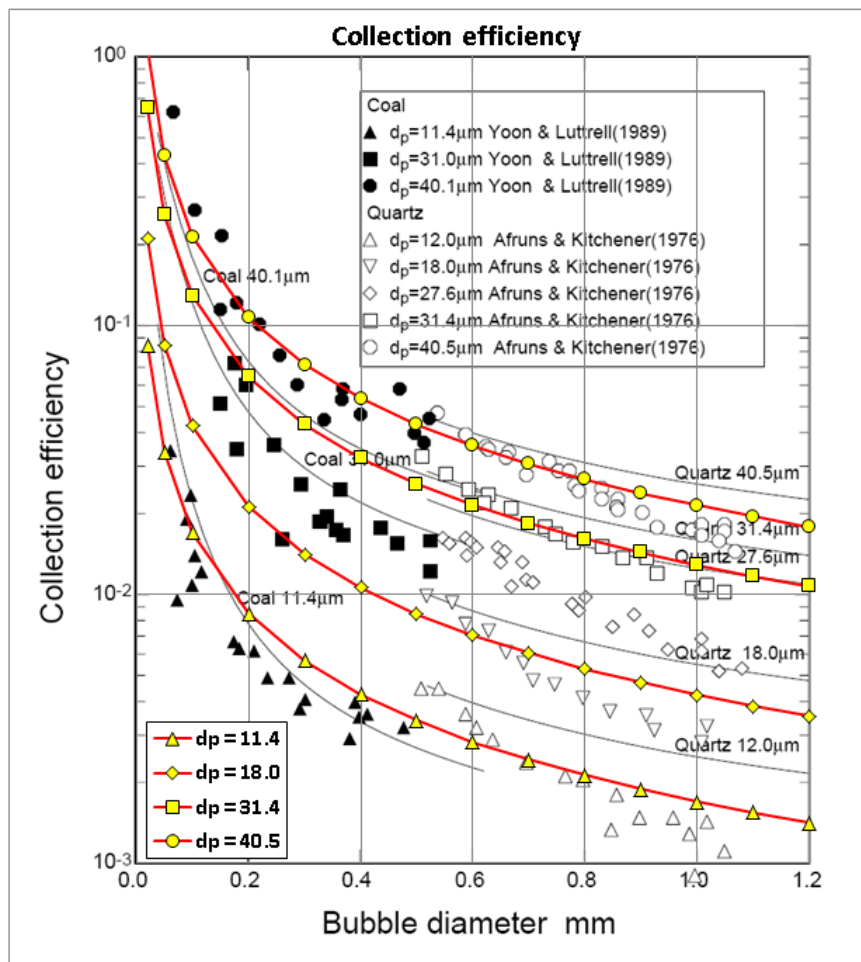


Figure 2-81 Data of Yoon & Luttrell and Afruns & Kitchener and correlation

2.15.100 Records: 385XXX, Leaching Input Parameters for SC

This record defines leaching parameters. XXX is the 1-D Solid Heat Conductor reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : LILCRT Leaching model indicator.
 = 0 : no leaching is applied,
 = 1 : leaching is applied on the left boundary surface
 = 2 : leaching is applied on the right boundary surface
 = 3 : leaching is applied on both boundary surfaces
Acceptable range: 0, 1, 2, 3
Default value: 0
- W-2 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK. This isotope is being leached from the boundary surface of SC.
Acceptable range: must be a valid reference number
Default value: none.
- W-3 (R) : CALCRT Average initial concentration (mass fraction) of the isotope KKI, (-). The initial mass of the isotope of KKI is equal to the total mass of the material in the SC node multiplied by this number. The initial mass is set only in the cells with the same material as in the boundary cell (the leached alloy). If LLILCRT=3, then the material in both left and right boundary cells must be the same. The same concentration is applied in all nodes with the leached material, unless the concentrations are defined differently in the records 393XXX.
Acceptable range: $0.0 < \text{CALCRT} < 0.5$
Default value: none.
- W-4 (R) : TOLCRT Characteristic time (s) for the surface concentration to reach zero (Stage I).
Acceptable range: $10^2 \leq \text{TOLCRT} \leq 10^6$
Default value: 10^3

NOTE!

A sorption model must be activated on the surface on which the leaching model is applied. Furthermore, the parameter ISRLRT must be set to 2 (sorption in liquid). The sorption model must be a CF type. Two methods are available:

- If the diffusion coefficient of the surface material is defined, then the diffusion model is used and the Control Function is a dummy and the value of the CF is not important. In that case a fine nodalization must be used.
 - size of the nodes close to the boundary: $10^{-6} - 10^{-5}$ m (1 - 10 μm),
 - applied for at least: 5×10^{-4} m (50 μm) depth.
- If the diffusion coefficient of the surface material is not defined, then the value of surface mass flux is equal to the value of the CF. In lack of diffusion, the material will be leached from the boundary cell only. Therefore the boundary cell must be large enough. The following limits are set by the input procedures:

SPECTRA Code Manuals - Volume 2: User's Guide

- minimum required size of the boundary node: 10^{-4} m (100 μ m)
- recommended size of the boundary node: 10^{-3} m (1000 μ m)

The following limits are internally imposed on the value obtained from the CF:

- $CF \leq 0.0$
- $CF \geq -1.0 \times 10^{-6}$

Example:

The following example defines chromium leaching on the left surface of SC-991.

```
* ---- Leaching model
*   LEACRT KKI CALCRT TOLCRT
385991 1   191 0.07  1.0E3
*
* ---- Define stable isotope Cr-52, Isotope 191, member of vapor class 7
F05191 Cr-52
*   M-core MW beta gamma yield
880191 0.0  52 0.0 0.0 0.0
885191 07 * release class
886191 07 * vapor class
*
* ---- Sorption definition
*   LEFT   RIGHT
*   SET MULT. SET MULT.
395991 1 0.0  0 0.0
*
*Vap-7: model ISRLRT
895107 -100 2 * cf-100, ISRLRT=2 (LIQUID)
*
705100 SORPTION CF (dummy)
*   Group Number Fact. Const.
700100 1   1   1.0  0.0
*   Arguments
* Pointers: (1) (2) (3) (4) Fact. Const
710100 9 000 1 0 1.0  0.0 * time
```

2.15.101 Records: 386000, Leaching Model General Parameters

W-1 (R) : TMLCRT Minimum temperature (K) for the reaction. The reaction is not proceeding if the surface temperature is smaller than TMLCRT. An interpolation zone of DTLCRT is assumed. The diffusion-controlled reaction reaches full speed if the temperature exceeds TMLCRT+DTLCRT.

Acceptable range: $273.0 \leq TMLCRT \leq 10,000.0$

Default value: 850.0

W-2 (R) : DTLCRT Interpolation temperature range (K) for the reaction. The diffusion-controlled reaction reaches full speed if the temperature exceeds TMLCRT+DTLCRT.

Acceptable range: $10.0 \leq DTLCRT \leq 100.0$

Default value: 50.0

2.15.102 Records: 8970XX, List of RT Isotopes Mapped to CV Gases

XX is the list number. Usually isotopes are treated as trace species; the isotope mass is not considered in the CV Package. Using this list, the user may link the RT isotope masses to the CV gas masses for the cases when the effect of gas pressurization is considered non-negligible. A mass source referring to this list must be specified in the records 13YXXX. The maximum number of lists is 20 (=NGMXFL).

W-1 (I) : I Gas number The built-in gases are: 0=water (liquid), 1=H₂, 2=He, 3=steam, 4=N₂, 5=O₂, 6=CO₂.
Acceptable range: 1 ≤ I ≤ NGASCV ≤ NGMXFL = 20
Default value: none.

W-2 (I) : KKI(1) Reference number of the first isotope on this list, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be an existing isotope
Default value: none.

W-3 (I) : KKI(2) Reference number of the second isotope on this list, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be an existing isotope
Default value: none.

... until all isotopes are defined. The maximum number of isotopes on one list is 20.

An example is shown below. The example shows how to link Xenon and Krypton isotopes in the RT Package to Xenon and Krypton gases in the FL Package.

```
*      Xe isotopes -> Xe gas (user-defined gas number 11)
*      Gas   Xe-131m Xe-131   Xe-132   Xe-133m Xe-134   Xe-135m Xe-135   Xe-137
897001 11   015      016      023      035      043      052      053      061
*
*      Kr isotopes -> Kr gas (user-defined gas number 10)
*      Gas   Kr-85m   Kr-85      Kr-90
897002 10   083      084      091
```

The gases must be defined in the FL input. An example of such input is shown in:

```
\Z-INPUTS\FL\GAS\CO-Ar-Ne-Kr-Xe-H2.ATT
```

The example above is valid if all built-in isotope chains are used (see 2.15.111). If additional isotopes are defined in the RT input, the list above must be appended accordingly. An example of additional isotope inputs for Xe and Kr isotopes is shown in:

```
\Z-INPUTS\RT\DECAY-CHAINS
```

2.15.103 Records: 898000, Selection of Sorption Processes on Aerosol Particles

The sorption on aerosol particles, defined in this record, is applied for all aerosol particles, including the particles deposited on structures.

W-1 (I) : IASRRT(1) Number of sorption set (defined in records 895YXX) to be used on the surface of the aerosol particles in a Control Volume, either atmosphere

SPECTRA Code Manuals - Volume 2: User's Guide

or pool of CV. The input parameter ISRLRT (record 895YXX) determines if sorption occurs in the gas or the liquid phase.

Acceptable range: must be one of existing sorption sets, if nonzero

Default value: 0

W-2 (R) : YASRRT(1) Multiplier for the sorption model applied on the aerosol particles in a Control Volume. The sorption rate that is calculated by the sorption model selected by the previous word, is multiplied by this value.

Acceptable range: $0.0 \leq \text{YASRRT}(1) \leq 10.0$. For the sorption model 2 (see 895YXX) only 1.0 and 0.0 may be used. Zero may be used to disable the sorption model but keep track of the penetrated and reversibly-bound molecules (the latter may for example be washed by water pool).

Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0).

W-3 (I) : IASRRT(2) Number of sorption set (defined in records 895YXX) to be used on the surface of the aerosol particles deposited on the surfaces of 1-D Solid Heat Conductors, either on the uncovered or on the pool-covered surface. The input parameter ISRLRT (record 895YXX) determines if sorption occurs in the gas or the liquid phase. It is recommended to use the same set on all aerosol particles, IASRRT(2) = IASRRT(1).

Acceptable range: must be one of existing sorption sets, if nonzero

Default value: 0

W-4 (R) : YASRRT(2) Multiplier for the sorption model applied on the aerosol particles deposited on the surfaces of 1-D Solid Heat Conductors. The sorption rate that is calculated by the sorption model selected by the previous word, is multiplied by this value.

Acceptable range: $0.0 \leq \text{YASRRT}(2) \leq 10.0$. For the sorption model 2 (see 895YXX) only 1.0 and 0.0 may be used. Zero may be used to disable the sorption model but keep track of the penetrated and reversibly-bound molecules (the latter may for example be washed by water pool).

Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0).

W-5 (I) : IASRRT(3) Number of sorption set (defined in records 895YXX) to be used on the surface of the aerosol particles deposited on the surfaces of 2-D Solid Heat Conductors, either on the uncovered or on the pool-covered surface. The input parameter ISRLRT (record 895YXX) determines if sorption occurs in the gas or the liquid phase. It is recommended to use the same set on all aerosol particles, IASRRT(3) = IASRRT(2) = IASRRT(1).

Acceptable range: must be one of existing sorption sets, if nonzero

Default value: 0

W-6 (R) : YASRRT(3) Multiplier for the sorption model applied on the aerosol particles deposited on the surfaces of 2-D Solid Heat Conductors. The sorption rate that is calculated by the sorption model selected by the previous word, is multiplied by this value.

SPECTRA Code Manuals - Volume 2: User's Guide

Acceptable range: $0.0 \leq \text{YASRRT}(3) \leq 10.0$. For the sorption model 2 (see 895YXX) only 1.0 and 0.0 may be used. Zero may be used to disable the sorption model but keep track of the penetrated and reversibly-bound molecules (the latter may for example be washed by water pool).

Default value: 1.0 (a small number, $<10^{-50}$, sets the value to 0.0).

W-7 (I) : IAFPRT Apply adjustment of fission products adsorbed on aerosol particles:
=1: Adjustment is applied. At the end of a time step, the penetrated mass is set to the total mass and the reversible mass is set to zero for those vapor classes for which model other than the Model 2 (PATRAS/SPATRA model) is applied.
=2: Adjustment is not applied.
Acceptable range: 1 or 2
Default value: 1

2.15.104 Records: 197XXX, Initial Masses of Isotopes on Aerosol Particles

XXX is the CV reference number, $001 \leq \text{XXX} \leq 999$.

W-1 (I) : ITP Data type indicator, 1=airborne aerosol particles, 2=particles deposited in the pool. The data specified by the Words below is applied for either airborne or pool-deposited particles depending on ITP
Acceptable range: 1 or 2
Default value: none.

W-2 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.

If ITP = 1:

W-3 (R) : YN5CRT(1) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 1 in the Control Volume XXX, (-).
Acceptable range: $0.0 \leq \text{YN5CRT}(1) \leq 1.0$
Default value: 0.0

W-4 (R) : YP5CRT(1) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 1 in the Control Volume XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $\text{YP5CRT}(1) \leq \text{YN5CRT}(1)$ for sorption model 2
 $\text{YP5CRT}(1) = \text{YN5CRT}(1)$ for other model
Default value: 0.0

SPECTRA Code Manuals - Volume 2: User's Guide

W-5 (R) : YN5CRT(2) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 2, present in the Control Volume XXX, (-).

Acceptable range: $0.0 \leq \text{YN5CRT}(2) \leq 1.0$

Default value: 0.0

W-6 (R) : YP5CRT(2) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 2 in the Control Volume XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001)

Acceptable range: $\text{YP5CRT}(2) \leq \text{YN5CRT}(2)$ for sorption model 2
 $\text{YP5CRT}(2) = \text{YN5CRT}(2)$ for other model

Default value: 0.0

. . . until data for all size sections is specified.

If ITP = 2:

W-3 (R) : YN6CRT(1) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 1, deposited in the pool of Control Volume XXX, (-).

Acceptable range: $0.0 \leq \text{YN6CRT}(1) \leq 1.0$

Default value: 0.0

W-4 (R) : YP6CRT(1) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 1 deposited in the pool of Control Volume XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).

Acceptable range: $\text{YP6CRT}(1) \leq \text{YN6CRT}(1)$ for sorption model 2
 $\text{YP6CRT}(1) = \text{YN6CRT}(1)$ for other model

Default value: 0.0

W-5 (R) : YN6CRT(2) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 2, deposited in the pool of Control Volume XXX, (-).

Acceptable range: $0.0 \leq \text{YN6CRT}(2) \leq 1.0$

Default value: 0.0

W-6 (R) : YP6CRT(2) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 2, deposited in the pool of the Control Volume XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).

Acceptable range: $\text{YP6CRT}(2) \leq \text{YN6CRT}(2)$ for sorption model 2
 $\text{YP6CRT}(2) = \text{YN6CRT}(2)$ for other model

Default value: 0.0

. . . until data for all size sections is specified.

The data sets for different isotopes should be entered in different records with the same number. For each aerosol size sections the sum of fractions entered in these records must be smaller than or equal to 1.0.

2.15.105 Records: 397XXX, Initial Masses of Isotopes on Particles Deposited on SC

XXX is the SC reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : IBC Boundary surface number, 1=left surface, 2=right surface. The data specified by the Words below is applied for the aerosol particles that are initially deposited on the boundary surface IBC.
Acceptable range: 1 or 2
Default value: none.
- W-2 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.
- W-3 (R) : YN7FRT(1) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 1, deposited on the boundary surface IBC of the 1-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YN7FRT(1) \leq 1.0$
Default value: 0.0
- W-4 (R) : YP7FRT(1) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 1, deposited on the boundary surface IBC of the 1-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YP7FRT(1) \leq YN7FRT(1)$ for sorption model 2
 $YP7FRT(1) = YN7FRT(1)$ for other model
Default value: 0.0
- W-5 (R) : YN7FRT(2) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 2, deposited on the boundary surface IBC of the 1-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YN7FRT(2) \leq 1.0$
Default value: 0.0
- W-6 (R) : YP7FRT(2) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 2, deposited on the boundary surface IBC of the 1-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YP7FRT(2) \leq YN7FRT(2)$ for sorption model 2
 $YP7FRT(2) = YN7FRT(2)$ for other model
Default value: 0.0

. . . until data for all size sections is specified. The data sets for different boundary surfaces and different isotopes should be entered in different records with the same number. For each aerosol size section the sum of fractions entered in these records must be smaller than or equal to 1.0.

2.15.106 Records: 497XXX, Initial Masses of Isotopes on Particles Deposited on TC

XXX is the TC reference number, $001 \leq XXX \leq 999$.

- W-1 (I) : IBC Boundary cell number. The data specified by the Words below is applied for the aerosol particles that are initially deposited on the surface of the boundary cell IBC.
Acceptable range: 1 or 2
Default value: none.
- W-2 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.
- W-3 (R) : YN8FRT(1) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 1, deposited on the surface of the boundary cell IBC of the 2-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YN8FRT(1) \leq 1.0$
Default value: 0.0
- W-4 (R) : YP8FRT(1) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 1, deposited on the boundary cell IBC of the 2-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YP8FRT(1) \leq YN8FRT(1)$ for sorption model 2
 $YP8FRT(1) = YN8FRT(1)$ for other model
Default value: 0.0
- W-5 (R) : YN8FRT(2) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 2, deposited on the surface of the boundary cell IBC of the 2-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YN8FRT(2) \leq 1.0$
Default value: 0.0
- W-6 (R) : YP8FRT(2) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 2, deposited on the boundary cell IBC of the 2-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YP8FRT(2) \leq YN8FRT(2)$ for sorption model 2
 $YP8FRT(2) = YN8FRT(2)$ for other model
Default value: 0.0

. . . until data for all size sections is specified. The data sets for different boundary surfaces and different isotopes should be entered in different records with the same number. For each aerosol size section the sum of fractions entered in these records must be smaller than or equal to 1.0.

2.15.107 Records: 198XXX, Isotopes on External Sources of Aerosols

XXX is the CV reference number, $001 \leq XXX \leq 999$. The external sources of aerosols are specified in records 175XXX. The present records may be used to define the isotopes that are present in the aerosols coming from the external sources.

- W-1 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.
- W-2 (R) : YNSCRT(1) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 1, coming from the external source defined in the record 175XXX into the Control Volume XXX, (-).
Acceptable range: $0.0 \leq \text{YNSCRT}(1) \leq 1.0$
Default value: 0.0
- W-3 (R) : YPSCRT(1) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 1, coming from the external source defined in the record 175XXX into the Control Volume XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $\text{YPSCRT}(1) \leq \text{YNSCRT}(1)$ for sorption model 2
 $\text{YPSCRT}(1) = \text{YNSCRT}(1)$ for other models
Default value: 0.0
- W-4 (R) : YNSCRT(2) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 2, coming from the external source defined in the record 175XXX into the Control Volume XXX, (-).
Acceptable range: $0.0 \leq \text{YNSCRT}(2) \leq 1.0$
Default value: 0.0
- W-3 (R) : YPSCRT(2) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 2, coming from the external source defined in the record 175XXX into the Control Volume XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $\text{YPSCRT}(2) \leq \text{YNSCRT}(2)$ for sorption model 2
 $\text{YPSCRT}(2) = \text{YNSCRT}(2)$ for other models
Default value: 0.0

... until data for all size sections is specified. The data sets for different isotopes should be entered in different records with the same number. For each aerosol size section the sum of fractions entered in these records must be smaller than or equal to 1.0.

2.15.108 Records: 398XXX, Isotopes on External Sources of SC-Deposited Aerosols

XXX is the SC reference number, $001 \leq XXX \leq 999$. The external sources of aerosols are specified in records 375XXX. The present records may be used to define the isotopes that are present in the aerosols coming from the external sources.

W-1 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.

W-2 (R) : YNS7RT(1) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 1, coming from the external source defined in the record 375XXX onto the surfaces of 1-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YNS7RT(1) \leq 1.0$
Default value: 0.0

W-3 (R) : YPS7RT(1) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 1, coming from the external source defined in the record 375XXX onto the surfaces of 1-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YPS7RT(1) \leq YNS7RT(1)$ for sorption model 2
 $YPS7RT(1) = YNS7RT(1)$ for other models
Default value: 0.0

W-4 (R) : YNS7RT(2) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 2, coming from the external source defined in the record 375XXX onto the surfaces of 1-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YNS7RT(2) \leq 1.0$
Default value: 0.0

W-3 (R) : YPS7RT(2) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 2, coming from the external source defined in the record 375XXX onto the surfaces of 1-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YPS7RT(2) \leq YNS7RT(2)$ for sorption model 2
 $YPS7RT(2) = YNS7RT(2)$ for other models
Default value: 0.0

... until data for all size sections is specified. The data sets for different isotopes should be entered in different records with the same number. For each aerosol size section the sum of fractions entered in these records must be smaller than or equal to 1.0.

2.15.109 Records: 498XXX, Isotopes on External Sources of TC-Deposited Aerosols

XXX is the TC reference number, $001 \leq XXX \leq 999$. The external sources of aerosols are specified in records 475XXX. The present records may be used to define the isotopes that are present in the aerosols coming from the external sources.

W-1 (I) : KKI Reference number of the isotope, where KK is the chain reference number and I is the isotope number within the chain KK.
Acceptable range: must be a valid reference number if nonzero
Default value: none.

W-2 (R) : YNS8RT(1) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 1, coming from the external source defined in the record 475XXX onto the surfaces of 2-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YNS8RT(1) \leq 1.0$
Default value: 0.0

W-3 (R) : YPS8RT(1) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 1, coming from the external source defined in the record 475XXX onto the surfaces of 2-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YPS8RT(1) \leq YNS8RT(1)$ for sorption model 2
 $YPS8RT(1) = YNS8RT(1)$ for other models
Default value: 0.0

W-4 (R) : YNS8RT(2) Initial mass fraction of the isotope KKI (both reversibly-bound and penetrated) present in the aerosol particles of the size section 2, coming from the external source defined in the record 475XXX onto the surfaces of 2-D Solid Heat Conductor XXX, (-).
Acceptable range: $0.0 \leq YNS8RT(2) \leq 1.0$
Default value: 0.0

W-3 (R) : YPS8RT(2) Initial fraction of the penetrated mass of the isotope KKI present in the aerosol particles of the size section 2, coming from the external source defined in the record 475XXX onto the surfaces of 2-D Solid Heat Conductor XXX, (-). Used only if the sorption model 2 is used for the aerosol particles (sorption set is selected in the record 898001).
Acceptable range: $YPS8RT(2) \leq YNS8RT(2)$ for sorption model 2
 $YPS8RT(2) = YNS8RT(2)$ for other models
Default value: 0.0

. . . until data for all size sections is specified. The data sets for different isotopes should be entered in different records with the same number. For each aerosol size section the sum of fractions entered in these records must be smaller than or equal to 1.0.

2.15.110 Records: 199XXX, Radiation Exposure and Dose Parameters

XXX is the Control Volume reference number, $001 \leq \text{XXX} \leq 999$.

W-1 (R) : CG1DRT Multiplier $C_{\gamma,1}$ (-), in the formula for the γ -radiation flux. The full formula is (see Volume 1 for detailed explanation):

$$\varphi_{\gamma,i} = C_{\gamma,1} \cdot \frac{0.620}{V_{CV}^{2/3}} \cdot S_{i,CV} + C_{\gamma,2} \cdot \frac{0.207}{V_{CV}^{2/3}} \cdot \left(S_{i,CV-pool} + \sum_{SC \in CV} S_{i,SC} + \sum_{TC \in CV} S_{i,TC} \right)$$

Acceptable range: $10^{-6} \leq \text{CG1DRT} \leq 10^6$
Default value: 1.0

W-2 (R) : CG2DRT Multiplier $C_{\gamma,2}$ (-), in the formula for the γ -radiation flux.
Acceptable range: $10^{-6} \leq \text{CG2DRT} \leq 10^6$
Default value: 1.0

W-3 (R) : CB1DRT Multiplier $C_{\beta,1}$ (-), in the formula for the γ -radiation flux. The full formula is (see Volume 1 for detailed explanation):

$$\varphi_{\beta,i} = C_{\beta,1} \cdot \frac{S_{i,CV} \cdot \rho}{(\mu_{a,\beta} / \rho)} \cdot (1 - \exp[-(\mu_{a,\beta} / \rho) \cdot (\rho R)]) +$$

$$+ C_{\beta,2} \cdot \frac{0.207}{V_{CV}^{2/3}} \cdot \left(S_{i,CV-pool} + \sum_{SC \in CV} S_{i,SC} + \sum_{TC \in CV} S_{i,TC} \right) \cdot \exp[-(\mu_{a,\beta} / \rho) \cdot (\rho R)]$$

Acceptable range: $10^{-6} \leq \text{CB1DRT} \leq 10^6$
Default value: 1.0

W-4 (R) : CB2DRT Multiplier $C_{\beta,2}$ (-), in the formula for the γ -radiation flux.
Acceptable range: $10^{-6} \leq \text{CB2DRT} \leq 10^6$
Default value: 1.0

W-5 (R) : QFGMRT Quality factor for the γ -radiation, Q_γ . Used to calculate the dose equivalent, H :

$$H = D_\gamma \cdot Q_\gamma + D_\beta \cdot Q_\beta$$

Acceptable range: $10^{-6} \leq \text{QFGMRT} \leq 10^6$
Default value: 1.0

W-6 (R) : QFBTRT Quality factor for the β -radiation, Q_β .
Acceptable range: $10^{-6} \leq \text{QFBTRT} \leq 10^6$
Default value: 1.0

2.15.111 Built-in Fission Product Chains (Decay Chains)

The built-in decay chains are shown in Figure 2-83 through Figure 2-92. Isotopes are shown in colours depending on their decay half-life time, T . The red colour is used for the short-life isotopes (T of order of minutes). The stable isotopes are shown in blue. The applied colour scale is shown in Figure 2-82. List of all built-in isotopes and their reference numbers is given in Table 2-47.

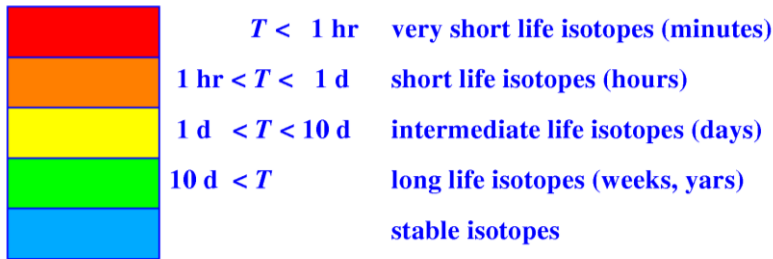


Figure 2-82 Decay chains, colour legend.

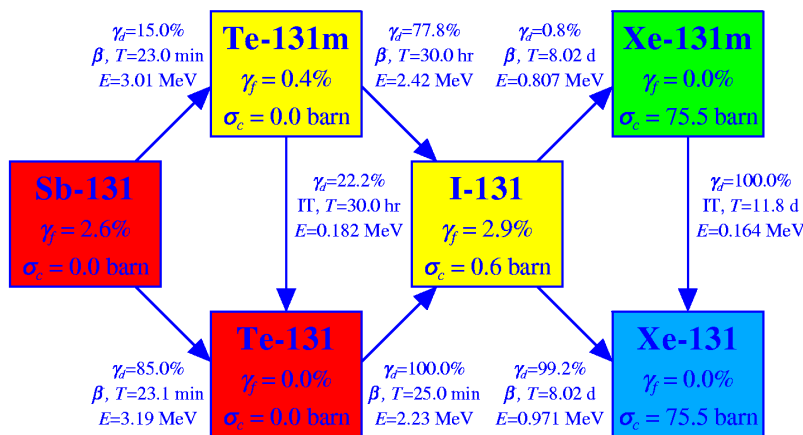


Figure 2-83 Decay chain, $M_w = 131$.

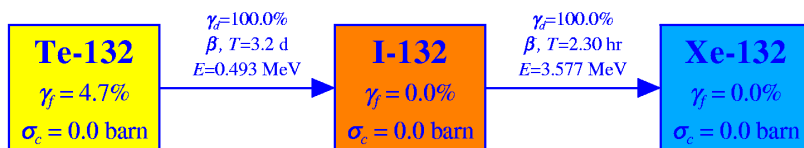


Figure 2-84 Decay chain, $M_w = 132$.

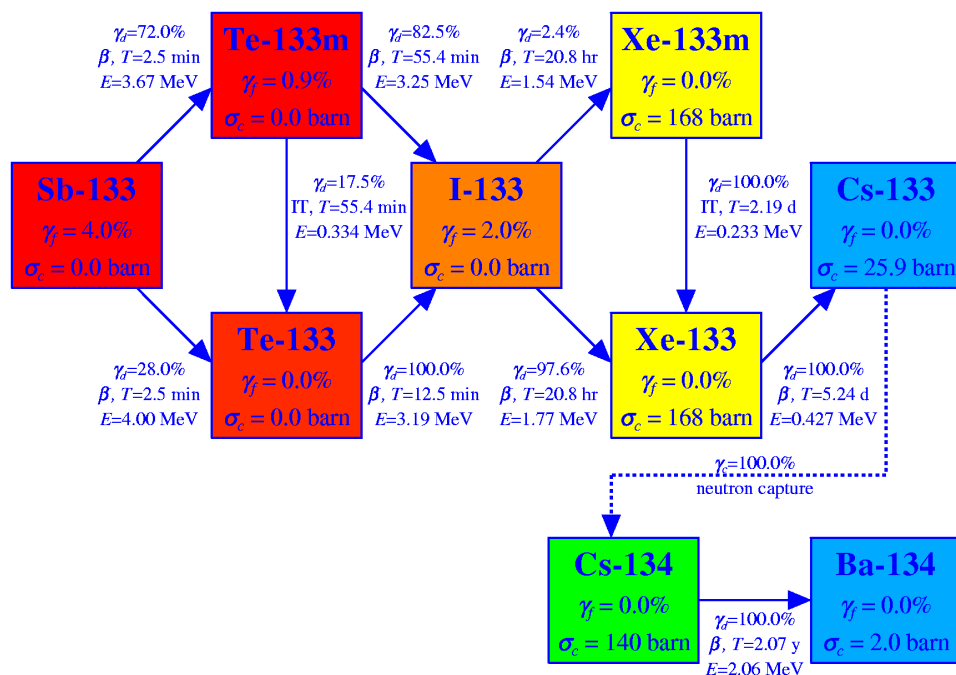


Figure 2-85 Decay chain, $M_w = 133$.

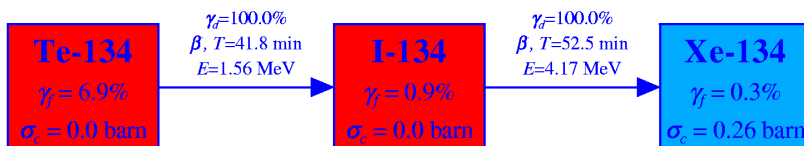


Figure 2-86 Decay chain, $M_w = 134$.

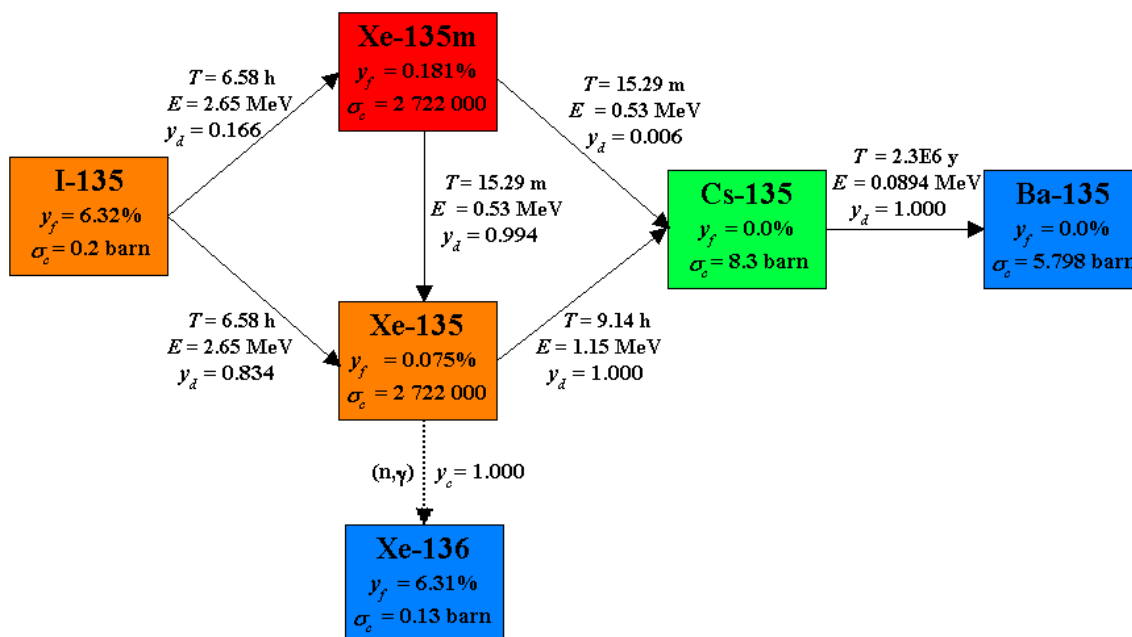


Figure 2-87 Decay chain, $M_w = 135 / 136$.

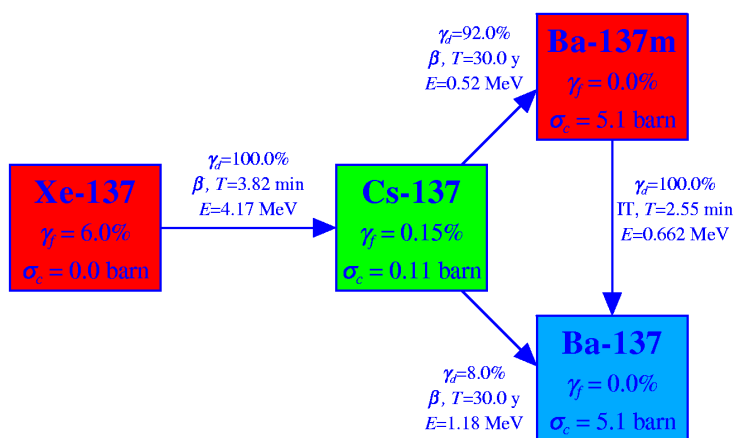


Figure 2-88 Decay chain, $M_w = 136$.

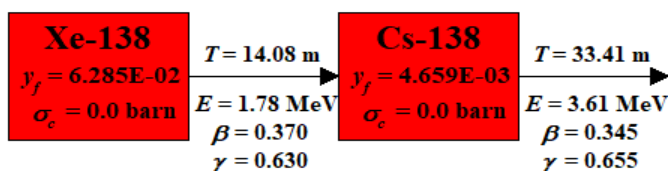


Figure 2-89 Decay chain, $M_w = 138$.

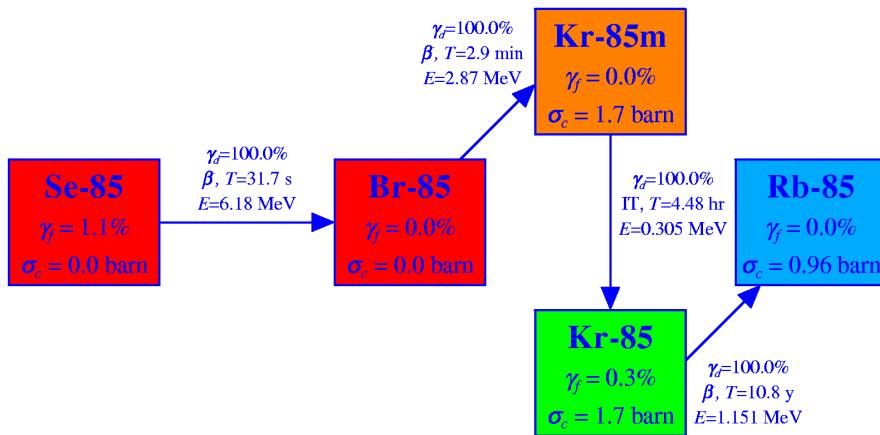


Figure 2-90 Decay chain, $M_w = 85$.

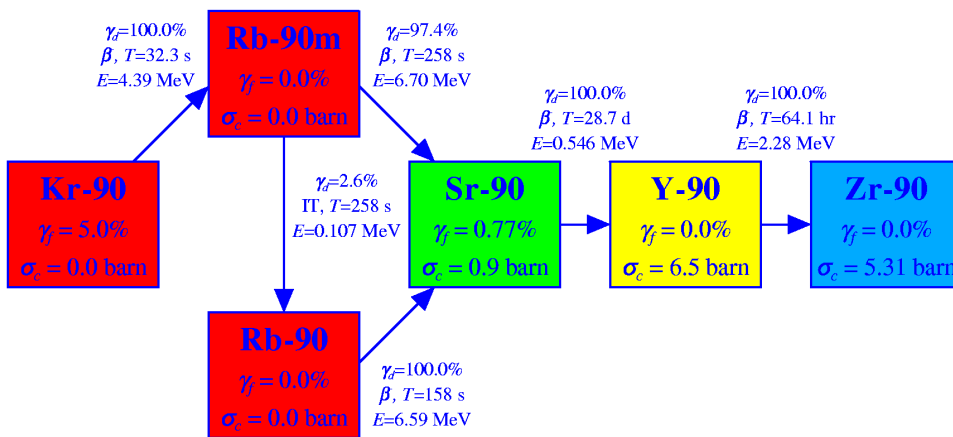


Figure 2-91 Decay chain, $M_w = 90$.

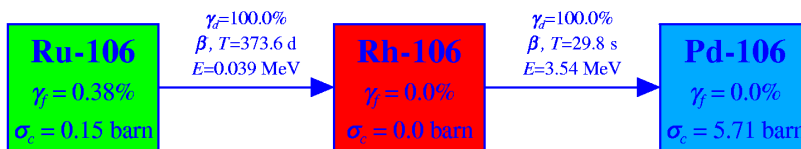


Figure 2-92 Decay chain, $M_w = 106$.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-4 (R) : DTPLT Plot frequency, (s). A negative value results in plot point being written every time step.
Acceptable range: $DTMAX \leq DTPLT \leq 10^{10}$ or $DTPLT < 0.0$
Default value: $(TENDI(i) - TSTART) / 200$, if $i=1$,
 $(TENDI(i) - TENDI(i-1)) / 200$, if $i>1$,
 where i is the time step domain number.
- W-5 (R) : TENDI End time for this domain, (s). The end time for the last domain determines the time when the transient calculations are terminated. Calculations can also be terminated at any time using the SPECTRA Stop File, “*.STP” (see section 3.8). This is done as follows. The stop file has to be put in the directory where the run is performed. The program will (among others) ask for the new end time. If zero is entered the current value will be unchanged. If a positive value is entered, it will be used provided that it is not smaller the current time and not larger than the end of the next time step domain (if exists).
Acceptable range: End time values must increase. Thus the value must be greater than the value of TENDI for the previous domain.
Default value: none.
- W-6 (I) : IOPSL Solver options valid for this domain. Using this input entry the user can deactivate the thermal-hydraulic packages, such as CV, JN, etc. This means the conditions in all Control Volumes, Junctions, etc. will be frozen during the whole time domain. This option is useful if the thermal-hydraulic packages require a lot of computing time (for example small Courant Limit), while the user needs a long calculation, with quasi-stationary thermal-hydraulic conditions. This may be the case if for example the user wishes to calculate a long term behavior (days, months, or even years) with practically constant thermal-power (long term operation with nominal power). In such run the parameters of interest may be:
Reactor Kinetics related parameters:
- depletion of fuel,
- accumulation of fission product poisons following start-up
- re-loading rate,
Radioactive Particle Transport Related parameter:
- accumulation of dust particles in various parts of the system during normal operation,
- accumulation of radioactive isotopes in various parts of the system during normal operation
The meaning of IOPSL is as follows:
IOPSL = 0 : normal calculations (all packages active)
IOPSL = 1 : deactivate CV/JN/H2 package.
IOPSL = 2 : deactivate CV/JN/H2 and SC/TC/TR/OX packages

IOPSL = 3 : deactivate CV/JN/H2 and SC/TC/TR/OX and TF/CF packages. Only the TF-YYY or the CF-YYY (see below) is recalculated.
IOPSL = 1YYY: the option is defined by a Tabular Function TF-YYY, where YYY = IOPSL-1000. The value of TF-YYY is rounded to the nearest integer and set to the range between 0 and 3. If the value is 3, then the TF/CF packages are deactivated with the exception of TF-YYY.

IOPSL = 2YYY: the option is defined by a Control Function CF-YYY, where YYY = IOPSL-2000. The value of CF-YYY is rounded to the nearest integer and set to the range between 0 and 3. If the value is 3, then the TF/CF packages are deactivated with the exception of CF-YYY and any TF that is being used by the CF-YYY.

Acceptable range: 0, 1, 2, or reference to a Tabular Function

Default value: 0

- W-7 (I) : IRKSL Additional action for the reactor kinetics model in case of deactivated thermal-hydraulic packages. This input entry determines the behavior of the Reactor Kinetics Package in case when IOPSL > 0.
- 1 : the RK is active; the reactivity is kept constant.
 - 2 : the RK is active; the reactor total power is kept constant by using a power controller. If this option is used, the constants in the PI power controller are defined in the record 761000. This option is not recommended. If the power is to be kept constant it is recommended to use option 1 or 4.
 - 3 : the RK is active; no specific actions are taken to ensure constant power or reactivity.
 - 4 : the RK is inactive; the reactor fission power is kept constant. However, changes in the isotope concentrations are calculated. The macroscopic fission cross section (RK-000-SigF-0000) and, consequently, the neutron density and the neutron flux (RK-000-Neut-0000, RK-000-Flux-0000) as well as the DNP concentrations (RK-000-Cpre-00nn) are updated to obtain the stationary state values corresponding to the current SigF.
- In the case of circulating fuel (IFTORK=2) two chains, DNP and DHG, are excluded from the solution (the concentrations are kept constant). This is because these chains contain short living isotopes. The flow solution for these isotopes would not be accurate for time steps significantly larger than the Courant limit.
- Acceptable range:* 1, 2, 3, 4
Default value: 4
- W-8 (I) : ICVSL Additional action for the Control Volumes with time dependent conditions in case of deactivated thermal-hydraulic packages. This input entry determines the behavior of Control Volumes for which ITYPECV ≠ 0 (record 100XXX) and parameters are defined by Tabular or Control Functions (record 125XXX).
- 1 : do not recalculate conditions in these Control Volumes (keep the parameters constant) when IOPSL > 0.
 - 2 : recalculate conditions in these Control Volumes (use the Tabular or Control Function Values) when IOPSL > 0.
- Acceptable range:* 1, 2
Default value: 1

SPECTRA Code Manuals - Volume 2: User's Guide

W-9 (R) : DTRST Restarting frequency, (s).
Acceptable range: $DTMAX \leq DTRST \leq 10^{10}$.
Default value: $(TENDI(i) - TSTART) / 2$ for $i=1$
 $(TENDI(i) - TENDI(i-1)) / 2$ for $i>1$
 where i is the time step domain number. If the value obtained from the above formulae is smaller than $1000 \times DTMAX$, it is set to $1000 \times DTMAX$. This is done to avoid excessive restarts when for short time domains.

Example inputs with the use of non-standard Solver options is presented below: In the first run a PBMR fuel reloading rate needed at nominal power is being determined. The computation time was set at 1 month (2.6×10^6 s). In the second run transport and deposition of radioactive isotopes during normal operation is analysed. The analysis time is 1 year (3.2×10^7 s).

```
*      Max.dt  Min.dt  Print  Plot  End time  Solver options
*      (s)      (s)      (s)      (s)      (s)      IOPSL IRKSL ICVSL
900001  0.1      1.0E-6  0.0      0.0      1000.0    0      0      0 * 1000 s to get stable conditions
900002 1000.     1.0E-6  0.0      0.0      2.6E+6    1      3      0 * 1 month analysis, keep feedback
*                                     * from SC (fuel temperatures),
*                                     * do not control power -
*                                     * the fuel reloading will keep
*                                     * the power constant
```

```
*      Max.dt  Min.dt  Print  Plot  End time  Solver options
*      (s)      (s)      (s)      (s)      (s)      IOPSL IRKSL ICVSL
900001  0.1      1.0E-6  0.0      0.0      1000.0    0      0      0 * 1000 s to get stable conditions
900002 1000.     1.0E-6  0.0      0.0      3.2E+7    2      4      0 * 1 year simulation with large dt
*                                     * and deactivated CV/JN/...
*                                     * to compute fission product
*                                     * transport and accumulation
*                                     * during normal operation
```

2.16.3 Record: 905000, Read Initial Conditions from a File

W-1 (A) : ICFILE File name containing initial conditions. The extension (default: ".ICF") must be included in the name.
Every time a calculation is finished, the program writes the current conditions (pressures, temperatures, fluid velocities, etc.) to a file with extension ".ICF" . This file may be used to overwrite the initial conditions entered in the input deck.

Typically an input model of a power plant is prepared, and then steady state calculations are performed until all parameters are stable. If the steady state calculations are long, then it is convenient to store the calculated parameters, and use them as a starting point for subsequent accident analyses. Then, to perform the accident analysis, user has to:

- attach the base model (see ATTACH statement, page 1-1),
- use this record to read initial conditions from a file, and
- define accident specific records.

In an example shown below, the base model of a NPP is stored as a file "BASE". Example of the steady state input deck is shown below.

The analyzed accident is a leak from the primary system (CV-001) to the environment (CV-030). The leak is defined by adding one Junction (JN-051). The input deck is shown below.

It is important to note the principal differences between using restart (see section 2.20), and using the initial condition file. Those differences are listed below.

1.) *Restart*

With restart all variables from all program data bases are saved and then read in binary format. When calculations are stopped and then restarted, then, unless the time steps are altered on restart, the results obtained after the restart are identical to those which would be obtained if the job proceeded without stopping. Very few numbers can be altered on restart (time step size, end time, diagnostics printout). The restart option is intended to allow continuation of a run that for some reason has been stopped. When a job is restarted no input processing is performed.

2.) *Initial Condition File (ICF)*

With ICF only the initial conditions are saved and read from a file. The file is in text format, thus the initial conditions can be altered by the user. When a job is stopped and then started again using ICF, the results are slightly different from those which would be obtained without stopping, because data is stored in formatted file, and not all data base is stored. With ICF the user can change practically anything in his input deck. Node numbers should not be changed because the values stored on ICF would then fall into wrong nodes. A limited re-nodalization with number changes is possible, but the user has then to manually fix the ICF, to make it appropriate for the new nodalization. When ICF is

SPECTRA Code Manuals - Volume 2: User's Guide

used, the whole input processing is performed as usually. At the end of the input processing phase ICF is read, and the initial conditions for CVs, JNs, SCs, CFs, and isotopes, stored in the ICF, replace those present in the input deck.

The values stored in ICF are used only for those nodes for which the option "use entered values" is selected. The appropriate options for JNs, SCs, CFs, and isotopes are read in records 201XXX, 301XXX, 701XXX, 740000 respectively. The value of 2 in records 201XXX, 301XXX, 701XXX, and the value of 1 in the record 740000 mean "use enter value". In such cases the value entered in input file or read from ICF is used.

Acceptable range: any string of up to 50 characters.

Default value: none.

Example of a (steady state) run with the base model stored in a file "BASE"

```
= Input file for steady state run (file: STEADY)
*
ATTACH BASE * Attach base model of NPP
*
* Define time steps
* Maximum dt Minimum dt Print dt Plot dt End time
* (s) (s) (s) (s) (s)
900001 0.1 0.0001 100.0 10.0 1000.0 * 1000 s of steady state run
```

Example input of a simple accident scenario (LOCA), using the base model BASE.

```
= Input file for accident analysis (LOCA from CV-001 to CV-030)
*
ATTACH BASE * Attach base model of NPP
*
905000 STEADY.ICF * Read initial conditions calculated in steady state run
*
* Define time steps
* Maximum dt Minimum dt Print dt Plot dt End time
* (s) (s) (s) (s) (s)
900001 0.1 0.0001 500.0 10.0 5000.0 * 5000 s of transient run
*
* Define leak (note that the initial condition data for this JN is not present in ICF)
205051 Leak model
* From To Area Elevation Length
200051 001 030 0.01 2.5 1.0
```

2.16.4 Record: 910000, Advancement Message Frequency, Extended Diagnostics

- W-1 (R) : DTSCR Screen (terminal) message frequency, (s). The information about current model time, time step and the CPU time used so far is written to the screen approximately every DTSCR seconds of the processor time. If not entered, or the entered value is out of the acceptable range it is automatically reset to the default value.
Acceptable range: $1.0 \leq \text{DTSCR} \leq 600.0$
Default value: 1.0
- W-2 (I) : NADIA Advancement message frequency, (-). At the end of each time step advancement, the information is available what time step (s) was used and how many iterations were performed. This information may be written to the diagnostics file. NADIA is the number of advancements between messages written to the diagnostics file. If not entered, or the entered value is out of the acceptable range it is automatically reset to the default value.
Acceptable range: $1 \leq \text{NADIA} \leq 100,000$
Default value: 1 for analysis times: $t \leq 10^4$ s
 10 for analysis times: 10^4 s < $t \leq 10^6$ s
 100 for analysis times: 10^6 s < $t \leq 10^8$ s
 1000 for analysis times: 10^8 s < $t \leq 10^{10}$ s
 10000 for analysis times: 10^{10} s < t
- W-3 (I) : IEXDIA Request for extended SOLVER diagnostics output. If a number different than zero is entered, then the following information is written to the diagnostics file in case of non-convergent iterations: the values of those variables that didn't converge, including values assumed and calculated for the last two iterations.
 The extended diagnostics can also be requested during the run using the SPECTRA Stop File, “*.STP” (see section 3.8). This is done as follows. The stop file has to be put in the directory where the run is performed. The program will (among others) ask if the extended diagnostics should be activated in the next part of the run. If the answer is "Y" then the extended diagnostics will be activated. Any other answer will result in suppressing the extended diagnostics. The extended diagnostics can only be requested if the diagnostics file is not suppressed (see section 2.16.7, below).
Acceptable range: all integers.
Default value: 0
- W-4 (I) : XDEBUG Request for debug print-out. If XDEBUG is greater than zero then the debug printout is written to the diagnostics file. The debug printout consists of the values of all iterated variables, controlled by the SOLVER. Values assumed and calculated in each iteration are printed for all iterations, for times greater than TDEBUG (s), where TDEBUG is defined as: $\text{TDEBUG} = \text{XDEBUG} - 1.0 \times 10^6$.
 The debug printout writes large amount of data to the diagnostics file and thus should be used with care.
 The debug printout can also be requested during the run using the SPECTRA Stop File, “*.STP” (see section 3.8). This is done as follows.

The stop file has to be put in the directory where the run is performed. The program will ask if the user wishes to terminate the calculation. The user should answer 'N' (no). Then the program will (among others) ask if the debug printout should be activated in the next part of the run. If the answer is "Y" then the debug printout will be activated. Any other answer will result in suppressing the debug printout. The debug printout can only be requested if the diagnostics file is not suppressed (see section 2.16.7, below).

Acceptable range: XDEBUG > 0.9×10^6 if non-zero. Thus the debug printout can be activated for the times greater than: -100,000 (s).

Default value: 0

W-5 (I) : IMESAG Message write option. Messages on changes of valve status, pump status may be written to a message file (*.MES) and the screen.
=1: messages are written to the message file
=2: messages are written to the message file and the screen
Acceptable range: 1, 2
Default value: 1

2.16.5 Record: 920000, Iteration Parameters

The parameters listed below control the numerical solution procedure. All of them have their default values. Any change in those parameters should be done with caution, since it may result in slowing down the solution or even causing the code to crash.

W-1 (I) : MAXITR Number of iterations to cut the time step. If the solution does not converge in MAXITR iterations then SOLVER repeats the advancement with a reduced time step. The value of the new, reduced time step, is determined by the time step reduction factor, DTREDN, (Word 3, below).
Acceptable range: $10 \leq \text{MAXITR} \leq 200$
Default value: 50

W-2 (I) : MINITR Number of iterations to increase the time step. If, due to non-convergent iterations or failure, the time step has been reduced below the maximum value (DTMAX, section 2.16.2) in previous advancements, then during subsequent advancements SOLVER tries to increase the time step to reach again DTMAX. This increase is attempted only if the last advancement has been solved in less than MINITR iterations.
Acceptable range: $10 \leq \text{MINITR} \leq 50$,
MINITR \leq MAXITR,
MINITR > ITMNSL (Word 14)
Default value: 20

W-3 (R) : DTREDN Time step reduction ratio in case of non-convergent iterations. If the solution does not converge in MAXITR (Word 1 above) iterations, then SOLVER attempts to repeat the advancement with a new, reduced time step. The reduced time step is obtained as: $\Delta t' = \Delta t / \text{DTREDN}$, where Δt is the time step for which the solution did not converge. If DTREDN is

too large, then time step reduction may be unnecessarily too severe, thus increasing the execution time.

Acceptable range: $2.0 \leq \text{DTREDN} \leq 16.0$

Default value: 4.0

W-4 (R) : DTREDF Time step reduction ratio in case of failure. Failure may occur for a number of reasons. For example, water property routines may be called with temperatures beyond the data range, a linear equation solver may fail (singular matrix), etc. If such failure occurs, then a recovery from the failure is possible. On recovery, the advancement is repeated with a new, reduced time step. The reduced time step is obtained as: $\Delta t' = \Delta t / \text{DTREDF}$, where Δt is the time step for which the failure occurred. Because the number of recoveries is limited (see Word 7, below), the time step reduction should be significant, to limit the possibility that the failure will occur again, forcing to use more recovery processes.

Acceptable range: $4.0 \leq \text{DTREDF} \leq 32.0$

Default value: 8.0

W-5 (R) : DTINC Maximum time step increase factor, (-). If, due to non-convergent iterations or failure, the time step had been reduced below the maximum value (DTMAX) in previous advancements then during subsequent advancements SOLVER tries to increase the time step to reach again DTMAX. This increase is attempted only if the last advancement was solved in less than MINITR (Word 2, above) iterations, and is limited to the ratio defined by DTINC. Thus the new time step is obtained as: $\Delta t' = \Delta t * \text{DTINC}$, where Δt is the time step at which solution converged in less than MINITR iterations.

The DTINC is not used in case the code runs with maximum time step and a new time step domain is reached. In that case SOLVER tries to use the new maximum time step, no matter how different it might be from the previous maximum time step. When this attempt is unsuccessful, it will try to reduce the time step.

Acceptable range: $1.001 \leq \text{DTINC} \leq 10^6$

Default value: 1.30278... This particular value was selected to allow the code to come back to the same end-of-advancement time points after a reduction of the time step by a factor of 2 (or multiple factors of 2). For example: suppose the maximum time step is 1.0. The end-of-advancement time points are: 1.0, 2.0, 3.0, etc. At certain moment, say 3.0 s, SOLVER cuts the time step by half. Then, if it increases the time step using the default value of DTINC, the following end-of-advancements time points will be: 3.5, 4.1514, 5.0, 6.0, etc. Thus when the maximum time step is re-reached (5.0 s), then the end-of-advancement time points will be exactly the same as if the reduction of time step did not occur. The exact value is defined by the positive root of the following quadratic equation:

$$\text{DTINC}^2 + \text{DTINC} - 3.0 = 0.0$$

SPECTRA Code Manuals - Volume 2: User's Guide

- W-6 (I) : IACTFL Action to be taken on failure. The value determines the kind of action that will be taken in case a failure occurs during calculations.
- IACTFL=1 : write output, plot, and diagnostics edits, restart file, and terminate the run.
- IACTFL=2 : continue calculations with reduced time step. The new time step is defined by the factor DTREDF (Word 4, above).
- Acceptable range: $1 \leq \text{IACTFL} \leq 2$
- Default value: 1
-
- W-7 (I) : LSTACK Limit in recovery from failure. If the value of IACTFL (Word 6, above) is equal to 2, then in case of failure the recovery procedure is applied, and the run is continued with reduced time step. This recovery procedure is invoked only up to LSTACK times. If failure occurs more than LSTACK times then the run is terminated. Increased value of LSTACK will allow more error recoveries. However, the number of error recoveries is also limited by the FORTRAN stack limit. If LSTACK is made too large, then the program may stop on the stack limit. If the stack is exceeded, then the FORTRAN run-time error message is printed: "Program stack exceeded", and the run is immediately terminated. This should be avoided, because if this happens neither the diagnostics message nor the output and plot edits from SPECTRA are available at the time of the crash. The acceptable range and the default value were set based on experience with the Lahey FORTRAN compiler [12], and may be different for other compilers.
- Acceptable range: $10 \leq \text{LSTACK} \leq 20$
- Default value: 15
-
- W-8 (I) : IACSFL Action to be taken on failure during initial state calculations. Sometimes convergence failure may occur during the initial state calculations, when SC or TC temperatures need to be initialized (INTSC=1 - section 2.3.3, or INTTC=1 - section 2.4.3) in a steady-state step. One solution is to initialize SCs manually (set INTSC, INTTC to 2 and provide the initial temperatures in the input deck). Other solution is to ignore the failure, and start the transient calculations from the obtained conditions. Ignoring the failure is often the best choice, since even un-converged calculated SC temperatures are typically better than can be obtained by manual initialization.
- IACSFL=1 : write output edit and terminate the run.
- IACSFL=2 : ignore the failure and continue.
- Acceptable range: $1 \leq \text{IACSFL} \leq 2$
- Default value: 1

Solver Convergence Criteria

- **It is not recommended to change the Solver convergence criteria.**
- **If frequent time step cuts are observed, but the values of un-converged parameters (printed if the extended diagnostic option is used – record 910000, Word 3) do not change much from iteration to iteration, then an increase of the convergence criteria may be considered as a method of speeding up the calculations.**

W-9 (R) :	CCCASL	Solver convergence criterion on the difference between the assumed and calculated value. The criterion is satisfied if the relative difference between the parameter value assumed for the iteration and calculated during this iteration, is smaller than CCCASL. <i>Acceptable range:</i> $10^{-5} \leq \text{CCCASL} \leq 10^{-1}$ <i>Default value:</i> 10^{-3}
W-10 (R) :	CCAASL	Solver convergence criterion on the difference between the assumed and previously assumed value. The criterion is satisfied if the relative difference between the parameter value assumed for the last iteration and the value assumed for the previous iteration, is smaller than CCAASL. <i>Acceptable range:</i> $10^{-6} \leq \text{CCAASL} \leq 10^{-2}$ <i>Default value:</i> 10^{-4}
W-11 (R) :	ABSLSL	Absolute limit on a parameter value. The Solver convergence criteria, defined by Words 9 and 10 above, are bypassed for a given parameter, if the absolute value of the parameter is smaller than ABSLSL. <i>Acceptable range:</i> $10^{-20} \leq \text{ABSLSL} \leq 1.0$ <i>Default value:</i> 10^{-10}
W-12 (R) :	CMCASL	Multiplier on CCCASL for the reactor kinetics model. <i>Acceptable range:</i> $1.0 \leq \text{CMCASL} \leq 100.0$ <i>Default value:</i> 1.0
W-13 (R) :	CMAASL	Multiplier on CCAASL for the reactor kinetics model. <i>Acceptable range:</i> $1.0 \leq \text{CMAASL} \leq 100.0$ <i>Default value:</i> 1.0
W-14 (I) :	ITMNSL	Minimum number of iterations to accept the solution. <i>Acceptable range:</i> $1 \leq \text{ITMNSL} \leq 20$ <i>Default value:</i> 3 5 if decay chains are used, i.e. if NDCHRT > 0 9 if LFM is used, i.e. if MSFMJN = 2
W-15 (I) :	DISTIN	Initial disturbance (relative) to start the solution procedure. <i>Acceptable range:</i> $10^{-10} \leq \text{DISTIN} \leq 10^{-1}$ <i>Default value:</i> 10^{-2}

Solver Convergence Criteria for FP Masses

- **The accuracy of the FP solution is judged by a global mass balance for fission products. If the mass error becomes large, the calculations are stopped. In such case it is best to eliminate the mass error using the AMFPRT > 0 option. The user may also try to reduce time step or decrease the convergence criteria. The recommended values are given in the descriptions below and summarized in Table 2-48.**
- **The default values were set to provide fast but less accurate solutions. The values were successfully tested for time steps up to 10⁵ s.**

W-16 (R) :	FCCASL	Solver convergence criterion applied for fission product masses in the gas space of Control Volumes. Same as CCCASL (Word 9) but applied for fission product masses. <i>Acceptable range:</i> $10^{-4} \leq \text{FCCASL} \leq 10^{+10}$ <i>Default value:</i> 10^{+1} . If a large mass error is encountered, then it is recommended to use 10^{-1} . This will increase accuracy at the expense of computing time.
W-17 (R) :	FCAASL	Solver convergence criterion applied for fission product masses in the gas space of Control Volumes. Same as CCAASL (Word 10) but applied for fission product masses. <i>Acceptable range:</i> $10^{-5} \leq \text{FCAASL} \leq 10^{+10}$ <i>Default value:</i> 10^0 . If a large mass error is encountered, then it is recommended to use 10^{-2} . This will increase accuracy at the expense of computing time.
W-18 (R) :	FABLSL	Absolute limit on a parameter value applied for fission product masses in the gas space of Control Volumes. Same as ABSLSL (Word 11) but applied for fission product masses. <i>Acceptable range:</i> $10^{-40} \leq \text{FABLSL} \leq 1.0 \times 10^{-10}$ <i>Default value:</i> 10^{-30}
W-19 (I) :	ITMXSL	Maximum number of iterations to accept the fission product solution. <i>Acceptable range:</i> $\text{ITMNSL} < \text{ITMXSL} \leq \text{MAXITR}$ <i>Default value:</i> 15. If a large mass error is encountered, then it is recommended to use 40. This will increase accuracy at the expense of computing time.
W-20 (I) :	IFPESL	Indicator for fission product (FP) mass error treatment. = 0: calculations are stopped when the FP mass error exceeds 10%, > 0: calculations are stopped when the error exceeds IFPESL %, < 0: calculations are never stopped because of FP mass error. Note that FP mass error may be eliminated by using the AMFPRT > 0 (input record 880000). It is usually best to use the AMFPRT > 0 option. Note: mass conservation is possible only if: (1) fission products cannot flow to/from time-dependent CVs (2) there is no sorption on surfaces linked to time-dependent CVs (3) all daughter products of radioactive decay are tracked (full radioactive chains) If (1), (2), or (3) is not fulfilled, IFPESL should be set to < 0. <i>Acceptable range:</i> all integers

SPECTRA Code Manuals - Volume 2: User's Guide

Default value: -1 if (1), (2), or (3) is not fulfilled
 0 otherwise

Table 2-48 Recommended convergence criteria for fission product mass

Calculation type	Parameter		
	FCCASL	FCAASL	ITMXSL
Fast but less accurate	10 ¹	10 ⁰	15
Accurate but slow	10 ⁻¹	10 ⁻²	40

2.16.6 Record: 925000, Reduction of Solid Material Specific Heat for Steady State

Calculations are often started with an approach to steady state. Such approach may be significantly accelerated by reducing the volumetric heat capacity ($\rho \times c_p$) of materials present in the model. Using this record, the user may reduce the volumetric heat capacity of all solid materials (used by SC and TC). The fluid properties in Control Volumes remain unaltered.

- W-1 (R) : CREDSL Reduction factor, (-). The reduction factor is applied if a positive value is entered.
Acceptable range: 0.001 ≤ CREDSL ≤ 1.0, if non-zero
Default value: none
- W-2 (R) : TREDSL End-time, (s), to apply the reduction factor CREDSL. For times greater than TREDSL the reduction is not applied (the reduction factor is set to 1.0).
Acceptable range: TREDSL > TSTART (start time, record 900000)
Default value: none

2.16.7 Record: 930000, Suppressing the Diagnostics File

- W-1 (I) : IDIAFL Indicator defining whether the warning and error messages are printed into the diagnostics file.
 If IDIAFL=0 then warning and error messages are printed into the diagnostics file. In some cases this may result in very large diagnostics file.
 If IDIAFL≠0 then warning and error messages suppressed. No information is printed to the diagnostics file during the calculations. The diagnostics file is closed at the end of input processing phase. This option saves the disk space and speeds up the calculations. The disadvantage of using this option is the lack of diagnostics messages in case of severe numerical problems.
 If IDIAFL≠0 then the extended diagnostics and the debug printout are automatically suppressed (IEXDIA and XDEBUG are set to zero - see section 2.16.4).
Acceptable range: any integer.
Default value: 0 .

2.16.8 Record: 931000, Adjusting Time Step at the End of Time Domain

W-1 (I) : ITSNSL Indicator defining whether the time step should be adjusted at the end of each time step domain to finish each domain at exactly the specified time point.

1 : Do not adjust time step. In the example shown in section 2.16.11 the first time step domain ends at 100.0 s. If the code is at 99.3 s and runs with the maximum time step of 1.0 s, then it will finish this domain and proceed to the next one at the time of 100.3 s.

2 : Adjust the time step to finish each time step domain at exactly the specified time point. In the example shown in section 2.16.11 the first time step domain ends at 100.0 s. If the code is at 99.3 s and runs with the maximum time step of 1.0 s, then it will automatically reduce this time step to 0.7 s, in order to finish this time step domain and proceed to the next one at exactly 100.0 s. This option may be important if certain events (for example break opening, control system actions) need to occur at precisely the start of certain time domain.

Acceptable range: 1 or 2
Default value: 1

2.16.9 Record: 940000, Interactive Simulation Activation

W-1 (I) : ISIMUL Activator of an interactive simulation run. In a non-interactive run, the computations are entirely determined by the input deck.. The results may be viewed using the plot file *.PLT (or the output file, *.OUT), when the calculations are finished. In an interactive run the values of all Tabular Functions that are defined as interactive may be changed (by the simulation program, which writes appropriate commands to the *.TFD file). The results maybe viewed during the calculations because SPECTRA writes every plot point separately (file *.SIM). Additionally SPECTRA writes the headers (variable names) in the file *.SIN. The simulation program (VISOR) reads a single plot point, displays the current conditions on the screen, sends eventual signal to the *.TFD file and sends signal to SPECTRA to proceed (this signal is simply a removal of the *.SIM file with the current plot point). The full plot file, *.PLT, is produced as usual, so that the results can be viewed in the usual post-processing mode, after the run is finished.

0 : Interactive simulation inactive.

1 : Interactive simulation active, fast mode. Actions take effect with a delay of up to the time step between plots. Run is faster because SPECTRA proceeds to the next plot point without waiting for eventual signals from VISOR.

2 : Interactive simulation active, slow mode. Actions take effect immediately. Run may be slower because SPECTRA waits for eventual signals from the simulator before proceeding to the next plot point.

Acceptable range: 0, 1, or 2.
Default value: 0 .

2.16.10 Record: 950000, Scrambling Input Files

If an input file needs to be distributed to a non-licensed user (for example as a model that has to serve as demo, a simulator, etc.) the input file may be scrambled to prevent the non-licensed user from making changes in the model.

W-1 (I) : ISCRMB Scrambling indicator.
 =0: scrambling is not needed.
 =1: scrambling is needed. The scrambled file *.SCR is generated. The
 file *.SCR should be renamed into *.SPE and distributed to a non-
 licensed user.
 Acceptable range: 0 or 1
 Default value: 0

2.16.11 Example of Transient Solution and Output Frequency Data

The input shown below defines the SOLVER data, including the start time for the run and time step data for three domains. The start time of the analysis is -10.0 s. The first time domain is active from the start time to 100 seconds. The second domain is active for times between 100 s and 500 s. The third domain is active for times between 500 s and 10,000 s. The transient calculations are terminated at 10,000 seconds. The time steps, the print- and the plot-points, are more frequent at the beginning of the transient. The maximum time step size is used for plot edits (zeroes are entered). The advancement message frequency and the iteration parameters are not entered, thus default values are used.

```
*      Definition of time steps
*      =====
*
*      Start Time
930000  -10.0
*
*      Maximum dt      Minimum dt      Print dt      Plot dt      End time
*      (s)             (s)             (s)           (s)          (s)
900001  1.0            0.001        10.0          0.0          100.0
900002  2.0            0.001        50.0          0.0          500.0
900003  10.0          0.001        500.0         0.0          10000.0
*
```

2.17 Exporting Input Data to Other Programs

SPECTRA allows to export data to other system codes. The export option creates a file *.EXP, which contains geometry and initial conditions for the following elements of an input model:

- CV Control Volumes
- JN Junctions
- FL Fluid Property Data
- SC 1-D Solid Heat Conductors
- MP Material Property Data
- TF Tabular Functions
- CF Control Functions

The data can be exported to one of the following formats:

- Generic format. With this format all data such as volumes, flow areas, loss coefficients, etc, are exported in a general format, as columns of numbers with headers. This format may provide a significant help in producing an input decks for computer codes which have similar structure as SPECTRA (i.e. free nodalization, modeling based on interconnected fluid volumes convecting heat to solid structures), for example: MELCOR, RELAP, WAVCO, CONTAIN, etc.
- MELCOR format. This option produces MELCOR input. Note that the input is restricted to:
 - CV Control Volumes
 - FL Flow Paths
 - NCG Non-Condensable Gases
 - HS Heat Structures
 - MP Material Properties
 - TF Tabular Functions
 - CF Control Functions

Other elements of the model, such as time steps, modeling assumptions (for example hydrogen models, aerosol models, fission product models, etc.), boundary conditions (for example sources of hydrogen, aerosol, fission products, etc.), must be prepared manually.

- RELAP format. This option produces RELAP5 input. Note that the input is restricted to:
 - Control Volumes (set of single volumes are created, no pipes, branches, etc.)
 - Junctions (set of single junctions are created)
 - Heat Structures
 - Material Properties
 - General Tables
 - Control Variables

Other elements of the model, such as time steps, modeling assumptions, boundary conditions, must be prepared manually.

SPECTRA Code Manuals - Volume 2: User's Guide

parameter PRPDH2). In MELCOR propagation is a user-defined parameter, with default value of 0.0 (instantaneous propagation through Control Volumes). A positive value will slow down the propagation.

Acceptable range: $0.0 \leq \text{TFRCSL} \leq 1.0$

Default value: 0.7 (ratio between the burn propagation PRPDH2, and burn dimension DIMH2)

W-5 (R) : IFRMSL MELCOR input parameter IFRMAT, format flag for temperature node location data.
IFRMSL=1: Node location data is exported according to IFRMAT=1; location of a temperature node and the number of this node.
IFRMSL=2: Node location data is exported according to IFRMAT=2; length and the number of consecutive mesh intervals with this length.
Acceptable range: TFRCSL = 1 or 2
Default value: 2

If IEXTRT = 3 (exporting to RELAP)

W-3 (I) : IRADSL Option for exporting the vertical orientation of Control Volumes. Used only is IEXPSL = 3. In general there is no good way to convert elevations of CV and JN into RELAP. There are two options for automatic definition of vertical orientation of CV when exporting data to RELAP:
IRADSL=-1: All CV-s will be defined as horizontal (inclination angle will be set to 0.0, elevation change will be set to zero). The input deck will run but the vertical angles will not be correct and will have to be redefined manually.
IRADSL=+1: All CV-s will be defined as vertical (inclination angle will be set to +90.0, elevation change will be set to volume height). All vertical-up junctions will be connected to the outlet of the "from" CV to the inlet of the "to" CV. All horizontal JN will be defined as cross-flow JN. All vertical-down junctions will be connected to the inlet of the "from" CV to the outlet of the "to" CV. Input deck will be OK provided that in SPECTRA model the junctions are:
 ▪ vertical JN: connected at the top or bottom of the Control Volumes it connects.
 ▪ horizontal JN: connected at the middle of the Control Volumes it connects.
If these conditions are not fulfilled, the inclination angles will not be correct and will have to be redefined manually. It should be noted that in RELAP JN are connected to inlet, outlet, or middle (cross-flow) of a CV. Therefore unless JN elevation is at the bottom, top, or middle of CV, a one-to-one conversion to RELAP is not possible. In such cases re-nodalization of the model will be necessary.
Acceptable range: $-1 \leq \text{IRADSL} \leq +1$
Default value: +1

2.18 Requests for External Data Files

The External Data File (EDF) Package serves as a utility in SPECTRA to communicate with external data files. SPECTRA has two external data files:

- “Write-EDF”, and
- “Read-EDF”

The EDF written by SPECTRA may be used by another program as a source of data (e.g. as boundary conditions, etc.). The EDF read by SPECTRA may be used to supply data (e.g. boundary conditions, etc.) to SPECTRA. Such data could be generated by another program, spreadsheet, hand-calculations, etc.

Using the “Write-EDF” a set of variables from the SPECTRA data base may be sent to the EDF. Any variable in from the SPECTRA data base may be used. The full list of SPECTRA variables is provided in Table 2-23 through Table 2-32.

Using the “Read-EDF” a set of Tabular Function values may be read by SPECTRA. The reason why only Tabular Functions are read is the following. Other variables, such as for example Control Volume temperature or pressure, are being calculated by the SOLVER Package, and they cannot be redefined outside the SOLVER. If a user wishes to use a Control Volume with fixed, or time-specified pressure, then he has to use the time-specified CV (see section 2.1.14), where CV temperature, pressure, etc. are defined using either Tabular or Control Function. Therefore reading TF values is sufficient to provide every kind of boundary condition that the SPECTRA user may wish to define in his calculations.

There are two main options of using EDF:

- Normal run with EDF
- Synchronized run with EDF

If the first option is used, then the Write-EDF is created during the calculations (it is very similar to the plot file; the main difference is lack of variable identifiers (headers) in the EDF file (compare section 3.3 and 2.18.6). The Read-EDF must be present when SPECTRA is started, and the values from the Read-EDF are read during the run and assigned to the appropriate tabular functions. At the end of calculations both files contain full information from the run.

The second option is provided to allows interactively read/write EDF. With this option on, SPECTRA may run parallel with another program (or another model run by the SPECTRA code itself) and exchange information with selected data exchange time step.

In case of synchronized run each EDF contains data for a single (current) time step only. The following procedure is used. Once SPECTRA comes to the point when EDF must be written, it first checks if the EDF that has been written at the previous step still exists. If it does, then it waits until it disappears. Thus, the non-existence of the file is treated as a sign from the other program that the information has been successfully received and the other program is ready to receive new information.

Similarly, once SPECTRA comes to the point when EDF must be read, it first checks if it exists. If so, it reads the information and then deletes the file. Thus it gives the signal to the other code that the information has been successfully received and SPECTRA is ready to receive new information.

During both normal run and synchronized run the EDF information is written/read using the data exchange step not smaller than the maximum time step DTMAX, specified in the records 900XXX (see section 2.16.2). Therefore the maximum time step must be selected as not larger than the data exchange step for all time step domains.

2.18.1 Record: 9800000, EDF Main Data

- W-1 (I) : IEDFED EDF option:
 = 1: Normal run without EDF (EDF Package inactive).
 = 2: Normal run with Write EDF used.
 = 3: Normal run with Read EDF used.
 = 4: Normal run with both Read and Write EDF used.
 = 5: Synchronized run with both Read and Write EDF, explicit coupling.
 = 6: Synchronized run with both Read and Write EDF, implicit coupling.
 Note: In the case of implicit coupling, data is exchanged every time step.
 Sub-cycling (time step reduction) is not possible. The minimum time step must be set as equal to the maximum time step: DTMIN(i) = DDTMAX(i). The data exchange time step (Word 5 below) must be equal to the maximum time step: DTEXED = DTMAX(i).
 Acceptable range: 1, 2, 3, 4, 5, 6.
 Default value: 1.
- W-2 (I) : IROPED Error handling for the Read-EDF:
 = 1: Write a diagnostic and stop if errors are encountered in the Read-EDF (for example loss of time synchronism, improper data fields, insufficient data, etc.).
 = 2: Ignore the errors and continue calculations. However do not assign the erroneously read values to the Tabular Functions.
 Acceptable range: 1 and 2.
 Default value: 1.
- W-3 (I) : NNFMED Data format indicator for the Write-EDF. The number of data fields in a single line of the Write-EDF will be restricted to NNFMED. The data is written to the EDF using the format: N(1X,ES16.9), where N is equal to NNFMED.
 A negative number indicates CSV format, with maximum number of data columns equal to -NNFMED. The total number of variables in the Write EDF (NVAWED) cannot exceed -NNFMED
 A value of 1 or -1 will result in a free format, without leading spaces.
 If NNFMED = 1, numbers will be separated by a single space,
 if NNFMED = -1, numbers will be separated by a single comma.
 Acceptable range: 1 ≤ NNFTED ≤ 1000 if positive
 NNFTED ≥ -20 if negative
 Default value: 5.

W-4 (R) : **ERRSED** Maximum acceptable time mismatch in synchronized runs, explicit coupling. This is a fraction of the data exchange time step. If the time mismatch is smaller than the product: $ERRSED \times DTEXED$, then the data is exchanged without any time step modification. If the mismatch is larger, the time step is reduced (Figure 2-93). A small increase of time step (10%) is also permitted, in order to avoid severe Δt reduction in the subsequent step. Decreasing **ERRSED** will result in more accurate timing of data exchange, at the expense of time step reductions. The number of time step reductions and the mismatch in data exchange timings are printed in the output and the message file, if requested by **IMESED**, below.

Acceptable range: $0.0 < ERRSED \leq 1.0$
Default value: 0.1

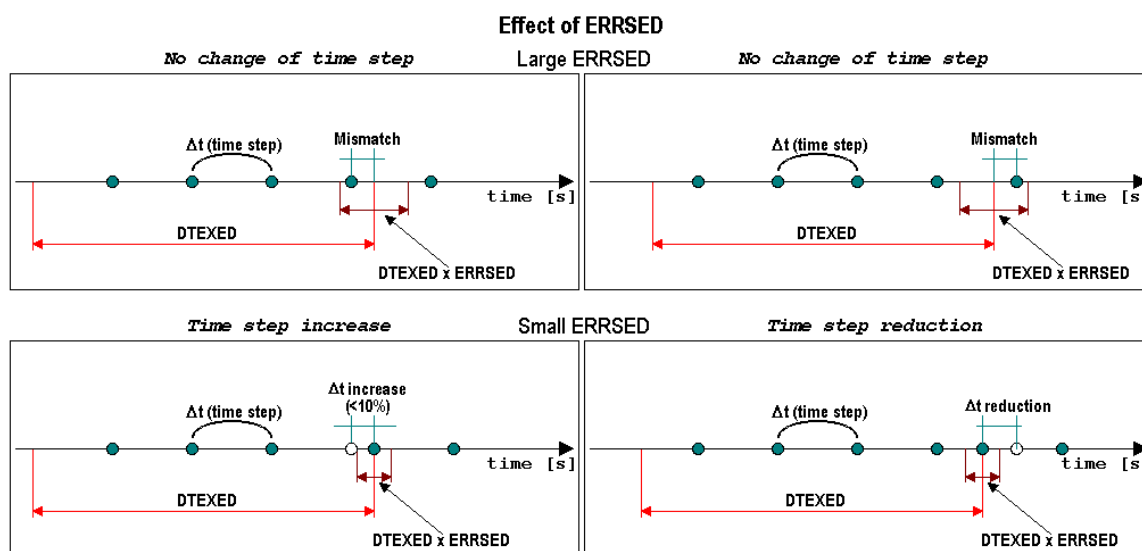


Figure 2-93 Effect of **ERRSED** (synchronized run, explicit coupling).

W-5 (R) : **DTEXED** Time step for data exchange, (s).

Acceptable range: $DTMAX(i) \leq DTEXED \leq 1.0E10$, or 0.0

Note: In the case of implicit coupling (**IEDFED**=6), data is exchanged every time step. Sub-cycling (time step reduction) is not possible. The minimum time step must be set as equal to the maximum time step: $DTMIN(i) = DDTMAX(i)$. The data exchange time step (Word 5 below) must be equal to the maximum time step: $DTEXED = DTMAX(i)$.

Default value: **DTMAX(i)**

Note: if zero or no value is entered, the data exchange time step will be equal to **DTMAX(i)**, so in general, it will be different in each time step domain. When a positive value is entered, a single value will be used throughout the run and it must be not smaller than the maximum value of **DTMAX(i)**, $i=1,N$.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-6 (I) : IMESED Option to write message about EDF transfers to the message file.
= 0 : do not write messages about EDF data transfers
= 1 : write a message whenever data is transferred through EDF
= 2 : write a message whenever time step is adjusted due to EDF
= 3 : write a message in both cases (EDF transfer or Δt adjustment)
= 4 : as above, additionally write the values of transferred data
Acceptable range: IMESED = 0, 1, 2, 3, 4
Default value: 0
- W-7 (I) : INITED Option to transfer data during initialization.
= 1 : Single data exchange, at the end of the iterations, is performed during initialization. This option may be required when a synchronized run is performed with another program.
= 2 : Two data exchanges are performed, first at the start of iterations and second at the end of iterations. Some data e.g. initial pressures, temperatures, etc. are available at the start of iteration and if these data are transferred it helps to pass them on to the other program already at the start of iterations. Other data, e.g. heat transfer coefficients, heat fluxes, etc., are available at the end of iterations, therefore the second data transfer is mandatory in order to achieve a complete data transfer.
Acceptable range: IMESED = 1, 2
Default value: 2
- W-8 (R) : EMICED Acceptable relative error in implicit coupling. Iterations continue until the relative errors of all exchanged parameters are smaller than EMICED. The relative error in iteration i is defined as:
$$\frac{|V_i - V_{i-1}|}{|V_i|} \quad \text{if } V_i \neq 0,$$
$$\frac{|V_i - V_{i-1}|}{|V_{i-1}|} \quad \text{if } V_{i-1} \neq 0,$$
$$0.0 \quad \text{otherwise.}$$
Here V_i is the value in iteration i , V_{i-1} is the value in iteration $i-1$.
EMICED < 10^{-50} means that the convergence is not checked within this run. In such case it must be checked by the other run.
Acceptable range: $0.0 \leq \text{EMICED} \leq 10^{-1}$
Default value: 10^{-3} (a small number, < 10^{-50} , disables convergence check in the current run)
- W-9 (I) : MIICED Maximum number of iterations. To avoid excessive number of iterations, a limit may be set here. If zero is entered, no limit is imposed.
Acceptable range: $0 \leq \text{MIICED} \leq 100$
Default value: 50
- W-10 (R) : XIMPED Implicit solution factor. In the case of implicit solution, the end-of time step value is multiplied by this factor. The applied value is set to: $V_{act} = V \times \text{XIMPED} + V_0 \times (1.0 - \text{XIMPED})$.
If a negative value is entered, the general Solver procedure is used to control the convergence of the parameter being sent to the Write-EDF. EMICED is still used, but somewhat differently and the iteration is a bit more complex. While with XIMPED = 1 two values are kept (the last and the previous iteration), Solver (XIMPED < 0) keeps four values: the assumed and the calculated values from the last two iterations. Based on these values, it determines a new assumed value for the next iteration.

SPECTRA Code Manuals - Volume 2: User's Guide

The convergence criterion, EMICED, is applied on the calculated values, while EMICED×0.1 is applied on the assumed values.

Acceptable range: XIMPED ≤ 1.0

Default value: -1.0 (a small number, <10⁻⁵⁰, sets the value to 0.0).

2.18.2 Record: E0500X, File Name of the Write-EDF

X is the EDF process number, XX = 0, 1, 2, ... Maximum number of EDF processes is 10.

W-1 (A) : WRFILE User defined name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.

Acceptable range: any string of up to 50 characters.

Default value: *.EDF, where * is the name of the input file.

2.18.3 Record: D0500X, File Name of the Read-EDF

X is the EDF process number, X = 0, 1, 2, ... Maximum number of EDF processes is 10.

W-1 (A) : RDFILE User defined name, length up to 50 characters. The name is read as a 50 character string, starting from the first non-blank character after the record identifier. There must be at least one blank character, separating the name from the record identifier.

Acceptable range: any string of up to 50 characters.

Default value: none (must be specified if IEDFED ≥ 3).

2.18.4 Records: 981000X, Definition of Variables Present in the Write-EDF

X is the EDF process number, X = 0, 1, 2, ... Maximum number of EDF processes is 10. Several records with the same number may be entered. Each record should contain a number of sets of six numbers, which in a unique way define the variable from SPECTRA data base.

W-1 (I) : IVW1ED First pointer for the first variable request.
(1) The value of this pointer defines the data base. The values are:
IVW1ED = 1: Control Volume Data Base.
IVW1ED = 2: Junction Data Base.
IVW1ED = 3: 1-D Solid Conductor Data Base.
IVW1ED = 4: 2-D Conductor Data Base.
IVW1ED = 5: Thermal Radiation Data Base.
IVW1ED = 6: Tabular Function Data Base.
IVW1ED = 7: Control Function or Reactor Kinetics Data Base.
IVW1ED = 8: Radioactive Particle Data Base
IVW1ED = 9: SOLVER Data Base.
Acceptable range: 1 ≤ IVW1ED ≤ 9.
Default value: none.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-5 (1) : IVW5ED Fifth pointer for the first variable request.
(1) This pointer is used for some parameters in the Radioactive Particle Transport Package - Table 2-28. For example, if the gravitational deposition velocity of aerosol particles is needed (IARG1C = 8, IARG3C = 53 or 74, see Table 2-28) then this pointer specifies the aerosol size section number. (Note that in this case the fourth pointer specifies the boundary cell number). The values of IARG5C, their interpretation and acceptable range, are shown in Table 2-28.
Acceptable range: indicated in Table 2-28.
Default value: none.
- W-6 (1) : IVW6ED Sixth pointer for the first variable request.
(1) This pointer is used for some parameters in the Radioactive Particle Transport Package - Table 2-28. For example, if the deposited fractions in given F_a -section (adhesion force section) is needed (IARG1C = 8, IARG3C = 65 or 86, see Table 2-28) then this pointer specifies F_a -section number. (Note that in this case the fifth pointer specifies the aerosol size section number and the fourth pointer specifies the boundary cell number). The values of IARG6C, their interpretation and acceptable range, are shown in Table 2-28.
Acceptable range: indicated in Table 2-28.
Default value: none.

The six words described above may be repeated. An arbitrary amount of sets of six words may be entered. Several records with the same number may be used but sets should not be split between records.

2.18.5 Records: 98200X, Definition of Variables Present in the Read-EDF

X is the EDF process number, X = 0, 1, 2, ... Maximum number of EDF processes is 10. Several records with the same number may be entered. Each record should contain reference number of the Tabular Functions that need to be read from the Read-EDF.

- W-1 (1) : IVR2ED Second pointer for the first variable request.
(1) IVR2ED = reference number of a Tabular Function,
Note that for the Read-EDF the first pointer is always equal to 6 (TF), the third pointer always equal to 1 (value of TF), and the fourth pointer always equal to 0 (un-used)
Acceptable range: must be a valid reference number of a Tabular Function, if non-zero.
Default value: none.
- W-2 (1) IVR2ED Second pointer for the second variable request. Meaning as above.
(2) an arbitrary amount of data words may be entered. Several records with the same number may be used.

2.18.6 Examples of EDF Input and Output

- **Write EDF**

The input shown below defines Write EDF data file which sends for plot parameters to the Write EDF ED-W.

```
*      EDF  ERROR  NNFMED  SYNCH  DT
9800000  2      1      5      0.0  0.25
E05000  ED-W
9810000  1 1 13 1 0 0      1 2 13 1 0 0      1 1 14 1 0 0      7 900 1 0 0 0
```

The EDF file ED-W is shown below.

```
4
0.000000000E+00  1.000000000E+05  1.000000000E+05  3.000000000E+02  0.000000000E+00
0.000000000E+00  1.000000000E+05  1.000000000E+05  3.000000000E+02  -1.000000000E+00
2.500000000E-01  1.000000000E+05  9.992427113E+04  3.000000000E+02  -7.500000000E-01
5.000000000E-01  1.000000000E+05  9.994008216E+04  3.000000000E+02  -5.000000000E-01
7.500000000E-01  1.000000000E+05  9.994139694E+04  3.000000000E+02  -2.500000000E-01
1.000000000E+00  1.000000000E+05  9.994128899E+04  3.000000000E+02  2.220446049E-16
1.250000000E+00  1.000000000E+05  9.994143062E+04  3.000000000E+02  2.500000000E-01
1.500000000E+00  1.000000000E+05  9.994157405E+04  3.000000000E+02  5.000000000E-01
1.750000000E+00  1.000000000E+05  9.994174764E+04  3.000000000E+02  7.500000000E-01
2.000000000E+00  1.000000000E+05  9.994192356E+04  3.000000000E+02  1.000000000E+00
```

- **Write EDF, CSV format**

The input shown below defines Write EDF data file which sends for plot parameters to the Write EDF ED-W.CSV, using the csv (comma-separated values) format (readable for excel).

```
      EDF  ERROR  NNFMED  SYNCH  DT
9800000  2      1      -5      0.0  0.25  * negative NNFMED defines CSV format
E05000  ED-W-CSV.CSV
9810000  1 1 13 1 0 0      1 2 13 1 0 0      1 1 14 1 0 0      7 900 1 0 0 0
```

The EDF (CSV) file is shown below.

```
TIME,CV-001-Pres-atms,CV-002-Pres-atms,CV-001-Temp-atms,CF-900-Valu-0000
0.000000000E+00, 1.000000000E+05, 1.000000000E+05, 3.000000000E+02, 0.000000000E+00
0.000000000E+00, 1.000000000E+05, 1.000000000E+05, 3.000000000E+02, -1.000000000E+00
2.500000000E-01, 1.000000000E+05, 9.992427113E+04, 3.000000000E+02, -7.500000000E-01
5.000000000E-01, 1.000000000E+05, 9.994008216E+04, 3.000000000E+02, -5.000000000E-01
7.500000000E-01, 1.000000000E+05, 9.994139694E+04, 3.000000000E+02, -2.500000000E-01
1.000000000E+00, 1.000000000E+05, 9.994128899E+04, 3.000000000E+02, 2.220446049E-16
1.250000000E+00, 1.000000000E+05, 9.994143062E+04, 3.000000000E+02, 2.500000000E-01
1.500000000E+00, 1.000000000E+05, 9.994157405E+04, 3.000000000E+02, 5.000000000E-01
1.750000000E+00, 1.000000000E+05, 9.994174764E+04, 3.000000000E+02, 7.500000000E-01
2.000000000E+00, 1.000000000E+05, 9.994192356E+04, 3.000000000E+02, 1.000000000E+00
```

The variables are written using fixed format (with a space for sign). On order to obtain the CSV file without spaces, the value of NNFMED should be set to -1:

```
      EDF  ERROR  NNFMED  SYNCH  DT
9800000  2      1      -1      0.0  0.25  * negative NNFMED defines CSV format
E05000  ED-W-CSV.CSV
9810000  1 1 13 1 0 0      1 2 13 1 0 0      1 1 14 1 0 0      7 900 1 0 0 0
```

SPECTRA Code Manuals - Volume 2: User's Guide

In this case the EDF (CSV) file is shown below.

```
TIME, CV-001-Pres-atms, CV-002-Pres-atms, CV-001-Temp-atms, CF-900-Valu-0000
.00000000, 100000.0000, 100000.0000, 300.000000, .00000000
.00000000, 100000.0000, 100000.0000, 300.000000, -1.000000000
.250000000, 100000.0000, 99924.2711, 300.000000, -.750000000
.500000000, 100000.0000, 99940.0822, 300.000000, -.500000000
.750000000, 100000.0000, 99941.3969, 300.000000, -.250000000
1.000000000, 100000.0000, 99941.2890, 300.000000, .222044605E-15
1.250000000, 100000.0000, 99941.4306, 300.000000, .250000000
1.500000000, 100000.0000, 99941.5741, 300.000000, .500000000
1.750000000, 100000.0000, 99941.7476, 300.000000, .750000000
2.000000000, 100000.0000, 99941.9236, 300.000000, 1.000000000
```

- **Synchronic run**

The input shown below defines EDF data for a synchronic run, where SPECTRA-calculated data will be sent out in the EDF file called "SPECTRA.DAT", while simultaneously an external data, calculated by other program (PANTHER) will be read from the file "PANTHER.DAT".

The following variables will be written to the SPECTRA.DAT file:

- Atmosphere temperature in CV-150.
- Atmosphere temperature in CV-160.
- Atmosphere pressures in CV-150.
- Atmosphere pressures in CV-160.

The following variables are read from the PANTHER.DAT file:

- Value of TF-151.
- Value of TF-152
- Value of TF-161.
- Value of TF-162.

```
*
*
*      =====
*      EDF Input Data
*      -----
*
*      Main data
*      Type(synch.)   Read option   Format
9800000   5             1             5
*
*
E05000   SPECTRA.DAT           * Write-EDF name
*                               * Write-EDF data:
* Pointers: (1) (2) (3) (4) * (1) (2) (3) (4)
9810000   1 150 13 1 * CV data base, CV-150, Temperature, Atmosphere
9810000   1 160 13 1 * CV data base, CV-160, Temperature, Atmosphere
9810000   1 150 14 1 * CV data base, CV-150, Pressure, Atmosphere
9810000   1 160 14 1 * CV data base, CV-160, Pressure, Atmosphere
*
*
D05000   PANTHER.DAT           * Read-EDF name
9820000  151 152 161 162 * Read-EDF data: reference numbers of TF
*
*      =====
```

An example of a Write-EDF file is presented below. It is important to note that the Write-EDF contains always:

- N integer number, defining the total number of variables, equal to NVAWED,

SPECTRA Code Manuals - Volume 2: User's Guide

- Time the current time,
- User-specified variables, NVAWED total.

An example of such file is shown below. The current time is in the file equal to 1.0 (s). The file SPECTRA.DAT for this time is:

```
4
1.00000E+00  2.93125D+02  2.93125D+02  1.01295D+05  1.01295D+05
```

The above example shows the EDF for a synchronized run, i.e. for a single time point. In case of a normal run, the file will contain all time dependent look something like:

```
4
0.00000E+00  2.93125D+02  2.93125D+02  1.01295D+05  1.01295D+05
1.00000E+00  2.93125D+02  2.93125D+02  1.01295D+05  1.01295D+05
2.00000E+00  2.93125D+02  2.93125D+02  1.01295D+05  1.01295D+05
3.00000E+00  2.93125D+02  2.93125D+02  1.01295D+05  1.01295D+05
4.00000E+00  2.93125D+02  2.93125D+02  1.01295D+05  1.01295D+05
...
```

SPECTRA expects the Read-EDF to have the same structure. The first number in the read EDF must determine the number of variables. This number must be equal to NVARED (record 9820000). If it is not, the run will be terminated unless ignoring read error is requested by setting IROPED to 2 (record 9800000). The next number is expected to be time. The time must be the same as the SPECTRA time. If it is not, the run will be terminated unless ignoring read error is requested by setting IROPED to 2 (record 9800000). Next, NVARED data fields are expected, providing data for the NVARED tabular functions, specified in the records 9920000. If the number of data fields is different or if any kind of read error is encountered, the run will be terminated unless ignoring read error is requested by setting IROPED to 2 (record 9800000).

Note that the Read-EDF is read by SPECTRA using the free format, so the number of data fields in a single line of the Read-EDF may be arbitrary. For example the Read-EDF file may look :

```
4
1.00  1.23  2.34  3.45  4.56
```

Alternatively in may have a form, for example:

```
4
1.00
1.23  2.34  3.45  4.56
```

This file will result in assigning the following values to tabular functions:

TF-151 = 1.23 TF-152 = 2.34 TF-161 = 3.45 TF-162 = 4.56

Again, the above example is for a synchronized run, i.e. it gives data for a single time point. In case of a normal run, the Read-EDF file should contain data for all time steps, and should look something like:

```
4
0.00  1.23  2.34  3.45  4.56
1.00  1.23  2.34  3.45  4.56
2.00  1.23  2.34  3.45  4.56
3.00  1.23  2.34  3.45  4.56
4.00  1.23  2.34  3.45  4.56
5.00  12.3  23.4  34.5  45.6
6.00  12.3  23.4  34.5  45.6
...
```

SPECTRA Code Manuals - Volume 2: User's Guide

The values in the first column represent the time, t . The values in the next columns define the values of the tabular functions at the time t . In the example presented above, during the first 4 second the tabular functions will be equal to:

TF-151 = 1.23
TF-152 = 2.34
TF-161 = 3.45
TF-162 = 4.56

During the next second (between $t = 4.0$ s and $t = 5.0$ s) the values will increase (linearly) to:

TF-151 = 12.3
TF-152 = 23.4
TF-161 = 34.5
TF-162 = 45.6

These values are kept constant for the next second, that means until $t = 6.0$ s.

- **Multiple EDFs**

Below an example of multiple EDF processes. The data exchanged are the same as in the example above, but the data concerning CV-150, TF-151, TF-152 are going to/from the first EDF process, while the data concerning CV-160, TF-161, TF-162 are going to/from the second EDF process. In general, one job may exchange data interactively with several (up to 10) other jobs.

```
*
*      =====
*      EDF Input Data for multiple EDF processes
*      -----
*
*      Main data
*      Type(synch.)   Read option   Format
9800000      5             1             5
*
E05000  SPECTRA-1.DAT      * Write-EDF name
*                               * Write-EDF data:
* Pointers: (1) (2) (3) (4) * (1)           (2)           (3)           (4)
9810000      1  150  13   1 * CV data base, CV-150, Temperature, Atmosphere
9810000      1  150  14   1 * CV data base, CV-150, Pressure, Atmosphere
*
E05001  SPECTRA-2.DAT      * Write-EDF name
*                               * Write-EDF data:
* Pointers: (1) (2) (3) (4) * (1)           (2)           (3)           (4)
9810001      1  160  13   1 * CV data base, CV-160, Temperature, Atmosphere
9810001      1  160  14   1 * CV data base, CV-160, Pressure, Atmosphere
*
D05000  PANTHER-1.DAT      * Read-EDF name
9820000  151  152          * Read-EDF data: reference numbers of TF
*
D05001  PANTHER-2.DAT      * Read-EDF name
9820001  161  162          * Read-EDF data: reference numbers of TF
*
```

2.19 Requests for Plot Variables

By default all plottable data is dumped into the plot file every time the plot edit is written (every DTPLT seconds). This may result in a very large size of the plot file produced during the run. Not only it creates the danger of filling the whole disk space, but also it increases the overall run time, since the I/O operations are relatively slow. The user can reduce the size of the plot file by two methods: reducing the plot frequency (thus making intervals between plot points - DTPLT - larger), or selecting only certain amount of variables he is interested in. The selection of plot variables is done using the records described in this section.

2.19.1 Record: 9900000, Full Plot File Option

W-1 (I) : IPLOT Full plot file indicator. If the value is equal to zero, or this record is missing, then the full plot file is written (all plottable variables will be present in the plot file). However, if the plot requests (records 991000, 992000, 993000 below) are entered, then the full plot file option is suppressed (IPLOT is set to 1 independently of the value entered in this record).
If IPLOT is different than zero, then only the requested variables (via records 991000, 992000, 993000) are written to the plot file. If no requests are present then the plot file is empty.
Acceptable range: all integers.
Default value: 0 (by default all plottable variables are dumped into the plot file if no requests are present, and only the requested variables if the requests are present).

2.19.2 Record: 9910000, Requests for Specific Component

These records may be used to request all plottable data for a specific component, for example all plottable data may be selected for one or several Control Volumes, one or several Solid Conductors, etc. Multiple records with the same number may be entered.

Note that the "summed quantities" (giving mass, energy, etc., summed for all components) are not obtained using these records. These records request all data related to a specific component (for example, specific Control Volume), while "summed quantities" are related to all components in the problem (for example all Control Volumes).

Each record should contain a number of pairs of data, defining the component for which all plottable variables need to be dumped into the plot file.

W-1 (I) : IPLC1(1) First pointer for the first component request. The value of this pointer defines the data base. The values are:
IPLC1 = 1: Control Volume Data Base.
IPLC1 = 2: Junction Data Base.
IPLC1 = 3: 1-D Solid Conductor Data Base.
IPLC1 = 4: 2-D Conductor Data Base.

SPECTRA Code Manuals - Volume 2: User's Guide

IPLV1 = 5: Thermal Radiation Data Base.
IPLV1 = 6: Tabular Function Data Base.
IPLV1 = 7: Control Function or Reactor Kinetics Data Base.
IPLC1 = 8: Radioactive Particle Data Base
Acceptable range: $1 \leq \text{IPLV1} \leq 7$.
Default value: none.

W-2 (I) : IPLV2(1) Second pointer for the first variable request. This pointer defines the type of variable in the data base. The values of IPLV2 and their interpretation are the same as in case of the Control Function argument pointer IARG3C, which are shown in tables Table 2-23 through Table 2-32. For example, if IPLV1 = 1 (Control Volume Data Base) then IPLV2 = 14 points to the CV temperatures (see Table 2-23).

Acceptable range:
 $1 \leq \text{IPLV3} \leq 131$ if IPLV1 = 1,
 $1 \leq \text{IPLV3} \leq 47$ if IPLV1 = 2,
 $1 \leq \text{IPLV3} \leq 43$ if IPLV1 = 3,
 $1 \leq \text{IPLV3} \leq 59$ if IPLV1 = 4,
 $1 \leq \text{IPLV3} \leq 8$ if IPLV1 = 5,
IPLV3 = 1 if IPLV1 = 6,
 $1 \leq \text{IPLV3} \leq 25$ if IPLV1 = 7,
 $1 \leq \text{IPLV2} \leq 323$ if IPLV1 = 8,
 $1 \leq \text{IPLV3} \leq 8$ if IPLV1 = 9.
Default value: none.

W-3 (I) : IPLV3(1) Third pointer for first variable request. This is an additional pointer, needed sometimes to specify for which material the data is needed. The values of IPLV3 and their interpretation are the same as in case of the Control Function argument pointer IARG4C, which are shown in Table 2-23 through Table 2-32. For example, if the Control Volume temperature is needed (IPLV1 = 1, IPLV2 = 14; see Table 2-23) then this pointer specifies whether the temperature of the atmosphere gas (IPLV3 = 1), atmosphere droplets (IPLV3 = 2), pool liquid (IPLV3 = 3), or pool bubbles (IPLV3 = 4), is used.

The values of IPLV3, their interpretation and acceptable ranges, are shown in tables Table 2-23 through Table 2-32 (as IARG4C).
Acceptable range: indicated in Table 2-23 through Table 2-32.
Default value: none.

W-4 (I) IPLV1(2) First pointer for the second component request. Meaning as above.

W-5 (I) IPLV2(2) Second pointer for the second component request. Meaning as above.

W-6 (I) IPLV3(2) Third pointer for the second component request. Meaning as above.

... ... an arbitrary amount of sets of three words may be entered. Several records with the same number may be used but sets should not be split between records.

SPECTRA Code Manuals - Volume 2: User's Guide

$1 \leq \text{IPLCV3} \leq 8$ if $\text{IPLCV1} = 5$,
 $\text{IPLCV3} = 1$ if $\text{IPLCV1} = 6$,
 $1 \leq \text{IPLCV3} \leq 25$ if $\text{IPLCV1} = 7$,
 $1 \leq \text{IPLCV2} \leq 323$ if $\text{IPLCV1} = 8$,
 $1 \leq \text{IPLCV3} \leq 8$ if $\text{IPLCV1} = 9$.
Default value: none.

- W-4 (I) : IPLCV4(1) Fourth pointer for the first individual request. This is an additional pointer, needed sometimes to specify for which material the data is needed. The values of IPLCV4 and their interpretation are the same as in case of the Control Function argument pointer IARG4C, which are shown in Table 2-23 through Table 2-32. For example, if the Control Volume temperature is needed ($\text{IPLCV1} = 1$, $\text{IPLCV3} = 14$; see Table 2-23) then this pointer specifies whether the temperature of the atmosphere gas ($\text{IPLCV4} = 1$), atmosphere droplets ($\text{IPLCV4} = 2$), pool liquid ($\text{IPLCV4} = 3$), or pool bubbles ($\text{IPLCV4} = 4$), is used. The values of IPLCV4, their interpretation and acceptable ranges, are shown in Table 2-23 through Table 2-32 (as IARG4C).
Acceptable range: indicated in Table 2-23 through Table 2-32.
Default value: none.
- W-5 (I) IPLCV1(2) First pointer for the second individual request. Meaning as above.
- W-6 (I) IPLCV2(2) Second pointer for the second individual request. Meaning as above.
- W-7 (I) IPLCV3(2) Third pointer for the second individual request. Meaning as above.
- W-8 (I) IPLCV4(2) Fourth pointer for the second individual request. Meaning as above.
- an arbitrary amount of sets of four words may be entered. Several records with the same number may be used but sets should not be split between records.

2.19.5 Example of Plot Requests Data

The input shown below requests for the following variables to be written to the plot file:

- All plottable variables for the Control Volume No. 003.
- Atmosphere pressures, for all Control Volumes.
- Atmosphere temperatures, for all Control Volumes.
- Heat transfer coefficient, for wall-atmosphere heat transfer on the left surface, for all Solid Conductors.
- Pool and bubble temperatures for the Control Volume No. 005.

```
*          =====
*
*      1.) Component requests
*      -----
*
*          Request for all plottable data for CV-003.
*
* Pointers: (1) (2) * (1)          (2)
9910000     1  3  * CV data base, CV No. 003
*
*      2.) Variable requests
*      -----
*
*          Request for atmosphere pressures and temperatures
*          for all Control Volumes, and heat transfer coefficient
*          from the left surface to the atmosphere for all Solid Conductors.
*
* Pointers: (1) (2) (3) * (1)          (2)          (3)
9920000     1 13  1  * CV data base, Pressure,   Atmosphere
9920000     1 14  1  * CV data base, Temperature, Atmosphere
9920000     3  4 -1  * SC data base, H.T.C.,     Left surface, atmosphere
*
*      3.) Individual requests
*      -----
*
*          Request for temperature of liquid pool and pool bubbles
*          in Control Volume No. 005.
*
* Pointers: (1) (2) (2) (3) * (1)          (2)          (3)          (4)
9930000     1 005 14  3  * CV data base, CV No. 005, Temperature, Pool
9930000     1 005 14  4  * CV data base, CV No. 005, Temperature, Bubbles
*
```

2.20 Restarting

The concept of restarting a terminated job is very simple and user convenient in the SPECTRA code. A restart file is written with specific frequency (by default 10 restart points per single time step domain - see section 2.16.2). Additionally a restart point is written every time a job is finished, either due to normal end, or terminated by the stop file, or terminated due to failure. Calculations may be resumed from any of these points. The restart point is not written if the job has crashed, for example when it's terminated by CTRL-C, in case of abnormal shutdown of the computer, for instance caused by operating system failure, power failure etc. This is one of the reasons why the user should avoid stopping a run with CTRL-C, and use the stop file instead (see section 3.8).

Restarting a job is interactive, and no input preparation is necessary. To restart a terminated job, one has to simply run the code in the directory where the results of the previous calculations exist, and, when prompted by the program, answer that restarting the previous run is indeed what he wishes to do. The program then reads the restart file, and interactively asks the user what changes he wants to make in the time step data (minimum, maximum time step, end time for the restarted run, see section 2.20.1 below). Next, the program lists sequentially the time points when restarts are available, and in each case asks if the user wants to restart from a given point (see section 3.4). Calculations are resumed at the requested restart point.

An input file (*.SPE) may be used on restart. If an input file is not present, then all data is read from the restart file (*.RST) and interactively (section 2.20.1). If an input file (*.SPE) is present, the Solver data (see section 2.16) and the Tabular Function data (see section 2.7) are read from the input file. The Solver data read from the input file replaces the Solver data read from the restart file. Thus all input parameters described in section 2.16 may be redefined on restart, using the SPECTRA input file (*.SPE). The TF data read from the input file replaces the TF data read from the restart file. New data points may be added to a Tabular Function or the existing data points may be replaced. However, no new TF can be defined on restart - only the data points for the existing Tabular Functions may be modified on restart using the SPECTRA input file (*.SPE). Currently only the TF data and the Solver data may be re-defined in the SPECTRA input file upon restart.

The output file and the diagnostics file, *.OUT, *.DIA, are appended when a job is restarted, so they contain all the information for the original run, followed by the information from the restarted job. The plot file, *.PLT, is appended from the restart point, so that the time argument in the plot file is increasing (eventual overlapping point are removed). If any of the files: *.OUT, *.DIA, *.PLT is not present, then the information prior to the restart will not be available in this file. The *.OUT and *.DIA files will start at the time of restart. The data in the *.PLT file will also start at the time of the restart, after the number of plot points and the headers (variable names) are written to it.

An example of using the restart option is shown in chapter 3, section 3.4. Interactive input entries for restart are described below, in section 2.20.1. Input entries read from an input file (*.SPE) on restart are described in section 2.16 and section 2.7.

2.20.1 Interactive Input on Restart

The following five values may be changed interactively on restart. The first three values may always be changed. The last two values may be changed only if the current status is "yes". The first three values are valid for the "current" time step domain, that means the time step domain in which the restart had been written.

SPECTRA Code Manuals - Volume 2: User's Guide

- W-1 (R) : DTMAX Maximum time step, (s).
Acceptable range: $DTMIN_R \leq DTMAX \leq 10 \cdot DTMAX_R$ (values with subscript "R" mean the old values, read from the restart file).
Default value: $DTMAX_R$ (old value, read from the restart file).
- W-2 (R) : DTMIN Minimum time step, (s).
Acceptable range: $10^{-10} \leq DTMIN \leq DTMIN_R$.
Default value: $DTMIN_R$ (old value, read from the restart file).
- W-3 (R) : DTPRT Printout (main edit) frequency, (s).
Acceptable range: $DTMAX \leq DTPRT \leq 10^{10}$.
Default value: $(TENDI(i) - TSTART) / 10$, if $i=1$,
 $(TENDI(i) - TENDI(i-1)) / 10$, if $i>1$,
 where i is the time step domain number.
- W-4 (R) : DTPLT Plot frequency, (s).
Acceptable range: $DTMAX \leq DTPLT \leq 10^{10}$.
Default value: $(TENDI(i) - TSTART) / 300$, if $i=1$,
 $(TENDI(i) - TENDI(i-1)) / 300$, if $i>1$,
 where i is the time step domain number.
- W-5 (R) : TENDI End time for this domain, (s).
Acceptable range: $TIME$ (current time) $\leq TENDI < TENDI_R^{next}$ (next time step domain) $- 1.0$. If the time step domain at the restart is the last one, then there is no upper limit for the end time.
Default value: $TENDI_R$ (old value, read from the restart file).
- W-6 (I) : IEXDIA If extended diagnostics had been previously requested then it may be switched off on the restart. The extended diagnostics can be switched on during the run, using the "SPECTRA Stop File" (see sections 2.16.4, 3.8).
Acceptable range: "Y", "y", "N", "n".
Default value: "N".
- W-7 (I) : XDEBUG If the debug printout had been previously requested then it may be switched off on the restart. The debug printout can be switched on during the run, using the "SPECTRA Stop File" (see sections 2.16.4, 3.8).
Acceptable range: "Y", "y", "N", "n".
Default value: "N".

2.21 Maximum Problem Size – Summary

The problems that are to be analyzed with the present SPECTRA version must be restricted according to the following limits.

- Thermal-hydraulics

Control volumes (CV):	550 (999 in LINUX version)	
Junctions (JN):	600 (999 in LINUX version)	50 in single CV
1-D solid heat conductors (SC):	500 (999)	Cells/SC: 100
2-D solid heat conductors (TC):	20 (or 2) ^(*)	Cells/TC: 51×51 = 2601
		Boundary Cells / TC: 4×50 = 200
Radiating systems (TR):	9	Surfaces / system: 90
Solid materials:	100	Data points / material: 100
Number of gases	20	Data points / gas: 100
Alternative fluids (liquid metals):	1	Data points / fluid: 1000
		heat transfer correlations: 100

- Material Oxidation (OX)

Oxidation models:	10 + 5 built-in models
-------------------	------------------------

- Reactor Kinetics (RK)

Delayed neutron precursor groups:	10	Reactivity functions:	50
Reactivity feedback data points:	50		
Weighting factors data points:	200	Core isotopes (IT):	200
Number of nodes in nodal point kin.	50		

- Radioactive Isotope Transport (RT)

Aerosol (dust) size sections:	20		
Resuspension models:	20	Adhesion force sections:	99
Inertial impaction surfaces per JN:	10		
Isotope chains:	24	Isotopes/chain:	11
Fission product release classes:	20	Isotopes/class:	100
Fission product vapor classes:	20	Isotopes/class:	100
Sorption models/class:	9		

- General Functions

Tabular functions (TF):	999	Data pairs / TF:	20,000
Control functions (CF):	999	Arguments / CF:	100

- External Data Files

Max. number of EDF processes:	10	Data channels / EDF:	200
-------------------------------	----	----------------------	-----

- Solver data (SL)

Time step domains:	999
--------------------	-----

^(*) Note that when the RT Package is used, the maximum number of TC-s is restricted to 2

2.22 Applicability Restrictions

The code can be delivered with restrictions, i.e. not all input parameters described in the previous sections can be used. The applicability restrictions are defined by the applicability code AppC. The parameter AppC has the format of four digits: *abcd*, determining restrictions for any of the four main types of nuclear reactors:

AppC(1) = <i>a</i>	-	Light Water Reactors (LWR)
AppC(2) = <i>b</i>	-	High Temperature Reactors (HTR)
AppC(3) = <i>c</i>	-	Liquid Metal Reactors (LMR)
AppC(4) = <i>d</i>	-	Molten Salt Reactors (MSR)

A value of zero means no restriction. A value of one means that the code version has restrictions for a particular reactor type. For example:

AppC = 0000 means no restrictions
AppC = 1000 means restrictions for LWR analyses

The applicability code AppC is printed in the output and diagnostics file, directly below the code version identifier - see section 3.1.1. Details on particular restrictions are described below.

- ***a* = 1: LWR restrictions**

In this case the following LWR-specific models are disabled:

- Fission product release models specific to LWRs: CORSOR-M (MFPRRT = 1) and ARSAP (MFPRRT = 2).
- Oxidation models specific to LWRs: Cathcart model (IOXLSC/IOXRSC/IOXBTC = -1) , Urbanic-Heidreich model (IOXLSC/IOXRSC/IOXBTC = -2), Benjamin model (IOXLSC/IOXRSC/IOXBTC = -4).

- ***b* = 1: HTR restrictions**

In this case the following HTR-specific models are disabled:

- Fission product release model specific to HTRs: HTR-FPR model (MFPRRT = 3).
- Oxidation model specific to HTRs: Roes model (IOXLSC/IOXRSC/IOXBTC = -5).

- ***c* = 1: LMR restrictions**

In this case the following LMR-specific model is disabled:

- Alternative fluid availability (IFLDFL > 1).

- ***d* = 1: MSR restrictions**

In this case the following MSR-specific model is disabled:

- Point kinetics model for circulating fuel (IFTORK =2).

3 Description of the Output Files

During calculations the SPECTRA program produces the following output files:

- *.OUT Printed output. The printouts are made with user-requested time intervals.
- *.PLT Plot file, used for graphs or visualization. The plot points are made with user-requested time intervals.
- *.DIA Diagnostics file. Contains all warning and error messages.
- *.RST Restart file. The restart is written only at the end of the calculations.

Additionally several files may optionally be used during calculations:

- *.ICF "Initial Condition File". It contains values of all time dependent parameters in the model. This file provides an easy way to start computations from earlier calculated conditions. The *.ICF file, like the *.RST file, is being written only at the end of the calculations.
- *.MES Message File contains messages about certain events, for example valve opening/closing, pump startup/shutdown, etc. - see input parameter IMESAG, input record 910000.
- *.TFD Tabular Function Data file may be used to change interactively a value of any Tabular Function that is defined as interactive (see section 2.7.5).
- *.EDF External data files (section 2.18).
- *.EXP Export of the model to Generic, MELCOR, or RELAP format (section 2.17).
- *.SIN *.SIM Interactive simulator files (section 2.16.9).
- *.SCR Scrambled input file (section 2.16.10).
- *.STP The SPECTRA Stop file (see section 3.8) may be used to interactively terminate the calculations.

3.1 Description of the Printed Output (*.OUT)

This section describes the main output file, "*.OUT", produced by SPECTRA during calculations. The file is arranged in several parts, described below:

- Part 1 Echo of the input file.
- Part 2 Printout of all input data. It contains code interpretation of all input parameters. Keyword to find the header of this part is "**=SPE=**".
The printout contains data for each package, keyword to find the header of each package is the package abbreviation within = signs, for example **=CV=** for Control Volumes.
Within each package the data is written for each component, keyword to find the header of each component is the component number preceded by = sign, for example **=CV-123** for control volume number 123.

SPECTRA Code Manuals - Volume 2: User's Guide

- Part 3 Printout at user defined frequency. The printout contains all transient parameters at given time point. Keyword to find the header of this part is “=SPE=”.
The printout contains data for each package, keyword to find the header of each package is the package abbreviation within = signs, for example =CV= for Control Volumes.
Within each package the data is written for each component, keyword to find the header of each component is the component number preceded by = sign, for example =CV-123 for control volume number 123.

An output that is given within the Part 2 (input processing) and the Part 3 (transient) from each Package is discussed separately in the subsequent sections.

3.1.1 SPECTRA Main Program Output

Control Volume outputs may be easily found in the output file by searching for the string: =SPE=. This output provides the code version (number and date) and the operating system platform (Windows or Linux). Furthermore, restrictions (if any) of this code version are given, including:

- Validity time limit: MM/YYYY
- Applicability code: AppC. The AppC has the format of four digits: *abcd*, determining restrictions for any of the four main types of nuclear reactors
 - a* - Light Water Reactors (LWR)
 - b* - High Temperature Reactors (HTR)
 - c* - Liquid Metal Reactors (LMR)
 - d* - Molten Salt Reactors (MSR)

A value of zero means no restriction. A value of one means that the code version has restrictions for a particular reactor type. For example:

AppC = 0000 means no restrictions
AppC = 1000 means restrictions for LWR analyses

Details on particular restrictions are described in section 2.22.

Typically the code is delivered without any restrictions (AppC = 0000). A restriction may be placed for a particular country or customer.

Example of printout is shown below:

```
=====
=SPE= SPECTRA Version 3.61, Jan. 2020, Windows

Sophisticated
Plant
  Evaluation
  Code for
    Thermal-hydraulic
    Response
    Assessment
-----
Validity: 06/2021,   Applicability: AppC = 0000
-----
```


3.1.2 Control Volume Output

Control Volume outputs may be easily found in the output file by searching for the string: =CV=. The first CV printout brings the input data printout. An example of the input printout for a Control Volume is shown below. The printout mainly reflects the data entered in the input file and is quite self-explanatory.

```
=CV= =====CV-001===== Example_problem,_volume_1_____

=CV= TYPE           : NORMAL CV

      BOTTOM ELEVATION= 0.00000E+00 m
      TOP ELEVATION  = 1.00000E+01 m
      TOTAL HEIGHT   = 1.00000E+01 m
      TOTAL VOLUME   = 1.00000E+01 m3
      HORIZONTAL AREA = 1.00000E+00 m2
      VERTICAL AREA   = 1.00000E+01 m2
      POOL SURF.C.DIM.= ( POOL SURF.AREA )**(1/2)

      NO DENSITY STRATIFICATION OF ATMOSPHERE

      NO THERMAL STRATIFICATION OF ATMOSPHERE

      NO THERMAL STRATIFICATION OF POOL

=CV= CV-001, SEGMENT DATA
      ELEV-BOTTOM  ELEV-TOP    HEIGHT    AREA      VOLUME
SEG.  (m)          (m)        (m)      (m2)      (m3)
  1    0.00000E+00 1.00000E+01 1.00000E+01 1.00000E+00 1.00000E+01

=CV= CV-001, MASS SOURCES
      Elevation    Area      Diameter    Source    Temper.    Pressure
No.   (m)          (m2)      (m)         Table     Table      Table
  1    0.00000E+00 1.00000E-03 1.00000E-02 TF-001    TF-002    TF-003
  2    1.00000E+01 1.00000E-03 1.00000E-02 TF-001    TF-005    TF-003

      MASS SOURCES - OVERALL COMPOSITION
No.   Water      Gas
  1    0.0000E+00 1.0000E+00
  2    1.0000E+00 0.0000E+00

      MASS SOURCES - GAS COMPOSITION
No.   H2         He         H2O        N2         O2         CO2
  1    0.0000E+00 0.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00
  2    0.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00

      PLUME MODEL FOR MASS SOURCES
No.   Atmosphere Pool
  1    No          No
  2    No          No

=CV= CV-001, ENERGY SOURCES
No.   Elevation    Source
      (m)          Table
  1    1.00000E+00 TF-006

      PLUME MODEL FOR ENERGY SOURCES
No.   Atmosphere Pool
  1    No          No

=CV= CV-001, DROP AND BUBBLY FLOW REGIME MODEL PARAMETERS

                        Droplets                      Bubbles
                        vertical horizontal          vertical horizontal
-----
Drift flux constant  CO    0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
Terminal velocity    v-inf 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
```

SPECTRA Code Manuals - Volume 2: User's Guide

```
Exponent          x      0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
De-entrainment    D      1.00000E+00  0.00000E+00

=CV= CV-001,      Surface area for droplet vertical de-entrainment
                  is always equal to the actual pool surface area

                  Surface area for bubble vertical de-entrainment
                  is always equal to the actual pool surface area

=CV= CV-001,      ANNULAR FLOW MODEL: DEFAULT

=CV= CV-001,      BUBBLE COLLAPSE MODEL

At Junction mass sources : active
At SC boiling surfaces   : active, off at: DTBCCV= 1.00000E+00 K
At tabular mass sources : active

=CV= CV-001,      DROPLET AND BUBBLE ACTIVATORS

Droplets creation at Junctions      : inactive
Bubbles creation at Junctions       : active
Boiling bubbles are created not deeper than: DMBLCV = 5.00000E+00 m
Non-eq. bubbles are created not deeper than: DMNBCV = 2.00000E+00 m
Droplet diameter at Junctions and TMS : Taylor instability model
Limits on diameter of droplets and bubbles
created at Junctions and TMS:
                                DMIN (m)      DMAX (m)
Droplets   : 1.00000E-03    2.00000E-02
Bubbles    : 1.00000E-03    9.00000E-02

=CV= CV-001,      VELOCITY CHANGE LIMITS

Atms : dVatms/dt = 1.00000E+02
Drop : dVdrop/dt = 1.00000E+02
Pool : dVpool/dt = 1.00000E+00
Bubb : dVbubb/dt = 1.00000E+00

=CV= CV-001,      CV DISPERSED COMPONENT OPTION: IWATCV = 3

Droplet diameter (m) : 1.00000E-02
Bubble diameter (m) : 1.60000E-02
Droplet position (-) : 7.00000E-01
Bubble position (-) : 8.00000E-01
Alpha-1 bubb.-annu. (-) : 7.50000E-01
Alpha-2 bubb.-annu. (-) : 8.00000E-01

=CV= CV-001,      DISTRIBUTION PARAMETER, C0, MODEL: ZUBER AND FINDLAY

=CV= CV-001,      NON-EQUILIBRIUM MASS TRANSFER MODEL

CONSTANT IN N-E BOILING MODEL : Cbb = 5.00000E-03
CONSTANT IN N-E CONDEN. MODEL : Cbc = 5.00000E-03

STEAM FROM N-E BOILING IS PLACED IN THE POOL AS BUBBLES
WATER FROM N-E CONDEN. IS PLACED AT THE INTERPHASE

N-E MASS TRANSFER IN DROPLETS : INACTIVE
N-E MASS TRANSFER IN BUBBLES  : INACTIVE

=CV= CV-001,      INTERPHASE HEAT AND MASS TRANSFER MODEL

AT POOL-ATMS INTERPHASE : ACTIVE
AT DROP-ATMS INTERPHASE : ACTIVE
AT BUBB-POOL INTERPHASE : ACTIVE

=CV= CV-001,      DE-ENTRAINMENT CALCULATION

DROPLET DE-ENTRAINMENT : IMPLICIT
BUBBLE DE-ENTRAINMENT  : IMPLICIT
```

SPECTRA Code Manuals - Volume 2: User's Guide

Below the individual Control Volume printouts, the total volume is printed (sum of the volumes for all CVs present in the model), as well as the volume data for the three largest volumes in the model. In the presented example the largest volume is CV-005 with 10,000 m³. The volume of the remaining CVs is 8,020 m³. The next in size is CV-003, with 5,000 m³. The volume of the remaining CVs (excluding CV-005 and CV-003) is 3,020 m³. The third in size is CV-004, with 3,000 m³. The volume of the remaining CVs (excluding CV-005, CV-003, CV-004) is 20 m³.

At the bottom of the CV input printout the internal CV numbering scheme is given. All printouts, diagnostic messages, plots, etc., are made using the reference numbers, which are chosen by the user. The calculations are performed using the internal, consecutive numbers. The user typically does not need to know the internal numbers. They might be helpful in case of some debugging sessions. The internal numbers are printed at the bottom of the input data printouts for every package.

```
=CV= ALL CONTROL VOLUMES -----
TOTAL VOLUME = 1.80200E+04 (m3)

DATA FOR 3 LARGEST CVs :
                                VOL. OF
                                REMAINING
CV VOLUME CVs
CV-005 Environment 1.0000E+04 8.0200E+03
CV-003 Larger_building 5.0000E+03 3.0200E+03
CV-004 Smaller_building 3.0000E+03 2.0000E+01
=====
=CV= CONTROL VOLUME INTERNAL NUMBERING SCHEME
=====

  Int. Ref.  Int. Ref.  Int. Ref.  Int. Ref.  Int. Ref.
  No.  No.    No.  No.    No.  No.    No.  No.    No.  No.
  ---  ---    ---  ---    ---  ---    ---  ---
    1  CV-001    2  CV-002    3  CV-003    4  CV-004    5  CV-005
=====
```

An example of the transient printout for a Control Volume is shown below. The printout consists of several blocks. The discussion of the data printed in each block is given below the printout.

```
=CV= =====CV-001===== Example_problem,_volume_1_____
=CV= CV-001, POOL SURFACE DATA AT TIME : 5.10000E+00 (s)

Elevation, m 5.24442E+00
Velocity, m/s 4.36009E-02
Surface area, m2 1.00000E+00
Char. dimension m 1.00000E+00
Volume above, m3 4.75558E+00
Volume below, m3 5.24442E+00
Ver. area above, m2 4.75558E+00
Ver. area below, m2 5.24442E+00
Droplet vol.frac.- 1.57989E-05
Bubble vol.frac.- 1.15936E-01

=CV= CV-001, STRATIFICATION DATA AT TIME : 5.10000E+00 (s)

Atmosphere, DSP - 0.00000E+00
Atmosphere, TSP - 0.00000E+00
Pool, PSP - 0.00000E+00

=CV= CV-001, THERMODYNAMIC DATA AT TIME : 5.10000E+00 (s)

Quantity Units Atms-Gas Atms-Drop Pool-Liq Pool-Bub
-----
-----
```

SPECTRA Code Manuals - Volume 2: User's Guide

Pressure,	Pa	1.10120E+05	1.10120E+05	1.10120E+05	1.20355E+05
Temperature,	K	3.19267E+02	3.46641E+02	3.15027E+02	3.14969E+02
Sat. Temp.,	K	3.03730E+02	3.75410E+02	3.75410E+02	3.03825E+02
Sat. Pressure	Pa	1.02054E+04	3.63343E+04	8.21047E+03	8.18488E+03
Volum. Fraction	-	9.99991E-01	9.45904E-06	9.53471E-01	4.65287E-02
Mass Fraction	-	9.92231E-01	7.76872E-03	9.99937E-01	6.25613E-05
Volume	m3	4.75553E+00	4.49832E-05	5.00041E+00	2.44016E-01
Mass	kg	5.60581E+00	4.38911E-02	4.95750E+03	3.10167E-01
Energy	J	1.65252E+06	1.35010E+04	8.69274E+08	9.26118E+04
Vert. Velocity	m/s	-3.53274E-02	6.37435E+00	2.19100E-02	3.02792E-01
Horiz. Velocity	m/s	8.01850E-03	8.01850E-03	0.00000E+00	0.00000E+00

=CV= CV-001, FLUID PROPERTY DATA AT TIME : 5.10000E+00 (s)

Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
Specific Volume	m3/kg	8.48322E-01	1.02489E-03	1.00866E-03	7.86725E-01
Density	kg/m3	1.17880E+00	9.75718E+02	9.91419E+02	1.27109E+00
Internal Energy	J/kg	2.94787E+05	3.07602E+05	1.75345E+05	2.98587E+05
Enthalpy	J/kg	3.88205E+05	3.07715E+05	1.75456E+05	3.93266E+05
Viscosity	kg/m/s	1.89376E-05	3.85890E-04	6.30334E-04	1.81697E-05
Conductivity	W/m/K	2.71931E-02	6.65713E-01	6.33102E-01	2.67289E-02
Cp	J/kg/K	1.03715E+03	4.18921E+03	4.18204E+03	1.06371E+03
Cv	J/kg/K	7.44339E+02	4.18767E+03	4.17939E+03	7.62893E+02
Prandtl Number	-	7.22283E-01	2.42833E+00	4.16376E+00	7.23085E-01
Expansion coef.	1/K	3.13217E-03	5.96484E-04	4.03462E-04	3.17491E-03
Diffusion coef.	m2/s	2.68263E-05			2.38757E-05
Surface tension	N/m		6.38645E-02	6.92942E-02	

=CV= CV-001, ATMOSPHERE GAS COMPOSITION AT TIME : 5.10000E+00 (s)

GAS No.	Id.	MASS kg	MASS FRACTION	PRESSURE Pa	VOLUME FRACTION
3	H2O	1.44357E-01	2.57513E-02	4.40575E+03	4.00086E-02
4	N2	4.21256E+00	7.51464E-01	8.39371E+04	7.62233E-01
5	O2	1.24889E+00	2.22785E-01	2.17771E+04	1.97758E-01
Totals:		5.60581E+00	1.00000E+00	1.10120E+05	1.00000E+00

Relative humidity (-) : 4.31709E-01

=CV= CV-001, POOL BUBBLE GAS COMPOSITION AT TIME : 5.10000E+00 (s)

GAS No.	Id.	MASS kg	MASS FRACTION	PRESSURE Pa	VOLUME FRACTION
3	H2O	7.55277E-03	2.43507E-02	4.43183E+03	3.68229E-02
4	N2	3.02614E-01	9.75649E-01	1.15923E+05	9.63177E-01
Totals:		3.10167E-01	1.00000E+00	1.20355E+05	1.00000E+00

Relative humidity (-) : 5.41465E-01

=CV= CV-001, PARTICLE DATA AT TIME : 5.10000E+00 (s)

Quantity	Units	Droplets	Bubbles
No. of particles	-	8.59416E+01	1.11749E+05
Average position	m	3.33196E+00	4.19205E+00
Average diameter	m	1.00000E-02	1.60000E-02
Average volume	m3	5.23607E-07	2.14469E-06

=CV= CV-001, MASS SOURCE DATA AT TIME : 5.10000E+00 (s)

Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
1) JN flows:	Wm	-5.04322E-02	-6.44212E-04	0.00000E+00	0.00000E+00
	Hm	-1.81391E+04	-1.98234E+02	0.00000E+00	0.00000E+00
2) SC/TC:	Wm	-1.48023E-04	0.00000E+00	1.48023E-04	0.00000E+00
	Hm	-3.59136E+02	0.00000E+00	1.08455E+01	0.00000E+00

SPECTRA Code Manuals - Volume 2: User's Guide

3) Non-equil:	Wm	kg/s	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	Hm	W	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4) Interph.:	Wm	kg/s	6.30413E-04	-5.70856E-04	-2.11194E-03	2.05239E-03
	Hm	W	1.65598E+03	-1.75618E+02	-3.70337E+02	5.28847E+03
5) De-entrm:	Wm	kg/s	4.46211E-02	-9.89443E-02	9.89443E-02	-4.46211E-02
	Hm	W	1.75480E+04	-3.04466E+04	3.04466E+04	-1.75480E+04
6) Mass Src.:	Wm	kg/s	0.00000E+00	1.00000E-01	-1.02918E-03	1.01029E-01
	Hm	W	0.00000E+00	3.21779E+04	-1.80468E+02	3.65650E+04
7) H2 burn:	Wm	kg/s	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	Hm	W	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8) Oxidation:	Wm	kg/s	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	Hm	W	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

=CV= CV-001, ENERGY SOURCE DATA AT TIME : 5.10000E+00 (s)

Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub	
1) SC/TC:	Qn	W	-3.68093E+01	0.00000E+00	-2.71160E+00	0.00000E+00
2) Th.Rad.:	Qn	W	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3) Inerph.:	Qn	W	6.80487E+01	-1.39926E+03	-4.22855E+03	-8.38738E+02
4) Bub.coll.:	Qn	W	0.00000E+00	0.00000E+00	3.62667E+03	0.00000E+00
5) Energy s.:	Qn	W	0.00000E+00	0.00000E+00	1.00000E+05	0.00000E+00
6) H2 burn:	Qn	W	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7) Turb/Comp:	Qn	W	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Work: p*dV/dt	W		-4.79847E+03	-1.79734E-02	1.18542E+01	4.78664E+03

=CV= CV-001, MASS SOURCE DATA FROM INDIVIDUAL SOURCES

=CV= CV-001, JUNCTION FLOW DATA AT TIME : 5.10000E+00 (s)

JN	Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
001	Flow (in)	kg/s	-5.04322E-02	-6.44212E-04	0.00000E+00	0.00000E+00
	Enthalpy	W	-1.81391E+04	-1.98234E+02	0.00000E+00	0.00000E+00
	Elevation	m	3.00000E+00	3.00000E+00	5.24442E+00	5.24442E+00
	Rel. Elev.	-	-1.30838E-01	-1.30838E-01	-5.00000E-01	-5.00000E-01
	Part.dia.	m		1.00000E-02		0.00000E+00
	Part.vol.	m3		5.23607E-07		0.00000E+00
	Part. src	1/s		-1.26096E+00		0.00000E+00

Individual gas mass sources (kg/s),

GAS	ATMOSPHERE	POOL
No.	Id.	kg/s
3	H2O	-6.57333E-04
4	N2	-3.83836E-02
5	O2	-1.13913E-02

=CV= CV-001, SOLID CONDUCTOR DATA AT TIME : 5.10000E+00 (s)

SC	Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
011L	Mass tr.	kg/s	-7.40114E-05	7.40114E-05	0.00000E+00	0.00000E+00
	Enthalpy	W	-1.79568E+02	5.42273E+00	0.00000E+00	0.00000E+00
	Elevation	m	3.00000E+00	4.75558E+00	0.00000E+00	0.00000E+00
	Rel. Elev.	-	-1.30838E-01	-5.00000E-01	5.00000E-01	5.00000E-01
	Part.dia.	m		4.99407E-03		0.00000E+00
	Part.vol.	m3		6.52182E-08		0.00000E+00
	Part. src	1/s		1.14005E+00		0.00000E+00

SC	Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
012L	Mass tr.	kg/s	-7.40114E-05	7.40114E-05	0.00000E+00	0.00000E+00
	Enthalpy	W	-1.79568E+02	5.42273E+00	0.00000E+00	0.00000E+00
	Elevation	m	1.00000E+00	4.75558E+00	0.00000E+00	0.00000E+00
	Rel. Elev.	-	2.89721E-01	-5.00000E-01	5.00000E-01	5.00000E-01
	Part.dia.	m		4.99407E-03		0.00000E+00
	Part.vol.	m3		6.52182E-08		0.00000E+00
	Part. src	1/s		1.14005E+00		0.00000E+00

=CV= CV-001, NON-EQUILIBRIUM MASS TRANSFER DATA AT TIME : 5.10000E+00 (s)

SPECTRA Code Manuals - Volume 2: User's Guide

Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
Volume	m3	4.75553E+00	4.49832E-05	5.00041E+00	2.44016E-01
Mass transfer	kg/m3/s	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Enthalpy	W/m3	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Elevation	m	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Relative Elev.	-	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Part. diameter	m	0.00000E+00		0.00000E+00	
Part. volume	m3	0.00000E+00		0.00000E+00	
Part. source	1/s/m3	0.00000E+00		0.00000E+00	

=CV= CV-001, INTERPHASE MASS TRANSFER DATA AT TIME : 5.10000E+00 (s)

Quantity	Units	Atms-Pool	Atms-Drop	Pool-Bub
Area	m2	1.00000E+00	2.69993E-02	8.98737E+00
Mass tr. coeff.	m/s	2.51628E-03	9.10617E-02	9.81888E-03
Mass transfer	kg/m2/s	5.95570E-05	2.11433E-02	2.28363E-04
Enthalpy - gas	W/m2	1.53463E+02	5.56500E+04	5.88433E+02
Enthalpy - liq	W/m2	1.04435E+01	6.50452E+03	4.00444E+01
Conv HTC	W/m2/K	1.01679E+00	9.79059E+01	7.85572E+03
Conv heat flux	W/m2	-4.31159E+00	2.68008E+03	4.55065E+02
Mass tr. heat fl.	W/m2	1.43019E+02	4.91455E+04	5.48389E+02
Liquid temperat.	K	3.15027E+02	3.46641E+02	3.15027E+02
Gas temperat.	K	3.19267E+02	3.19267E+02	3.14969E+02
Gas volume fractions:				
	H2O	4.00086E-02	4.00086E-02	3.68229E-02
	N2	7.62233E-01	7.62233E-01	9.63177E-01
	O2	1.97758E-01	1.97758E-01	0.00000E+00

=CV= CV-001, DE-ENTRAINMENT DATA AT TIME : 5.10000E+00 (s)

Quantity	Units	Drop ver	Drop hor	Bubble ver
Mass transfer	kg/s	9.89443E-02	0.00000E+00	4.46211E-02
Enthalpy	W	3.04466E+04	0.00000E+00	1.75480E+04
Elevation	m	4.75558E+00	0.00000E+00	5.24442E+00
Relative Elev.	-	-5.00000E-01	0.00000E+00	-5.00000E-01
Volume fraction	-	1.57989E-05	0.00000E+00	1.15936E-01

=CV= CV-001, TABULAR MASS SOURCE DATA AT TIME : 5.10000E+00 (s)

Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
Mass flux	kg/s	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E-01
Temperature	K	0.00000E+00	0.00000E+00	0.00000E+00	3.74000E+02
Pressure	Pa	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E+05
Enthalpy	W	0.00000E+00	0.00000E+00	0.00000E+00	4.00112E+04
Elevation	m	4.75558E+00	4.75558E+00	0.00000E+00	0.00000E+00
Relative Elev.	-	-5.00000E-01	-5.00000E-01	5.00000E-01	5.00000E-01
Part. diameter	m		0.00000E+00		2.00000E-02
Part. volume	m3		0.00000E+00		4.18885E-06
Part. source	1/s		0.00000E+00		1.66983E+04

Bubble collapse parameters

Collapse time	s	0.00000E+00
Bubble flow time	s	2.00000E+01
Pool bypas frac.	-	0.00000E+00
Heat transfer c.	W/m2/K	7.24499E+03
Heat flux	W/m2	-2.28236E+06
Heat to pool	W	3.62667E+03

Quantity	Units	Before coll.	After coll.
Gas flow	kg/s	1.00000E-01	1.01029E-01
Liquid flow	kg/s		-1.02918E-03
Gas enthalpy	W	4.00112E+04	3.65650E+04
Liquid enthalpy	W		-1.80468E+02
Bubble diameter	m	2.00000E-02	1.89838E-02
Bubble temperat.	K	3.74000E+02	3.15027E+02
Gas volume fractions, (-):			

SPECTRA Code Manuals - Volume 2: User's Guide

```

H2      0.00000E+00  0.00000E+00
He      0.00000E+00  0.00000E+00
H2O     0.00000E+00  1.01870E-02
N2      1.00000E+00  9.89813E-01
O2      0.00000E+00  0.00000E+00
CO2     0.00000E+00  0.00000E+00
    
```

```

Mass source No.:      2
Quantity              Units      Atms-Gas      Atms-Drop      Pool-Liq      Pool-Bub
-----
Mass flux             kg/s      0.00000E+00  1.00000E-01  0.00000E+00  0.00000E+00
Temperature           K        0.00000E+00  3.50000E+02  0.00000E+00  0.00000E+00
Pressure              Pa        0.00000E+00  1.00000E+05  0.00000E+00  0.00000E+00
Enthalpy              W        0.00000E+00  3.21779E+04  0.00000E+00  0.00000E+00
Elevation             m        0.00000E+00  0.00000E+00  5.24442E+00  5.24442E+00
Relative Elev.        -        5.00000E-01  5.00000E-01 -5.00000E-01 -5.00000E-01
Part. diameter        m        1.23804E-02  0.00000E+00  0.00000E+00  0.00000E+00
Part. volume          m3      9.93590E-07  0.00000E+00  0.00000E+00  0.00000E+00
Part. source          1/s      1.03362E+02  0.00000E+00  0.00000E+00  0.00000E+00
    
```

=CV= CV-001, ENERGY SOURCE DATA FROM INDIVIDUAL SOURCES

=CV= CV-001, SC CONVECTION DATA AT TIME : 5.10000E+00 (s)

```

SC Side  Quantity  Units  Atms-Gas  Atms-Drop  Pool-Liq  Pool-Bub
-----
001 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.76151E-01  0.00000E+00
002 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.76151E-01  0.00000E+00
003 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.76151E-01  0.00000E+00
004 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.76151E-01  0.00000E+00
005 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.76151E-01  0.00000E+00
006 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.75947E-01  0.00000E+00
007 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.75747E-01  0.00000E+00
008 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.84397E-01  0.00000E+00
009 Left  Heat flux  W      0.00000E+00  0.00000E+00 -2.86623E-01  0.00000E+00
010 Left  Heat flux  W     -2.42513E-01  0.00000E+00 -2.08127E-01  0.00000E+00
011 Left  Heat flux  W     -1.82834E+01  0.00000E+00  0.00000E+00  0.00000E+00
012 Left  Heat flux  W     -1.82834E+01  0.00000E+00  0.00000E+00  0.00000E+00
    
```

=CV= CV-001, TABULAR ENERGY SOURCE DATA AT TIME : 5.10000E+00 (s)

```

ES  Quantity  Units  Atms-Gas  Atms-Drop  Pool-Liq  Pool-Bub
---
001 Heat flux  W      0.00000E+00  0.00000E+00  1.00000E+05  0.00000E+00
    
```

The first block contains the data related to the pool surface, including elevation (above bottom of CV), velocity (upwards), area, characteristic dimension, volumes above and below the pool surface, vertical cross section area above and below the pool surface, and volume fractions of bubbles and droplets at the pool surface.

The second block contains the current values of the stratification parameters: DSP, TSP, PSP. If there is a thermal stratification of atmosphere or pool then the temperatures at the bottom and at the top of atmosphere or pool are printed.

The third block contains printout of thermodynamic data for all components that may be present in a Control Volume: atmosphere (gas), droplets, pool (liquid), and bubbles. If a given component is currently not present in the Control Volume then its column is filled with zeroes. **The volume and the mass fractions, printed in this block, always refer to the sum of the continuous and the corresponding discontinuous component.** For example, the bubble volumetric fraction (4.65287×10^{-2}) is equal to the volume of bubbles ($2.44016 \times 10^{-1} \text{ m}^3$) divided by the sum of the volume of water in the pool (5.00041 m^3) and the volume of bubbles. The droplet volumetric fraction

(9.45904×10^{-6}) is equal to the volume of droplets ($4.4983250 \times 10^{-5} \text{ m}^3$) divided by the sum of volumes of the atmosphere (4.75553 m^3) and the droplets.

It is important to note that the positive direction for the vertical velocities is always towards the atmosphere-pool interphase. Thus **for pool and bubbles positive velocity means upwards, for atmosphere and droplets positive velocity means downwards.**

The next block contains fluid property data for all components present in a Control Volume: atmosphere (gas), droplets, pool (liquid), and bubbles. If a given component is currently not present in the Control Volume then its column is filled with zeroes.

The fourth block contains the data on the atmosphere gas composition. The atmosphere is assumed to be composed of a mixture of gases. This block gives masses, mass fractions, partial pressures, and volume fractions, for all gases in the atmosphere, as well as the relative humidity for the atmosphere. This block is printed only if atmosphere is present in the Control Volume.

The next block contains the data on the bubble gas composition. The bubbles are assumed to be composed of a mixture of gases. This block gives masses, mass fractions, partial pressures, and volume fractions, for all gases in the bubbles, as well as the relative humidity for the bubble gas. This block is printed only if bubbles are present in the Control Volume.

The next block contains particle data, including number of particles, position, diameter and volume of the average particle. Note that the position inside the Control Volume is defined differently for droplets and bubbles: **In case of bubbles the average position is measured from the bottom of CV, in case of droplets the average position is measured from the top of CV.** In case particles are not present in a CV their average position is assumed to be zero.

The next block contains mass source data for CV, including mass fluxes and corresponding enthalpy fluxes for all components. In the example case there is a mass source due to Junction flows, evaporation or condensation on Solid Conductors, interphase mass transfer, de-entrainment, and tabular mass sources. The values printed there are explained in the paragraph discussing the printout of individual mass sources, below.

The next block contains data on energy sources in CV, including energy fluxes for all components. In the example case there is an energy transfer due to convection from Solid Conductors, interphase energy transfer, bubble collapse, and tabular energy sources.

The following blocks contain data on individual mass sources. The first block in this group contains data on Junction flows. This block contains mass sources for all components (atmosphere, droplets, pool and bubbles) caused by the Junction flows. Note that the values printed in this block are positive if the flow is into the CV, regardless what is the positive Junction direction. In the example case JN-001 is the only Junction connected to the Control Volume. Consequently the mass flow printed in this block is equal to the JN mass source, W_m , printed under point 1.) in the block "mass source data". If more Junctions were connected to the CV then the value W_m , printed in the "mass source data", would be equal to the sum of the mass flows for all Junctions connected to a given CV.

Apart from the mass and enthalpy sources the block contains data on the source absolute and relative "elevations". The definitions of those "elevations" are given in Volume 1. **In case of pool and bubbles, the absolute elevations are defined as the distances from the bottom of a CV to a given place in the pool. in case of atmosphere and droplets, the absolute elevations are defined as the distances from the top of a CV to a given place in the atmosphere.** The relative elevations are

defined as the distances from the center of the continuous component (atmosphere, pool) to a given place in CV, divided by the height of the continuous component.

In the example case only gas flows through the Junction, thus there is a non-zero source only for the atmosphere. Total height of the CV is 10.0 m and the center point of the Junction is located at 7.0 m above the floor of the CV. Thus, for atmosphere and droplets the absolute elevation of the source is 3.0 m. The pool surface level is 5.24442 m, thus the height of the atmosphere is $10.0 - 5.24442 = 4.75558$ m. The relative elevations for atmosphere and droplet, which are measured from the atmosphere center point, are equal to: $(4.75558/2.0 - 3.0) / 4.75558 = -1.30838 \times 10^{-1}$.

In case of pool and bubble there is no mass source since the Junction is located in the atmosphere space. Nevertheless the values of the elevations are still printed. The absolute elevation is set to the elevation of the pool surface (5.24442 m). Note that if the pool level was somewhat above the lowermost point of the Junction (6.9 m), say at 6.96 m, then the source location would be in the center of the water cover area: $(6.9+6.96)/2 = 6.93$ m. If the pool level was above the uppermost point of the Junction (7.1 m), then the source location would be always at the Junction center point (7.0 m) which would then be the same as the center of the water covered area. Thus the source elevation is a continuous function of the pool level. Relative elevations are obtained in the same manner as above, but this time they are related to the center point of the pool: $(5.24442/2.0 - 5.24442) / 5.24442 = -0.50$. Note that the relative elevations are always within the range: $(-0.5, +0.5)$.

The next part of this block contains data on the diameters and volumes of a single particle (bubbles, droplets), and the source strength (number of particles created per second). In the present case the source is negative, that means droplets are transported out of CV through the Junction. The following part gives the gas composition in case of gas sources (atmosphere, bubbles).

At the bottom of the Junction mass source printout the bubble collapse parameters are printed if bubble collapse occurs. In this case bubble collapse does not occur (there is no positive gas mass source below the pool level) and the bubble collapse data is not printed (an example of bubble collapse printout is given below, in the Tabular Mass Source output description).

The following blocks contain data on Solid Conductor sources, belonging to the group of the individual mass sources. These blocks contain mass transfer (boiling / condensation) on Solid Conductors. In the example case there is a mass transfer (condensation) on the left surfaces of SC-011 and SC-012. There is a negative mass source for the atmosphere gas and a positive mass source for the droplets. Note that in the block "mass source data" the value of mass source, W_m , printed under point 2.) is equal to the sum of the individual values for SC-011 and SC-012, printed here. This block contains the usual information on the absolute and relative elevations. The way those are defined is discussed in the description of the Junction flows block, above. Note that in case of atmosphere the elevation of the gas mass sink is equal to the elevation of the center point of the SC surface, while the elevation of the droplet mass source is equal to the elevation of the lowermost point of the Conductor. Again it should be noted that in case of pool and bubbles the absolute elevations are measured from the bottom of CV, in case of atmosphere and droplets the absolute elevations are measured from the top of CV.

In the presented example the center points are: SC-011: 7.0 m, SC-012: 9.0. The height of both surfaces is 1.0 m. Thus the absolute elevations, for atmosphere and droplet sources, measured from the top of CV, are equal to, for the center points: 3.0 m, and 1.0 m; for the lowermost points: 3.5 m, and 1.5 m, for SC-011 and SC-012 respectively. In the present example however the elevations of the droplet sources are not equal to 3.5 and 1.5 m. This is because the default value of the condensate drainage parameter (CFDLSC) is used, which results in depositing droplets from condensing surfaces directly in the pool (see description of CFDLSC in sections 2.3.11 and 2.3.12). The droplet source

elevation is therefore set to the pool level, measured from the top of CV: $10.0 - 5.24442 = 4.75558$. To obtain a mechanistic treatment of droplets falling from the condensing surfaces one would have to set CFDLSC to the height of the SC (1.0 m). Then the droplet source elevation would indeed be equal to 3.5 m and 1.5 m for SC-011 and SC-012 respectively.

The next part of this block contains data on the diameters and volumes of a single particle (bubbles, droplets), and the source strength (number of particles created per second). In the presented example the condensate forms droplets of the diameter of about half centimeter, at the rate of about one droplet per second. In the present example those droplets are not suspended in the atmosphere but deposited directly in the pool, because of the default value of the CFDLSC parameter, mentioned above. This particular choice of the default value of the CFDLSC and CFDRSC parameters was motivated by the observation that typically calculations are faster, without any practical difference in the results. Therefore mechanistic treatment of droplets from condensing surface is an option that must be activated by the user, if he wishes to use it.

At the bottom of the Solid Conductor mass source printout the bubble collapse parameters are printed if the bubble collapse occurs. In this case the bubble collapse does not occur (there is no boiling) and the bubble collapse data is not printed.

The following block contains data on Non-equilibrium mass transfer, belonging to the group of the individual mass sources. In the presented example there is no non-equilibrium mass transfer and the only non-zero values are the component volumes.

The following block contains data on Interphase mass transfer, belonging to the group of the individual mass sources. The data is printed for the three inter-phases: pool-atmosphere, atmosphere-droplet, and pool-bubble. The data include: interphase areas, mass fluxes, corresponding enthalpy fluxes, and the heat fluxes: convective heat flux and mass transfer heat flux. The mass transfer heat flux is simply the difference between the gas enthalpy flux and the liquid enthalpy flux (approximately equal to the latent heat of evaporation multiplied by the mass transfer rate). The following comments can be made in relation to the interphase mass transfer data for the presented example.

In case of pool-atmosphere interphase there is a small negative (atmosphere-to-pool) convective heat flux. It is caused by the fact that the atmosphere temperature (3.19267×10^2 K) is slightly higher than the pool surface temperature (3.15027×10^2 K). The mass transfer rate (as well as the mass transfer heat flux) is positive indicating that evaporation takes place. This evaporation is caused by the fact that the atmosphere is relatively dry (relative humidity of about 4.31709×10^{-1}).

In case of atmosphere-droplet interphase there is a positive (droplet-to-atmosphere) convective heat flux, and mass transfer flux, caused by the fact that droplets (created at the tabular mass source) are relatively warm (3.46641×10^2 K). In case of bubbles there is positive mass flux (evaporation into bubbles). The bubbles, injected by Tabular Mass Source, are initially dry (pure nitrogen bubble source).

The relation between the heat and mass transfer rates printed in this block and the values printed in the mass source data and heat source data, printed above, is not trivial and is shortly explained here. The values of interphase heat and mass transfer are discussed below sequentially for: droplets, bubbles, atmosphere, and pool.

Droplets

The total mass transfer for droplet-atmosphere transfer, printed in the mass source data for droplets, W_m , in point 4), is equal to:

SPECTRA Code Manuals - Volume 2: User's Guide

$$W_m = -\text{Area} (2.69993 \times 10^{-2} \text{ m}^2) \cdot \text{Mass transfer rate} (2.11433 \times 10^{-2} \text{ kg/m}^2/\text{s}) = -5.70856 \cdot 10^{-4} \text{ kg/s.}$$

The minus sign comes from the convention that positive interphase mass transfer means evaporation. Therefore, when the mass transfer is positive, the droplet mass decreases.

The corresponding enthalpy source for the droplets, H_m , in point 4) is equal to:

$$H_m = -\text{Area} (2.69993 \times 10^{-2} \text{ m}^2) \cdot \text{Enthalpy-liq} (6.50452 \times 10^3 \text{ W/m}^2) = -1.75618 \times 10^3 \text{ W.}$$

The heat source, printed in the energy source data for droplets, Q_n , in point 3), is equal to:

$$Q_n = -\text{Area} (2.69993 \times 10^{-2} \text{ m}^2) \cdot \text{Convective heat flux} (2.68008 \times 10^3 \text{ W/m}^2) - \\ - \text{Area} (2.69993 \times 10^{-2} \text{ m}^2) \cdot \{ \text{Enthalpy-gas} (5.56500 \times 10^4 \text{ W/m}^2) - \\ \text{Enthalpy-liq} (6.50452 \times 10^3 \text{ W/m}^2) \} = -1.39926 \times 10^3 \text{ W}$$

The first term represents the true heat transfer at the droplet surface, the second term represents the heat consumed during evaporation (enthalpy of the created steam minus enthalpy of the disappearing liquid). The minus sign in the first term comes from the convention that positive interphase heat transfer means heat from liquid to gas.

Bubbles

The total mass transfer for bubble-atmosphere transfer, printed in the mass source data for bubbles, W_m , in point 4), is equal to:

$$W_m = +\text{Area} (8.98737 \text{ m}^2) \cdot \text{Mass transfer rate} (2.28363 \times 10^{-4} \text{ kg/m}^2/\text{s}) = 2.05239 \times 10^{-3} \text{ kg/s.}$$

The plus sign comes from the convention that positive interphase mass transfer means evaporation. Therefore, when the mass transfer is positive, the bubble mass increases.

The corresponding enthalpy source for the bubbles, H_m , in point 4) is equal to:

$$H_m = \text{Area} (8.98737 \text{ m}^2) \cdot \text{Enthalpy-gas} (5.88433 \times 10^2 \text{ W/m}^2) = 5.28847 \times 10^3 \text{ W.}$$

The heat source, printed in the energy source data for bubbles, Q_n , in point 3), is equal to:

$$Q_n = +\text{Area} (8.98737 \text{ m}^2) \cdot \text{Convective heat flux} (4.55065 \times 10^2 \text{ W/m}^2) - \\ - \text{Area} (8.98737 \text{ m}^2) \cdot \{ \text{Enthalpy-gas} (5.88433 \times 10^2 - \text{Enthalpy-liq} (4.00444 \times 10^1) \} = \\ = -8.38738 \times 10^2 \text{ W}$$

The first term represents true heat transfer at the bubble surface; the second term represents the heat consumed during evaporation (enthalpy of the created steam minus enthalpy of the disappearing liquid). The plus sign in the first term comes from the convention that positive interphase heat transfer means heat from liquid to gas.

Atmosphere

The total mass transfer, printed in the mass source data for atmosphere, W_m , in point 4), is the sum of pool-atmosphere (p-a) and droplet-atmosphere (d-a) mass transfers, and is equal to:

$$W_m = + \text{Area}_{p-a} (1.0 \text{ m}^2) \cdot \text{Mass transfer rate}_{p-a} (5.95570 \times 10^{-5} \text{ kg/m}^2/\text{s}) + \\ + \text{Area}_{d-a} (2.69993 \times 10^{-2} \text{ m}^2) \cdot \text{Mass transfer rate}_{d-a} (2.11433 \times 10^{-2} \text{ kg/m}^2/\text{s}) = \\ = 6.30413 \times 10^{-4} \text{ kg/s}$$

The plus sign comes from the convention that positive interphase mass transfer means evaporation. Thus when mass transfer is positive the atmosphere mass increases.

The corresponding enthalpy source for atmosphere, H_m , in point 4) is equal to:

$$H_m = \text{Area}_{p-a} (1.0 \text{ m}^2) \cdot \text{Enthalpy-gas}_{p-a} (1.53463 \times 10^2 \text{ W/m}^2) + \\ + \text{Area}_{d-a} (2.69993 \times 10^{-2} \text{ m}^2) \cdot \text{Enthalpy-gas}_{d-a} (5.56500 \times 10^4 \text{ W/m}^2) = 1.65598 \times 10^3 \text{ W}$$

The heat source, printed in the energy source data for droplets, Q_n , in point 3), is the sum of pool-atmosphere (p-a) and droplet-atmosphere (d-a) heat transfers, and is equal to:

$$Q_n = +\text{Area}_{p-a} (1.0 \text{ m}^2) \cdot \text{Convective heat flux}_{p-a} (-4.31159 \text{ W/m}^2) + \\ + \text{Area}_{d-a} (2.69993 \times 10^{-2} \text{ m}^2) \cdot \text{Convective heat flux}_{d-a} (2.68008 \times 10^3 \text{ W/m}^2) = 6.80487 \times 10^2 \text{ W}$$

The minus signs come from the convention that positive interphase heat transfer means heat from liquid to gas.

Pool

The total mass transfer, printed in the mass source data for pool, W_m , in point 4), is the sum of pool-atmosphere (p-a) and pool-bubble (p-b) mass transfers, and is equal to:

$$W_m = -\text{Area}_{p-a} (1.0 \text{ m}^2) \cdot \text{Mass transfer rate}_{p-a} (5.95570 \times 10^{-5} \text{ kg/m}^2/\text{s}) - \\ - \text{Area}_{p-b} (8.98737 \text{ m}^2) \cdot \text{Mass transfer rate}_{p-b} (2.28363 \times 10^{-4} \text{ kg/m}^2/\text{s}) = -2.11194 \times 10^{-3} \text{ kg/s}$$

The minus sign comes from the convention that positive interphase mass transfer means evaporation. Thus when mass transfer is positive the pool mass decreases.

The corresponding enthalpy source for pool, H_m , in point 4) is equal to:

$$H_m = -\text{Area}_{p-a} (1.0 \text{ m}^2) \cdot \text{Enthalpy-liq}_{p-a} (1.04435 \times 10^1 \text{ W/m}^2) - \\ - \text{Area}_{p-b} (8.98737 \text{ m}^2) \cdot \text{Enthalpy-liq}_{p-b} (4.00444 \times 10^1 \text{ W/m}^2) = -3.70337 \times 10^2 \text{ W}$$

The heat source, printed in the energy source data for droplets, Q_n , in point 3), is the sum of pool-atmosphere (p-a) and droplet-atmosphere (d-a) heat transfers, as well as the heat consumed during evaporation from the pool surface, and is equal to:

$$Q_n = -\text{Area}_{p-a} (1.0 \text{ m}^2) \cdot \text{Convective heat flux}_{p-a} (-4.31159 \text{ W/m}^2) - \\ - \text{Area}_{p-b} (8.98737 \text{ m}^2) \cdot \text{Convective heat flux}_{p-b} (4.55065 \times 10^2 \text{ W/m}^2) - \\ - \text{Area}_{p-a} (1.0 \text{ m}^2) \cdot \{ \text{Enthalpy-gas}_{p-a} (1.53463 \times 10^2 \text{ W/m}^2) - \\ - \text{Enthalpy-liq}_{p-a} (1.04435 \times 10^1 \text{ W/m}^2) \} = -4.22855 \times 10^3 \text{ W}$$

The minus sign in the first two terms come from the convention that positive interphase heat transfer means heat from liquid to gas.

The following block contains data on De-entrainment, belonging to the group of the individual mass sources. Three de-entrainment processes may be taken into account. For droplets these are vertical de-entrainment (when droplets hit the pool surface or CV floor) and horizontal de-entrainment (when droplets hit a wall). For bubbles only vertical de-entrainment is modelled (when bubbles hit the pool surface). In the presented example the droplet horizontal de-entrainment model is not used, thus zeroes are printed in the second column of this block. Droplet vertical de-entrainment mass transfer is $9.89443 \times 10^{-2} \text{ kg/s}$. This is a negative mass source for the droplets and a positive mass source for the

SPECTRA Code Manuals - Volume 2: User's Guide

pool (see mass source data printout, H_m, point 5). The bubble vertical de-entrainment is equal to 4.46211×10^{-2} kg/s. This is a negative source of mass for the bubbles and a positive mass source for the atmosphere (see mass source data printout, H_m, point 5).

The following blocks contain data on Tabular mass sources, belonging to the group of the individual mass sources. The tabular mass sources are treated quite similarly to the Junction flow sources and the printout is the same as in case of the Junction flow sources, discussed above. In the presented example there are two tabular sources.

The first tabular source is a source of gas, placed at the bottom of the CV. This gas constitutes a source for the pool bubbles. The mass flow is 0.1 kg/s. The injected stream breaks into bubbles of the diameter of 2.00000×10^{-2} m. The bubble source strength is equal to about $1.66983 \times 10^{+4}$ bubbles per second.

At the bottom of the printout bubble collapse parameters are printed if the bubble collapse occurs. During the "bubble collapse" phase the bubble temperature ($3.74000 \times 10^{+2}$ K) equilibrates with the pool temperature ($3.15027 \times 10^{+2}$ K). Simultaneously some water is evaporated into the bubble. After bubble collapse, the bubble diameter is reduced from 2.00000×10^{-2} m to 1.89838×10^{-2} m).

The second tabular source is a source of liquid, placed at the top of the CV. This liquid constitutes a source for the atmosphere droplets. The mass flow is 1.00000×10^{-1} kg/s. The injected stream breaks into droplets of the diameter of 1.23804×10^{-2} m. The droplet source strength is equal to 1.03362×10^2 droplets per second.

Next hydrogen burn and oxidation data may be printed. Since neither of these processes occurs in the present example, these blocks are not printed and zeroes are printed in the mass source data, H_m, points 7) and 8), and energy source data Q_n, point 6).

The following blocks contains data on individual energy sources. The first block in this group contains data on Solid Conductor convection. This block contains heat fluxes from all SC surfaces present in the CV. In the presented example nine SCs (SC-001 - SC-009) convect heat to the pool. One SC (SC-010) is partly immersed in pool and convects heat to both pool and atmosphere. Two SCs (SC-011, SC-012) convect heat to the atmosphere gas.

The following block contains data on Tabular energy sources, belonging to the group of the individual energy sources. In the presented example there is a single tabular energy source, placed below the pool surface in the CV.

At the bottom of the CV output the "summed quantities" (data summed for all Control Volumes) are printed. The example output is given below.

```
=====
=CV=  DATA SUMMED FOR ALL CV M & E SOURCES AT TIME :  5.10000E+00 (s)
=====
```

Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
Mass (M Src.)	kg	0.00000E+00	4.05000E-01	0.00000E+00	4.05000E-01
Energy (M Src.)	J	0.00000E+00	1.30320E+05	0.00000E+00	1.62045E+05
Energy (E Src.)	J	0.00000E+00	0.00000E+00	5.10000E+05	0.00000E+00

Quantity	Units	Total Value
Mass (M Src.)	kg	8.1000000E-01
Energy (M Src.)	J	2.9236565E+05
Energy (E Src.)	J	5.1000000E+05
Energy (M&E S.)	J	8.0236565E+05

SPECTRA Code Manuals - Volume 2: User's Guide

```
=====
=CV= DATA SUMMED FOR ALL CONTROL VOLUMES AT TIME : 5.10000E+00 (s)
=====
```

Summed mass of gases in atmosphere and pool bubbles

GAS	MASS, ATMS.	MASS, POOL	MASS, TOTAL
No. Id.	kg	kg	kg
3 H2O	1.77702E+00	7.55277E-03	1.78457E+00
4 N2	1.01171E+04	3.02614E-01	1.01174E+04
5 O2	2.58999E+00	0.00000E+00	2.58999E+00

Quantity	Units	Atms-Gas	Atms-Drop	Pool-Liq	Pool-Bub
Volume	m3	9.00976E+03	4.49832E-05	9.01000E+03	2.44016E-01
Mass	kg	1.01214E+04	4.38911E-02	8.93278E+06	3.10167E-01
Energy	J	2.49218E+09	1.35010E+04	1.56531E+12	9.26118E+04

Total values:

* Current = at time: 5.10000E+00 (s)
 * C-I = current value minus initial value
 * C-I-M&E = current minus initial minus M&E, H2 burn, and Oxidation sources
 * C-I-M&E-SC = current minus initial minus M&E, H2 burn, and Oxidation sources
 minus total integrated heat flux from all 1-D and 2-D SCs

Quantity	Units	Current	C - I	C-I-M&E	C-I-M&E-SC
Volume	m3	1.80200E+04	-3.63798E-12		
Mass	kg	8.94290E+06	8.10000E-01	5.21541E-10	
Energy	J	1.56780E+12	8.00420E+05	-1.94526E+03	-9.72949E-05

If there are no flows to or from inactive CVs (CVs in which conditions are held constant) then C-I-M&E and C-I-M&E-SC can be used to check M&E balance:

Relative mass error = C-I-M&E / Current

Relative energy error = C-I-M&E-SC / Current

Typically relative errors are ~1E-14 (governed by round-off error of double precision numbers, which is ~1E-15).

When Thermal Radiation model is active the energy error depends on the accuracy in view factors and thus may be relatively large: up to ~1E-6 (TR package requires view factor inaccuracy to be not bigger than 1E-7).

=====

This data contains two parts. The first part gives summed quantities for all mass and energy sources. The second part gives summed quantities for the whole system.

Summed quantities for mass and energy sources

This output consists of the following two blocks:

First block. For all components: atmosphere, droplets, pool, and bubbles, the following summed quantities are given:

- integrated mass (kg) from all mass sources,
- integrated energy (J) accompanying mass sources, from all mass sources,
- integrated energy (J), from all energy sources.

Second block. The following summed quantities are given:

- total integrated mass from all mass sources (kg),
- total integrated energy (J) accompanying mass sources, from all mass sources,
- total integrated energy from all energy sources (J).
- total integrated energy (J), all mass and energy sources.

The first three values are equal to their corresponding values in the first block, summed over all components. The last value is equal to the sum of the second and the third value.

Summed quantities for all Control Volumes

This output consists of the following three blocks:

First block. For all gases, which are present in atmosphere and bubbles, the mass of each individual gas, summed over all Control Volumes is printed in this block.

Second block. For all components: atmosphere, droplets, pool, and bubbles, the following summed quantities are given: volume, mass, and energy. Note that the atmosphere mass printed in this block is equal to the sum of the atmosphere individual masses printed in the first block, and the bubble mass printed in this block is equal to the sum of the individual bubble masses, printed in the first block.

Third block. The following summed quantities are given: volume, mass, and energy. The printed values are:

- Current values. Note that in the column "Current" each quantity is equal to the sum over all components of the same quantity printed in the second block.
- Current minus initial.
- Current minus initial minus integrated mass and energy sources. This column contains data for mass and energy. The value of mass in this column represents the "**mass error**".
- Current minus initial minus integrated mass and energy sources minus integrated heat flux from all 1-D and 2-D Solid Heat Conductors. This column contains data for energy only. The value represents the "**energy error**".

The values printed in this block can be considered as the mass and energy errors only in case when there are no flows to or from inactive Control Volumes (CVs in which conditions are held constant - ITYPECV≠0, see section 1.1.1). Typically relative errors (the value of error, divided by the "Current" value) are of order of 10^{-14} (governed by round-off error of double precision numbers). When the Thermal Radiation model is active the energy error depends on the accuracy in view factors and thus may be relatively large: up to 10^{-6} (the TR package requires view factor inaccuracy to be smaller than 10^{-7}).

3.1.3 Junction Output

The Junction outputs may be easily found in the output file by searching for the string: =JN=. The first JN printout brings the input data printout. An example of the input printout for a Junction is shown below. The printout mainly reflects the data entered in the input file and is quite self-explanatory.

```
=JN= =====JN-001===== Example_problem,_Junction_1_(CV-001_-_CV-002)____  
  
CONNECTION      : FROM CV-001 TO CV-002  
AREA            m2: 1.00000E+00  
ELEVATION       m: 5.00000E+00  
LENGTH (MOM)   m: 5.00000E+00  
EDGES INDICATOR : 0.00000E+00  
DIAMETER        m: 1.12838E+00  
HEIGHT          m: 1.12838E+00  
FLOW DIRECTION  : HORIZONTAL  
ELEVATIONS      IN CV-001      IN CV-002  
TOP            m: 5.56419E+00  5.56419E+00
```

SPECTRA Code Manuals - Volume 2: User's Guide

```

BOTTOM m: 4.43581E+00 4.43581E+00

=JN= JN-001, INITIAL VELOCITIES: INPUT VALUES ARE USED
      Vatms = 0.00000E+00 (m/s)
      Vpool = 0.00000E+00 (m/s)

=JN= JN-001, FRICTION DATA AND COEFFICIENTS
FR. LENGTH m: 5.00000E+00
ROUGHNESS m: 1.00000E-05
DIAMETER m: 1.12838E+00
FORM LOSS (F) -: 1.00000E+00
FORM LOSS (R) -: 1.00000E+00
Rf (2-ph, F) -: 1.00000E+00
Rf (2-ph, R) -: 1.00000E+00
CMOODY -: 7.00000E-01
1-PHASE MODEL : COLEBROOK-WHITE
2-PHASE MODEL : HANCOX-NICOLL

=JN= JN-001, VALVE DATA
MOTOR VALVE : TF-006
(1/A)*(dA/dt): 1.00000E+00
CHECK VALVE : NONE
INITIAL FR.OPEN : 0.00000E+00
MIN OPEN (LEAK) : 0.00000E+00
MAX OPEN (LIMIT): 1.00000E+00
VALVE COEFF. CV : 5.00000E+00

=JN= JN-001, FLOW CONTROL
GAS : MOMENTUM EQ.
LIQUID : MOMENTUM EQ.

=JN= JN-001, FLOW COMPOSITION PARAMETER (FCP) DATA
GAS: 1 FCP: 1.00000E+00
GAS: 2 FCP: 1.00000E+00
GAS: 3 FCP: TF-004
GAS: 4 FCP: 1.00000E+00
GAS: 5 FCP: 1.00000E+00
GAS: 6 FCP: 1.00000E+00

=JN= JN-001, ENTRAINMENT INDICATORS
E-atms : 0.00000E+00
E-drop : 1.00000E+00
E-pool : 0.00000E+00
E-bubb : 1.00000E+00

=JN= JN-001, DROP AND BUBBLY FLOW REGIME MODEL PARAMETERS

```

		Droplets		Bubbles	
		vertical	horizontal	vertical	horizontal
-----	-----	-----	-----	-----	-----
Drift flux constant	C0	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Terminal velocity	v-inf	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Exponent	x	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

```

=JN= JN-001, ANNULAR FLOW MODEL: DEFAULT

=JN= JN-001, COUNTER-CURRENT FLOW MODEL CONSTANTS

Vertical flow: CCFVJN = 1.00000E-01
Horizontal flow: CCFHJN = 1.00000E+01

```

Below the individual Junction printouts, several blocks are printed containing data valid for all Junctions. Next the Junction connectivity data is printed, which lists all Junctions connected to every Control Volume. This output helps the user to verify the correctness of his model. Finally, the internal numbering scheme for Junctions is printed. The example printout is given below.

```

=====
=JN= JUNCTION OPTIONS: VELOCITIES AND ELEVATIONS

```


SPECTRA Code Manuals - Volume 2: User's Guide

```
=====
MINIMUM VELOCITY FOR CRITICAL FLOW TEST: 1.00000E+01      m/s

JUNCTION ELEVATIONS ARE CHECKED
WHETHER THEY ARE TOO CLOSE TO CV BOTTOM OR TOP
THIS IS DEFAULT OPTION, USED FOR TWO-PHASE SYSTEMS

=====
=JN= JUNCTION PACKAGE FLOW SOLUTION
=====

JUNCTION FLOW MATRIX IS SOLVED USING:
- LU DECOMPOSITION,      IF NUMBER OF ACTIVE JN. <=1000
- BICONJUGATE GRADIENT M., IF NUMBER OF ACTIVE JN. >=1001

JUNCTION MATRIX IS RE-SOLVED DURING ITERATIONS

MAX. NO. OF MATRIX SOLUTIONS PER TIME STEP:      2

MIN.VELOCITY FOR Cf, XCFMJN = 1.00000E-03

COURANT L. GAS COMP. CLCMJN = 1.00000E-01

COURANT LIMIT, ATMS, CLMAJN = 5.00000E-01

COURANT LIMIT, POOL, CLMPJN = 5.00000E-01

COURANT L. ENERGY S. CLCEJN = 1.00000E-01

COURANT L. PUMPS/CM. CLCPJN = 5.00000E-01

VELOCITY LIMIT MULT. CVCLJN = 5.00000E-01

VELOCITY LIMIT      VVCLJN = 1.00000E+01

GAS COMPOSITION CALCULATION : EXPLICIT

=====
=JN= JN REFERENCE DATA FOR      2 CONTROL VOLUMES
=====

=JN= Connect. of: CV-001 Example_problem,_volume_1_____
           JN-001 Example_problem,_Junction_1_(CV-001_->_CV-002)_____
           leads to CV-002 Example_problem,_volume_2_____

=JN= Connect. of: CV-002 Example_problem,_volume_2_____
           JN-001 Example_problem,_Junction_1_(CV-001_->_CV-002)_____
           leads from CV-001 Example_problem,_volume_1_____

=====
=JN= MAXIMUM DSP DATA FOR      2 CONTROL VOLUMES
=====

CV-001 : DSPmax = 9.28468E-01 , SET BY JN-001
CV-002 : DSPmax = 9.28468E-01 , SET BY JN-001

=====
=JN= JUNCTION INTERNAL NUMBERING SCHEME
=====

Int. Ref.
No.   No.
---  -----
  1  JN-001

=====
=JN= END OF JUNCTION DATA
=====
```

SPECTRA Code Manuals - Volume 2: User's Guide

An example of the transient printout for a Junction is shown below.

```

=====
=JN= =====JN-001===== Example_problem,_Junction_1_(CV-001_-_>_CV-002)_____
=JN= JN-001, CONNECTION DATA : CV-001 ---> CV-002
=JN= JN-001, COMPONENT DATA AT TIME : 5.10000E+00 (s)

Quantity      Units      Atms-Gas    Atms-Drop    Pool-Liq     Pool-Bub
-----
Velocity,     m/s       7.13455E-01 7.13455E-01 2.49976E-04 0.00000E+00
Mass flow,    kg/s      5.50493E-01 5.91827E-02 1.24306E-01 0.00000E+00
Area,         m2        4.98339E-01 8.50670E-05 5.01576E-01 0.00000E+00
Temperature,  K         3.79741E+02 3.47634E+02 3.15024E+02 0.00000E+00
Density,      kg/m3     1.54832E+00 9.75140E+02 9.91420E+02 0.00000E+00
Enthalpy,    J/kg      4.19062E+05 3.11940E+05 1.75510E+05 0.00000E+00
Cv            J/kg      7.30838E+02 4.18774E+03 4.17785E+03 0.00000E+00
Cp            J/kg      1.02477E+03 4.19014E+03 4.18204E+03 0.00000E+00

=JN= JN-001, ATMOSPHERE AND BUBBLE GAS COMPOSITION AT TIME : 5.10000E+00 (s)

      GAS                ATMOSPHERE GAS                POOL BUBBLE GAS
      No. Id.           MASS FRAC.    VOL. FRAC.    MASS FRAC.    VOL. FRAC.
      3  H2O            8.97921E-03   1.38889E-02   0.00000E+00   0.00000E+00
      4  N2             8.73394E-01   8.82148E-01   0.00000E+00   0.00000E+00
      5  O2             1.17627E-01   1.03963E-01   0.00000E+00   0.00000E+00

=JN= JN-001, OVERALL DATA AT TIME : 5.10000E+00 (s)

      Area, (m2)  Flow, (kg/s)  Enth. (J/kg)  Velocity (m/s)
Gas   :  4.98339E-01 5.50493E-01 4.19062E+05 7.13455E-01
Liquid:  5.01661E-01 1.83489E-01 2.19514E+05 3.70915E-04
Total :  1.00000E+00 7.33981E-01 3.69177E+05

      P-up, (Pa)  P-down, (Pa)  dP, (Pa)  Reynolds No. Friction F.
Atms  :  1.74557E+05 1.74554E+05 3.85425E+00 5.84932E+04 2.02134E-02
Pool  :  1.77314E+05 1.77313E+05 1.36456E+00 4.43942E+02 1.44163E-01

Pool level, (m) : 5.00178E+00
Cp/Cv for gas, (-) : 1.40219E+00
Density of gas, (kg/m3) : 1.54832E+00

=JN= JN-001, OVERALL GAS COMPOSITION AT TIME : 5.10000E+00 (s)

      No. Id.           MASS FRACTION
      3  H2O            8.97921E-03
      4  N2             8.73394E-01
      5  O2             1.17627E-01

=JN= JN-001, VALVE DATA AT TIME : 5.10000E+00 (s)

      A(full)      A(actual)      Frac.open      K-for      K-rev
TF/CF (m2) (m2) (-) (-) (-)
006  1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00

```

The printout consists of the following blocks.

The first block contains printout of component data. Current values are printed in four columns, for the four components that may share the same flow path: atmosphere (gas), droplets, pool (liquid), and bubbles.

SPECTRA Code Manuals - Volume 2: User's Guide

The second block contains printout of the atmosphere and bubble gas composition, including mass fractions and volumetric fractions.

The third block contains the overall data. The overall data output consists of three parts. The first part gives flow area, mass flow and enthalpy, for the gas, liquid and the total flow. The overall values of the areas and flows are defined as the sums of the individual component data. For example, the overall gas flow, W_{gas} , is equal to the sum of the atmosphere flow, W_{atms} and the bubble flow, W_{bubb} :

$$W_{gas} = W_{atms} + W_{bubb}$$

The overall enthalpies are defined as the averages of the component values, weighted by the component mass flows. For example, the overall gas enthalpy, h_{gas} , is equal to:

$$h_{gas} = \frac{W_{atms}h_{atms} + W_{bubb}h_{bubb}}{W_{atms} + W_{bubb}}$$

where h_{atms} and h_{bubb} are the enthalpies of the atmosphere and the bubbles respectively.

The second part gives pressures upstream and downstream the Junction, pressure differences, Reynolds numbers, and friction factors, for both atmosphere flow and pool flow. Pressure differences are calculated by the program always for both atmosphere and pool, even if the flow of one of those components is zero. These values are needed in case a counter-current flow should occur.

The third part of this block gives the pool level in the Junction, the ratio of specific heats, $(c_p/c_v)_{gas}$, for gas, as well as the gas density, ρ_{gas} . Those values are calculated as the averages of the component values, weighted by the absolute values of the component flows, as shown below.

Ratio of specific heats:

$$\left(\frac{c_p}{c_v}\right)_{gas} = \frac{|W_{atms}|c_{p,atms} + |W_{bubb}|c_{p,bubb}}{|W_{atms}|c_{v,atms} + |W_{bubb}|c_{v,bubb}}$$

- $c_{p,atms}$ specific heat at constant pressure for the atmosphere gas,
- $c_{v,atms}$ specific heat at constant volume for the atmosphere gas,
- $c_{p,bubb}$ specific heat at constant pressure for the bubble gas,
- $c_{v,bubb}$ specific heat at constant volume for the bubble gas.

Gas density:

$$\rho_{gas} = \frac{|W_{atms}|\rho_{atms} + |W_{bubb}|\rho_{bubb}}{|W_{atms}| + |W_{bubb}|}$$

- ρ_{atms} density of atmosphere,
- ρ_{bubb} density of bubbles.

The values of $(c_p/c_v)_{gas}$ and ρ_{gas} are used by the program for the critical flow calculations.

The fourth block contains overall gas composition (mass fractions) defined as:

SPECTRA Code Manuals - Volume 2: User's Guide

$$c_{i,gas} = \frac{|W_{atms}|c_{i,atms} + |W_{bubb}|c_{i,bubb}}{\sum (|W_{atms}|c_{i,atms} + |W_{bubb}|c_{i,bubb})}$$

where: $c_{i,atms}$ - concentration (mass fraction) of the gas No. i, in the atmosphere,
 $c_{i,bubb}$ - concentration of the gas No. i, in the bubbles.

The summation is performed over all gases.

The fifth block contains valve data: the total open area and open fraction, as well as the actual friction coefficient (which depends on the open area), are given. This block is printed only if the valve option is used for a given Junction.

If the flow is critical then an informational message is printed at the bottom of the printout for the given Junction.

3.1.4 1-D Solid Heat Conductor Output

The 1-D Solid Heat Conductor outputs may be easily found in the output file by searching for the string: =SC=. The first SC printout brings the input data printout. An example of the input printout for a 1-D Solid Heat Conductor is shown below. The printout mainly reflects the data entered in the input file and is quite self-explanatory.

```
=SC= =====SC-001===== Rectangular,_fins_on_left_side,_spines_on_right___

SC GROUP NUMBER : 1
GEOMETRY TYPE : RECTANGULAR
CONDUCTOR SIZE : 1.00000E+00
LEFT COORDINATE : 0.00000E+00
THICKNESS (m) : 2.00000E-02
ELEVATION (m) : 5.00000E+00
VERTICAL ORIENT.: VERTICAL
POWER SOURCE : 0.00000E+00
NO.OF CONDUCTORS: 1.00000E+00
INITIAL TEMP. : INPUT VALUES
TRANSIENT TEMP. : CONDUCTION EQUATION
SOLUTION SCHEME : TEMPERATURE NODES AT CELL CENTERS (NIMISC = 1)

      WIDTH      VOLUME      MASS      MATERIAL
CELL   [m]        [m3]        [kg]      NUMBER
  1  1.00000E-03  1.20000E-05  5.76000E-02  MP-001
  2  2.00000E-03  2.40000E-05  1.15200E-01  MP-001
  3  2.00000E-03  2.40000E-05  1.15200E-01  MP-001
  4  2.00000E-03  2.40000E-05  1.15200E-01  MP-001
  5  1.00000E-03  1.20000E-05  5.76000E-02  MP-001

      REL.POWER      POWER
CELL   DENSITY      FRACTION
  1  0.00000E+00  0.00000E+00
  2  0.00000E+00  0.00000E+00
  3  0.00000E+00  0.00000E+00
  4  0.00000E+00  0.00000E+00
  5  0.00000E+00  0.00000E+00

      NODE POS.      TEMPERATURE
NODE   [m]          [K]
  1  0.00000E+00  3.00000E+02
  2  2.00000E-03  3.00000E+02
  3  4.00000E-03  3.00000E+02
```

SPECTRA Code Manuals - Volume 2: User's Guide

```

4 6.00000E-03 3.00000E+02
5 8.00000E-03 3.00000E+02

TOTAL THICK. OF SC, [m] : 8.00000E-03

TOTAL VOLUME OF SC, [m3]: 9.60000E-05
TOTAL INITIAL MASS, [kg]: 4.60800E-01

      B O U N D A R Y   C O N D I T I O N S
                        LEFT      RIGHT
                        -----
Heat transfer area, m2 : 1.20000E-02 1.20000E-02
Area per single SC, m2 : 1.20000E-02 1.20000E-02
Height of surface, m : 1.09545E-01 1.09545E-01
Elevation of center, m : 0.00000E+00 0.00000E+00
Lowest point elev. m : -5.47723E-02 -5.47723E-02
Highest point elev. m : 5.47723E-02 5.47723E-02

Control Volume No. : None CV-001
Tabular Heat Transfer C.: TF-001 TF-003
Tabular Temperature : TF-002 None
Non-convective Heat Flux: None None

Natural conv. config. : VERTICAL WALL VERTICAL WALL
Natural conv. dim., m : 1.09545E-01 2.00000E-02

Forced conv. config. : INTERNAL INTERNAL
Forced conv. dim., m : 1.09545E-01 1.20000E-02

Boiling model : ACTIVE ACTIVE
Nucl. boiling model : CHEN CHEN
Nucl. boiling, Csf : 1.30000E-02 1.30000E-02
CHF model : ZUBER-U.A.S. ZUBER-U.A.S.
Film boiling config. : VERTICAL WALL VERTICAL WALL
Film boiling dim., m : 1.09545E-01 2.00000E-02

Condensation config. : VERTICAL VERTICAL
Condensation dim., m : 1.09545E-01 2.00000E-02
Noncondensables model : MODIFIED OGG MODIFIED OGG
Condensate film drain. : POOL OR RAIN POOL OR RAIN
Edge elev./Edge SC no. : 0.00000E+00 -1.00000E+00

CV horizontal flow is : PARALLEL PARALLEL
Contact angle deg : 9.6000E+01 9.60000E+01
Rod bundle multiplier : 0.00000E+00 0.00000E+00
Oxidation model : None None

RIGHT SIDE FIN/SPINE DATA
Type : FINS
Half thickness, m : 1.00000E-03
Length, m : 2.00000E-02
Distance (effective) m : 1.20000E-02
Thermal conduct. W/m/K : MP-001
Area increase - : 4.33333E+00
Volume increase - : 4.33333E+00

=SC= SC-001, BOUNDARY FLUID TEMPERATURE USED FOR POOL:

      T(fluid) = T(CV,pool)

=SC= SC-001, VELOCITY MULTIPLIER: 1.00000E+00

=SC= SC-001, Maximum fraction of surface area covered by pool
      to allow simultaneous heat transfer to pool and atmosphere:
      - LEFT SURFACE, PMXLSC: 0.00000E+00
      - RIGHT SURFACE, PMXRSC: 0.00000E+00

=SC= SC-001, FAILURE: NOT CALCULATED

=SC= SC-001, AXIAL HEAT TRANSFER: NOT CALCULATED

```

SPECTRA Code Manuals - Volume 2: User's Guide

At the bottom of the 1-D Solid Conductor data printout the data valid for all heat conductors are printed. Next the SC reference data is printed for all Control Volumes, which are used as boundary conditions for SC. Finally, the internal numbering scheme is printed.

```
=SC= ALL 1-D SOLID HEAT CONDUCTORS -----
CHF AND MINIMUM FILM BOILING PARAMETERS:
- MINIMUM VALUE OF T(CHF)-T(MFB): TFMNSC = 5.00000E+00
- MAXIMUM VALUE OF T(CHF)-T(MFB): TFMXSC = 1.00000E+03
- MAXIMUM VALUE OF SLIP FOR CHF : SMAXSC = 1.00000E+02
- MULTIPLIER FOR COUNTER-FLOW TA: CMN1SC = 1.00000E-02
- MULTIPLIER FOR CO-FLOW TA      : CMN2SC = 1.00000E+00

=====
=SC= SC REFERENCE DATA FOR 2 CONTROL VOLUMES
=====

=SC= SC surfaces in CV-001 Room

SC-001 right side 1-D finned wall, Aluminum
SC-002 right side 1-D finned wall, Stainless Steel
SC-003 right side 1-D NON-finned wall, Aluminum

=SC= ALL 1-D SOLID HEAT CONDUCTORS -----

SC-S IN SEQUENTIAL ORDER                                LEFT AREA  RIGHT AREA
                                                         [m2]       [m2]
SC-001 1-D finned wall, Aluminum                       1.2000E-02 1.2000E-02
SC-002 1-D finned wall, Stainless Steel                 1.2000E-02 1.2000E-02
SC-003 1-D NON-finned wall, Aluminum                   1.2000E-02 1.2000E-02

SC-S SORTED BY THE RIGHT SURFACE SIZE :                LEFT AREA  RIGHT AREA
                                                         [m2]       [m2]
SC-003 1-D NON-finned wall, Aluminum                   1.2000E-02 1.2000E-02
SC-002 1-D finned wall, Stainless Steel                 1.2000E-02 1.2000E-02
SC-001 1-D finned wall, Aluminum                       1.2000E-02 1.2000E-02

TOTAL AREA, SURFACES CONNCTED TO CV :    LEFT      RIGHT      TOTAL
TOTAL AREA, SURFACES NOT CONNCTED TO CV: 3.6000E-02 0.0000E+00 3.6000E-02

=SC= SOLID HEAT CONDUCTORS OF GROUP : 1 -----

SC-S IN SEQUENTIAL ORDER                                LEFT AREA  RIGHT AREA
                                                         [m2]       [m2]
SC-001 1-D finned wall, Aluminum                       1.2000E-02 1.2000E-02
SC-002 1-D finned wall, Stainless Steel                 1.2000E-02 1.2000E-02
SC-003 1-D NON-finned wall, Aluminum                   1.2000E-02 1.2000E-02

TOTAL AREA, SURFACES CONNCTED TO CV :    LEFT      RIGHT      TOTAL
TOTAL AREA, SURFACES NOT CONNCTED TO CV: 3.6000E-02 0.0000E+00 3.6000E-02

=SC= TOTAL VOLUME AND MASS -----

TOTAL VOLUME = 2.8800E-04 [m3]
TOTAL MASS   = 1.6704E+00 [kg]

No. Material                V [m3]      V [%]
1 _____                1.9200E-04  66.7
2 _____                9.6000E-05  33.3

No. Material                M [kg]      M [%]
1 _____                9.2160E-01  55.2
2 _____                7.4880E-01  44.8

=SC= TOTAL VOLUME AND MASS FOR SC GROUP : 1 -----
```

SPECTRA Code Manuals - Volume 2: User's Guide

TOTAL VOLUME = 2.8800E-04 [m3]
 TOTAL MASS = 1.6704E+00 [kg]

No.	Material	V [m3]	V [%]
1		1.9200E-04	66.7
2		9.6000E-05	33.3

No.	Material	M [kg]	M [%]
1		9.2160E-01	55.2
2		7.4880E-01	44.8

=====

=SC= 1-D SOLID HEAT CONDUCTOR INTERNAL NUMBERING SCHEME

=====

Int. No.	Ref. No.
1	SC-001

=====

=SC= END OF 1-D SOLID HEAT CONDUCTOR DATA

=====

An example of the transient printout for a Solid Conductor is shown below.

=SC= =====SC-001===== Rectangular, _fins_on_left_side, _spines_on_right__

=SC= SC-001, NODE TEMPERATURES AT TIME : 5.00000E+01 (s)

Node	Position, (m)	T, (K)
1	0.00000E+00	3.88156E+02
2	2.00000E-02	3.78728E+02

=SC= SC-001, BOUNDARY CONDITIONS AT TIME : 5.00000E+01 (s)

Vol	H.T. Area Fractions	Twall (K)	Tfluid (K)	h (W/m2/K)	H.T. Mode
Left : 001	atms 1.00000E+00	3.88156E+02	3.89768E+02	1.16412E+04	CONDEN
	pool 0.00000E+00	3.88156E+02	0.00000E+00	0.00000E+00	
	repr 1.00000E+00	3.88156E+02	3.89768E+02	1.16412E+04	
Right: 002	atms 4.99983E-01	3.78728E+02	3.70262E+02	5.70140E+01	FC-LAM
	pool 5.00017E-01	3.78728E+02	3.70005E+02	4.27029E+03	NUC-B
	repr 1.00000E+00	3.78728E+02	3.70008E+02	2.16372E+03	

=SC= SC-001, BOUNDARY HEAT FLUXES AT TIME : 5.00000E+01 (s)

Vol	q(conv) (W/m2)	Q(conv) (W)	q(rad) (W/m2)	Q(rad) (W)
Left : 001	atms -1.87579E+04	-1.87579E+04	0.00000E+00	0.00000E+00
	pool 0.00000E+00	0.00000E+00		
	repr -1.87579E+04	-1.87579E+04	0.00000E+00	0.00000E+00
Right: 002	atms 4.82693E+02	2.41338E+02	0.00000E+00	0.00000E+00
	pool 3.72528E+04	1.86270E+04		
	repr 1.88684E+04	1.88684E+04	0.00000E+00	0.00000E+00

=SC= SC-001, FLUID VELOCITIES AT TIME : 5.00000E+01 (s)

Vol	v-atms (m/s)	v-pool (m/s)	v-bubb (m/s)
Left : 001	1.12097E-04	0.00000E+00	0.00000E+00
Right: 002	0.00000E+00	0.00000E+00	0.00000E+00

=SC= SC-001, FLUID COMPOSITION AT TIME : 5.00000E+01 (s)

		LEFT SURFACE		RIGHT SURFACE	
Gas No.	Gas Id.	MASS FRACTION	VOLUME FRACTION	MASS FRACTION	VOLUME FRACTION

SPECTRA Code Manuals - Volume 2: User's Guide

```

-----
atms  3  H2O  8.50851E-01  8.99092E-01  8.61549E-01  9.07416E-01
atms  4  N2   1.16011E-01  8.07261E-02  1.07689E-01  7.40670E-02
atms  5  O2   3.31379E-02  2.01815E-02  3.07617E-02  1.85168E-02
-----
atms  droplets  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
pool  bubbles   1.00000E+00  1.00000E+00  0.00000E+00  8.00380E-05

=SC=  SC-001,  CONDENSATION PARAMETERS AT TIME :  5.00000E+01 (s)
      Mass flux  Liq.enth.  Vap.enth.  Cond.film  f(NC)  f(SH)
      Vol  (kg/m2/s)  (W/m2)  (W/m2)  (m)  (-)  (-)
-----
Left :  1  8.4675E-03  4.1159E+03  2.2874E+04  2.6777E-05  2.897E-01  1.000E+00

=SC=  SC-001,  BOILING PARAMETERS AT TIME :  5.00000E+01 (s)
      Mass flux  Liq.enth.  Vap.enth.  Tsat  qCHF
      Vol  (kg/m2/s)  (W/m2)  (W/m2)  (K)  (W/m2)
-----
Right:  2  1.2673E-02  5.1427E+03  3.3915E+04  3.7343E+02  1.4619E+06

=SC=  SC-001,  LEFT SURFACE, FIN/SPINE DATA AT TIME :  5.00000E+01 (s)

ATMOSPHERE:
Fin/Spine Efficiency (-) : Eff = 3.62893E-02
Fin/Spine Enhancement (-) : E = 1.53304E+00
Heat/Mass Transfer      TRUE      EFFECTIVE
Heat tr. coeff. (W/m2/K) : h = 7.59350E+03  1.16412E+04
Heat flux (W/m2) : q = -1.22357E+04 -1.87579E+04
Mass tr. flux (kg/m2/s) : m = 5.52330E-03  8.46747E-03
Liquid enth. flux (W/m2) : Hliq= 2.68477E+03  4.11588E+03
Gas enth. flux (W/m2) : Hgas= 1.49205E+04  2.28738E+04

=SC=  SC-001,  RIGHT SURFACE, FIN/SPINE DATA AT TIME :  5.00000E+01 (s)

ATMOSPHERE:
Fin/Spine Efficiency (-) : Eff = 6.43304E-01
Fin/Spine Enhancement (-) : E = 6.13217E+00
Heat/Mass Transfer      TRUE      EFFECTIVE
Heat tr. coeff. (W/m2/K) : h = 9.29753E+00  5.70140E+01
Heat flux (W/m2) : q = 7.87148E+01  4.82693E+02

POOL:
Fin/Spine Efficiency (-) : Eff = 3.85625E-02
Fin/Spine Enhancement (-) : E = 1.27004E+00
Heat/Mass Transfer      TRUE      EFFECTIVE
Heat tr. coeff. (W/m2/K) : h = 3.36232E+03  4.27029E+03
Heat flux (W/m2) : q = 2.93319E+04  3.72528E+04
Mass tr. flux (kg/m2/s) : m = 9.97843E-03  1.26730E-02
Liquid enth. flux (W/m2) : Hliq= 4.04924E+03  5.14270E+03
Gas enth. flux (W/m2) : Hgas= 2.67038E+04  3.39149E+04

```

The first block contains the printout of the node temperatures for all nodes of the given Conductor. The first node is located on the left surface of the Conductor. The last node is located on the right surface of the conductor. The location of each node is printed in the input diagnostics printout.

The second block contains boundary conditions for the left and right surfaces. Three values are printed: for atmosphere ("atms"), pool ("pool"), and representative ("repr"). The representative values are used as boundary conditions for the Solid Conductor transient conduction equation. The heat transfer mode identifiers, which may be printed in this block are: NC-LAM - natural convection, laminar flow, NC-TUR - natural convection, turbulent flow, FC-LAM - forced convection, laminar flow, FC-TRN - forced convection, transition flow, FC-TUR - forced convection, turbulent flow, NUC-B - nucleate boiling, TRAN-B - transition boiling, FILM-B - film boiling, CONDEN - condensation, INSUL - insulation, TAB-F. - heat transfer coefficient specified by a Tabular Function, CON-F. - heat transfer coefficient specified by a Control Function.

It is important to note that the heat transfer coefficient printed in this block is always related to the heat flux by the following equation:

$$q = h (T_{wall} - T_{fluid})$$

Which means that the heat transfer coefficient is equal to:

$$h = \frac{|q|}{|T_{wall} - T_{fluid}|}$$

In case of condensation the usual definition of the condensation heat transfer coefficient is:

$$h = \frac{|q|}{\Delta T_{sat}} = \frac{|q|}{(T_{sat} - T_{wall})}$$

Therefore the condensation heat transfer coefficient can be obtained as follows:

$$h_{cond} = h \frac{T_{fluid} - T_{wall}}{T_{sat} - T_{wall}}$$

For pure steam or nearly pure steam mixtures $h \approx h_{cond}$. However if the gas contains a large amount of noncondensables, the gas temperature (T_{fluid}) may be significantly different from saturation temperature (T_{sat}). In such cases to obtain the true value of the condensation heat transfer coefficient the above formula must be used. For example, let's try to obtain the condensation heat transfer coefficient for SC-001 in the example shown above. The value of h is 7.59350×10^3 W/m²/K. (Note that if fins or spines are present then the "true" heat transfer coefficient must be used, and not the "effective" h.t.c. - see description of fin/spine data below). The fluid temperature is 3.89768×10^2 K. The wall surface temperature is 3.88156×10^2 K. The saturation temperature is found in the CV output as the "Sat. temp." for the "atms-gas" component. In the present example the saturation temperature is very close to the fluid temperature: $3.89811 \times 10^{+2}$ K. Therefore:

$$\begin{aligned} h_{cond} &= 7.59350 \times 10^{+3} \times (3.89768 \times 10^{+2} - 3.88156 \times 10^{+2}) / (3.89811 \times 10^{+2} - 3.88156 \times 10^{+2}) = \\ &= 7.47879 \times 10^{+3} \text{ W/m}^2/\text{K}. \end{aligned}$$

The third block contains convective and radiative boundary heat fluxes for the left and right surfaces. Convective heat fluxes are given again for the atmosphere, pool, and as the representative values. In case of radiative heat fluxes there is only atmosphere flux; the value of the representative flux is always equal to the atmosphere flux. Note that the radiative fluxes are non-zero not only in case when the thermal radiation model is active, but also in case when a user prescribed heat flux, defined by a Tabular or a Control Function, is used (input parameters IQRLSC, IQRRSC, sections 2.3.11, 2.3.12).

The fourth block contains fluid velocities at the left and right surfaces. Both atmosphere and pool velocities are given.

The fifth block contains fluid composition at the left and right surfaces. First the volume and mass fractions of the atmosphere gases are printed. The values are appropriate for the center point of this part of the surface, which is above the pool surface.

Next the volume and mass fractions of the droplets and bubbles are printed. The droplet fractions are appropriate for the center point of this part of the surface, which is above the pool surface. The bubble fractions are appropriate for the center point of this part of the surface, which is below the pool surface.

The next block contains condensation parameters, including film thickness, non-condensable degradation factor, condensation mass flux, and the enthalpy fluxes associated with the appearing water and the disappearing steam. This block is printed only if condensation occurs on either of the Conductor surfaces.

The next block contains boiling parameters, including boiling mass flux, and the enthalpy fluxes associated with the disappearing water and the appearing steam. This block is printed only if boiling occurs on either of the Conductor surfaces.

The next blocks contain extended surface data. Extended surface (fin/spine) data is printed only if fins/spines are present at the surface. If the surface is exposed to a single environment (i.e. either atmosphere or pool) then this printout consists of only a single block - left surface in the example case. If, on the other hand, the surface is partly covered by pool (as it is on the right surface), then two blocks are printed. The first block gives data for the part of the SC surface above the pool. The second block gives the data for the part below the pool surface.

The printout gives the following information:

- Fin/spine efficiency, defined as the ratio of heat transferred over the total fin/spine area to that which would be transferred if the fins/spines were isothermal (see [14], section 3.B.2.b, page 3-115). The efficiency is always smaller than one and it is close to 1.0 if the heat transfer coefficient is small.
- Fin/spine enhancement, defined as the ratio of average heat transferred through the wall surface (at the base of fins/spines) to that which would be transferred through the same surface if there were no fins/spines. Thus the enhancement is calculated as:

$$E = \frac{A_{base, no\ fin} + A_{fin} \eta}{A_{base}} = \left(\frac{A_{base, no\ fin}}{A_{base}} \right) + \left(\frac{A_{fin}}{A_{base, fin}} \right) \cdot \left(\frac{A_{base, fin}}{A_{base}} \right) \cdot \eta$$

where:

A_{base}	-	surface area at the fin/spine base (equal to the sum: $A_{base, no\ fin} + A_{base, fin}$), (m ²).
A_{fin}	-	area of heat/mass transfer of the fin/spine, (m ²).
η	-	efficiency of fin, (-).
$A_{base, no\ fin}$	-	this part of the surface area at the fin/spine base, which is not covered by fin/spine, (m ²), (Figure 3-1).
$A_{base, fin}$	-	this part of the surface area at the fin/spine base, which is covered by fin/spine, (m ²), (Figure 3-1).

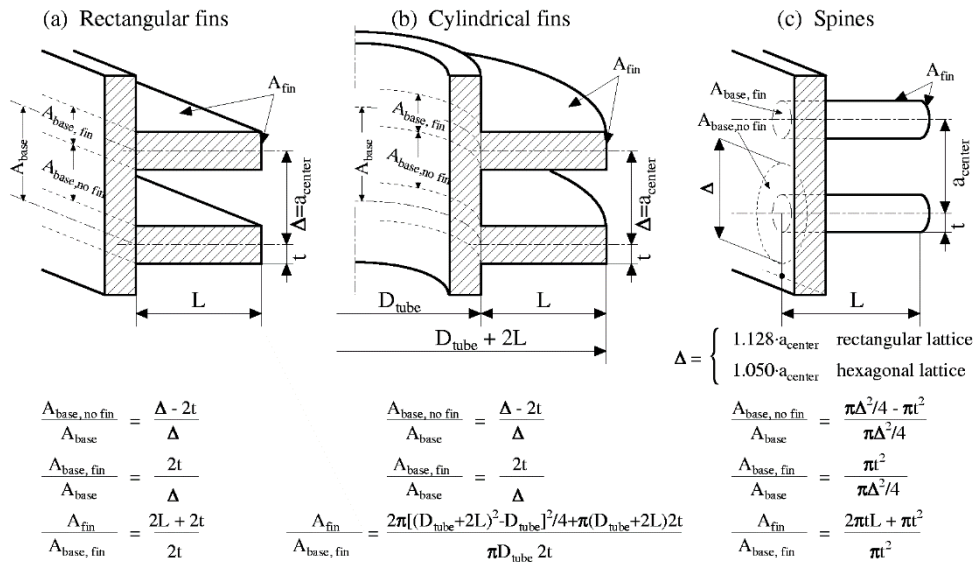


Figure 3-1 Fins and spines

- True and effective values of heat transfer coefficients, heat and mass fluxes. The true values are those calculated by the Heat Transfer Package, using appropriate correlation (convection, boiling, condensation). The effective values are obtained by multiplying the true values by the fin/spine enhancement factor, E. Note that the effective values are those, which are used as Solid Conductor boundary conditions by the 1-D Solid Conductor Package. Thus for example the values of heat transfer coefficient, printed in the second (Boundary Conditions) block are the same as the effective heat transfer coefficients printed in the fin/spine output.

At the bottom of the SC output the summed quantities (data summed for all 1-D Solid Conductors) are printed. An example printout is shown below.

```

=====
=SC= DATA SUMMED FOR ALL 1-D SOLID CONDUCTORS AT TIME : 0.00000E+00 (s)
=====

The heat fluxes and integrated heat fluxes printed below
are summed over those surfaces which transfer heat to
normal Control Volumes (those CVs for which conditions
are not held constant).

                Heat Flux      Integrated
                W              Heat Flux
                W              J
-----
Convective : -5.40977E+04   0.00000E+00
Radiative  : 0.00000E+00   0.00000E+00
Total      : -5.40977E+04   0.00000E+00
=====
    
```

This output gives heat fluxes (W), and integrated heat fluxes (J), summed over all 1-D Solid Conductors. Three values are given:

- Convective heat fluxes.

- Radiative heat fluxes.
- Total (convective + radiative) heat fluxes. Note that the total integrated heat flux (J) should be equal to the value of the total energy "Current - Initial - M&E sources", printed at the bottom of the CV output.

3.1.5 2-D Solid Heat Conductor Output

The 2-D Solid Heat Conductor outputs may be easily found in the output file by searching for the string: =TC=. The first TC printout brings the input data printout. An example of the input printout for a 2-D Solid Heat Conductor is shown below. The example consists of the structure shown in Figure 3-2.

The printout below mainly reflects the data entered in the input file and is quite self-explanatory.

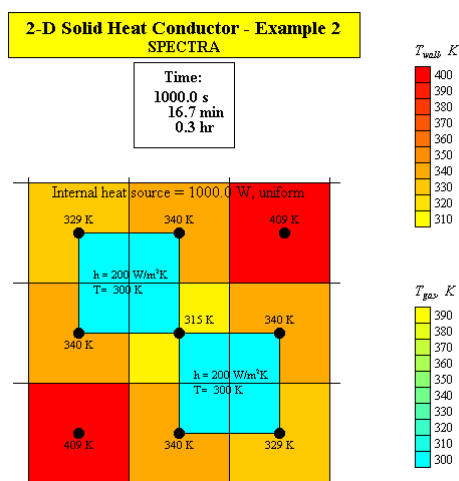


Figure 3-2 Example of a 2-D Solid Heat Conductor

```
=TC= =====TC-100=====  Steady_state_with_heat_sourc_-_rectangular,_2-D___

GEOMETRY TYPE      :  RECTANGULAR
CONDUCTOR SIZE     :  1.00000E+00
LEFT COORDINATE    :  0.00000E+00
ELEVATION (m)     :  0.00000E+00
VERTICAL ORIENT.  :  VERTICAL
POWER SOURCE       :  1.00000E+03
NO.OF CONDUCTORS  :  1.00000E+00
INITIAL TEMP.     :  INPUT VALUES
TRANSIENT TEMP.   :  CONDUCTION EQUATION

=TC=  TC-100,   X, Y MESH CELL SIZES OF THE 2-D SOLID HEAT CONDUCTOR

X-COORDINATE      :  3  MESH CELLS
Y-COORDINATE      :  3  MESH CELLS
```

SPECTRA Code Manuals - Volume 2: User's Guide

X-COORDINATE CELL DATA

Cell No. (K)	Cell half width (m)	Cell center X-coord. (m)
1	1.00000E-02	1.00000E-02
2	1.00000E-02	3.00000E-02
3	1.00000E-02	5.00000E-02

Y-COORDINATE CELL DATA

Cell No. (L)	Cell half width (m)	Cell center Y-coord. (m)
1	1.00000E-02	0.00000E+00
2	1.00000E-02	2.00000E-02
3	1.00000E-02	4.00000E-02

=TC= TC-100, CELL TYPE MAP OF THE 2-D SOLID HEAT CONDUCTOR

```

\K: 1 2 3
L\-----
1 |XX|XX|XX|
  |X |X|XX|
-----
2 |X |X|XX|
  |XX|X |X|
-----
3 |XX|X |X|
  |XX|XX|XX|
-----

```

=TC= TC-100, MATERIAL MAP OF THE 2-D SOLID HEAT CONDUCTOR

```

\ K: 1 2 3
L \ --- --- ---
1  001 001 001
2  001 001 001
3  001 001 001

```

=TC= TC-100, TOTAL NUMBER OF ACTIVE CELLS IS: 9

=TC= TC-100, CELL NUMBERING MAP

```

\ K: 1 2 3
L \ --- --- ---
1  001 002 003
2  004 005 006
3  007 008 009

```

=TC= TC-100, TOTAL NUMBER OF BOUNDARY CELLS IS: 7

=TC= TC-100, BOUNDARY CELL NUMBERING MAP

```

\ K: 1 2 3
L \ --- --- ---
1  001 002 000
2  003 004 005
3  000 006 007

```

=TC= TC-100, INVERSE CELL NUMBERING MAP

I = CONSECUTIVE CELL NO.
K = X COORDINATE CELL NO.
L = Y-COORDINATE CELL NO.

(I K L)	(I K L)	(I K L)	(I K L)	(I K L)
001 01 01	002 02 01	003 03 01	004 01 02	005 02 02
006 03 02	007 01 03	008 02 03	009 03 03	

=TC= TC-100, CELL DATA

TC-100, Cell No.: 1, K = 1, L = 1

```

-----
Volume of cell,      m3 : 3.00000E-04
Cell center X-coord. m : 1.00000E-02
Cell center Y-coord. m : 0.00000E+00

```

SPECTRA Code Manuals - Volume 2: User's Guide

Power fraction, - : 1.07143E-01
Input temperature, K : 3.00000E+02
BOUNDARY CELL No.: 1 -----
Heat transfer area, m2 : 2.00000E-02
Height of surface, m : 1.00000E-02
Bottom elevation, m : -1.00000E-02
Top elevation, m : 0.00000E+00
Control Volume No. : None
Tabular Heat Transfer C.: TF-001
Tabular Temperature : TF-002
Non-conv. Heat Flux : None

TC-100, Cell No.: 2, K = 2, L = 1

Volume of cell, m3 : 3.00000E-04
Cell center X-coord. m : 3.00000E-02
Cell center Y-coord. m : 0.00000E+00
Power fraction, - : 1.07143E-01
Input temperature, K : 3.00000E+02
BOUNDARY CELL No.: 2 -----
Heat transfer area, m2 : 2.00000E-02
Height of surface, m : 1.00000E-02
Bottom elevation, m : -1.00000E-02
Top elevation, m : 0.00000E+00
Control Volume No. : None
Tabular Heat Transfer C.: TF-001
Tabular Temperature : TF-002
Non-conv. Heat Flux : None

TC-100, Cell No.: 3, K = 3, L = 1

Volume of cell, m3 : 4.00000E-04
Cell center X-coord. m : 5.00000E-02
Cell center Y-coord. m : 0.00000E+00
Power fraction, - : 1.42857E-01
Input temperature, K : 3.00000E+02
Internal cell - no boundary conditions

TC-100, Cell No.: 4, K = 1, L = 2

Volume of cell, m3 : 3.00000E-04
Cell center X-coord. m : 1.00000E-02
Cell center Y-coord. m : 2.00000E-02
Power fraction, - : 1.07143E-01
Input temperature, K : 3.00000E+02
BOUNDARY CELL No.: 3 -----
Heat transfer area, m2 : 2.00000E-02
Height of surface, m : 1.00000E-02
Bottom elevation, m : -2.00000E-02
Top elevation, m : -1.00000E-02
Control Volume No. : None
Tabular Heat Transfer C.: TF-001
Tabular Temperature : TF-002
Non-conv. Heat Flux : None

TC-100, Cell No.: 5, K = 2, L = 2

Volume of cell, m3 : 2.00000E-04
Cell center X-coord. m : 3.00000E-02
Cell center Y-coord. m : 2.00000E-02
Power fraction, - : 7.14286E-02
Input temperature, K : 3.00000E+02
BOUNDARY CELL No.: 4 -----
Heat transfer area, m2 : 2.00000E-02
Height of surface, m : 0.00000E+00
Bottom elevation, m : 0.00000E+00
Top elevation, m : 0.00000E+00
Control Volume No. : None
Tabular Heat Transfer C.: TF-001
Tabular Temperature : TF-002
Non-conv. Heat Flux : None

SPECTRA Code Manuals - Volume 2: User's Guide

TC-100, Cell No.: 6, K = 3, L = 2

Volume of cell, m3 : 3.00000E-04
Cell center X-coord. m : 5.00000E-02
Cell center Y-coord. m : 2.00000E-02
Power fraction, - : 1.07143E-01
Input temperature, K : 3.00000E+02
BOUNDARY CELL No.: 5 -----
Heat transfer area, m2 : 2.00000E-02
Height of surface, m : 1.00000E-02
Bottom elevation, m : -3.00000E-02
Top elevation, m : -2.00000E-02
Control Volume No. : None
Tabular Heat Transfer C.: TF-001
Tabular Temperature : TF-002
Non-conv. Heat Flux : None

TC-100, Cell No.: 7, K = 1, L = 3

Volume of cell, m3 : 4.00000E-04
Cell center X-coord. m : 1.00000E-02
Cell center Y-coord. m : 4.00000E-02
Power fraction, - : 1.42857E-01
Input temperature, K : 3.00000E+02
Internal cell - no boundary conditions

TC-100, Cell No.: 8, K = 2, L = 3

Volume of cell, m3 : 3.00000E-04
Cell center X-coord. m : 3.00000E-02
Cell center Y-coord. m : 4.00000E-02
Power fraction, - : 1.07143E-01
Input temperature, K : 3.00000E+02
BOUNDARY CELL No.: 6 -----
Heat transfer area, m2 : 2.00000E-02
Height of surface, m : 1.00000E-02
Bottom elevation, m : -4.00000E-02
Top elevation, m : -3.00000E-02
Control Volume No. : None
Tabular Heat Transfer C.: TF-001
Tabular Temperature : TF-002
Non-conv. Heat Flux : None

TC-100, Cell No.: 9, K = 3, L = 3

Volume of cell, m3 : 3.00000E-04
Cell center X-coord. m : 5.00000E-02
Cell center Y-coord. m : 4.00000E-02
Power fraction, - : 1.07143E-01
Input temperature, K : 3.00000E+02
BOUNDARY CELL No.: 7 -----
Heat transfer area, m2 : 2.00000E-02
Height of surface, m : 1.00000E-02
Bottom elevation, m : -4.00000E-02
Top elevation, m : -3.00000E-02
Control Volume No. : None
Tabular Heat Transfer C.: TF-001
Tabular Temperature : TF-002
Non-conv. Heat Flux : None

At the bottom of the 2-D Solid Conductor data printout, the data valid for all 2-D heat conductors is printed. Next the TC reference data is printed for all Control Volumes, which are used as boundary conditions for TC (not present in the current example because no CV were used). Finally, the internal numbering scheme is printed.

=TC= ALL 2-D SOLID HEAT CONDUCTORS -----

SPECTRA Code Manuals - Volume 2: User's Guide

```

CHF AND MINIMUM FILM BOILING PARAMETERS:
- MINIMUM VALUE OF T(CHF)-T(MFB) : TFMNTC = 5.00000E+00
- MAXIMUM VALUE OF T(CHF)-T(MFB) : TFMXTC = 1.00000E+03
- MAXIMUM VALUE OF SLIP FOR CHF : SMAXTC = 1.00000E+02

=====
=TC= 2-D SOLID HEAT CONDUCTOR INTERNAL NUMBERING SCHEME
=====

Int.  Ref.
No.   No.
---  -
1    TC-100

=====
=TC= END OF 2-D SOLID HEAT CONDUCTOR DATA
=====

```

An example of the transient printout for a Solid Conductor is shown below. The output consists of the node temperature printout, followed by the printouts for all boundary cells. The printout for the boundary cells is very similar to the printout of left and right surface for 1-D heat conductors.

```

=TC= =====TC-100=====  Steady_state_with_heat_sourc_-_rectangular,_2-D___

=TC= TC-100,  NODE TEMPERATURES AT TIME : 1.00000E+03 (s)
\ K:  1      2      3
L \  -----
1   329.  340.  409.
2   340.  315.  340.
3   409.  340.  329.

=TC= TC-100,  BOUNDARY CONDITIONS AT TIME : 1.00000E+03 (s)

BOUNDARY DATA AT TIME : 1.00000E+03 (s)
-----
TC-100,  Boundary Cell: IBC = 1,  Cell: I = 1 (K,L) = (01,01)
-----

Temperatures and heat transfer coefficients at the boundary surface
Vol      H.T.Area      Twall      Tfluid      h      H.T.
-----  Fractions      (K)        (K)         (W/m2/K)  Mode
-----
000 atms  0.00000E+00  3.29330E+02  0.00000E+00  0.00000E+00
pool    0.00000E+00  3.29330E+02  0.00000E+00  0.00000E+00
repr    1.00000E+00  3.29330E+02  3.00000E+02  2.00000E+02  TAB-F.

Heat fluxes at the boundary surface
Vol      q(conv)      Q(conv)      q(rad)      Q(rad)
-----  (W/m2)      (W)          (W/m2)      (W)
-----
000 atms  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
pool    0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
repr    5.86603E+03  1.17321E+02  0.00000E+00  0.00000E+00

Fluid velocities at the boundary surface
Vol comp      v
-----  (m/s)
-----
000 atms  0.00000E+00
000 pool  0.00000E+00
000 bubb  0.00000E+00

Gas composition at the boundary surface
Gas Gas      MASS      VOLUME
No. Id.      FRACTION  FRACTION
-----

```


SPECTRA Code Manuals - Volume 2: User's Guide

```

-----
atms droplets 0.00000E+00 0.00000E+00
pool bubbles 0.00000E+00 0.00000E+00

```

BOUNDARY DATA AT TIME : 1.00000E+03 (s)

TC-100, Boundary Cell: IBC = 2, Cell: I = 2 (K,L) = (02,01)

Temperatures and heat transfer coefficients at the boundary surface

Vol	H.T.Area Fractions	Twall (K)	Tfluid (K)	h (W/m2/K)	H.T. Mode
000 atms	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00	
pool	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00	
repr	1.00000E+00	3.39665E+02	3.00000E+02	2.00000E+02	TAB-F.

Heat fluxes at the boundary surface

Vol	q(conv) (W/m2)	Q(conv) (W)	q(rad) (W/m2)	Q(rad) (W)
000 atms	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
pool	0.00000E+00	0.00000E+00		
repr	7.93303E+03	1.58661E+02	0.00000E+00	0.00000E+00

Fluid velocities at the boundary surface

Vol comp	v (m/s)
000 atms	0.00000E+00
000 pool	0.00000E+00
000 bubb	0.00000E+00

Gas composition at the boundary surface

Gas No.	Gas Id.	MASS FRACTION	VOLUME FRACTION
atms droplets		0.00000E+00	0.00000E+00
pool bubbles		0.00000E+00	0.00000E+00

BOUNDARY DATA AT TIME : 1.00000E+03 (s)

TC-100, Boundary Cell: IBC = 3, Cell: I = 4 (K,L) = (01,02)

Temperatures and heat transfer coefficients at the boundary surface

Vol	H.T.Area Fractions	Twall (K)	Tfluid (K)	h (W/m2/K)	H.T. Mode
000 atms	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00	
pool	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00	
repr	1.00000E+00	3.39665E+02	3.00000E+02	2.00000E+02	TAB-F.

Heat fluxes at the boundary surface

Vol	q(conv) (W/m2)	Q(conv) (W)	q(rad) (W/m2)	Q(rad) (W)
000 atms	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
pool	0.00000E+00	0.00000E+00		
repr	7.93303E+03	1.58661E+02	0.00000E+00	0.00000E+00

Fluid velocities at the boundary surface

Vol comp	v (m/s)
000 atms	0.00000E+00
000 pool	0.00000E+00
000 bubb	0.00000E+00

Gas composition at the boundary surface

Gas No.	Gas Id.	MASS FRACTION	VOLUME FRACTION
atms droplets		0.00000E+00	0.00000E+00
pool bubbles		0.00000E+00	0.00000E+00

SPECTRA Code Manuals - Volume 2: User's Guide

No.	Id.	FRACTION	FRACTION
atms	droplets	0.00000E+00	0.00000E+00
pool	bubbles	0.00000E+00	0.00000E+00

BOUNDARY DATA AT TIME : 1.00000E+03 (s)

TC-100, Boundary Cell: IBC = 4, Cell: I = 5 (K,L) = (02,02)

Temperatures and heat transfer coefficients at the boundary surface

Vol	H.T.Area Fractions	Twall (K)	Tfluid (K)	h (W/m2/K)	H.T. Mode
000	atms	0.00000E+00	3.15067E+02	0.00000E+00	0.00000E+00
	pool	0.00000E+00	3.15067E+02	0.00000E+00	0.00000E+00
	repr	1.00000E+00	3.15067E+02	3.00000E+02	2.00000E+02 TAB-F.

Heat fluxes at the boundary surface

Vol	q(conv) (W/m2)	Q(conv) (W)	q(rad) (W/m2)	Q(rad) (W)
000	atms	0.00000E+00	0.00000E+00	0.00000E+00
	pool	0.00000E+00	0.00000E+00	0.00000E+00
	repr	3.01344E+03	6.02687E+01	0.00000E+00

Fluid velocities at the boundary surface

Vol comp	v (m/s)	
000	atms	0.00000E+00
000	pool	0.00000E+00
000	bubb	0.00000E+00

Gas composition at the boundary surface

Gas No.	Gas Id.	MASS FRACTION	VOLUME FRACTION
atms	droplets	0.00000E+00	0.00000E+00
pool	bubbles	0.00000E+00	0.00000E+00

BOUNDARY DATA AT TIME : 1.00000E+03 (s)

TC-100, Boundary Cell: IBC = 5, Cell: I = 6 (K,L) = (03,02)

Temperatures and heat transfer coefficients at the boundary surface

Vol	H.T.Area Fractions	Twall (K)	Tfluid (K)	h (W/m2/K)	H.T. Mode
000	atms	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00
	pool	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00
	repr	1.00000E+00	3.39665E+02	3.00000E+02	2.00000E+02 TAB-F.

Heat fluxes at the boundary surface

Vol	q(conv) (W/m2)	Q(conv) (W)	q(rad) (W/m2)	Q(rad) (W)
000	atms	0.00000E+00	0.00000E+00	0.00000E+00
	pool	0.00000E+00	0.00000E+00	0.00000E+00
	repr	7.93303E+03	1.58661E+02	0.00000E+00

Fluid velocities at the boundary surface

Vol comp	v (m/s)	
000	atms	0.00000E+00
000	pool	0.00000E+00
000	bubb	0.00000E+00

SPECTRA Code Manuals - Volume 2: User's Guide

Gas composition at the boundary surface

Gas No.	Gas Id.	MASS FRACTION	VOLUME FRACTION
atms	droplets	0.00000E+00	0.00000E+00
pool	bubbles	0.00000E+00	0.00000E+00

BOUNDARY DATA AT TIME : 1.00000E+03 (s)

TC-100, Boundary Cell: IBC = 6, Cell: I = 8 (K,L) = (02,03)

Temperatures and heat transfer coefficients at the boundary surface

Vol	H.T. Area Fractions	Twall (K)	Tfluid (K)	h (W/m2/K)	H.T. Mode
000	atms	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00
	pool	0.00000E+00	3.39665E+02	0.00000E+00	0.00000E+00
	repr	1.00000E+00	3.39665E+02	3.00000E+02	2.00000E+02 TAB-F.

Heat fluxes at the boundary surface

Vol	q(conv) (W/m2)	Q(conv) (W)	q(rad) (W/m2)	Q(rad) (W)
000	atms	0.00000E+00	0.00000E+00	0.00000E+00
	pool	0.00000E+00	0.00000E+00	0.00000E+00
	repr	7.93303E+03	1.58661E+02	0.00000E+00

Fluid velocities at the boundary surface

Vol comp	v (m/s)	
000	atms	0.00000E+00
000	pool	0.00000E+00
000	bubb	0.00000E+00

Gas composition at the boundary surface

Gas No.	Gas Id.	MASS FRACTION	VOLUME FRACTION
atms	droplets	0.00000E+00	0.00000E+00
pool	bubbles	0.00000E+00	0.00000E+00

BOUNDARY DATA AT TIME : 1.00000E+03 (s)

TC-100, Boundary Cell: IBC = 7, Cell: I = 9 (K,L) = (03,03)

Temperatures and heat transfer coefficients at the boundary surface

Vol	H.T. Area Fractions	Twall (K)	Tfluid (K)	h (W/m2/K)	H.T. Mode
000	atms	0.00000E+00	3.29330E+02	0.00000E+00	0.00000E+00
	pool	0.00000E+00	3.29330E+02	0.00000E+00	0.00000E+00
	repr	1.00000E+00	3.29330E+02	3.00000E+02	2.00000E+02 TAB-F.

Heat fluxes at the boundary surface

Vol	q(conv) (W/m2)	Q(conv) (W)	q(rad) (W/m2)	Q(rad) (W)
000	atms	0.00000E+00	0.00000E+00	0.00000E+00
	pool	0.00000E+00	0.00000E+00	0.00000E+00
	repr	5.86603E+03	1.17321E+02	0.00000E+00

Fluid velocities at the boundary surface

Vol comp	v (m/s)	
000	atms	0.00000E+00
000	pool	0.00000E+00

SPECTRA Code Manuals - Volume 2: User's Guide

```
000 bubb 0.00000E+00

Gas composition at the boundary surface
      Gas Gas      MASS      VOLUME
      No. Id.  FRACTION  FRACTION
-----
atms droplets 0.00000E+00 0.00000E+00
pool bubbles 0.00000E+00 0.00000E+00
```

At the bottom of the TC output the summed quantities (data summed for all 2-D Solid Conductors) are printed. An example printout is shown below.

```
=====
=TC=  DATA SUMMED FOR ALL 2-D SOLID CONDUCTORS AT TIME : 1.00000E+03 (s)
=====

The heat fluxes and integrated heat fluxes printed below
are summed over those surfaces which transfer heat to
normal Control Volumes (those CVs for which conditions
are not held constant).

      Heat Flux      Integrated
      W              J
-----
Convective : 0.00000E+00 0.00000E+00
Radiative  : 0.00000E+00 0.00000E+00
Total      : 0.00000E+00 0.00000E+00
=====
```

3.1.6 Thermal Radiation Output

The Thermal Radiation outputs may be easily found in the output file by searching for the string: **=TR=**. The first TR printout brings the input data printout. An example of the thermal radiation input printout is shown below.

```
=====
=TR=  INPUT DATA FOR 1 RADIATING SYSTEMS
=====

=TR=  SYSTEM No.: 1      Example_problem_-_thermal_radiation_____
=TR=  MODEL:  Grey Enclosure with Participating Gas
=TR=  INPUT DATA FOR 4 RADIATING SURFACES

i      TR      SC/TC      Emissivity      Pool option
---
1  TR-101  SC-001 Left  TF-007          No
2  TR-102  SC-002 Right TF-007          No
3  TR-103  SC-003 Right TF-007          No
4  TR-104  SC-004 Right TF-007          Yes

=TR=  View Factors, (-), F (i->j)
\ j      1      2      3      4
```

SPECTRA Code Manuals - Volume 2: User's Guide

```

i \ -----
1  1.171565E-01  9.248080E-02  3.951813E-01  3.951813E-01
2  2.774424E-01  0.000000E+00  3.612788E-01  3.612788E-01
3  2.963860E-01  9.031970E-02  0.000000E+00  6.132943E-01
4  2.963860E-01  9.031970E-02  6.132943E-01  0.000000E+00

```

```

I  Sum { F(i->j) j=1..N }
1  1.000000E+00
2  1.000000E+00
3  1.000000E+00
4  1.000000E+00

```

```

=TR= Beam Lengths, (m), L (i->j)
\ j      1      2      3      4
i \ -----|CV  -----|CV  -----|CV  -----|CV
1  1.98E+01|001  1.30E+01|Seq  7.30E+00|001  7.30E+00|001
2  1.30E+01|Seq  0.00E+00|000  7.30E+00|Seq  7.30E+00|Seq
3  7.30E+00|001  7.30E+00|Seq  0.00E+00|000  6.50E+00|001
4  7.30E+00|001  7.30E+00|Seq  6.50E+00|001  0.00E+00|000

```

=TR= Radiation Beams Passing Through Multiple CV-s:

```

Beam      : TR-101 -> TR-102
CV-s on the Beam: CV-001  CV-002
Beam Lengths : 6.50E+00  6.50E+00

```

```

Beam      : TR-102 -> TR-101
CV-s on the Beam: CV-001  CV-002
Beam Lengths : 6.50E+00  6.50E+00

```

```

Beam      : TR-102 -> TR-103
CV-s on the Beam: CV-002  CV-001
Beam Lengths : 3.65E+00  3.65E+00

```

```

Beam      : TR-102 -> TR-104
CV-s on the Beam: CV-002  CV-001
Beam Lengths : 3.65E+00  3.65E+00

```

```

Beam      : TR-103 -> TR-102
CV-s on the Beam: CV-002  CV-001
Beam Lengths : 3.65E+00  3.65E+00

```

```

Beam      : TR-104 -> TR-102
CV-s on the Beam: CV-002  CV-001
Beam Lengths : 3.65E+00  3.65E+00

```

```

=====
=TR= RADIATION PROPERTIES OF 6 GASES
=====

```

=TR= EMISSIVITY

```

Gas  Emissivity Correlation
---  -----
1  No absorption/emission
2  No absorption/emission
3  Kostowski Correlation for H2O
4  No absorption/emission
5  No absorption/emission
6  Kostowski Correlation for CO2

```

=TR= ABSORPTIVITY

```

Gas  Absorptivity Correlation
---  -----
1  No absorption/emission
2  No absorption/emission
3  A = E ( Tw, pL(Tw/Tg) ) ( Tg/Tw )** 4.500E-01
4  No absorption/emission
5  No absorption/emission
6  A = E ( Tw, pL(Tw/Tg) ) ( Tg/Tw )** 6.500E-01

```

SPECTRA Code Manuals - Volume 2: User's Guide

```

=====
=TR=  RADIATING SURFACE INTERNAL NUMBERING SCHEME
=====

=TR=  RADIATING SYSTEM No.:  1           Example_problem_-_thermal_radiation_____

      Int. Ref.   Int. Ref.   Int. Ref.   Int. Ref.
      No.  No.    No.  No.    No.  No.    No.  No.
      ---  ---    ---  ---    ---  ---    ---  ---
      1  TR-101   2  TR-102   3  TR-103   4  TR-104

=====
=TR=  END OF THERMAL RADIATION DATA
=====

```

The radiation model applied is printed at the top of this printout. Then the following blocks are printed:

The first block contains associations of radiating surfaces with the Solid Conductor surfaces (left or right). It also prints the indication of how the surface emissivity is defined, and whether the pool option is used.

The second block contains all view factors, $F_{i \rightarrow j}$, and the sums:

$$S_i = \sum_j F_{j \rightarrow i}$$

All values of S_i must be equal to one; otherwise an input error is signaled.

The following blocks are printed only if the radiation model with participating gas is chosen. The first block contains all mean beam lengths, $L_{i \rightarrow j}$. Also the Control Volumes, through which the beam passes, are given. If the beam passes through a sequence of several Control Volumes, then the letters "Seq" are printed instead of the volume number. In such case the beams passing multiple Control Volumes are listed next, including the lengths the beam passes in each Control Volume.

The next part of the printout contains enclosure data. This data is printed only to give the user a qualitative verification of his beam length data. This block is printed only if there are no beams passing through multiple Control Volumes (only then the logic identifying enclosures is used). Since in the example case above beams pass multiple Control Volumes, the enclosure data printout is not included there. A printout from another example is included below.

```

=TR=  Enclosure(s) description

=TR=  Enclosure  Fluid  Radiating  Pool
      No.       Volume Surfaces   option
      -----  -----  -
      01       CV-001
                TR-101    No
                TR-102    No
                TR-103    No
                TR-104    Yes

=TR=  AVERAGED OVER ENCLOSURES VALUES OF GEOMETRIC MEAN BEAM LENGTHS
      Enclosure average beam l.= average L(i->j), weighted by: A(i)*F(i->j)
      Engineering beam length = 4*V/A           V - gas volume of enclosure
                                           A - total surface area

      Enclosure  Fluid  Average  Engineering
      No.       Volume Beam L. (m) Beam L. (m)
      -----  -----  -

```

SPECTRA Code Manuals - Volume 2: User's Guide

01 CV-001 7.60 6.67

For each identified enclosure an average value of mean beam length is calculated, from the formula:

$$L_{ave} = \frac{\sum_{i=1}^N \sum_{j=1}^N A_i F_{i \rightarrow j} L_{i \rightarrow j}}{\sum_{i=1}^N \sum_{j=1}^N A_i F_{i \rightarrow j}}$$

where: A_i - area of surface i, (m²),
 $F_{i \rightarrow j}$ - view factor between surface i and j, (-),
 $L_{i \rightarrow j}$ - mean beam length between surface i and j, (m),
 N - number of radiating surfaces in given enclosure.

The average value is compared with an "engineering estimation" of mean beam length in an enclosure, which is ([14] page 15-65):

$$L_{ave} = \frac{4V}{A}$$

where: V - total volume of the enclosure, (m³), (equal to the volume above the pool for the Control Volume associated with the enclosure),
 A - total surface area of the enclosure, (m²), (equal to the sum of surface areas of all radiating surfaces associated with the enclosure, ΣA_i).

An example of the Thermal Radiation transient printout is shown below.

```

=====
=TR=  OUTPUT DATA FOR   1  RADIATING SYSTEMS AT TIME: 1.00000E+03
=====

=TR=  SYSTEM No.:   1           Example_problem_-_thermal_radiation_____

=TR=  Surface data
Surface      SC              T              Emis.              q              Q
-----      -              -              -              -              -
              (K)              (-)              (W/m2)              (W)
TR-101      SC-001 Left      3.58045E+02      9.50000E-01      -4.89554E+00      -2.30697E+03
TR-102      SC-002 Right     3.58096E+02      9.50000E-01      -1.24244E+01      -1.95161E+03
TR-103      SC-003 Right     3.58046E+02      9.50000E-01      -4.66802E+00      -2.93300E+03
TR-104      SC-004 Right     3.57988E+02      9.60000E-01      -5.43003E+00      -3.41179E+03

=TR=  Gas Emissivity,  (CV)
\ j          1          2          3          4
i \  -----|CV  -----|CV  -----|CV  -----|CV
1   7.30E-01|001  9.08E-01|Seq  7.11E-01|001  7.11E-01|001
2   9.08E-01|Seq  0.00E+00|000  8.57E-01|Seq  8.57E-01|Seq
3   7.11E-01|001  8.57E-01|Seq  0.00E+00|000  6.96E-01|001
4   7.11E-01|001  8.57E-01|Seq  6.96E-01|001  0.00E+00|000

=TR=  Gas Absorptivity,  (CV)
\ j          1          2          3          4
i \  -----|CV  -----|CV  -----|CV  -----|CV
1   7.30E-01|001  9.08E-01|Seq  7.11E-01|001  7.11E-01|001
2   9.08E-01|Seq  0.00E+00|000  8.58E-01|Seq  8.58E-01|Seq
3   7.11E-01|001  8.58E-01|Seq  0.00E+00|000  6.96E-01|001
4   7.11E-01|001  8.58E-01|Seq  6.96E-01|001  0.00E+00|000

=TR=  Gas Temperature,  (CV)
\ j          1          2          3          4

```

SPECTRA Code Manuals - Volume 2: User's Guide

```

i \ -----|CV -----|CV -----|CV -----|CV
1  3.59E+02|001  3.60E+02|Seq  3.59E+02|001  3.59E+02|001
2  3.60E+02|Seq  0.00E+00|000  3.60E+02|Seq  3.60E+02|Seq
3  3.59E+02|001  3.60E+02|Seq  0.00E+00|000  3.59E+02|001
4  3.59E+02|001  3.60E+02|Seq  3.59E+02|001  0.00E+00|000

```

```

=TR= Gas Heat Absorp., (CV)
\ j      1      2      3      4
i \ -----|CV -----|CV -----|CV -----|CV
1  -2.39E+02|001 -6.11E+02|Seq -7.47E+02|001 -7.47E+02|001
2  -5.75E+02|Seq  0.00E+00|000 -7.03E+02|Seq -7.03E+02|Seq
3  -7.48E+02|001 -7.47E+02|Seq  0.00E+00|000 -1.52E+03|001
4  -8.23E+02|001 -7.76E+02|Seq -1.67E+03|001  0.00E+00|000

```

=TR= Data for Radiation Beams Passing Through Multiple CV-s:

```

Beam      : TR-101 -> TR-102
CV-s on the Beam: CV-001 CV-002
Gas Emissivity : 6.96E-01 6.96E-01
Gas Absorptivity: 6.96E-01 6.98E-01
Gas Temperature : 3.59E+02 3.61E+02

```

```

Beam      : TR-102 -> TR-101
CV-s on the Beam: CV-001 CV-002
Gas Emissivity : 6.96E-01 6.96E-01
Gas Absorptivity: 6.96E-01 6.98E-01
Gas Temperature : 3.59E+02 3.61E+02

```

```

Beam      : TR-102 -> TR-103
CV-s on the Beam: CV-002 CV-001
Gas Emissivity : 6.22E-01 6.22E-01
Gas Absorptivity: 6.23E-01 6.22E-01
Gas Temperature : 3.61E+02 3.59E+02

```

```

Beam      : TR-102 -> TR-104
CV-s on the Beam: CV-002 CV-001
Gas Emissivity : 6.22E-01 6.22E-01
Gas Absorptivity: 6.23E-01 6.22E-01
Gas Temperature : 3.61E+02 3.59E+02

```

```

Beam      : TR-103 -> TR-102
CV-s on the Beam: CV-002 CV-001
Gas Emissivity : 6.22E-01 6.22E-01
Gas Absorptivity: 6.23E-01 6.22E-01
Gas Temperature : 3.61E+02 3.59E+02

```

```

Beam      : TR-104 -> TR-102
CV-s on the Beam: CV-002 CV-001
Gas Emissivity : 6.22E-01 6.22E-01
Gas Absorptivity: 6.23E-01 6.22E-01
Gas Temperature : 3.61E+02 3.59E+02

```

=====

The thermal radiation transient printout consists of the following blocks.

The first block contains printout of the surface data, including temperature, emissivity, heat flux, as well as heat power emitted from all radiating surfaces. If the radiation model with non-absorbing/non-emitting gas is chosen, then this is the only printout from the thermal radiation model.

The next blocks are printed if the radiation model with participating gas is chosen. The first block here contains the gas emissivities for all radiation paths. It also gives the number of a Control Volume, if the beam passes through a single Control Volume, or the letters "Seq", if the beam passes through

several Control Volumes. If the beam passes through single Control Volume, then this is the emissivity calculated for the gas composition and temperature in this CV:

$$\varepsilon_{i \rightarrow j} = f(pL_{i \rightarrow j})$$

where $(pL_{i \rightarrow j})$ is the optical length in the CV. If the beam passes through multiple Control Volumes, then the average emissivity is obtained from:

$$\varepsilon_{i \rightarrow j} = 1 - \prod_m (1 - \varepsilon_m)$$

where ε_m is the individual emissivity in the m -th CV, where the beam optical length is pL_m , $\varepsilon_m = \varepsilon_m(pL_m)$. The multiplication is performed over all Control Volumes on the beam length. The total beam length between surfaces i and j must of course be equal to the sum of individual lengths, so the following relation is always true (if not, this is flagged as an input error):

$$L_{i \rightarrow j} = \sum_m L_m$$

The symbols ε_m , L_m should be, strictly speaking, $\varepsilon_{m, i \rightarrow j}$, $L_{m, i \rightarrow j}$, but for the sake of clarity the indexes i , j were skipped.

The next block contains the gas absorptivities for all radiation paths. It also gives the number of a Control Volume, if the beam passes a single Control Volume, or the letters "Seq", if the beam passes several Control Volumes. The average absorptivity of the beam passing through multiple Control Volumes is calculated, similarly as in case of emissivity, from:

$$a_{i \rightarrow j} = 1 - \prod_m (1 - a_m)$$

This means, the overall transmittance is equal to the product of individual transmittances. Again, individual absorptivities a_m depend on the individual optical lengths, pL_m , $a_m = a_m(pL_m)$.

Next the gas temperatures are printed. If the beam passes a single Control Volume, then the value printed here is of course identical to the CV atmosphere temperature. For example, the printout for $i=1, j=1$: **3.59E+02 | 001**, means the gas temperature is 359 K and it is equal to the atmosphere temperature in CV-001. If the beam passes several Control Volumes, then this is the averaged temperature. For example, the printout for $i=1, j=2$: **3.60E+02 | Seq**, means the gas average temperature is 360 K, and it is averaged over the full sequence of Control Volumes through which the beam passes. The temperature averaging is performed as follows:

$$T_{i \rightarrow j} = \left(\frac{\sum_m (\varepsilon_m \cdot T_m^4)}{\sum_m \varepsilon_m} \right)^{1/4}$$

where L_m is the beam length in the m -th CV and the summation is performed over all Control Volumes on the beam length.

Finally the heat absorbed (emitted) by the gas is printed. If the beam passes a single Control Volume, then the absorbed (emitted) heat (calculated by the Thermal Radiation Package) is of course deposited in (removed from) this Control Volume. If the beam passes several Control Volumes, then the net heat transfer to gas, obtained from the Thermal Radiation Package, is partitioned among all Control Volumes using the following formula.

$$Q_m = Q_{i \rightarrow j} \cdot \left(\frac{\varepsilon_m}{\sum_m \varepsilon_m} \right) - A_i F_{i \rightarrow j} \sigma \varepsilon_m (T_m^4 - T_{i \rightarrow j}^4)$$

Where $Q_{i \rightarrow j}$ is the total heat exchanged with gas on the radiation beam $i \rightarrow j$. Again the subscript m should be, strictly speaking, replaced by $m, i \rightarrow j$, since all values are those for the radiation beam from the surface i to the surface j . The extra subscripts were skipped for clarity. Note that the above formulation fulfils the following important relations.

- If the gas emissivity in given CV is zero, then the part of total heat assigned to that volume is zero:

$$Q_m = 0.0 \quad \text{if} \quad \varepsilon_m = 0.0$$

This can easily be proved by substituting zero for ε_m in the above formula.

- The sum of all heats is equal to the total heat:

$$\sum_m Q_m = Q_{i \rightarrow j}$$

This can be proved by performing the summation and substituting the formula for the average temperature, $T_{i \rightarrow j}$:

$$\begin{aligned} \sum_m Q_m &= Q_{i \rightarrow j} \cdot \left(\frac{\sum_m \varepsilon_m}{\sum_m \varepsilon_m} \right) - A_i F_{i \rightarrow j} \sigma \sum_m \varepsilon_m (T_m^4 - T_{i \rightarrow j}^4) = \\ &= Q_{i \rightarrow j} - A_i F_{i \rightarrow j} \sigma \left(\sum_m \varepsilon_m T_m^4 - T_{i \rightarrow j}^4 \sum_m \varepsilon_m \right) = \\ &= Q_{i \rightarrow j} - A_i F_{i \rightarrow j} \sigma \left(\sum_m \varepsilon_m T_m^4 - \frac{\sum_m \varepsilon_m T_m^4}{\sum_m \varepsilon_m} \sum_m \varepsilon_m \right) = \\ &= Q_{i \rightarrow j} - A_i F_{i \rightarrow j} \sigma \left(\sum_m \varepsilon_m T_m^4 - \sum_m \varepsilon_m T_m^4 \right) = \\ &= Q_{i \rightarrow j} \end{aligned}$$

3.1.7 Tabular Function Output

The Tabular Function outputs may be easily found in the output file by searching for the string: =TF=. The first TF printout brings the input data printout. An example of a Tabular Function input printout is shown below.

```
=TF= =====TF-001===== Example_1_of_Tabular_Function_____
1.) TABULAR FUNCTION DEFINITION AND LIMITS:

Addit.const. Multiplier Interpolation
-----
0.00000E+00 1.00000E+00 Linear (1-st order)

Limits Minimum Maximum
-----
TF(t) -1.00000E+99 1.00000E+99
dTF(t)/dt -1.00000E+99 1.00000E+99
MESSAGE TF(t) -1.00000E+99 1.00000E+99
MESSAGE dTF(t)/dt -1.00000E+99 1.00000E+99

2.) INTERACTIVE TABULAR FUNCTION

At any time of calculations the TF value may be modified in the *.TFD file

If there is no data in the file, then the tabulated points are used.

Reset option not used. To get back to tabulated points,
the TF definition must be removed from *.TFD file
manually or by an external program

3.) TF DATA VALUES

TOTAL NUMBER OF DATA POINTS: 7

N X Y
---
1 5.00000E+00 1.00000E-01
2 1.00000E+01 1.10000E+00
3 1.50000E+01 1.10000E+00
4 2.50000E+01 2.00000E-01
5 3.00000E+01 2.50000E+00
6 3.50000E+01 1.00000E+00
7 4.50000E+01 1.00000E+00
---
```

At the bottom of the TF data the internal numbering scheme is printed:

```
=====
=TF= TABULAR FUNCTION INTERNAL NUMBERING SCHEME
=====

Int. Ref. Int. Ref.
No. No. No. No.
---
1 TF-001 2 TF-002

=====
=TF= END OF TABULAR FUNCTION DATA
=====
```

An example of the Tabular Function transient printout is shown below.

```
=====
=TF= OUTPUT DATA FOR 2 TABULAR FUNCTIONS, AT TIME : 5.00000E+01 (s)
=====

Function Value Name
```

SPECTRA Code Manuals - Volume 2: User's Guide

```
TF-001  1.00000E+00  Example_1_of_Tabular_Function_____
TF-002  3.00000E+00  Example_2_of_Tabular_Function_____
```

3.1.8 Control Function Output

The Control Function outputs may be easily found in the output file by searching for the string: =CF=. The first CF printout brings the input data printout. An example of a Control Function input printout is shown below.

```
=CF= =====CF-100===== 2-D General Tabular Function

A.) CONTROL FUNCTION DEFINITION AND LIMITS:

CF TYPE      : TABULAR FUNCTION
Initial value : to be calculated

Addit.const. Multiplier  CF Type
-----
0.00000E+00  1.00000E+00  TABULAR FUNCTION

Limits      Minimum      Maximum
-----
CF(t)       -1.00000E+99  1.00000E+99
dCF(t)/dt   -1.00000E+99  1.00000E+99
MESSAGE CF(t)       -1.00000E+99  1.00000E+99
MESSAGE dCF(t)/dt   -1.00000E+99  1.00000E+99

B.) CF ARGUMENTS DESCRIPTION:

No.  Addit.const.  Multiplier  Variable  Comment
---  -
1.   0.00000E+00  1.00000E+00  JN-500-PVf1-pool-m3/s  X (1-ST INDEPENDENT VAR.)
2.   0.00000E+00  1.00000E+00  TF-101-Valu-0000-      TF VALUE FOR THE ARGUMENT X
3.   0.00000E+00  1.00000E+00  TF-102-Valu-0000-      TF VALUE FOR THE ARGUMENT X
4.   0.00000E+00  1.00000E+00  TF-103-Valu-0000-      TF VALUE FOR THE ARGUMENT X
5.   0.00000E+00  1.00000E+00  JN-500-PSpd-pool-1/s   Y (2-ND INDEPENDENT VAR.)

2-D INTERPOLATION IS PERFORMED, CF IS DEFINED AS:

CF(t) = f(x,y)

where: x - first argument, defined as: x = JN-500-PVf1-pool-m3/s
       y - second argument, defined as: y = JN-500-PSpd-pool-1/s

x-interpolation is performed for all tabular functions -> TF(x)
y-interpolation is performed using the following data points:

1  y = 2.00000E+01  g(y) = 1.00000E+00 * TF-101(x) + 0.00000E+00
2  y = 4.00000E+01  g(y) = 1.00000E+00 * TF-102(x) + 0.00000E+00
3  y = 5.00000E+01  g(y) = 1.00000E+00 * TF-103(x) + 0.00000E+00

Argument values : implicit
```

At the bottom of the CF data printout the method of calculating all Control Functions is printed. In the present example the functions are included in the implicit solution scheme. This means iteration will be continued until the required convergence is reached for all parameters, including values of all Control Functions. The other option, "CF not included" means that the values of CF will be updated by the solver in the main iteration, along with all other solution parameters, but the convergence criterion will not be checked for the CF. If all other parameters converge, the solver will complete the

SPECTRA Code Manuals - Volume 2: User's Guide

advancement and proceed to the next one, independently of the convergence of the CF. Finally, the internal numbering scheme is printed.

```
=CF= ALL CONTROL FUNCTIONS -----  
      CF SOLUTION IS INCLUDED IN THE IMPLICIT ITERATION  
=====
```

Int. No.	Ref. No.	Int. No.	Ref. No.	Int. No.	Ref. No.	Int. No.	Ref. No.
1	CF-001	2	CF-002	3	CF-003	4	CF-004

```
=====
```

An example of the Control Function transient printout is shown below.

```
=====
```

Function	Value	Name
=CF-001	3.80000E+02	Maximum_temperature_of_SC-001
=CF-002	3.42000E+02	Average_temperature_of_SC-001
=CF-003	6.50000E+01	Constant_value_of_15.0
=CF-004	3.80000E+02	Tmax_for_t < 15_s, Tave_for_t > 15_s

```
=====
```

SPECTRA Code Manuals - Volume 2: User's Guide

3.1.9 Reactor Kinetics Output

The Reactor Kinetics outputs may be easily found in the output file by searching for the string: **=RK=**. The first RK printout brings the input data printout. An example of a Reactor Kinetics (including the Isotope Transformation) input printout is shown below.

```

=====
=RK=  INPUT DATA FOR THE REACTOR KINETICS MODEL
=====

=RK=  POWER CALCULATED BY THE REACTOR KINETICS MODEL
      IS AVAILABLE AS CONTROL FUNCTION: CF-001

      IN CASE OF SOLID FUEL (IFTORK=1) THE POWER INCLUDES:
      - FISSION POWER (RT-000-Qfis-000)
      - DECAY    POWER (RT-000-Qdec-000)

      IN CASE OF LIQUID FUEL (IFTORK=2) THE POWER INCLUDES:
      - FISSION POWER (RT-000-Qfis-000)
      THE DECAY POWER IS IN SUCH CASE CALCULATED BY
      THE RT PACKAGE AND ADDED AUTOMATICALLY TO THE CV POOL

=RK=  NODE-INDEPENDENT DATA:
      NO. OF NEUTRONS PER FISSION      [-] : XNPFK = 2.50000E+00
      HEAT RELEASE PER FISSION         [J] : QFISRK = 3.09026E-11
      THERMAL NEUTRON VELOCITY         [m/s] : CTHNRK = 2.56000E+03
      FAST FISSION FACTOR               [-] : EPSRK = 1.02000E+00
      RESONANCE ESCAPE PROBABILITY      [-] : PRESRK = 8.70000E-01
      FAST NONLEAKAGE PROBABILITY       [-] : PFNLRK = 8.80000E-01
      THERMAL NONLEAKAGE PROBABILITY    [-] : PTNLRK = 8.80000E-01
      K-INF                             [-] :          1.29132E+00
      MULTIPLIER ON DECAY HEAT          [-] : QDMLRK = 1.00000E+00
      MINIMUM MACROSCOPIC FISSION CS. [1/m] : SIGMRK = 1.00000E-06
      DO NOT INCLUDE P*EPS IN THE REACTIVITY EFFECT CALCULATION, (IPERRK=1)

=RK=  NODE-DEPENDENT DATA:

      NODE      PNGTRK
      No.      [s]
      ----
      1      6.00000E-04

      NODE      SIGFRK      RVOLRK      PINIRK      IINIRK      RINIRK
      [1/m]      [m3]      [W]      [-]      [$]
      ----
      1      8.40000E-01  5.15000E+00  3.75000E+07  1      0.00000E+00

      POINT KINETICS INITIALIZATION : INONRK = 0
      PLOT REQUEST, REACTIVITY VS. K: IRPLRK = 1

=RK=  DELAYED NEUTRON PRECURSOR DATA

      Yield          Decay          Half-life
      Group  Absolute  Relative  Constant  T(1/2)
      No.    [1/fis]    [-]      [1/s]     [s]
      1      2.20000E-04  3.38462E-02  1.24000E-02  5.58990E+01
      2      1.42000E-03  2.18462E-01  3.05000E-02  2.27261E+01
      3      1.27000E-03  1.95385E-01  1.11000E-01  6.24457E+00
      4      2.57000E-03  3.95385E-01  3.01000E-01  2.30281E+00
      5      7.50000E-04  1.15385E-01  1.14000E+00  6.08024E-01
      6      2.70000E-04  4.15385E-02  3.01000E+00  2.30281E-01
      ----
      Sum:   6.50000E-03  1.00000E+00

=RK=  EXTERNAL NEUTRON SOURCES

      NODE  SOURCE [1/s]
  
```

SPECTRA Code Manuals - Volume 2: User's Guide

```

1 NO EXTERNAL SOURCE

=RK= EXTERNAL REACTIVITY DATA

      NODE REACTIVITY [$]
      1 NO EXTERNAL REACTIVITY

=RK= REACTIVITY FEEDBACK DATA

      Fuel Temper.  Reactivity
No.    [K]          [$]
  1    0.00000E+00  0.00000E+00
  2    1.00000E+04 -1.00000E+02

      Moderator T.  Reactivity
No.    [K]          [$]
  1    0.00000E+00  0.00000E+00
  2    1.00000E+04  1.50000E+01

      Void Fraction Reactivity
No.    [-]          [$]
  1    0.00000E+00  0.00000E+00
  2    1.00000E+00  0.00000E+00

=RK= FULL REACTIVITY FEEDBACK DATA FOR 2 x 2 x 2 DATA POINTS

----- Void Fraction = 0.000E+00

      \Tfuel 0.000E+00 1.000E+04
      Tmod.\
0.000E+00 0.000E+00 -1.000E+02
1.000E+04 1.500E+01 -8.500E+01

----- Void Fraction = 1.000E+00

      \Tfuel 0.000E+00 1.000E+04
      Tmod.\
0.000E+00 0.000E+00 -1.000E+02
1.000E+04 1.500E+01 -8.500E+01

=RK= WEIGHTING FACTOR DATA FOR 1 NODES

---- NODE No.: 1

-Tf- Fuel Temperature Weighting Factors

No. Component number and variable description      Weighting factor
--  -----
  1 SC-001 Temperature of Nodes: 1 - 5             1.00000E+00
--  -----
Total                                             1.00000E+00

The average fuel temperature is obtained from:

Tfuel = SUM( Wi * Ti ) / SUM ( Wi )

Normalization is performed because all factors are positive

=RK= SOURCE DENSITY DATA FOR CIRCULATING FUEL (USED ONLY FOR IFTORK = 2)

-Qf- Fraction of isotopes generated in core regions

No. Location                                     Power factor
--  -----
  1 CV-001 Pool volume                           1.00000E+00
--  -----
Total                                             1.00000E+00

Normalization is performed

-Tm- Moderator Temperature Weighting Factors

```

SPECTRA Code Manuals - Volume 2: User's Guide

No.	Component number and variable description	Weighting factor
1	SC-001 Temperature of Nodes: 1 - 6	1.00000E+00
	Total	1.00000E+00

The average moderator temperature is obtained from:

$$T_{mod} = \text{SUM}(W_i * T_i) / \text{SUM} (W_i)$$

Normalization is performed because all factors are positive

-Vf- Void fraction Weighting Factors

No.	Component number and variable description	Weighting factor
1	SC-001 Local bubble fraction at right surface	1.00000E+00
	Total	1.00000E+00

The average void fraction is obtained from:

$$\text{VOID} = \text{SUM}(W_i * \text{VOID}_i) / \text{SUM} (W_i)$$

Normalization is performed because all factors are positive

=RK= REACTOR CONTROL WHEN CV/JN/H2 PACKAGES ARE DISABLED
OR DURING INITIALIZATION OF THE NODAL POINT KINETICS (INONRK=1) :
- CONSTANT IN THE PROPORTIONAL CONTROLLER: CPCVRK = 1.00000E+00
- CONSTANT IN THE INTEGRATING CONTROLLER: CICVRK = 1.00000E+00

=RK= REACTIVITY EFFECT OF ISOTOPE CONCENTRATION CHANGES: YES (IREIRK=1)

=RK= FUEL TYPE: SOLID FUEL (IFTORK = 1)

ISOTOPE MAPPING TO RT : NOT REQUESTED (IMAPRK = 0)

=====
=RK= ISOTOPE TRANSFORMATION MODEL
=====

=RK= INITIAL ISOTOPE CONCENTRATIONS:
EQUILIBRIUM CONCENTRATIONS OF NON-FISSILE ISOTOPES
ARE CALCULATED IF NO VALUE IS SPECIFIED IN INPUT

=RK= INITIAL DATA FOR 34 ISOTOPES

i	Isotope	Input Initial Concentr. [1/m3]	Multiplier on Reactivity [-]
101	Th-232	0.00000E+00	1.00000E+00
102	Th-233	0.00000E+00	1.00000E+00
103	Th-234	0.00000E+00	1.00000E+00
104	Pa-233	0.00000E+00	1.00000E+00
105	Pa-234	0.00000E+00	1.00000E+00
106	U-233	0.00000E+00	1.00000E+00
107	U-234	0.00000E+00	1.00000E+00
108	U-235	1.66337E+25	1.00000E+00
201	U-238	1.49703E+26	1.00000E+00
202	U-239	0.00000E+00	1.00000E+00
203	U-240	0.00000E+00	1.00000E+00
204	Np-239	0.00000E+00	1.00000E+00
205	Np-240	0.00000E+00	1.00000E+00
206	Pu-239	0.00000E+00	1.00000E+00
207	Pu-240	0.00000E+00	1.00000E+00
208	Pu-241	0.00000E+00	1.00000E+00
301	I-135	0.00000E+00	1.00000E+00
302	Xe-135	0.00000E+00	1.00000E+00
401	Nd-149	0.00000E+00	1.00000E+00
402	Pm-149	0.00000E+00	1.00000E+00
403	Sm-149	0.00000E+00	1.00000E+00

SPECTRA Code Manuals - Volume 2: User's Guide

501	Eu-157	0.00000E+00	1.00000E+00
502	Gd-157	0.00000E+00	1.00000E+00
601	DHG-01	0.00000E+00	1.00000E+00
602	DHG-02	0.00000E+00	1.00000E+00
603	DHG-03	0.00000E+00	1.00000E+00
604	DHG-04	0.00000E+00	1.00000E+00
605	DHG-05	0.00000E+00	1.00000E+00
606	DHG-06	0.00000E+00	1.00000E+00
607	DHG-07	0.00000E+00	1.00000E+00
608	DHG-08	0.00000E+00	1.00000E+00
609	DHG-09	0.00000E+00	1.00000E+00
610	DHG-10	0.00000E+00	1.00000E+00
611	DHG-11	0.00000E+00	1.00000E+00

=RK= DECAY DATA FOR 34 ISOTOPES

i	Isotope	Decay Heat [J/decay]	Decay Heat [MeV/decay]	Decay Constant [1/s]	Decay Yield Fraction(s) Isotope Yield [-]
101	Th-232	0.00000E+00	0.00000E+00	0.00000E+00	
102	Th-233	1.99000E-13	1.24220E+00	5.23000E-04	Pa-233 1.00000E+00
103	Th-234	4.37000E-14	2.72784E-01	3.33000E-07	Pa-234 1.00000E+00
104	Pa-233	9.15000E-14	5.71161E-01	2.93000E-07	U-233 1.00000E+00
105	Pa-234	3.52000E-13	2.19725E+00	2.87000E-05	U-234 1.00000E+00
106	U-233	0.00000E+00	0.00000E+00	0.00000E+00	
107	U-234	0.00000E+00	0.00000E+00	0.00000E+00	
108	U-235	0.00000E+00	0.00000E+00	0.00000E+00	
201	U-238	0.00000E+00	0.00000E+00	0.00000E+00	
202	U-239	2.03000E-13	1.26717E+00	5.02000E-04	Np-239 1.00000E+00
203	U-240	6.22000E-14	3.88265E-01	1.38000E-05	Np-240 1.00000E+00
204	Np-239	1.16000E-13	7.24095E-01	3.44000E-06	Pu-239 1.00000E+00
205	Np-240	3.52000E-13	2.19725E+00	1.93000E-04	Pu-240 1.00000E+00
206	Pu-239	0.00000E+00	0.00000E+00	0.00000E+00	
207	Pu-240	0.00000E+00	0.00000E+00	0.00000E+00	
208	Pu-241	3.36000E-15	2.09738E-02	1.67000E-09	
301	I-135	4.24000E-13	2.64669E+00	2.93000E-05	Xe-135 1.00000E+00
302	Xe-135	1.84000E-13	1.14856E+00	2.10700E-05	
401	Nd-149	2.71000E-13	1.69164E+00	9.63000E-05	Pm-149 1.00000E+00
402	Pm-149	1.71000E-13	1.06742E+00	3.57000E-06	Sm-149 1.00000E+00
403	Sm-149	0.00000E+00	0.00000E+00	0.00000E+00	
501	Eu-157	2.18000E-13	1.36080E+00	1.27000E-05	Gd-157 1.00000E+00
502	Gd-157	0.00000E+00	0.00000E+00	0.00000E+00	
601	DHG-01	3.84000E-13	2.39700E+00	1.77000E+00	DHG-02 1.00000E+00
602	DHG-02	3.84000E-13	2.39700E+00	5.77000E-01	DHG-03 1.00000E+00
603	DHG-03	3.84000E-13	2.39700E+00	6.74000E-02	DHG-04 1.00000E+00
604	DHG-04	3.84000E-13	2.39700E+00	6.21000E-03	DHG-05 6.02000E-01
605	DHG-05	3.84000E-13	2.39700E+00	4.74000E-04	DHG-06 5.54000E-01
606	DHG-06	3.84000E-13	2.39700E+00	4.81000E-05	DHG-07 3.58000E-01
607	DHG-07	3.84000E-13	2.39700E+00	5.34000E-06	DHG-08 7.10000E-01
608	DHG-08	3.84000E-13	2.39700E+00	5.73000E-07	DHG-09 7.00000E-01
609	DHG-09	3.84000E-13	2.39700E+00	1.04000E-07	DHG-10 5.06000E-01
610	DHG-10	3.84000E-13	2.39700E+00	2.96000E-08	DHG-11 1.00000E-01
611	DHG-11	3.84000E-13	2.39700E+00	7.59000E-10	

=RK= NEUTRON CAPTURE DATA FOR 34 ISOTOPES

i	Isotope	N. Capture cross sec. [barn]	N. Capture cross sec. [m2]	N. Capture Yield Fraction(s) Isotope Yield [-]
101	Th-232	6.54100E+00	6.54100E-28	Th-233 1.00000E+00
102	Th-233	1.40000E+03	1.40000E-25	Th-234 1.00000E+00
103	Th-234	0.00000E+00	0.00000E+00	
104	Pa-233	3.60600E+01	3.60600E-27	Pa-234 1.00000E+00
105	Pa-234	0.00000E+00	0.00000E+00	
106	U-233	4.18400E+01	4.18400E-27	U-234 1.00000E+00
107	U-234	9.06100E+01	9.06100E-27	U-235 1.00000E+00
108	U-235	8.64400E+01	8.64400E-27	
201	U-238	1.87867E+01	1.87867E-27	U-239 1.00000E+00
202	U-239	2.20000E+01	2.20000E-27	U-240 1.00000E+00
203	U-240	0.00000E+00	0.00000E+00	
204	Np-239	3.28600E+01	3.28600E-27	Np-240 1.00000E+00
205	Np-240	0.00000E+00	0.00000E+00	

SPECTRA Code Manuals - Volume 2: User's Guide

206	Pu-239	2.74800E+02	2.74800E-26	Pu-240	1.00000E+00
207	Pu-240	2.63000E+02	2.63000E-26	Pu-241	1.00000E+00
208	Pu-241	3.28200E+02	3.28200E-26		
301	I-135	0.00000E+00	0.00000E+00		
302	Xe-135	2.72200E+06	2.72200E-22		
401	Nd-149	0.00000E+00	0.00000E+00		
402	Pm-149	1.24300E+03	1.24300E-25		
403	Sm-149	6.15300E+04	6.15300E-24		
501	Eu-157	1.68600E+02	1.68600E-26		
502	Gd-157	1.91600E+05	1.91600E-23		
601	DHG-01	0.00000E+00	0.00000E+00		
602	DHG-02	0.00000E+00	0.00000E+00		
603	DHG-03	0.00000E+00	0.00000E+00		
604	DHG-04	0.00000E+00	0.00000E+00		
605	DHG-05	0.00000E+00	0.00000E+00		
606	DHG-06	0.00000E+00	0.00000E+00		
607	DHG-07	0.00000E+00	0.00000E+00		
608	DHG-08	0.00000E+00	0.00000E+00		
609	DHG-09	0.00000E+00	0.00000E+00		
610	DHG-10	0.00000E+00	0.00000E+00		
611	DHG-11	0.00000E+00	0.00000E+00		

=RK= FISSION DATA FOR 34 ISOTOPES

i	Isotope	Fission cross sec. [barn]	Fission cross sec. [m2]	Isotope	Fission Yield Fraction(s) Yield [-]
101	Th-232	0.00000E+00	0.00000E+00		
102	Th-233	0.00000E+00	0.00000E+00		
103	Th-234	0.00000E+00	0.00000E+00		
104	Pa-233	0.00000E+00	0.00000E+00		
105	Pa-234	0.00000E+00	0.00000E+00		
106	U-233	4.64700E+02	4.64700E-26	I-135	4.41000E-02
				Xe-135	1.47000E-02
				Nd-149	7.60000E-03
				Eu-157	6.70000E-05
				Gd-157	7.20000E-08
				DHG-01	2.39200E-01
				DHG-02	4.20800E-01
				DHG-03	5.80000E-01
				DHG-04	3.08000E-01
				-----	-----
				Total:	1.61447E+00
107	U-234	0.00000E+00	0.00000E+00		
108	U-235	5.05000E+02	5.05000E-26	I-135	6.32000E-02
				Xe-135	2.60000E-03
				Nd-149	1.05000E-02
				Eu-157	6.30000E-05
				Gd-157	2.20000E-09
				DHG-01	2.39200E-01
				DHG-02	4.20800E-01
				DHG-03	5.80000E-01
				DHG-04	3.08000E-01
				-----	-----
				Total:	1.62436E+00
201	U-238	0.00000E+00	0.00000E+00		
202	U-239	1.40000E+01	1.40000E-27	I-135	6.32000E-02
				Xe-135	2.60000E-03
				Nd-149	1.05000E-02
				Eu-157	6.30000E-05
				Gd-157	2.20000E-09
				DHG-01	2.39200E-01
				DHG-02	4.20800E-01
				DHG-03	5.80000E-01
				DHG-04	3.08000E-01
				-----	-----
				Total:	1.62436E+00
203	U-240	0.00000E+00	0.00000E+00		
204	Np-239	0.00000E+00	0.00000E+00		

SPECTRA Code Manuals - Volume 2: User's Guide

205 Np-240	0.00000E+00	0.00000E+00		
206 Pu-239	6.98900E+02	6.98900E-26	I-135	6.19000E-02
			Xe-135	1.04000E-02
			Nd-149	1.25000E-02
			Eu-157	7.50000E-04
			Gd-157	3.00000E-07
			DHG-01	1.60000E-01
			DHG-02	3.00000E-01
			DHG-03	5.80000E-01
			DHG-04	3.08000E-01
			-----	-----
			Total:	1.43355E+00

207 Pu-240	0.00000E+00	0.00000E+00		
208 Pu-241	9.46100E+02	9.46100E-26	I-135	7.07000E-02
			Xe-135	2.10000E-03
			Nd-149	1.46000E-02
			Eu-157	2.70000E-03
			Gd-157	4.30000E-08
			DHG-01	1.60000E-01
			DHG-02	3.00000E-01
			DHG-03	5.80000E-01
			DHG-04	3.08000E-01
			-----	-----
			Total:	1.43810E+00

301 I-135	0.00000E+00	0.00000E+00
302 Xe-135	0.00000E+00	0.00000E+00
401 Nd-149	0.00000E+00	0.00000E+00
402 Pm-149	0.00000E+00	0.00000E+00
403 Sm-149	0.00000E+00	0.00000E+00
501 Eu-157	0.00000E+00	0.00000E+00
502 Gd-157	0.00000E+00	0.00000E+00
601 DHG-01	0.00000E+00	0.00000E+00
602 DHG-02	0.00000E+00	0.00000E+00
603 DHG-03	0.00000E+00	0.00000E+00
604 DHG-04	0.00000E+00	0.00000E+00
605 DHG-05	0.00000E+00	0.00000E+00
606 DHG-06	0.00000E+00	0.00000E+00
607 DHG-07	0.00000E+00	0.00000E+00
608 DHG-08	0.00000E+00	0.00000E+00
609 DHG-09	0.00000E+00	0.00000E+00
610 DHG-10	0.00000E+00	0.00000E+00
611 DHG-11	0.00000E+00	0.00000E+00

=RK= NO FUEL ELEMENT REMOVAL

=RK= FUEL LOADING FUNCTIONS

NODE	LOADING FUNCTION No.
No.	1
1	CF-002

=RK= INITIAL FUEL COMPOSITION DATA

i	Isotope	Initial Mass Fraction [-]	Initial Nuclide Concentration [1/m3]
106	U-233	0.00000E+00	0.00000E+00
108	U-235	1.00000E+00	1.66337E+25
202	U-239	0.00000E+00	0.00000E+00
206	Pu-239	0.00000E+00	0.00000E+00
208	Pu-241	0.00000E+00	0.00000E+00

=RK= RELOAD DATA FOR 1 LOADING FUNCTIONS

=RK= LOADING FUNCTION No.: 1

Concentration of Isotops in Assemblies Being Loaded During Transient

Concentration

SPECTRA Code Manuals - Volume 2: User's Guide

i	Isotope	[1/m3]
101	Th-232	0.00000E+00
102	Th-233	0.00000E+00
103	Th-234	0.00000E+00
104	Pa-233	0.00000E+00
105	Pa-234	0.00000E+00
106	U-233	0.00000E+00
107	U-234	0.00000E+00
108	U-235	3.32673E+25
201	U-238	1.33069E+26
202	U-239	0.00000E+00
203	U-240	0.00000E+00
204	Np-239	0.00000E+00
205	Np-240	0.00000E+00
206	Pu-239	0.00000E+00
207	Pu-240	0.00000E+00
208	Pu-241	0.00000E+00
301	I-135	0.00000E+00
302	Xe-135	0.00000E+00
401	Nd-149	0.00000E+00
402	Pm-149	0.00000E+00
403	Sm-149	0.00000E+00
501	Eu-157	0.00000E+00
502	Gd-157	0.00000E+00
601	DHG-01	0.00000E+00
602	DHG-02	0.00000E+00
603	DHG-03	0.00000E+00
604	DHG-04	0.00000E+00
605	DHG-05	0.00000E+00
606	DHG-06	0.00000E+00
607	DHG-07	0.00000E+00
608	DHG-08	0.00000E+00
609	DHG-09	0.00000E+00
610	DHG-10	0.00000E+00
611	DHG-11	0.00000E+00

Fuel Composition in Assemblies Being Loaded During Transient

i	Isotope	Mass Fraction [-]	Nuclide Concentration [1/m3]
106	U-233	0.00000E+00	0.00000E+00
108	U-235	2.00000E+00	3.32673E+25
202	U-239	0.00000E+00	0.00000E+00
206	Pu-239	0.00000E+00	0.00000E+00
208	Pu-241	0.00000E+00	0.00000E+00

=====
 =RK= ISOTOPE INTERNAL NUMBERING SCHEME
 =====

Int. No.	Ref. No.	Int. No.	Ref. No.	Int. No.	Ref. No.	Int. No.	Ref. No.	Int. No.	Ref. No.
1	IT-101	2	IT-102	3	IT-103	4	IT-104	5	IT-105
6	IT-106	7	IT-107	8	IT-108	9	IT-201	10	IT-202
11	IT-203	12	IT-204	13	IT-205	14	IT-206	15	IT-207
16	IT-208	17	IT-301	18	IT-302	19	IT-401	20	IT-402
21	IT-403	22	IT-501	23	IT-502	24	IT-601	25	IT-602
26	IT-603	27	IT-604	28	IT-605	29	IT-606	30	IT-607
31	IT-608	32	IT-609	33	IT-610	34	IT-611		

=====
 =RK= END OF REACTOR KINETICS DATA
 =====

An example of the Reactor Kinetics transient printout is shown below. The letter *f*, in the isotope printout, signifies a fissile isotope.

SPECTRA Code Manuals - Volume 2: User's Guide

=====

=RK= OUTPUT DATA FOR POINT REACTOR KINETICS MODEL, AT TIME : -8.64000E+04 [s]

=====

=RK= NEUTRON POWER (FISSION POWER) DATA

Node	Neutron Density [1/m3]	Neutron Velocity [m/s]	Neutron Flux [1/m2/s]	External Neutron Source [1/s]	Neutron Power [W]
1	1.09575E+14	2.56000E+03	2.80511E+17	0.00000E+00	3.75000E+07

=RK= REACTOR AVERAGE PARAMETERS

Node	Fuel Temperature [K]	Moderator Temperature [K]	Void Fraction [-]
1	1.37339E+03	1.34908E+03	1.00000E+00

=RK= REACTIVITY DATA

Node	Current Reactivity [\$]	Control Rod Reactivity [\$]	Temp.&Void Feedback [\$]	Isotope Change Feedback [\$]	Bias Reactivity [\$]
1	0.00000E+00	0.00000E+00	-1.17103E+01	2.92344E+01	-1.75241E+01

=RK= MULTIPLICATION FACTOR DATA

Node	K-eff [-]
1	1.00000E+00

=RK= MACROSCOPIC FISSION CROSS SECTION DATA

Node	SigmaF (1/m) [-]
1	8.40000E-01

=RK= DATA FOR 6 DELAYED NEUTRON PRECURSORS

Node No.: 1

Group No.	Concentration [1/m3]
1	3.24011E+15
2	8.50251E+15
3	2.08949E+15
4	1.55928E+15
5	1.20148E+14
6	1.63816E+13

=RK= DATA FOR 34 ISOTOPES AT TIME : -8.64000E+04 [s]

Node No.: 1

i	Isotope	Nuclide Density [1/m3]	Decay Heat [W/m3]	Reactivity [\$]	Reactivity Change [\$]
101	Th-232	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
102	Th-233	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
103	Th-234	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
104	Pa-233	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
105	Pa-234	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
106 f	U-233	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
107	U-234	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
108 f	U-235	1.66337E+25	0.00000E+00	6.07781E+01	0.00000E+00
201	U-238	1.49703E+26	0.00000E+00	-2.66063E+01	0.00000E+00
202 f	U-239	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
203	U-240	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
204	Np-239	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
205	Np-240	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
206 f	Pu-239	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
207	Pu-240	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
208 f	Pu-241	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
301	I-135	5.08252E+20	6.31411E+03	0.00000E+00	0.00000E+00
302	Xe-135	1.59142E+20	6.16974E+02	-4.09802E+00	0.00000E+00
401	Nd-149	2.56917E+19	6.70483E+02	0.00000E+00	0.00000E+00
402	Pm-149	6.86324E+20	4.18980E+02	-8.07054E-03	0.00000E+00

SPECTRA Code Manuals - Volume 2: User's Guide

```

403 Sm-149 1.41958E+21 0.00000E+00 -8.26322E-01 0.00000E+00
501 Eu-157 1.16843E+18 3.23493E+00 -1.86365E-06 0.00000E+00
502 Gd-157 2.76107E+18 0.00000E+00 -5.00467E-03 0.00000E+00
601 DHG-01 3.18432E+16 2.16432E+04 0.00000E+00 0.00000E+00
602 DHG-02 2.69524E+17 5.97179E+04 0.00000E+00 0.00000E+00
603 DHG-03 4.33502E+18 1.12197E+05 0.00000E+00 0.00000E+00
604 DHG-04 5.87366E+19 1.40066E+05 0.00000E+00 0.00000E+00
605 DHG-05 4.63253E+20 8.43195E+04 0.00000E+00 0.00000E+00
606 DHG-06 2.52907E+21 4.67130E+04 0.00000E+00 0.00000E+00
607 DHG-07 8.15546E+21 1.67233E+04 0.00000E+00 0.00000E+00
608 DHG-08 5.39626E+22 1.18735E+04 0.00000E+00 0.00000E+00
609 DHG-09 2.08119E+23 8.31146E+03 0.00000E+00 0.00000E+00
610 DHG-10 3.70003E+23 4.20560E+03 0.00000E+00 0.00000E+00
611 DHG-11 1.44296E+24 4.20560E+02 0.00000E+00 0.00000E+00
-----
1.68426E+26 5.14215E+05 2.92344E+01 0.00000E+00

```

=RK= MISCELLANEOUS DATA

Node	Fission Cross-sec. [1/m]	Fission Power [W]	Decay Power [W]	Total Power [W]
1	8.40000E-01	3.75000E+07	2.64821E+06	4.01482E+07

=RK= FUEL LOADING FUNCTIONS

Node Reload rates [1/s] for: 1 functions

Node	Reload rates [1/s]
1	0.00000E+00

=====

3.1.10 Material Property Output

An example of a Material Property data printout is shown below.

```

=MP= =====MP-002===== Stainless_steel,_SS-304_____

MULTIPLIERS
- THERMAL CONDUCTIVITY: TCMLMP = 1.00000E+00
- DENSITY : RHMLMP = 1.00000E+00
- SPECIFIC HEAT : CPMLMP = 1.00000E+00

MP-CON (K) (W/M/K )
3.00000E+02 1.35000E+01
8.00000E+02 2.30000E+01
1.30000E+03 3.20000E+01

MP-RHO (K) (KG/M3 )
3.00000E+02 7.80000E+03
8.00000E+02 7.60000E+03
1.30000E+03 7.35000E+03

MP-CP (K) (J/KG/K)
3.00000E+02 4.10000E+02
5.00000E+02 4.50000E+02
8.00000E+02 5.00000E+02
1.30000E+03 5.50000E+02

MP-CV (K) (J/M3/K)
3.00000E+02 3.19800E+06
5.00000E+02 3.47400E+06
8.00000E+02 3.80000E+06
1.30000E+03 4.04250E+06

```

3.1.11 Transient Solution (SOLVER) Data

An example of a the SOLVER input data printout is shown below.

```
=====
=SL= SOLVER INPUT DATA FOR 1 TIME STEP DOMAINS
=====

=SL= TIME STEP DOMAIN NO.: 1
      MAXIMUM TIME STEP FOR THIS DOMAIN: 1.00000E-01 (S)
      MINIMUM TIME STEP FOR THIS DOMAIN: 1.00000E-04 (S)
      PRINT FREQUENCY FOR THIS DOMAIN  : 5.00000E+00 (S)
      PLOT FREQUENCY FOR THIS DOMAIN   : 1.00000E+00 (S)
      END TIME FOR THIS DOMAIN         : 5.00000E+00 (S)

=====
=SL= SOLVER INPUT DATA
=====

=SL= START TIME: -8.64000E+04

=SL= SCREEN MESSAGE FREQUENCY: 1.00000E+00

=SL= ADVANCEMENT MESSAGE FREQUENCY: 10

=SL= EXTENDED DIAGNOSTICS NOT REQUESTED

=SL= DEBUG PRINTOUT NOT REQUESTED

=SL= MESSAGES WRITTEN TO *.MES FILE

=SL= ITERATION DATA
      MAX.NO.OF ITER. TO CUT TIME STEP BY DTREDN, MAXITR = 50
      MIN.NO.OF ITER. TO INCREASE TIME STEP BY DTINC, MINITR = 20
      MINIMUM NO.OF ITER. TO ACCEPT THE SOLUTION, ITMNSL = 3
      TIME STEP REDUCTION FACTOR IN CASE OF NONCONV. DTREDN = 4.00000E+00
      TIME STEP REDUCTION FACTOR IN CASE OF FAILURE, DTREDF = 8.00000E+00
      TIME STEP INCREASE FACTOR IF ITER < MINITR, DTINC = 1.30278E+00
      ACTION ON FAILURE DURING TRANSIENT : TERMINATE THE RUN
      ACTION ON FAILURE DURING INITIAL STATE: TERMINATE THE RUN

      MAIN CONVERGENCE CRITERIA :
      - CALCULATED-ASSUMED : CCCASL = 1.00000E-03
      - ASSUMED-ASSUMED : CCAASL = 1.00000E-04
      - RK MULT. CAL.-ASS. : CMCASL = 1.00000E+00
      - RK MULT. ASS.-ASS. : CMAASL = 1.00000E+00
      - ABSOLUTE LIMIT : ABSLSL = 1.00000E-10
      - INITIAL DISTURBANCE: DISTIN = 1.00000E-02
      FISSION PRODUCT CONVERGENCE CRITERIA :
      - CALCULATED-ASSUMED : FCCASL = 1.00000E+01
      - ASSUMED-ASSUMED : FCAASL = 1.00000E+00
      - ABSOLUTE LIMIT : FABLSL = 1.00000E-30
      - MAX. ITERATIONS : ITMXSL = 15
      - MASS ERROR TREATM. : IFPESL = -1 (MASS ERROR ALLOWED)

=SL= IDIAFL = 0 : WARNING AND ERROR MESSAGES ARE WRITTEN
      TO THE DIAGNOSTICS FILE DURING THE CALCULATIONS

=SL= ITSNSL = 1 : TIME STEP IS NOT ADJUSTED AT THE END OF EACH TIME STEP DOMAIN

=SL= SIMULATOR OPTION : INACTIVE (ISIMUL<=0)

=SL= SCRAMBLING OF INPUT: NOT NEEDED (ISCRMB<=0)

=SL= MODEL EXPORTING : NOT NEEDED (IEXPSL=0)

=SL= INITIAL CONDITIONS ARE READ FROM THE
      INITIAL CONDITION FILE: ./SS-CP.ICF
```

SPECTRA Code Manuals - Volume 2: User's Guide

```
=====
=SL=  END OF NUMERICAL SOLVER DATA
=====
```

An example of the SOLVER transient output is shown below.

```
=====
=SL=  SOLVER OUTPUT AT TIME:  5.10000E+00,  ADVANCEMENT NUMBER:      51
=====
```

```
=SL=  MAIN ITERATION PARAMETERS
```

PACKAGE	VARIABLE	ITERATIONS TO CONVERGE
Control Volume	Atms mass, kg,	4
Control Volume	Bubble mass, kg,	5
Control Volume	Droplet mass, kg,	4
Control Volume	Pool mass, kg,	3
Control Volume	Energy, J/kg,	6
Control Volume	No.of bubb. -,	4
Control Volume	No.of drops, -,	3
Control Volume	Bubb.posit. m,	3
Control Volume	Droplet pos. m,	3
Control Volume	Pressure Pa,	1
CV Junction	Velocity, m/s,	1
CV Junction	Pressure, Pa,	1
1-D H. Conductor	T(left), K,	3
1-D H. Conductor	T(right), K,	3
2-D H. Conductor	T(boundary), K,	1
Control Function	CF value,	1
Reactor Kinetics	Neutron concent.	1
Reactor Kinetics	Precur. concent.	1

```
=====
```

At the end of the calculations SOLVER prints the run statistics. An example of this printout is shown below.

```
=====
=SL=  RUN STATISTICS
```

```
-----
Analyzed model time (s) :  5.10      ( 0.142E-02 (hrs) )
CPU time (s)           :  0.734     ( 0.204E-03 (hrs) )
Warp factor (model/CPU) :  6.94
Minimum time step (s) :  0.100
Maximum time step (s) :  0.100
Average time step (s) :  0.100
No. of advancements      :  51
CPU per advancement (s) :  0.144E-01
=====
```


3.2 Description of the Diagnostics File (*.DIA)

An example of the diagnostics file is shown below. The diagnostics file contains all warning and error messages produced during:

- input processing,
- transient calculations.

All error messages are preceded by “*****”. All warning messages are preceded by “* * *”.

Furthermore, the diagnostics file contains information about every time step advancement, including:

- advancement number,
- time at the start of the advancement, (s),
- time at the end of the advancement, (s),
- time step, (s),
- number of iterations required to complete the advancement,
- CPU time and run time (s).

When the run is terminated, the run statistics is written to the diagnostics file.

```
=====
SPECTRA - Sophisticated Plant Evaluation Code for
          Thermalhydraulic Response Assessment
          Version 2.00 (c) MSt, October 2003
-----
Input data diagnostics
=====

* * * =IN= WARNING: TOO MANY ENTRIES IN RECORD: 302001
          EXCESSIVE ITEMS ( 2 - 2) OMITTED
          ***** NOTE !
          THIS WARNING INDICATES THAT THERE MIGHT BE AN ERROR
          IN THIS RECORD. CHECK CAREFULLY THE ENTIRE INPUT RECORD.

-----
SPECTRA - Sophisticated Plant Evaluation Code for
          Thermalhydraulic Response Assessment
          Version 2.00 (c) MSt, October 2003
-----
Transient diagnostics for the problem:
-----
CV example
=====

Adv:      0 T(beg)= 0.000E+00 T(end)= 0.000E+00 dT= 1.000E+99 Iter:   4 CPU= 0.000E+00
Adv:      1 T(beg)= 0.000E+00 T(end)= 1.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.125E-01
Adv:      2 T(beg)= 1.000E-01 T(end)= 2.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.281E-01
Adv:      3 T(beg)= 2.000E-01 T(end)= 3.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.281E-01
Adv:      4 T(beg)= 3.000E-01 T(end)= 4.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.438E-01
Adv:      5 T(beg)= 4.000E-01 T(end)= 5.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.438E-01
Adv:      6 T(beg)= 5.000E-01 T(end)= 6.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.438E-01
Adv:      7 T(beg)= 6.000E-01 T(end)= 7.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.594E-01
Adv:      8 T(beg)= 7.000E-01 T(end)= 8.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.594E-01
Adv:      9 T(beg)= 8.000E-01 T(end)= 9.000E-01 dT= 1.000E-01 Iter:   7 CPU= 3.594E-01
Adv:     10 T(beg)= 9.000E-01 T(end)= 1.000E+00 dT= 1.000E-01 Iter:   7 CPU= 3.750E-01

* * * =CV= WARNING IN EQM6CV, CALCULATING CV TABULAR MASS SOURCES:
          CV-001, MASS SOURCE:      1
          POSITIVE MASS SOURCE, Wtotal = 5.00000E-02
          SOURCE PRESSURE BELOW CV PRESSURE
          P(Source) = 1.00000E+05
          P( CV )   = 1.05000E+05

          WARNING FOR : Control Volume No.:      1

-----
* * * =CV= WARNING IN EQM6CV, CALCULATING CV TABULAR MASS SOURCES:
          CV-001, MASS SOURCE:      2
          POSITIVE MASS SOURCE, Wtotal = 5.00000E-02
          SOURCE PRESSURE BELOW CV PRESSURE
          P(Source) = 1.00000E+05
          P( CV )   = 1.05000E+05

          WARNING FOR : Control Volume No.:      1
```

SPECTRA Code Manuals - Volume 2: User's Guide

```

-----
Adv:      11  T (beg)= 1.000E+00  T (end)= 1.100E+00  dT= 1.000E-01  Iter:   14  CPU= 3.906E-01
Adv:      12  T (beg)= 1.100E+00  T (end)= 1.200E+00  dT= 1.000E-01  Iter:   15  CPU= 4.062E-01
Adv:      13  T (beg)= 1.200E+00  T (end)= 1.300E+00  dT= 1.000E-01  Iter:   12  CPU= 4.062E-01
Adv:      14  T (beg)= 1.300E+00  T (end)= 1.400E+00  dT= 1.000E-01  Iter:   10  CPU= 4.219E-01
Adv:      15  T (beg)= 1.400E+00  T (end)= 1.500E+00  dT= 1.000E-01  Iter:    9  CPU= 4.219E-01
Adv:      16  T (beg)= 1.500E+00  T (end)= 1.600E+00  dT= 1.000E-01  Iter:    9  CPU= 4.375E-01
Adv:      17  T (beg)= 1.600E+00  T (end)= 1.700E+00  dT= 1.000E-01  Iter:   11  CPU= 4.531E-01
Adv:      18  T (beg)= 1.700E+00  T (end)= 1.800E+00  dT= 1.000E-01  Iter:   11  CPU= 4.531E-01
Adv:      19  T (beg)= 1.800E+00  T (end)= 1.900E+00  dT= 1.000E-01  Iter:   11  CPU= 4.688E-01
Adv:      20  T (beg)= 1.900E+00  T (end)= 2.000E+00  dT= 1.000E-01  Iter:   11  CPU= 4.844E-01
Adv:      21  T (beg)= 2.000E+00  T (end)= 2.100E+00  dT= 1.000E-01  Iter:    8  CPU= 4.844E-01
Adv:      22  T (beg)= 2.100E+00  T (end)= 2.200E+00  dT= 1.000E-01  Iter:    9  CPU= 5.000E-01
Adv:      23  T (beg)= 2.200E+00  T (end)= 2.300E+00  dT= 1.000E-01  Iter:    8  CPU= 5.000E-01
Adv:      24  T (beg)= 2.300E+00  T (end)= 2.400E+00  dT= 1.000E-01  Iter:    8  CPU= 5.156E-01
Adv:      25  T (beg)= 2.400E+00  T (end)= 2.500E+00  dT= 1.000E-01  Iter:    8  CPU= 5.156E-01
Adv:      26  T (beg)= 2.500E+00  T (end)= 2.600E+00  dT= 1.000E-01  Iter:    8  CPU= 5.312E-01
Adv:      27  T (beg)= 2.600E+00  T (end)= 2.700E+00  dT= 1.000E-01  Iter:    9  CPU= 5.312E-01
Adv:      28  T (beg)= 2.700E+00  T (end)= 2.800E+00  dT= 1.000E-01  Iter:   10  CPU= 5.469E-01
Adv:      29  T (beg)= 2.800E+00  T (end)= 2.900E+00  dT= 1.000E-01  Iter:    8  CPU= 5.469E-01
Adv:      30  T (beg)= 2.900E+00  T (end)= 3.000E+00  dT= 1.000E-01  Iter:    8  CPU= 5.625E-01
Adv:      31  T (beg)= 3.000E+00  T (end)= 3.100E+00  dT= 1.000E-01  Iter:    8  CPU= 5.625E-01
Adv:      32  T (beg)= 3.100E+00  T (end)= 3.200E+00  dT= 1.000E-01  Iter:    8  CPU= 5.781E-01
Adv:      33  T (beg)= 3.200E+00  T (end)= 3.300E+00  dT= 1.000E-01  Iter:    8  CPU= 5.781E-01
Adv:      34  T (beg)= 3.300E+00  T (end)= 3.400E+00  dT= 1.000E-01  Iter:    8  CPU= 5.938E-01
Adv:      35  T (beg)= 3.400E+00  T (end)= 3.500E+00  dT= 1.000E-01  Iter:    8  CPU= 5.938E-01
Adv:      36  T (beg)= 3.500E+00  T (end)= 3.600E+00  dT= 1.000E-01  Iter:    8  CPU= 6.094E-01
Adv:      37  T (beg)= 3.600E+00  T (end)= 3.700E+00  dT= 1.000E-01  Iter:    8  CPU= 6.094E-01
Adv:      38  T (beg)= 3.700E+00  T (end)= 3.800E+00  dT= 1.000E-01  Iter:    8  CPU= 6.250E-01
Adv:      39  T (beg)= 3.800E+00  T (end)= 3.900E+00  dT= 1.000E-01  Iter:    8  CPU= 6.250E-01
Adv:      40  T (beg)= 3.900E+00  T (end)= 4.000E+00  dT= 1.000E-01  Iter:    8  CPU= 6.406E-01
Adv:      41  T (beg)= 4.000E+00  T (end)= 4.100E+00  dT= 1.000E-01  Iter:    8  CPU= 6.406E-01
Adv:      42  T (beg)= 4.100E+00  T (end)= 4.200E+00  dT= 1.000E-01  Iter:    8  CPU= 6.562E-01
Adv:      43  T (beg)= 4.200E+00  T (end)= 4.300E+00  dT= 1.000E-01  Iter:    8  CPU= 6.562E-01
Adv:      44  T (beg)= 4.300E+00  T (end)= 4.400E+00  dT= 1.000E-01  Iter:    8  CPU= 6.719E-01
Adv:      45  T (beg)= 4.400E+00  T (end)= 4.500E+00  dT= 1.000E-01  Iter:    8  CPU= 6.719E-01
Adv:      46  T (beg)= 4.500E+00  T (end)= 4.600E+00  dT= 1.000E-01  Iter:    8  CPU= 6.875E-01
Adv:      47  T (beg)= 4.600E+00  T (end)= 4.700E+00  dT= 1.000E-01  Iter:    8  CPU= 6.875E-01
Adv:      48  T (beg)= 4.700E+00  T (end)= 4.800E+00  dT= 1.000E-01  Iter:    7  CPU= 7.031E-01
Adv:      49  T (beg)= 4.800E+00  T (end)= 4.900E+00  dT= 1.000E-01  Iter:    7  CPU= 7.031E-01
Adv:      50  T (beg)= 4.900E+00  T (end)= 5.000E+00  dT= 1.000E-01  Iter:    7  CPU= 7.188E-01
Adv:      51  T (beg)= 5.000E+00  T (end)= 5.100E+00  dT= 1.000E-01  Iter:    7  CPU= 7.344E-01

```

-> END OF CALCULATIONS.

-> RUN STATISTICS

```

-----
Analyzed model time (s) : 5.10      ( 0.142E-02 (hrs) )
CPU time (s)           : 0.734     ( 0.204E-03 (hrs) )
Warp factor (model/CPU) : 6.94
Minimum time step (s) : 0.100
Maximum time step (s) : 0.100
Average time step (s) : 0.100
No. of advancements    : 51
CPU per advancement (s) : 0.144E-01

```

In case when the debug printout is requested, the diagnostics file contains also the debug printout. It may be used in case of numerical problems, to find out how the iterations proceed. Debug printout is written to the diagnostics file every iteration. Thus an enormous amount of printout may be generated in a very short time. Therefore debug printout should be activated shortly before the time when the numerical problems are occurring.

An example of the debug printout is shown below. Debug printout gives four values for each variable controlled by the SOLVER: the assumed and obtained values, for the last two iterations.

Each variable that has not yet converged is distinguished in the output by the exclamation sign (!) in front of the variable name.

```

=====
=SL=  SOLVER DEBUG PRINTOUT
=====
ADV.:      51  T (beg)= 5.000E+00  T (end)= 5.100E+00  DT= 1.000E-01  ITER:    2
=====

```

SPECTRA Code Manuals - Volume 2: User's Guide

				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
Atms mass,	kg,	CV-001	H2	0.00000E+00	-1.00000E-04	0.00000E+00	0.00000E+00
Atms mass,	kg,	CV-001	He	0.00000E+00	-1.00000E-04	0.00000E+00	0.00000E+00
!Atms mass,	kg,	CV-001	H2O	1.44343E-01	1.44251E-01	1.44353E-01	1.44350E-01
!Atms mass,	kg,	CV-001	N2	4.21229E+00	4.21162E+00	4.21244E+00	4.21230E+00
!Atms mass,	kg,	CV-001	O2	1.24880E+00	1.24991E+00	1.24889E+00	1.24889E+00
Atms mass,	kg,	CV-001	CO2	0.00000E+00	-1.00000E-04	0.00000E+00	0.00000E+00
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
Bubble mass,	kg,	CV-001	H2	0.00000E+00	-1.00000E-04	0.00000E+00	0.00000E+00
Bubble mass,	kg,	CV-001	He	0.00000E+00	-1.00000E-04	0.00000E+00	0.00000E+00
!Bubble mass,	kg,	CV-001	H2O	7.40714E-03	7.35254E-03	7.55781E-03	7.55875E-03
!Bubble mass,	kg,	CV-001	N2	2.98931E-01	2.96938E-01	3.02737E-01	3.02877E-01
Bubble mass,	kg,	CV-001	O2	0.00000E+00	-1.00000E-04	0.00000E+00	0.00000E+00
Bubble mass,	kg,	CV-001	CO2	0.00000E+00	-1.00000E-04	0.00000E+00	0.00000E+00
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
!Droplet mass,kg,		CV-001	drop	4.38730E-02	4.39026E-02	4.38985E-02	4.38749E-02
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
!Pool mass,	kg,	CV-001	pool	4.95749E+03	4.95699E+03	4.95750E+03	4.95750E+03
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
!Energy,	J/kg,	CV-001	atms	2.94696E+05	2.94631E+05	2.94752E+05	2.94697E+05
!Energy,	J/kg,	CV-001	drop	3.07601E+05	3.07555E+05	3.07600E+05	3.07601E+05
!Energy,	J/kg,	CV-001	pool	1.75345E+05	1.75326E+05	1.75347E+05	1.75345E+05
!Energy,	J/kg,	CV-001	bubb	2.99227E+05	2.98155E+05	2.69266E+05	2.99819E+05
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
!No.of bubb.	-,	CV-001		1.10401E+05	1.09680E+05	1.11749E+05	1.11749E+05
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
!No.of drops,	-,	CV-001		8.59410E+01	8.59639E+01	8.59416E+01	8.59416E+01
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
!Bubb.posit.	m,	CV-001		4.19171E+00	4.18809E+00	4.19205E+00	4.19205E+00
				ASSUMED		CALCULATED	
				LAST ITER.	ITER-1	LAST ITER.	ITER-1
!Droplet pos.	m,	CV-001		3.33171E+00	3.33472E+00	3.33196E+00	3.33196E+00
				P (Pa)	T (K)		
Thermodynamics,		CV-001	atms	1.10030E+05	3.19146E+02		
				Atms. Velocity, (m/s)		Pool Velocity, (m/s)	
				LAST VALUE	PREV. VALUE	LAST VALUE	PREV. VALUE
Velocities,		JN-001		4.25023E-01	4.25139E-01	0.00000E+00	0.00000E+00
				Atms. Pressure, (Pa)		Pool Pressure, (Pa)	
				LAST VALUE	PREV. VALUE	LAST VALUE	PREV. VALUE
Pressures,		CV-001		1.10030E+05	1.09990E+05	1.10030E+05	1.09990E+05
				ASSUMED		CALCULATED	

SPECTRA Code Manuals - Volume 2: User's Guide

		LAST ITER.	ITER-1	LAST ITER.	ITER-1
		ASSUMED		CALCULATED	
		LAST ITER.	ITER-1	LAST ITER.	ITER-1
T(left),	K, SC-001	3.15002E+02	3.14971E+02	3.15002E+02	3.15002E+02
T(left),	K, SC-002	3.15002E+02	3.14971E+02	3.15002E+02	3.15002E+02
T(right),	K, SC-001	3.15002E+02	3.14970E+02	3.15002E+02	3.15002E+02
T(right),	K, SC-002	3.15002E+02	3.14970E+02	3.15002E+02	3.15002E+02
		ASSUMED		CALCULATED	
		LAST ITER.	ITER-1	LAST ITER.	ITER-1
Neutron concent.	NC-000	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

=====

3.3 Description of the Plot File (*.PLT)

The SPECTRA plot file is written in a readable, ASCII format. The structure of the file is shown below. A simple post processing program: S-GRAPH, is provided for quick extract of plot data and arranging the in columns for plotting (with EXCEL or other plotting program). Use of S-GRAPH is described in section 3.3.1. A convenient visualization tool, program VISOR, is available for graphical presentation of SPECTRA results. Use of VISOR is illustrated in section 3.3.2.

An example of the plot file is shown below. The first record of the plot file contains information on how many plot variables are present in the file. In the present example the number of plot variables (NPLT) is equal to 26. The value of NPLT is written to the plot file using the format: (' NPLT =',I7) and can be read using for example the format: (8X,I7) (8 characters, integer number 7 fields wide).

```
NPLT =      26
  1.  SL-000-Time-0000-s
  2.  CV-100-Pres-atms-Pa
  3.  CV-200-Pres-atms-Pa
  4.  CV-300-Pres-atms-Pa
  5.  CV-400-Pres-atms-Pa
  6.  CV-500-Pres-atms-Pa
  7.  CV-100-Temp-atms-K
  8.  CV-200-Temp-atms-K
  9.  CV-300-Temp-atms-K
 10.  CV-400-Temp-atms-K
 11.  CV-500-Temp-atms-K
 12.  CV-100-Temp-drop-K
 13.  CV-200-Temp-drop-K
 14.  CV-300-Temp-drop-K
 15.  CV-400-Temp-drop-K
 16.  CV-500-Temp-drop-K
 17.  CV-100-Temp-pool-K
 18.  CV-200-Temp-pool-K
 19.  CV-300-Temp-pool-K
 20.  CV-400-Temp-pool-K
 21.  CV-500-Temp-pool-K
 22.  CV-100-Temp-bubb-K
 23.  CV-200-Temp-bubb-K
 24.  CV-300-Temp-bubb-K
 25.  CV-400-Temp-bubb-K
 26.  CV-500-Temp-bubb-K

0.00000E+00  1.05000E+05  1.05000E+05  1.05000E+05  1.05000E+05  1.05000E+05  3.15000E+02  3.15000E+02  3.15000E+02  3.15000E+02
3.15000E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.15000E+02  3.15000E+02  3.15000E+02  3.15000E+02
3.15000E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

2.00000E-01  1.05001E+05  1.05001E+05  1.05001E+05  1.05001E+05  1.05001E+05  3.15001E+02  3.15001E+02  3.15001E+02  3.15001E+02
3.15001E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.15000E+02  3.15000E+02  3.15000E+02  3.15000E+02
3.15000E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

4.00000E-01  1.05001E+05  1.05001E+05  1.05003E+05  1.05003E+05  1.05003E+05  3.15001E+02  3.15001E+02  3.15003E+02  3.15003E+02
3.15003E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.15000E+02  3.15000E+02  3.15000E+02  3.15000E+02
3.15000E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

5.00000E-01  1.05001E+05  1.05001E+05  1.05003E+05  1.05003E+05  1.05003E+05  3.15001E+02  3.15001E+02  3.15003E+02  3.15003E+02
3.15003E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  3.15000E+02  3.15000E+02  3.15000E+02  3.15000E+02
3.15000E+02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
```

The following NPLT records are occupied by the alphanumeric identifiers of variables, one identifier in a single record. The identifiers are written using the format: (I9,'.',A25), and can be read using for example the format (12X,A25) (12 characters, alpha-numeric string 25 characters).

Each variable identifier is a 25 (or less) character string. For example, the identifier of the atmosphere pressure in the Control Volume No. 100, is:

CV-100-Pres-atms-Pa

Each identifier consists of the following parts:

- 2 char. Package identifier. For example 'CV' is the Control Volume Package.
- 1 char. dash (-)
- 3 char. Component number, written using three digits. If for example the package identifier is 'CV' then this is the Control Volume number.
- 1 char. dash (-)
- 4 char. Variable identifier. For example 'Pres' means pressure.
- 1 char. dash (-)
- 4 char. Additional variable identifier. For example 'atms' means atmosphere. If for a given variable the additional identifier is not used, then this part contains four zeroes.
- 1 char. dash (-)
- 8 char Units of the variable. This is a string of up to 8 characters. If it is shorter than 8 characters the remaining characters are left blank. If the variable is dimensionless then the string is empty.

The next part of the plot file, below the variable identifiers, contains the plot edits. Each plot edit is preceded by a single empty line. Each plot edit consists of NPLT numbers, giving the current values of the NPLT plot variables. The values of the plot variables are written using the format: **(10(ES12.5))** (ten real numbers, each 12 fields wide with 5 decimal places after the decimal point). The same format must be used to read the plot variables.

The full list of identifiers used by the SPECTRA plot file is presented in tables Table 2-23 through Table 2-32.

3.3.1 Using S-GRAPH to Make Plots

Convenient plot programs (a "mouse-click" type) are able to perform all necessary operations: extract the requested data from the plot file, display it on the screen, and finally make a hard-copy using a printer. Such program, called VISOR, is available for SPECTRA post-processing. Examples are shown in the next section. VISOR is a first choice tool make making graphs and presenting SPECTRA results. VISOR however is limited to a certain operating platform (i.e. Windows environment). For systems such as UNIX or LINUX or for Users who do not wish to use VISOR, a simple, but generally applicable program is provided, which helps to make graphs from SPECTRA results. The program name is S-GRAPH and is described below.

The program S-GRAPH extracts one, or several variables from the SPECTRA plot file, and writes those variables in a form of several columns of numbers. When the data is available in the form of columns than a general plot program, available on given computer system, may be used to make a graph.

The process is illustrated in Figure 3-3. When SPECTRA run is finished the plottable variables are available in the plot file (*.PLT). The program S-GRAPH reads the SPECTRA plot file and a so-called plot request file (*.PLR). The structure of the plot request file is described below. The plot request file tells S-GRAPH which variable (or variables) need to be extracted from the plot file, and stored in the form of data columns.

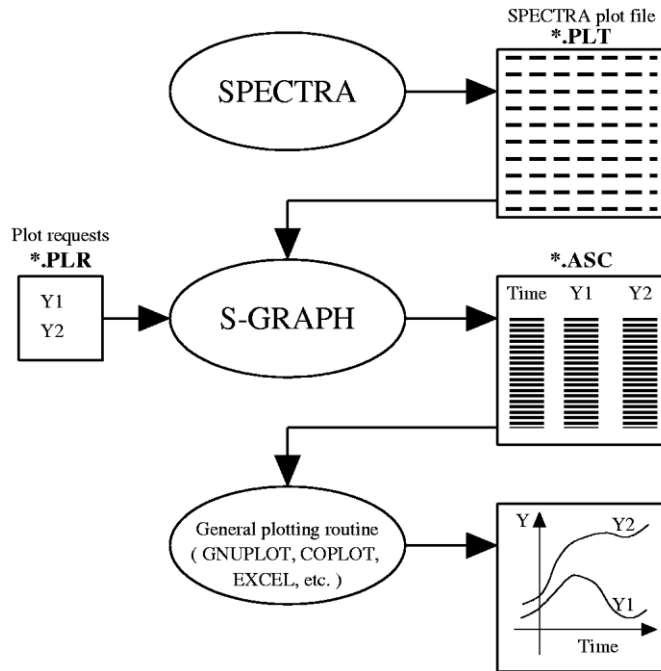


Figure 3-3 Use of the program S-GRAPH.

When S-GRAPH is finished the requested variable(s) are available in the S-GRAPH output file (*.ASC). Those data columns may be easily plotted using a general-purpose plot program available for a given system. Such programs (for example: GNUPLOT, XMGR, EXCEL, etc.) are easy to obtain for any particular system.

HOW TO USE S-GRAPH

The following steps, described below, need to be made to produce a graph with the help of the program S-GRAPH:

- Prepare requests for plot variable (or variables).
- Extract the variable data from the plot file using S-GRAPH.
- Make a graph using a plot program or a spreadsheet (EXCEL, GNUPLOT, COPLLOT).

A) Prepare the plot request file (*.PLR)

The plot request file tells S-GRAPH which variables need to be extracted from the SPECTRA plot file, and written as the columns of data. The first variable to be extracted is always time (s). It will be written in the first column. There is no need to request the time specifically in the *.PLR file.

The *.PLR file consists of one or more records (maximum is 99). Each record is a request for a single variable. There are three different formats, which can be used to request a variable:

Format 1:

The number of the variable in the plot file can be used. For example, in case of the plot file shown above, to request the CV-100 pressure one needs to write simply:

2

Format 2:

The "pointers" can be used. A set of pointers consists of four numbers. The first pointer is the package identifier. For example the CV Package has number 1. The second pointer is the component number within package. If for example the first pointer is equal to one, then the second pointer is the CV number. The third and fourth pointers indicate the variable. The values of those pointers are shown in Table 2-23 through Table 2-32. For example, in case of the CV Package the third pointer equal to 13 means pressure and the fourth pointer equal to one means atmosphere (Table 2-23). Thus, to request the same variable as above - the atmosphere pressure in CV-001, one needs to write:

1 100 13 1

Format 3:

The name of the variable can be used. To request the same variable as above one needs to write:

CV-100-Pres-atms-Pa

The units need not to be included, thus the same request may also look like:

CV-100-Pres-atms

Both strings shown above will extract the same variable from the plot file.

Any of the three formats shown above may be used. If the *.PLR file consists of a single record then it will produce two columns: time and the requested variable. If it consists of N records it will produce N+1 columns: time and the requested variables, in the same order in which they are requested, as shown in the examples shown below.

SPECTRA Code Manuals - Volume 2: User's Guide

Example 1:

The file 'PRES.PLR' contains the following lines:

```
CV-100-Pres-atms  
CV-300-Pres-atms  
CV-200-Pres-atms
```

It will produce four columns of data. The first column will contain time. The next three columns will contain atmosphere pressures in Control Volumes 100, 300 and 200 respectively. The data will be stored in the file 'PRES.ASC'

Example 2:

The file 'TEMP.PLR' contains the following lines:

```
CV-100-Temp-atms  
1 100 14 2  
CV-100-Temp-pool  
1 100 14 4
```

It will produce five columns of data: time and four temperatures: atmosphere, droplets, pool and bubbles, in CV-001. The data will be stored in the file 'TEMP.ASC'.

Example 3:

The file 'X.PLR' contains the following lines:

```
CV-100-Temp-atms  
4
```

It will produce three columns of data: time, atmosphere temperature in CV-001, and the variable that is stored with the number four in the plot file. The data will be stored in the file 'X.ASC'

B) Run S-GRAPH to extract the requested variables

Execute S-GRAPH in a directory in which the SPECTRA plot file (*.PLT) and a plot request file (*.PLR) exist.

If the directory contains only one file with the extension 'PLT', then S-GRAPH will automatically use this file as the plot file. If there are more plot files, it will display the list of all plot files present in the current directory, and ask the user to enter the file name (the extension need not be entered).

If the directory contains only one file with the extension 'PLR', then S-GRAPH will automatically use this file as the request file. If there are more request files it will display the list of all request files present in the current directory, and ask the user to enter the file name (the extension need not be entered).

S-GRAPH checks whether the requested variables are present in the plot file. If they are not it writes an appropriate error message and stops.

If the requests are valid it extracts the requested variables and stores them in the output file. The name of the S-GRAPH output file has always the extension 'ASC'. The first part of the name is the same as the name of the request file. Thus, if the name of the request file is for example: 'PRES.PLR', then the results will be written to the file 'PRES.ASC'.

The results are written in the ASCII format, in the following manner. The first line contains names of all variables (25 character strings) separated by spaces. The next records contain the values of all plot variables, separated by spaces. Some plot programs (COPLLOT) need the variable names to be written in the first record of the data file. Some other programs can only read columns of data and thus it may be necessary to delete the first record.

C) Make the graph using the file produced by S-GRAPH

In the last step a graph is made, using one of available general plot programs or spreadsheets, like EXCEL, GNUPLOT, COPLLOT, etc. If the plot program cannot read alphanumeric headers then the first record in the *.ASC file must be deleted before making a graph.

3.3.2 Using VISOR as a Post-Processor

VISOR is an excellent tool to visualise results of SPECTRA or other codes (currently VISOR may be used for RELAP, MELCOR, MAAP, as well as for data arranged in columns). Use of VISOR is described in the VISOR Manual, however the program is so user friendly and simple that may be used practically without any training. A beginner may simply start from working examples and modify them for his needs.

Some simple example pictures, made with VISOR are shown below in Figure 3-4 through Figure 3-7.

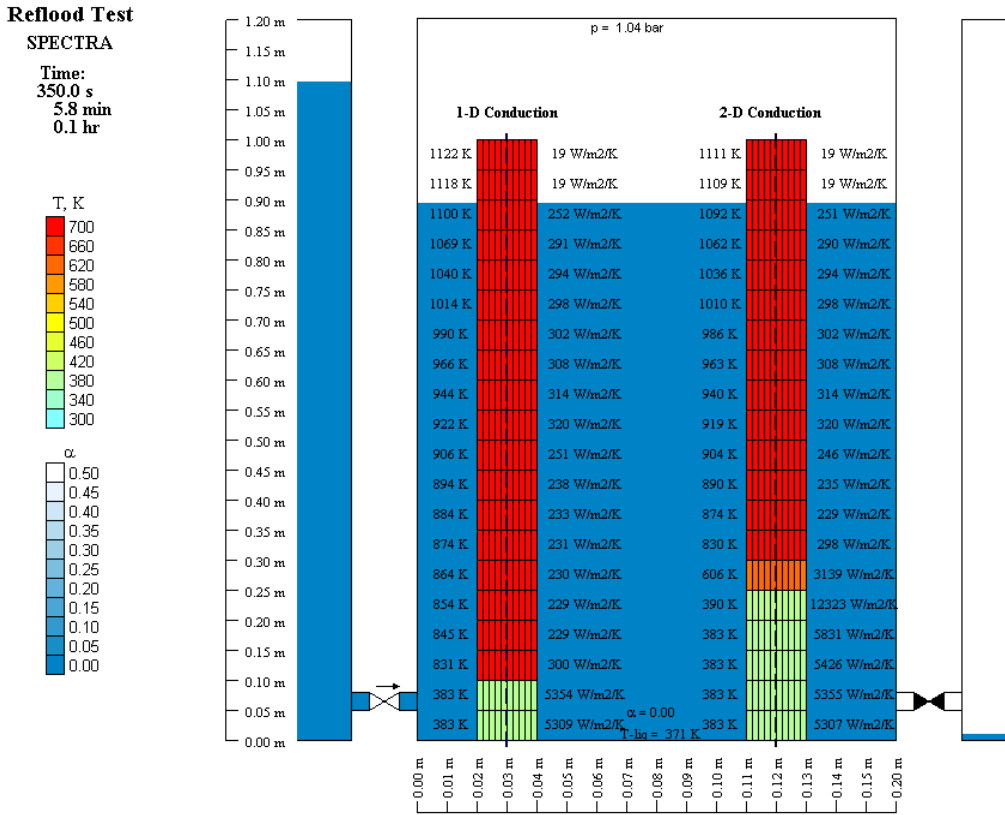


Figure 3-4 Example test case - REFLOOD.

Heat Exchanger Test

Temperature Averaging Option Applied

SPECTRA

Time: 300.1 s
5.0 min
0.1 hr

T, K
350
345
340
335
330
325
320
315
310
305
300

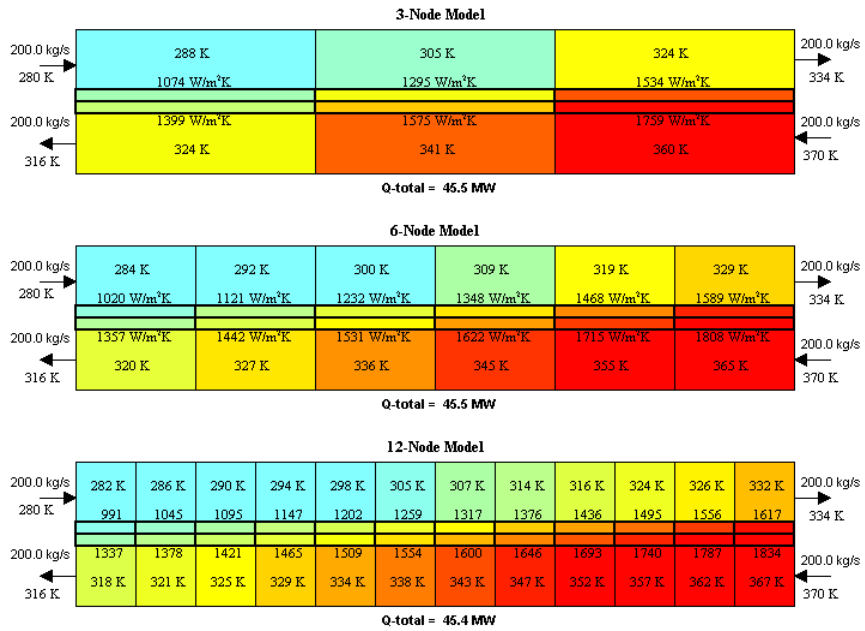


Figure 3-5 Example test case - HEX.

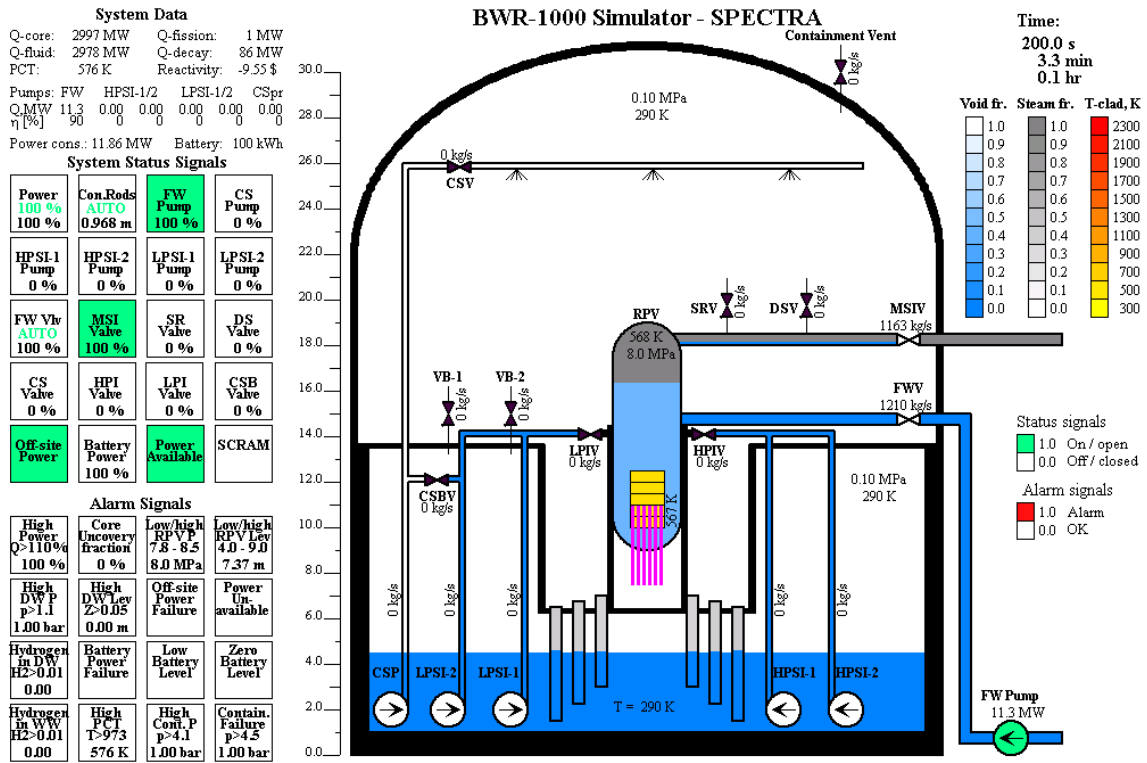


Figure 3-6 BWR-1000 simulator, reactor vessel, emergency systems, and containment.

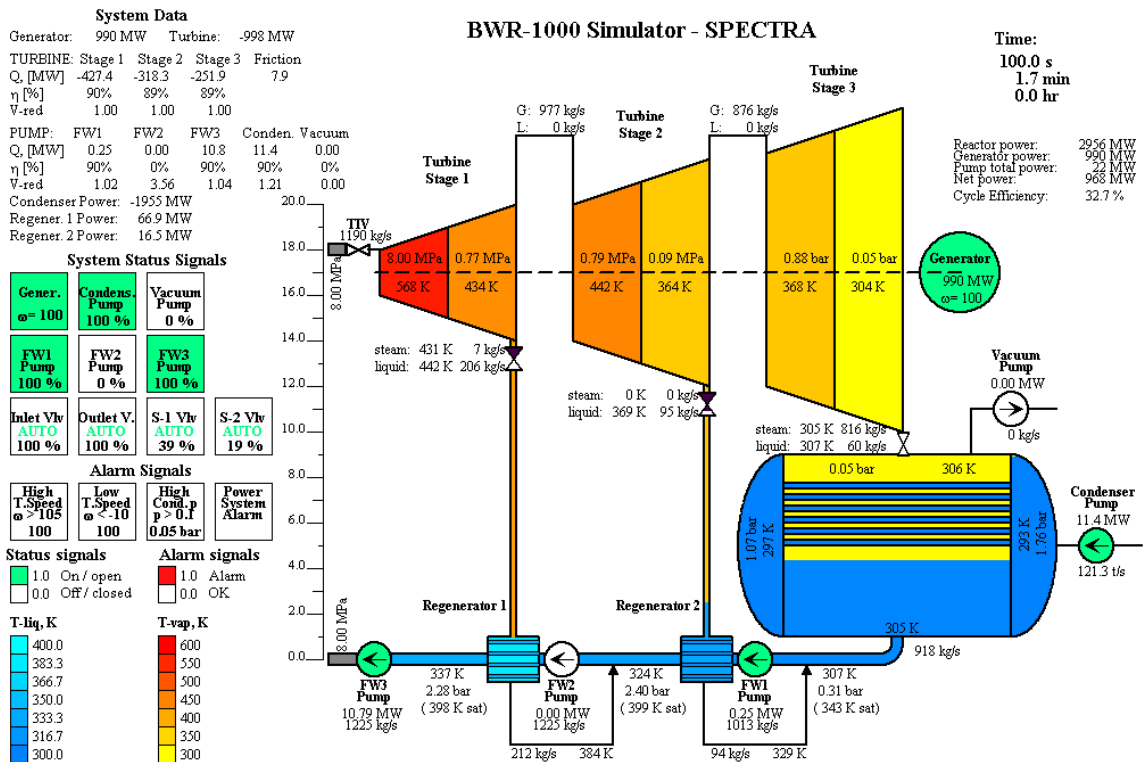


Figure 3-7 BWR-1000 simulator, turbine.

3.4 Restart File (*.RST)

The restart option is provided to allow continuing calculations, which have been terminated, either by normal termination, by stop file, or by failure. The restart file (*.RST) is a binary file, which contains values of all variables in all SPECTRA Common Blocks. When a job is restarted the values of all variables are read from the *.RST file and the calculations are continued. An example illustrating the restarting procedure is presented below.

Example

An example is provided in \Z-INPUTS\SL\Restarting\. The following input files are present:

- “Run12” Input file Run12.SPE - a “full-time” run, analysis time 0.0 – 2200 s.
- “Run1” Input file Run1.SPE - the same input, but the run time is 0 – 1100 s
- “Run2” Input file Run2.SPE - restart input – only time steps are provided
 - end time = 2200 s,
 - start time is determined interactively on restart, as shown below.

It is important to note that the input file for restarting should contain minimum input (as all input will be read from the restart file. In the present case, the input file Run2.SPE contains the following inputs:

```
*
*      DTMAX  DTMIN    DTPRT  DTPLT   TEND  *   Time step data
900001  0.1    1.0E-6   100.0  10.0   2200.0 *
*
```

The run script, provided in the test run location \Z-INPUTS\SL\Restarting\, the file “Run-all.bat” contains the following commands:

```
call C:\SPECTRA\Z-EXE\SPECTRA.EXE Run12.SPE
call C:\SPECTRA\Z-EXE\SPECTRA.EXE Run1.SPE

copy Run1.RST Run2.RST
copy Run1.OUT Run2.OUT
copy Run1.PLT Run2.PLT
copy Run1.MES Run2.MES
copy Run1.DIA Run2.DIA

call C:\SPECTRA\Z-EXE\SPECTRA.EXE Run2.SPE
```

The run script performs the following operations:

- First, it executes the full run, Run12.SPE (2200 s), which serves as reference run.
- Next, it executes the run Run1.SPE, which covers the first half of the transient (1100 s)
- Next it copies the results of the output files from run “Run1” to “Run2”
- Finally, it executes the Run2.SPE. When this one is executed, SPECTRA detects the presence of the restart file and starts the interactive restarting process, which is shown below.

SPECTRA Code Manuals - Volume 2: User's Guide

```
C:\Windows\System32\cmd.exe
=SPE= SPECTRA Version 22-04, Apr. 2022, Windows

Sophisticated
Plant
Evaluation
Code for
Thermal-hydraulic
Response
Assessment
-----
Validity: 12/2025, Applicability: AppC = 0000
-----

> INPUT DATA FILE : \> Run2.SPE

> RESTART FILE EXISTS. ENTER "R" TO RESTART, OTHER TO START : \> r

-> READING RESTART FILE
> CURRENT TIME: 5.00000E+02 [s], RESTART FROM THIS POINT (Y/N) : \> n
> CURRENT TIME: 1.10000E+03 [s], RESTART FROM THIS POINT (Y/N) : \> y

-> CURRENT TIME STEP DOMAIN NUMBER: 1
-> TIME STEPS AND END TIME
> MAXIMUM DT ( 1.00000E-01 [s] ), NEW: \> 0
> MINIMUM DT ( 1.00000E-06 [s] ), NEW: \> 0
> PRINT DT ( 1.00000E+02 [s] ), NEW: \> 0
> PLOT DT ( 1.00000E+01 [s] ), NEW: \> 0
> END TIME ( 2.20000E+03 [s] ), NEW: \> 0

-> TRANSIENT CALCULATIONS RESTARTED

t = 1.38E+03 ( 64%) dt = 1.00E-01 CPU = 2.34E-01 RUN = 1.00E+00 Iter: 4

-> END OF CALCULATIONS.

-> RUN STATISTICS
-----
Analyzed model time [s]: 0.230E+04 ( 0.639 [hrs] ) 100%
Processor time (CPU) [s]: 0.781 ( 0.217E-03 [hrs] )
Clock time (RUN) [s]: 1.55 ( 0.430E-03 [hrs] )
Warp factor (model/CPU) : 0.294E+04 ( 1 / 0.340E-03 )
Run ratio (RUN/model) : 0.673E-03 ( 1 / 0.149E+04 )
Minimum time step [s]: 0.100E+00
Maximum time step [s]: 0.100E+00
Average time step [s]: 0.100E+00
No. of advancements 23001
No. of iter. per advanc.: 4.20
CPU per advancement [s]: 0.340E-04
Run time per advanc. [s]: 0.673E-04
-----

-> =SPE= SPECTRA Version 22-04, Apr. 2022, Windows
FILES CLOSED ON : 20/10/2022, 18:29:21.68
```

When Run2.SPE is started, SPECTRA detects that the restart file exists for the requested job ("Run2.RST"). It therefore asks whether the user wishes to restart the job, or to start a new run. In this case the user wants to restart, therefore "r" (or "R") is entered.

Next, the program reads the restart file, prints the times of the restart points, and asks the user to restart the job. In this case the user wants to restart from the second point, at $t = 1100$ s.

Next, the program asks for the new time steps, print and plot intervals, and the end time for this time step domain. The values read from the restart file are the default values, and they are printed in brackets. For the present example the user does not wish to change the time steps; therefore, zeroes are entered.

SPECTRA Code Manuals - Volume 2: User's Guide

The output file and the diagnostics file are appended, so the information from the first run is not lost.

Note 1:

If the output/plot files are not copied, then the results of the Run2.SPE will contain only the data for times between 1100 s and 2200 s. The plot file will still be readable; in the case when no previous plot file is provided, SPECTRA will start the new plot file by writing variable names/ headers, so the plot file will be readable by the usual plotting programs.

Note 2:

During the restart the input file (in this case Run2.SPE), if exists, should contain only the Solver (time step) data and eventually the Tabular Function data that should replace the data in the restart file (see section 2.20). An example of the input file (Run2-TF.SPE) that may be used on restart to redefine an existing Tabular Function, TF-100, is presented below.

```
*
*          DTMAX  DTMIN    DTPRT  DTPLT   TEND  * Time step data
900001  0.1    1.0E-6    100.0   10.0   2200.0 *
*
605100  Downstream boundary pressure versus time, p(t)
600100   0.0    0.100E+5  1
600100 1000.0  10.000E+5  2
600100 1200.0  10.000E+5  3
600100 2000.0   1.000E+5  4
```

Compared to the original TF-100, the last value has been redefined from 0.1E+5 to 1.0E+5. The run Run2-TF may be executed in the same way as Run-2, i.e.

- The output files from “Run-1” should be copied to “Run-2-TF”
- The Run-2-TF.SPE should be executed and restarted from the second restart point.

In this case Run2-TF will be the same as Run2 until 1200 s. After that the results will be different as the values of TF-100 are different.

Summarizing, it should be noted that:

- The data that must always be entered interactively includes:
 - the restarting time point,
 - the time step data for the current time step domain (zeros may be entered to keep the old value).
- The data that may be entered in the SPECTRA input file (*.SPE) includes:
 - Solver data,
 - TF data.

Currently, only the Solver data and the TF data may be re-defined in the SPECTRA input file upon restart (see section 2.20).

SPECTRA Code Manuals - Volume 2: User's Guide

3.5 The Initial Condition File (*.ICF)

At the end of each calculations SPECTRA writes all current parameters (pressures, temperatures, fluid velocities, etc., into the *.ICF file. In contrast to the restart file, the ICF file is a text file, so it is easy for the user to manipulate. An example of an ICF file is shown below.

```
=CV= INITIAL CONDITION DATA FOR 5 CONTROL VOLUMES

CV DSP TSP PSP
001 0.00000000E+00 0.00000000E+00 0.00000000E+00
002 0.00000000E+00 0.00000000E+00 0.00000000E+00
003 0.00000000E+00 0.00000000E+00 0.00000000E+00
004 0.00000000E+00 0.00000000E+00 0.00000000E+00
005 0.00000000E+00 0.00000000E+00 0.00000000E+00

CV ATMS-PRES ATMS-TEMP POOL-LEVEL POOL-TEMP
001 1.10120002E+05 3.19267493E+02 5.24442099E+00 3.15027081E+02
002 1.10191625E+05 3.19314069E+02 5.00000195E+00 3.14999980E+02
003 1.05034461E+05 3.15032406E+02 4.99999897E+00 3.14999904E+02
004 1.05034460E+05 3.15032405E+02 4.99999897E+00 3.14999904E+02
005 1.05034461E+05 3.15032407E+02 4.99999897E+00 3.14999904E+02

CV ATMS GAS COMPOSITION
001 0.00000000E+00 0.00000000E+00 4.31708948E-01 7.62233365E-01 1.97758053E-01 0.00000000E+00
002 0.00000000E+00 0.00000000E+00 4.14391333E-01 7.59650039E-01 2.01874765E-01 0.00000000E+00
003 0.00000000E+00 0.00000000E+00 2.88037881E-03 9.99774778E-01 0.00000000E+00 0.00000000E+00
004 0.00000000E+00 0.00000000E+00 2.88038628E-03 9.99774778E-01 0.00000000E+00 0.00000000E+00
005 0.00000000E+00 0.00000000E+00 2.88036870E-03 9.99774779E-01 0.00000000E+00 0.00000000E+00

CV DROP.FRACTION TEMPERATURE DIAMETER POSITION
001 9.45904198E-06 3.46641497E+02 1.00000000E-02 3.33195737E+00
002 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
003 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
004 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
005 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00

CV BUBB.FRACTION TEMPERATURE DIAMETER POSITION
001 4.65286629E-02 3.14969153E+02 1.60000000E-02 4.19204872E+00
002 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
003 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
004 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
005 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00

CV BUBB GAS COMPOSITION
001 0.00000000E+00 0.00000000E+00 5.41465292E-01 9.63177081E-01 0.00000000E+00 0.00000000E+00
002 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
003 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
004 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
005 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00

=JN= INITIAL CONDITION DATA FOR 1 JUNCTIONS

JN ATMS-VELOCITY POOL-VELOCITY
001 4.25095714E-01 0.00000000E+00

JN VALVE OPEN FR. K-FORWARD K-REVERSE
001 1.00000000E+00 1.00000000E+00 1.00000000E+00

JN ATMS-PUMP-SPEED POOL-PUMP-SPEED ATMS-PUMP-FLOW POOL-PUMP-FLOW
001 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00

=SC= INITIAL CONDITION DATA FOR 12 1-D SOLID HEAT CONDUCTORS
CELL TEMPERATURES
SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
001 2 00 3.15002253E+02 3.15001981E+02
SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
002 2 00 3.15002253E+02 3.15001981E+02
SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
003 2 00 3.15002253E+02 3.15001981E+02
SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
004 2 00 3.15002253E+02 3.15001981E+02
SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
005 2 00 3.15002253E+02 3.15001981E+02
SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
006 2 00 3.15002252E+02 3.15001980E+02
SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
```


SPECTRA Code Manuals - Volume 2: User's Guide

```
007  2 00 3.15002251E+02 3.15001979E+02
      SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
008  2 00 3.15002258E+02 3.15001982E+02
      SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
009  2 00 3.15002262E+02 3.15001983E+02
      SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
010  2 00 3.15002964E+02 3.15002529E+02
      SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
011  2 00 2.77516768E+02 2.77324570E+02
      SC N K/L ----- 01 ----- ----- 02 ----- ----- 03 ----- ----- 04 ----- ----- 05 -----
012  2 00 2.77516768E+02 2.77324570E+02
```

```
SC OXIDATION DATA, METAL AND OXIDE THICKNESSES IN BOUNDARY CELLS
SC  LEFT METAL      LEFT OXIDE      RIGHT METAL      RIGHT OXIDE
001  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
002  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
003  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
004  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
005  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
006  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
007  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
008  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
009  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
010  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
011  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
012  0.00000000E+00  0.00000000E+00  0.00000000E+00  0.00000000E+00
```

=TC= INITIAL CONDITION DATA FOR 0 2-D SOLID HEAT CONDUCTORS

=CF= INITIAL CONDITION DATA FOR 0 CONTROL FUNCTIONS

=RK= REACTOR KINETICS CF NO.: 0 (CF-000)

This file may be used to provide initial conditions for another calculations. This is done in record 905000 (see section 2.16.3). When the ICF file is requested in record 905000, then all conditions that are present in the input deck are replaced by the values read from the ICF file. Therefore, **If the ICF file is used and the user wishes to change some parameter in the system, he cannot do it in the input deck! the parameter must be modified in the ICF file.** This is easily done, since the ICF is an ASCII file.

For example, the user needs to run a full power stationary state using the reactor kinetics model. The initial temperatures of fluid and structures, entered in the input deck, are usually not very accurate. Consequently the temperatures will change before steady state operation is reached. If the user starts the run directly with the reactor kinetics model, then the thermal feedback would cause large reactivity changes and would make it very difficult to keep the reactor at the desired power. To avoid this one can apply a two-step procedure:

1. Run the model with a constant reactor power (defined by a Tabular Function) for a time sufficiently long to obtain stable parameters in the analysed system. This Constant Power (CP) run will produce the file CP.ICF.
2. Start the reactor kinetics run (RK) using the initial conditions calculated in the CP run, by requesting the file CP.ICF in record 905000.

3.6 The Tabular Function Data File (*.TFD)

The TFD file may be used to change the value of any Tabular Function that is defined as interactive (see section 2.7.5). The interactive functions are used to run SPECTRA as a background code for a simulator.

In order to change the value of any function, one has simply to type the function number and the value. For example, the following record in the TFD file:

500 -2.37

will change the value of function TF-500 to -2.37. Note that the change will be restricted by the limits imposed on the function (see section 2.7.3).

If several definitions are present in the TFD file, then the last one is used. For example, if the following records are present in the TFD file:

```
500 -2.37
500 +1.23
500 0.0
500 1000.0
```

then the value of TF-500 will be set to 1000.0.

In order to switch back to the TF data tabulated in the input deck, one must remove all definitions of given TF from the TFD file. This can be done automatically using the automatic reset option - record 611XXX.

3.7 Message File (*.MES)

The message file contains messages about certain events. The following events are written to the message file:

- change of burn status within CV, change of burn propagation status,
- change of valve status (opening/closing),
- change of pump/turbine status (starting up/stopping),
- reaching user defined limits (min/max, rates of change) for TF/CF,
- EDF data transfers (optionally, if requested by the user),
- TF value read from the *.TFD file (timing and value read).

3.8 Stop File (*.STP)

Calculations can be terminated at any time using a SPECTRA Stop File. To do this user has to put a file, with the name "*.STP", in the directory where the run is performed.

When the program encounters the presence of the stop file it asks the user for confirmation (see the example printout below). If the termination is confirmed, the program writes the final edit in the output and plot files, writes the restart file, deletes the stop file (to avoid unintended stopping in the future), and terminates the calculations. Below, an example of the screen output is shown.

```
t = 5.13E+04 ( 0%) dt = 1.00E+01 CPU = 1.00E+01 RUN = 1.00E+01 Iter: 6
t = 7.15E+04 ( 0%) dt = 1.00E+01 CPU = 1.10E+01 RUN = 1.10E+01 Iter: 6

-> STOP SIGNAL ENCOUNTERED
```

SPECTRA Code Manuals - Volume 2: User's Guide

```
> ENTER "Y" TO CONFIRM TERMINATION OF THE RUN
> ENTER "N" TO CONTINUE AFTER INTERACTIVE MENU
> ENTER "F" TO REDIRECT INTERACTIVE MENU TO STOP FILE
> Y
> RUN TERMINATED BY THE STOP FILE

-> RUN STATISTICS
-----
Analyzed model time (s): 0.733E+05 ( 20.4 (hrs) ) 0%
Processor time (CPU) (s): 10.1 ( 0.281E-02 (hrs) )
Clock time (RUN) (s): 10.1 ( 0.281E-02 (hrs) )
Warp factor (model/CPU) : 0.724E+04 ( 1 / 0.138E-03 )
Run ratio (RUN/model) : 0.138E-03 ( 1 / 0.725E+04 )
Minimum time step (s): 1.000
Maximum time step (s): 10.00
Average time step (s): 4.49
No. of advancements 16347
No. of iter. per advanc.: 6.13
CPU per advancement (s): 0.619E-03
Run time per advanc. (s): 0.619E-03
-----

-> =SPE= SPECTRA Version 3.61, February 2016
FILES CLOSED ON : 22/02/2016, 22:04:59.26
```

The "stop file" may also be used to change time steps, activate the extended diagnostics or debug printout (section 2.16.2, 2.16.4). To change time steps or activate the extended diagnostics or debug printout, the user has to answer "N" or "n" when asked to confirm termination of the run (see the example output below). In this case the program will ask the user for the time steps, print and plot intervals, as well as the end time for this time step domain. If zeroes are entered then the current values are used (unchanged). Next, the program will ask whether the extended diagnostics or debug printout should be activated. If the transient diagnostics is suppressed (see section 2.16.7), then the program will ask first whether the transient diagnostics should be activated. Then, if the answer is yes, it will ask whether the user wishes to activate the extended diagnostics and the debug printout.

Finally, the program will ask whether to write a restart and the ICF data at the current time. Thus the STOP file may be used to obtain an extra restart point or ICF data (apart from the restarts that are being written in the restart frequency of DTRST - see section 2.16.2 and the ICF file which is always written at the termination of the run). Below, an example of the screen output is shown.

```
t = 7.25E+04 ( 0%) dt = 1.00E+01 CPU = 1.00E+01 RUN = 1.00E+01 Iter: 6
t = 8.33E+04 ( 0%) dt = 1.00E+01 CPU = 1.10E+01 RUN = 1.10E+01 Iter: 6

-> STOP SIGNAL ENCOUNTERED
> ENTER "Y" TO CONFIRM TERMINATION OF THE RUN
> ENTER "N" TO CONTINUE AFTER INTERACTIVE MENU
> ENTER "F" TO REDIRECT INTERACTIVE MENU TO STOP FILE
> N
> RUN WILL BE CONTINUED

> CURRENT TIME: 8.50324E+04 (s), CURRENT DOMAIN No.: 3
> MAXIMUM DT ( 1.00000E+01 (s) ), NEW:\> 0
> MINIMUM DT ( 1.00000E-05 (s) ), NEW:\> 0
> PRINT DT ( 9.00000E+03 (s) ), NEW:\> 0
> PLOT DT ( 5.00000E+02 (s) ), NEW:\> 0
> END TIME ( 1.00000E+05 (s) ), NEW:\> 0
> DO YOU WANT EXTENDED DIAGNOSTICS IN THE NEXT PART OF THE RUN (Y/N) :\> N
> DO YOU WANT DEBUG PRINTOUT IN THE NEXT PART OF THE RUN (Y/N) :\> N
> DO YOU WANT TO WRITE A RESTART AT THE CURRENT TIME POINT (Y/N) :\> N
> DO YOU WANT TO WRITE AN ICF AT THE CURRENT TIME POINT (Y/N) :\> N

-> TRANSIENT CALCULATIONS CONTINUED
```

SPECTRA Code Manuals - Volume 2: User's Guide

```
t = 8.50E+04 ( 0%) dt = 1.00E+01 CPU = 1.11E+01 RUN = 3.23E+01 Iter: 6
t = 1.17E+05 ( 1%) dt = 1.00E+02 CPU = 1.21E+01 RUN = 3.33E+01 Iter: 6
```

In some cases it is convenient to redirect the interactive menu into the content of the *.STP file. This can be done by pressing "F" or "f". The content of the *.STP file should look like:

```
N * DON'T STOP
O * MAX DT
O * MIN DT
O * PRINT DT
O * PLOT DT
O * END TIME
N * EXTENDED DIAGNOSTICS
N * DEBUG PRINTOUT
N * WRITE RESTART POINT
N * WRITE ICF
```

Below, an example of the screen output is shown for the above *.STP file.

```
t = 5.30E+04 ( 0%) dt = 1.00E+01 CPU = 8.99E+00 RUN = 9.00E+00 Iter: 6
t = 6.97E+04 ( 0%) dt = 1.00E+01 CPU = 9.98E+00 RUN = 1.00E+01 Iter: 6

-> STOP SIGNAL ENCOUNTERED
> ENTER "Y" TO CONFIRM TERMINATION OF THE RUN
> ENTER "N" TO CONTINUE AFTER INTERACTIVE MENU
> ENTER "F" TO REDIRECT INTERACTIVE MENU TO STOP FILE
> F

> RUN WILL BE CONTINUED

> CURRENT TIME: 7.78024E+04 (s), CURRENT DOMAIN No.: 3
> MAXIMUM DT ( 1.00000E+01 (s) ), NEW:\> 0.000000000000000E+000
> MINIMUM DT ( 1.00000E-05 (s) ), NEW:\> 0.000000000000000E+000
> PRINT DT ( 9.00000E+03 (s) ), NEW:\> 0.000000000000000E+000
> PLOT DT ( 5.00000E+02 (s) ), NEW:\> 0.000000000000000E+000
> END TIME ( 1.00000E+05 (s) ), NEW:\> 0.000000000000000E+000
> DO YOU WANT EXTENDED DIAGNOSTICS IN THE NEXT PART OF THE RUN (Y/N) :\> N
> DO YOU WANT DEBUG PRINTOUT IN THE NEXT PART OF THE RUN (Y/N) :\> N
> DO YOU WANT TO WRITE A RESTART AT THE CURRENT TIME POINT (Y/N) :\> N
> DO YOU WANT TO WRITE AN ICF AT THE CURRENT TIME POINT (Y/N) :\> N

-> TRANSIENT CALCULATIONS CONTINUED

t = 7.78E+04 ( 0%) dt = 1.00E+01 CPU = 1.05E+01 RUN = 1.59E+01 Iter: 6
t = 9.44E+04 ( 0%) dt = 1.00E+01 CPU = 1.15E+01 RUN = 1.69E+01 Iter: 6
```

4 SPECTRA Installation Guide

This chapter describes installation and verification of the SPECTRA code. Hardware requirements are given in section 4.1. Installation is discussed in section 4.2. Installation of the program should be followed by verification, which consists of rerunning the supplied test case with the newly installed program and comparing the obtained results with the supplied reference results. A short guide how to execute the program is provided in section 4.3. The reference results of the test case for verification of the installed code are described in section 4.4. Section 4.5 discusses the automatic verification. Section 4.6 discusses other possible verification runs.

4.1 Hardware and Software Requirements

SPECTRA may be run under Windows or Linux operating systems. Both Windows and Linux versions are delivered.

4.2 Installation of the SPECTRA Code

The SPECTRA distribution consists of the following parts:

- SPECTRA code
- Code manuals
- Utilities (inputs for V&V and test input files)

Installation procedure for SPECTRA:

- SPECTRA executable should be copied to a preferred location, for example:
 - Windows:
C:\SPECTRA\SPECTRA.EXE
 - Linux
~/SPECTRA/SPECTRA.X
- In Windows an appropriate link should be set, to be able to start SPECTRA calculations by simply double-clicking on a SPECTRA input file *.SPE. This may be done as follows:
 - Right-click on any SPECTRA input file, *.SPE
 - Select “open with”
 - Select “browse” (or “Look for another app on this PC”, depending on Windows version)
 - Select the SPECTRA code executable, located as selected in the previous step.

The post-processor/visualization tool for SPECTRA (also applicable for other codes, MELCOR, RELAP5, etc.), VISOR, is distributed together with the SPECTRA code. The distribution consists of the following parts:

- VISOR code
- User's manual

Installation procedure for VISOR:

SPECTRA Code Manuals - Volume 2: User's Guide

- VISOR can only be executed under Windows. It can read plot files created on both Windows and Linux machines. Visor should be copied to a preferred location, for example: C:\SPECTRA\VISOR.EXE
- An appropriate link should be set, to be able to start VISOR by simply double-clicking on a VISOR input file *.VSD. This may be done as follows:
 - Right-click on any Visor input file, *.VSD
 - Select “open with”
 - Select “browse” (or “Look for another app on this PC”, depending on Windows version)
 - Select the VISOR code executable, located as selected in the previous step.

4.3 Execution of the Code

If the links described in the previous section are set then:

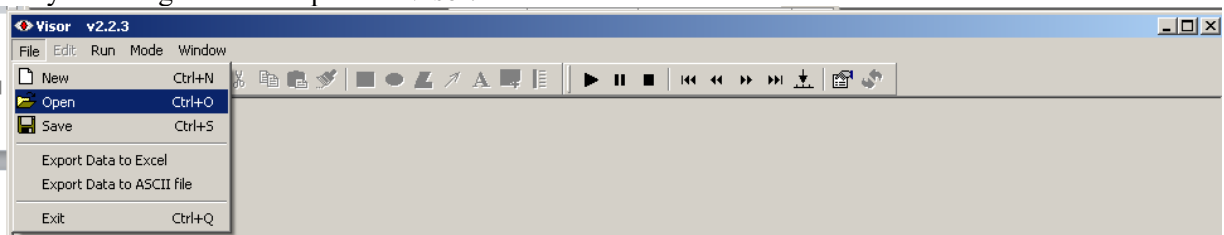
- SPECTRA can be started by simply double-clicking on a SPECTRA input file *.SPE
- VISOR can be started by simply double-clicking on a VISOR visualization file *.VSD

Alternatively, these programs can be started by double clicking on the executable files, followed by typing the SPECTRA input file name:

```
C:\SPECTRA.361\Z-EXE\SPECTRA-3-61.exe

=====  
=SPE= SPECTRA Version 3.61, Jan. 2020, Windows  
Sophisticated  
Plant  
Evaluation  
Code for  
Thermal-hydraulic  
Response  
Assessment  
=====  
Validity: 01/2022, Applicability: AppC = 0000  
=====  
> INPUT DATA FILE :>
```

or by selecting “File” - “Open” in Visor:



SPECTRA Code Manuals - Volume 2: User's Guide

Alternatively, a script may be written to start specific SPECTRA jobs. This method is more convenient if multiple jobs need to be started. For example, suppose we define a Windows script (e.g. as a file: Run-123.bat) as follows:

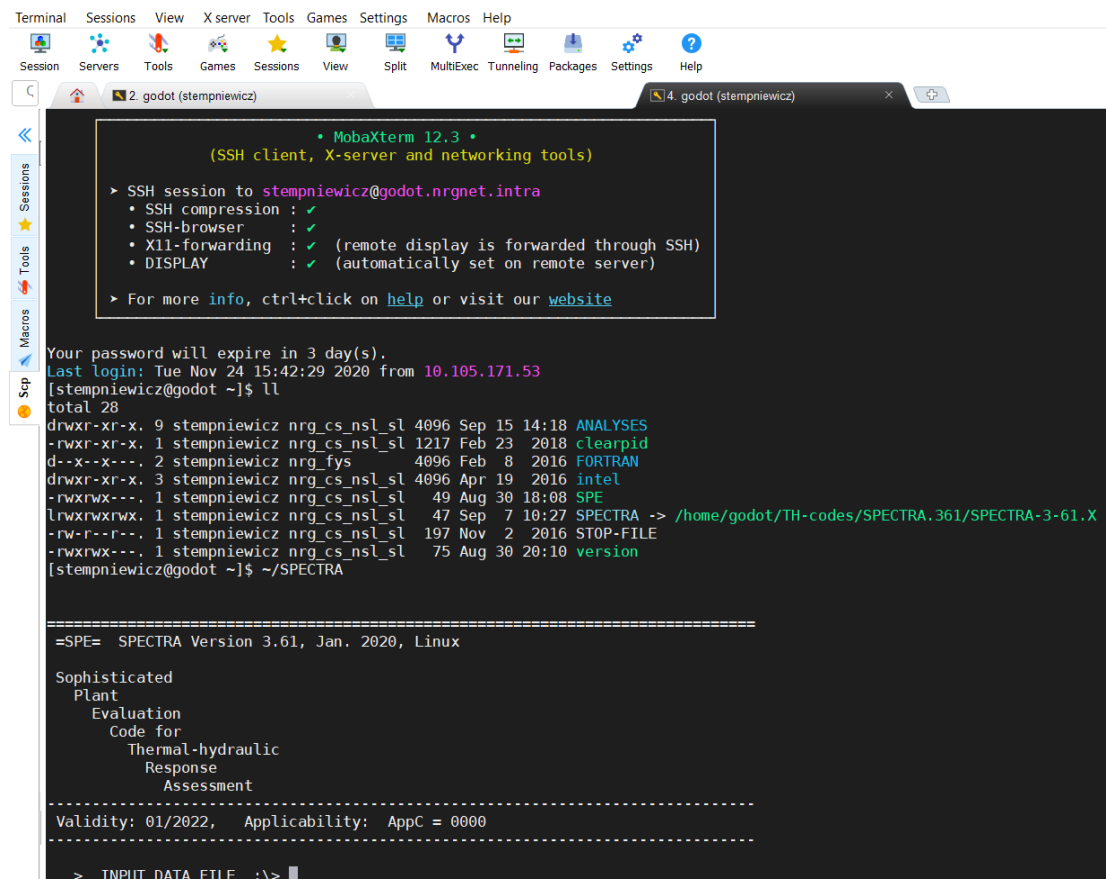
```
start C:\SPECTRA\SPECTRA.EXE JOB1.SPE
start C:\SPECTRA\SPECTRA.EXE JOB2.SPE
call C:\SPECTRA\SPECTRA.EXE JOB3.SPE
```

This will start simultaneously three calculations, with inputs defined as JOB1, JOB2, and JOB3. If we want to start runs subsequently, this can be done using the following script:

```
call C:\SPECTRA\SPECTRA.EXE Test1.SPE
call C:\SPECTRA\SPECTRA.EXE Test2.SPE
call C:\SPECTRA\SPECTRA.EXE Test3.SPE
```

The calculations will be performed in sequence, i.e. Test 2 will be started when Test 1 is finished, etc.

Similar ways are available in Linux. The code can be started by typing the full path to the code and then typing the input file name at the command prompt:



```
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help
2. godot (stempniewicz) 4. godot (stempniewicz)
• MobaXterm 12.3 •
  (SSH client, X-server and networking tools)
  > SSH session to stempniewicz@godot.nrgnet.intra
    • SSH compression : ✓
    • SSH-browser      : ✓
    • X11-forwarding   : ✓ (remote display is forwarded through SSH)
    • DISPLAY          : ✓ (automatically set on remote server)
  > For more info, ctrl+click on help or visit our website

Your password will expire in 3 day(s).
Last login: Tue Nov 24 15:42:29 2020 from 10.105.171.53
[stempniewicz@godot ~]$ ll
total 28
drwxr-xr-x. 9 stempniewicz nrg_cs_nsl_sl 4096 Sep 15 14:18 ANALYSES
-rwxr-xr-x. 1 stempniewicz nrg_cs_nsl_sl 1217 Feb 23 2018 clearpid
d--x--x---. 2 stempniewicz nrg_fys      4096 Feb  8 2016 FORTRAN
drwxr-xr-x. 3 stempniewicz nrg_cs_nsl_sl 4096 Apr 19 2016 intel
-rwxrwx---. 1 stempniewicz nrg_cs_nsl_sl  49 Aug 30 18:08 SPE
lrwxrwxrwx. 1 stempniewicz nrg_cs_nsl_sl  47 Sep  7 10:27 SPECTRA -> /home/godot/TH-codes/SPECTRA.361/SPECTRA-3-61.X
-rw-r--r---. 1 stempniewicz nrg_cs_nsl_sl 197 Nov  2 2016 STOP-FILE
-rwxrwx---. 1 stempniewicz nrg_cs_nsl_sl  75 Aug 30 20:10 version
[stempniewicz@godot ~]$ cd ~/SPECTRA

=====
=SPE= SPECTRA Version 3.61, Jan. 2020, Linux

Sophisticated
Plant
Evaluation
Code for
Thermal-hydraulic
Response
Assessment
-----
Validity: 01/2022, Applicability: AppC = 0000
-----

> INPUT DATA FILE : \>
```

SPECTRA Code Manuals - Volume 2: User's Guide

Linux jobs can be started in the background, using the `nohup` command. For example, suppose we define a script (e.g. as an executable file: `Run-123.x`) as follows:

```
nohup ~/SPECTRA/SPECTRA.X JOB1.SPE > JOB1.SCN &  
nohup ~/SPECTRA/SPECTRA.X JOB2.SPE > JOB2.SCN &  
nohup ~/SPECTRA/SPECTRA.X JOB3.SPE > JOB3.SCN &
```

This will start simultaneously three calculations, with inputs defined as `JOB1`, `JOB2`, and `JOB3`. The output that is normally sent to the screen, will be sent to the prescribed file, in this case `*.SCN`. The screen output is a short summary of an advancement, including the current time, the percentage advancement, the time step used, CPU Time and run (clock) time elapsed, and the number of iterations needed. An example of the screen output is shown below:

```
t =-9.90E+00 ( 0%) dt = 1.00E-01 CPU = 3.63E+00 RUN = 3.62E+00 Iter: 20  
t =-9.89E+00 ( 0%) dt = 4.71E-03 CPU = 4.84E+00 RUN = 4.83E+00 Iter: 5  
t =-9.85E+00 ( 0%) dt = 8.57E-03 CPU = 5.92E+00 RUN = 5.91E+00 Iter: 11  
t =-9.80E+00 ( 0%) dt = 8.56E-03 CPU = 7.16E+00 RUN = 7.15E+00 Iter: 5  
t =-9.76E+00 ( 0%) dt = 8.56E-03 CPU = 8.26E+00 RUN = 8.25E+00 Iter: 5
```

The jobs can also be started in the foreground, in which case they will be executed subsequently. For example, suppose we define a script (e.g. as an executable file: `Run-123.x`) as follows:

```
~/SPECTRA/SPECTRA.X Test1.SPE  
~/SPECTRA/SPECTRA.X Test2.SPE  
~/SPECTRA/SPECTRA.X Test3.SPE
```

The calculations will be performed in sequence, i.e. Test 2 will be started when Test 1 is finished, etc. It should be noted that Linux system is case-sensitive, so `Test1.SPE` is not the same as, for example, `test1.spe`. In Windows system the file names are not case sensitive.

During the calculations `SPECTRA` creates output files, described in Chapter 3. The output files are located in the same directory where the input file exist, and have the same name as the input file but with different extensions (see section 3).

4.4 Manual Verification

The manual verification test is provided in the directory:

```
\Z-INPUTS\Qualification-tests-EFP\
```

The full test “establishment of flow problem” (EFP) is described in detail in Volume 3. The verification test discussed here consists of the first 60 seconds of EFP Case A. Results of `SPECTRA` are compared to the results of `MELCOR`. The visualization picture for this test is provided in `EFP-SPE.VSD`. The end state ($t = 60$ s) is shown in Figure 4-1. In order to perform verification of calculated results the following steps should be taken.

- Run the file: `EFP-A.SPE` using the Windows or Linux version of `SPECTRA`.
- Compare the output file: `EFP-A.OUT`, with the source file delivered in:
 `\Z-INPUTS\Qualification-tests-EFP\Source\EFP-A.OUT` (Windows version)
 `\Z-INPUTS\Qualification-tests-EFP\Source-Linux\EFP-A.OUT` (Linux version)

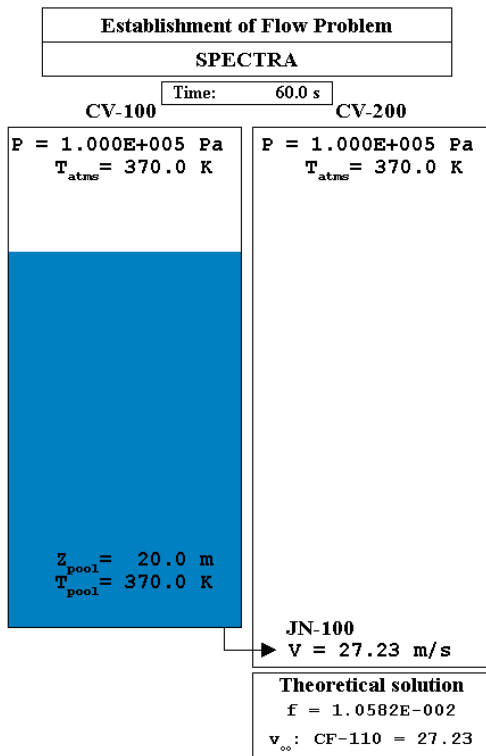


Figure 4-1 Test “establishment of flow” - visualization screen from EFP-SPE.VSD

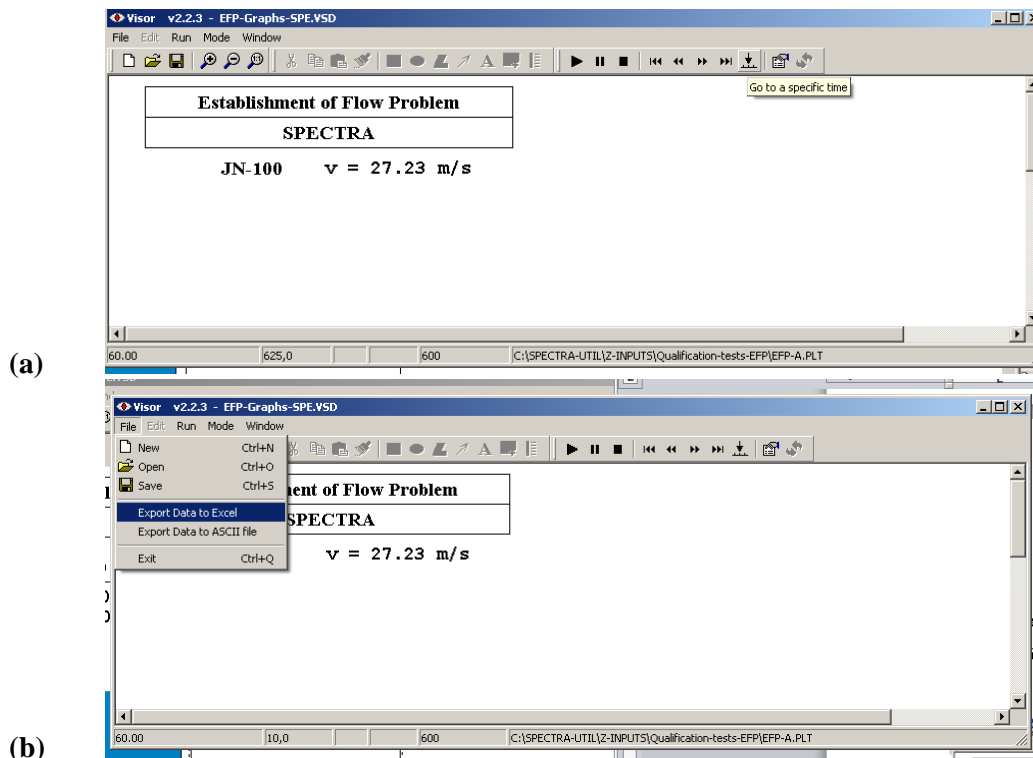
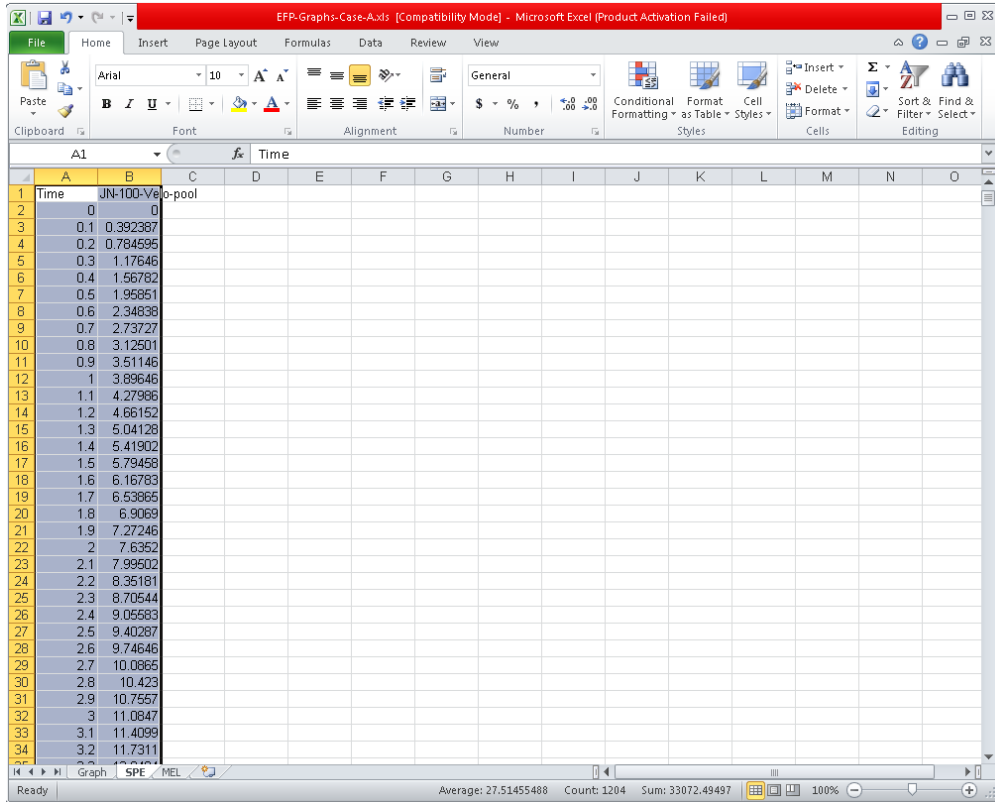
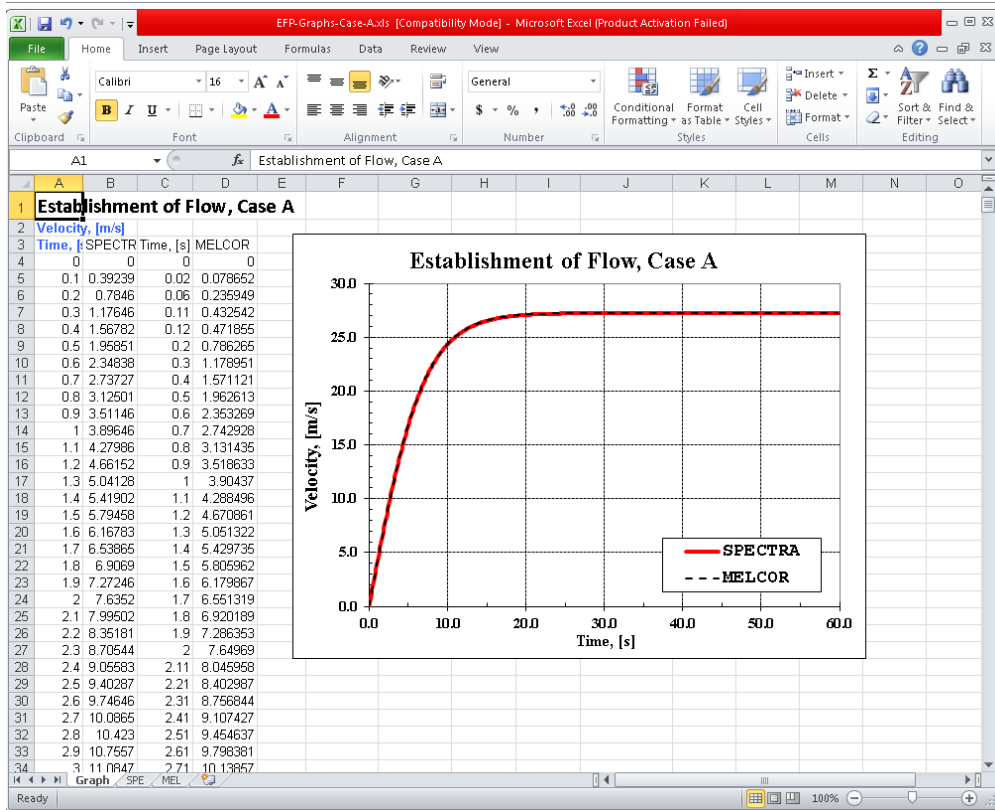


Figure 4-2 Test “establishment of flow” - export of data from EFP-Graphs-SPE.VSD

SPECTRA Code Manuals - Volume 2: User's Guide



(a)



(b)

Figure 4-3 Test “establishment of flow” - import of to data into EFP-Graphs-Case-A.xls

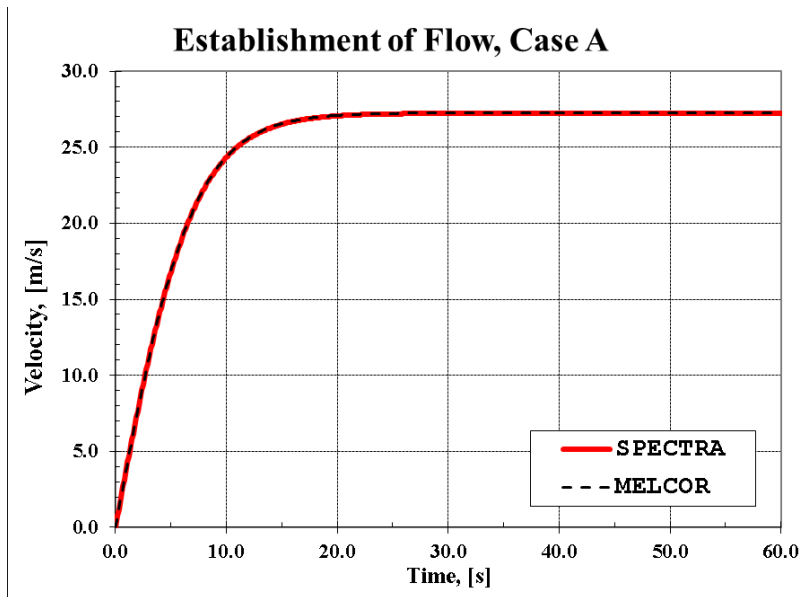


Figure 4-4 Reference test result - steam line flow versus time

The obtained results should be identical as the appropriate source results. Furthermore, it is recommended to compare the SPECTRA results with the reference (MELCOR) results for this case. This is done as follows:

- Open the file EFP-Graphs-SPE.VSD (double-click on this file).
- Check the end value, by clicking on “Go to a specific time” button - Figure 4-2 (a) and specifying 60.0 seconds. The velocity should read 27.23 m/s.
- Export the data to excel by pressing the button “Export Data to Excel” - Figure 4-2 (b). This will open a new excel file (with a default name, e.g. “Sheet1”).
- Open the file EFP-Graphs-Case-A.xls and copy the data from “Sheet1” into EFP-Graphs-Case-A, tab “SPE” - Figure 4-3 (a).
- View the graph provided in EFP-Graphs-Case-A, tab “Graph” - Figure 4-3 (b).

The SPECTRA results should be in good agreement with the MELCOR results (these are provided in EFP-Graphs-Case-A, tab “MEL”). The final graph is provided in Figure 4-4.

4.5 Automatic Verification

The base set of automatic verification tests is provided in the directory:
`\Z-INPUTS\Qualification-tests\`

The automatic verification is made based on the following property of the SPECTRA output file: The *.OUT file starts with an echo of input file, which is followed by an end-of-input marker (a period in the first column) and then followed by the output. If *.OUT from an earlier calculation is renamed to *.SPE and executed, then the code reads the input file, ignores everything which follows the end-of-input marker and performs calculations. If the calculations proceed in exactly the same way as the earlier calculation, the new *.OUT is exactly the same then the original *.OUT file. This procedure is illustrated in Figure 4-5. In short, the *.OUT file renamed into *.SPE and executed, should duplicate itself. If an Initial Condition File is used, then it must also be provided together with the renamed *.OUT file.

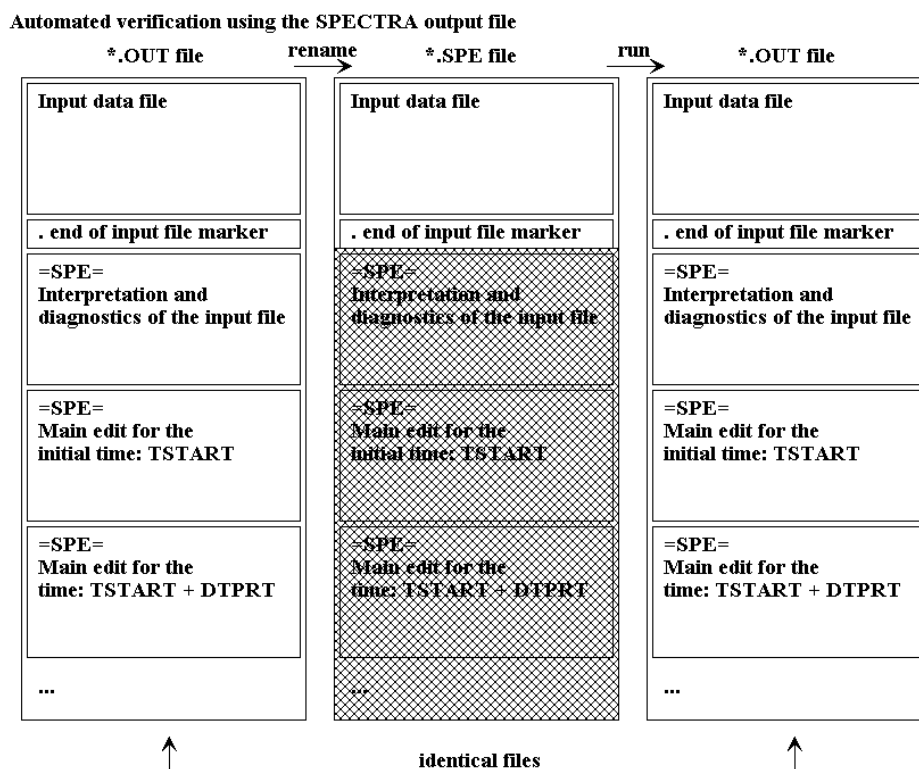


Figure 4-5 Automatic verification using the *.OUT file

The main directories contain subdirectories \Source, with output files from all test calculations. In order to activate the automatic testing one must activate the script:

```
Test-all.bat
```

This script performs the following actions:

- Extracts the original *.OUT and *.ICF files from the \Source subdirectory
- Renames *.OUT into *.SPE
- Executes all *.SPE files (Note: path to the source code may need to be redefined by the user. The current path is C:\SPECTRA\Z-EXE\SPECTRA.EXE)
- Compares the obtained results with the results stored in the \Source directory
- Writes the outcome of such comparison to the file “Results.txt”

When the test script is terminated, the user must check the file “Results.txt” If the test is successful there is no difference in all cases. The contents of the Results.txt file should be as shown below:

SPECTRA AUTOMATIC TEST SCRIPT EXECUTED ON:

```
USERNAME=STEMPNIEWICZ
COMPUTERNAME=P6014
```

```
Tue 11/24/2020
04:35 PM
```

SPECTRA Code Manuals - Volume 2: User's Guide

THE TEST IS SUCCESSFUL IF THERE ARE NO DIFFERENCES IN ALL CASES

Comparing files Butterfly-Valve.OUT and .\SOURCE\BUTTERFLY-VALVE.OUT
FC: no differences encountered

Comparing files CF.OUT and .\SOURCE\CF.OUT
FC: no differences encountered

Comparing files ED-RW.OUT and .\SOURCE\ED-RW.OUT
FC: no differences encountered

... etc.

Linux version of the same set of automatic verification tests is provided in the directory:
\Z-INPUTS\Qualification-tests-Linux\

The testing procedure is the same as described above for the Windows verification tests.

The automatic verification tests specific to HTRs is provided in the directory:
\Z-INPUTS\Qualification-tests-HTR\

The testing procedure is the same as described above for the base verification tests.

4.6 Other Verification Runs

Apart from the verification run, described above, the user may perform additional verification using any test cases described in the Volume 3 of the SPECTRA Code Manuals: "Verification & Validation". The SPECTRA Manuals are available in the subdirectory \Z-MANUALS\, which is supplied together with the SPECTRA code.

Almost all test cases that are described in Volume 3 are available in the subdirectory \Z-INPUTS\, which is supplied together with the SPECTRA code. In order to perform additional verification runs the user must perform the following steps:

- Select a test case in Volume 3. The user may find it important to perform additional verification of a selected part of the code, for example the 2-D conduction, the Radioactive Particle Transport, etc. In such case the user should select a test case from the appropriate chapter of Volume 3.
- The location of the input file is mentioned for each test described in Volume 3. In order to make it easier for the user to find the files, the file locations are always given in bold characters, for example the "CV" test case may be found in \Z-INPUTS\CV\CV.SPE. Thus, once the user selects the test, it should not be a problem to locate the appropriate input deck in the subdirectory \Z-INPUTS\.
- Once the input deck is located, calculations should be performed according to the instructions for code execution, mentioned in section 4.3.
- When the calculations are finished the results may be viewed using the provided visualization picture (Visor picture), for example \Z-INPUTS\CV\CV.VSD. Using Visor one can compare snapshots at given time points to corresponding snapshots presented in Volume 3, but also make time-dependent graphs for comparison with similar graphs provided in Volume 3.

Literature

- [1] "Reactor Physics Constants", ISBN-13: 978-0870794971, Argonne National Laboratory, ANL-5800, Second Edition, July 1963.
- [2] American Nuclear Society Standards Committee Working Group ANS-5.1, "Decay Heat Power in Light Water Reactors", ANSI/ANS-5.1-1979, La Grange Park, IL, 1979.
- [3] F. de Cachard, S. Lomperski, G.R. Monauni, "Thermal-Hydraulic Modelling of Finned Tube Containment Condensers", PSI Annual Report 1997, Annex IV, PSI Nuclear Energy and Safety Research, CH-5232 Villigen PSI.
- [4] R.A. Dimenna, J.R. Larson, R.W. Johnson, T.K. Larson, C.S. Miller, J.E. Streit, R.G. Hanson, D.M. Kiser, "RELAP5/MOD2 Models and Correlations", NUREG/CR-5194, EGG-2531, August 1988.
- [5] J.J. Duderstad, L.J. Hamilton, "Nuclear Reactor Analysis", ISBN 0-471-22363-8, John Wiley & Sons, Inc., New York, 1976.
- [6] "Chart of the Nuclides", <https://www.nndc.bnl.gov/chart/>.
- [7] Y.Y. Hsu, R.W. Graham, "Transport Processes in Boiling and Two-Phase Systems, Including Near-Critical Fluids", Hemisphere Publishing Corporation, ISBN 0-07-030637-0, 1976.
- [8] A.F. Henry, "Nuclear Reactor Analysis", ISBN 0-262-08081-8, Massachusetts Institute of Technology, Cambridge, 1975.
- [9] J.P. Holman, "Heat Transfer", Fourth Edition, ISBN 0-07-029598-0, McGraw Hill, New York, 1976.
- [10] I.E. Idelchik, "Handbook of Hydraulic Resistance" Second Edition, ISBN 3-540-15962-2, Hemisphere Publishing Corporation, 1986.
- [11] J.R. Lamarsh, A.J. Baratta, "Introduction to Nuclear Engineering", Third Edition, ISBN 0-201-82498-1, Prentice Hall, 2001.
- [12] FORTRAN 77 Compiler, Version 5.01, F77L-EM/32, Lahey Computer Systems, Inc., 1988-1992.
- [13] NuChart Version 4.0.0, July 1998. Nuclear data from NUDAT data files, release October 1997, produced by National Nuclear Data Center.
- [14] W.M. Rohsenow, J.P. Harnett, "Handbook of Heat Transfer", McGraw Hill, ISBN 0-07-053576-0, 1973.
- [15] "RELAP4/MOD5, A Computer Program for Transient Thermal-Hydraulic Analysis of Nuclear Reactors and Related Systems, User's Manual, RELAP4/MOD5 Description", ANCR-NUREG-1335, Idaho Nuclear Engineering Laboratory, Idaho Falls, ID, September, 1976.

SPECTRA Code Manuals - Volume 2: User's Guide

- [16] J.L. Rempe, et al., "Light Water Reactor Lower Head Failure Analysis", NUREG/CR-5642, EGG-2618, October 1993.
- [17] C.J. Dean, R.J. Perry, "The 1995 WIMS Nuclear Data Library", AEA Technology, Technical Service Division, AEA-TSD-0630, March 1995.
- [18] W.H. McAdams, "Heat Transmission", ISBN-13: 978-0898748765, Robert E. Krieger Publishing Company, third edition, Malabar, Florida, 1985.
- [19] L.A. Bromley, "Heat Transfer in Stable Film Boiling", *Chem. Eng. Prog. Ser.*, **46**, pp. 221-227, 1950.
- [20] P.J. Berenson, "Transition Boiling Heat Transfer from a Horizontal Surface", *Journal of Heat Transfer*, **83C**(3), pp. 351-358, 1961.
- [21] J.C. Chato, "Laminar condensation inside horizontal and inclined tubes", *J. Am. Soc. Heating Refrig. Aircond. Engrs.*, p.52, February 1962.
- [22] J. Gerstmann, P. Griffith, "Effect of Surface Instability on Laminar Film Condensation", MIT Heat Transfer Lab. Report 5050-36; *Int. Heat Mass Transfer*, **10**, p. 567, 1967.
- [23] W. Nusselt, "Die Oberflächenkondensation des Wasserdampfes", *Zeitschr. Ver. Deutsch. Ing.*, **60**, p. 541, 1916.
- [24] Kuhn S.Z., Schrock V. E., Peterson P.F., "An investigation of condensation from steam-gas mixtures flowing downward inside a vertical tube". *Nuclear Engineering and Design* **177** (1997) 53-69.
- [25] D.G. Ogg, "Vertical Downflow Condensation Heat Transfer in Gas-Steam Mixtures", MS thesis, University of California, Berkeley, 1991.
- [26] M.M. Stempniewicz, "Simulation of Containment Transient Response During Accidents in Advanced Reactor Types - The Computer Code SPECTRA", PhD Thesis at Silesian Technical University, Institute of Thermal Technology, Gliwice, Poland; NRG report 31437/00.52167, Arnhem, May 12, 2000.
- [27] K. Bemmert, P. Zehner, "Measurements of the Four-Quadrant Characteristics on a Multi-Stage Turbine", *Journal of Engineering for Power, Transactions of ASME*, Vol. **102**, pp. 316-321, April 1980.
- [28] R.E. Featherstone, C. Nalluri, "Civil Engineering Hydraulics - Essential Theory with Worked Examples", ISBN-13: 978-0632038633, Granada Publishing Limited, London, 1982.
- [29] E. Logan, "Handbook of Turbomachinery", Marcel Dekker Inc., New York, ISBN: 0-8247-9263-7, 1994, ISBN 0-8247-0995-0, 1995.
- [30] F.W. Dittus, L.M.K. Boelter, "Heat Transfer in Automobile Radiators of the Tubular Type", *Publications in Engineering*, University of California, Berkeley, Vol. 2, 443, 1930.

SPECTRA Code Manuals - Volume 2: User's Guide

- [31] B.H. McDonald, "Comparison of the physical models and numerical methods in the codes used for the GREY LWR code comparison exercise", CSNI report number 116, OECD Nuclear Energy Agency, Paris 1988.
- [32] M.M.R. Williams, S.K. Loyalka, "Aerosol Science Theory and Practice - with Special Application to the Nuclear Industry", ISBN 0-08-037209, Pergamon Press, First Edition, Oxford, 1991.
- [33] M.W. Reeks, D. Hall, "Kinetic models for particle resuspension in turbulent flows: theory and measurement", *Aerosol Science*, **32**, 1-31, 2001.
- [34] W.C. Hinds, "Aerosol Technology – Properties, Behaviour, and Measurement of Airborne Particles", John Wiley & Sons, Inc., ISBN 0-471-19410-7, New York, 1999.
- [35] R.O. Gauntt, et.al., "MELCOR Computer Code Manuals, Reference Manuals, Version 1.8.6, September 2005", NUREG/CR-6119, Vol. 2, Rev. 3, SAND 2005-5713, published: September 2005.
- [36] K.Y. Suh, R.J. Hammersley, "Modelling of Fission Product Release and Transport for Severe Fuel Damage Analyses", *Nuclear Science and Engineering*, Vol. **109**, pp.26-38, 1991.
- [37] P. Nanni, V. Buscaglia, G. Battilana, "E. Reudl, "Air Oxidation of a Mn-Cr austenitic steel of potential use for fusion reactor structural applications between 1073 and 1473 K at 10⁵ Pa", *Journal of Nuclear Materials*, Vol. **182**, pp. 118-127, 1991.
- [38] R. Nieder et al., "Chemie des Hochtemperaturreaktors", Jülich, November 1981, Jül-Conf-43, ISSN 0344-5798, pp. 30- 42: P. Kubaschewski, B. Heinrich: "Graphitkorrosion durch Wasserdampf, Hochtemperaturreaktorbau GmbH".
- [39] D.R. Lide, et al., "CRC Handbook of Chemistry and Physics, A Ready-Reference Book of Chemical and Physical Data", 72-nd edition, ISBN-0-8493-0472-5, CRC Press Inc., 1991-1992.
- [40] F.R. Larson, J. Miller, "A Time-Temperature Relationship for Rupture and Creep Stress", *Transactions of the ASME*, July 1952, pp. 765-775.
- [41] L.E. Herranz, C.L. Del Pra, A. Dehbi, "Major Challenges to Modelling Aerosol Retention Near a Tube Breach During Steam Generator Tube Rupture Sequences", *Nuclear Technology*, Vol. **158**, pp. 83 - 93, April 2007.
- [42] M.R. Sippola, W.W. Nazaroff, "Particle Deposition from Turbulent Flow: Review of Published Research and Its Applicability to Ventilation Ducts in Commercial Buildings", Lawrence Berkeley National Laboratory Report, LBNL - 51432, June, 2002.
- [43] R.C. Reid, J.M. Prausnitz, B.E. Poling, "The Properties of Gases and Liquids", Fourth Edition, ISBN 0-07-051799-1, McGraw Hill, New York, 1989.

SPECTRA Code Manuals - Volume 2: User's Guide

- [44] A. Ullman, R. Acharia, D.R. Olander, "Theretical accommodation coefficients of inert gases on stainless steel and UO₂", *J. Nucl. Mat.*, **51**, p 277, 1974.
- [45] A.M. Ross, R.L. Stoute, "Heat transfer coefficient between UO₂ and Zircaloy-2", AECL-1552, 1962.
- [46] A.E. Bergles, J.H. Leinhard V, G.E. Kendall, P. Griffith, "Boiling and Evaporation in Small Diameter Channels", *Heat Transfer Engineering*, **24**(1): 18-40, 2003.
- [47] S.G. Kandlikar, "Critical heat flux in subcooled flow boiling - an assessment of current understanding and future directions for research", *Multiphase Science and Technology*, **13**, (3): 207-232, 2001.
- [48] S.H. Kim, W.P. Baek, S.H. Chang, "Measurement of critical heat flux in narrow annuli submerged in saturated water", *Nuclear Engineering and Design*, **199**: 41-48, 2000.
- [49] M. Monde, Y. Mitsutake, "Critical heat flux of natural circulation boiling in vertical tube. Effect of oscillation and circulation on CHF", *International Journal of Heat and Mass Transfer*, **43**, 2002.
- [50] F.C. Engel, "Laminar, transition and turbulent parallel flow pressure drop across wire-wrap-spaced rod bundles", *Nuclear Science and Engineering*, Vol. **69**, pp. 290-296, 1979.
- [51] E. Bubelis, M. Schikorr, "Review and Proposal for Best-fit of Wire-wrapped Fuel Bundle Friction Factor and Pressure Drop Predictions Using Various Existing Correlations", *Nuclear Engineering and Design*, **238**, pp.3299–3320, 2008FZKA 7446, November 2008.
- [52] "Status Report on Spent Fuel Pools Under Loss Of Cooling and Loss of Coolant Accidents, Final Report", NEA/CSNI/R(2015)2, May 2015
- [53] H. Pruijboom, A. Tas, "Comparison of Thermohydraulic and Nuclear Aspects in a Standard HEU Core and a Typical LEU Core for the HFR Petten - a Case Study", https://inis.iaea.org/collection/NCLCollectionStore/_Public/36/023/36023776.pdf
- [54] D.E. Jacober, M.J. Matteson, "The Collection of Aerosols from Gas Streams by Impaction on Multiple Spherical Targets", *Aerosol Science and Technology* **4**, pp.:433-443, 1985.
- [55] P.N. Haubenreich, J.R. Engel, B.E. Price, H.C. Claiborne, "MSRE Design and Operations Report, Part III: Nuclear Analysis", ORNL-TM-730, Feb. 1964.
- [56] C. Constable, B. Lindley, G. Parks, "Maximising Discharge Burnup in an Open Cycle Molten Salt Reactor", PHYSOR2020, EPJ Web of Conferences 247, 12002 (2021), <https://doi.org/10.1051/epjconf/202124712002>.

SPECTRA Code Manuals - Volume 2: User's Guide

- [57] Ji-Hun Kim, Sejin Kwonb, Jinyoung Choi, Yong Jin Cho, “Concrete ablation analysis for molten corium-concrete interaction mitigation strategy”, *Annals of Nuclear Energy* 132 (2019) 615–627.
- [58] T. Sevón, “Molten Core - Concrete Interactions in Nuclear Accidents, Theory and Design of an Experimental Facility”, VTT Research Notes 2311, ESPOO 2005 <https://publications.vtt.fi/pdf/tiedotteet/2005/T2311.pdf>
- [59] L.L. Humphries, et.al., “MELCOR Computer Code Manuals, Vol. 1: Primer and User's Guide, Vol. 2: Reference Manuals, Version 2.1.6840”, SAND2015-6691R, Published: August 2015.
- [60] Woong Kee Kim, Ji Hoon Shim, Massoud Kaviani, “Thermophysical properties of liquid UO_2 , ZrO_2 and corium by molecular dynamics and predictive models”, *Journal of Nuclear Materials* 491 (2017) 126-137.
- [61] M. Ramacciotti, et.al., “Viscosity Models for Corium Melts, *Nuclear Engineering and Design* 204, 377-389, 2001.

appendix A Pump/Compressor Maps

Two models are available for pumps/compressors in SPECTRA. The first model (Type 1) simply sets the flow in junction based on the pressure difference across the junction and the user-defined maps. The second model (Type 2) calculates the pressure head based on the user-defined maps and then uses the general momentum equation to calculate the flow. Type 1 is seldom used. This was the first pump model applied in an early version of SPECTRA, and it is preserved in the code to keep compatibility with earlier input decks. Type 2 is generally recommended, because it is physically correct, while Type 1 is only an approximation valid for quasi-stationary conditions. Moreover Type 2 offers several additional capabilities, like:

- More flexible map generation (there are more map defining parameters that can be specified by the user - exponents a , b , c).
- Internal power calculation. When Type 1 is used, the user must define Control Functions to define power entering the fluid. A set of recommended functions had been provided in the manual to an early SPECTRA version. When Type 2 is used, the power that enters the fluid is calculated internally by the code, using efficiency tables.
- Speed can be calculated using a rotor inertia equation.

The discussion below explains how a pump/compressor map is defined using relatively few input parameters. The pump maps are discussed basically for the Type 2 pumps/compressors. The Type 1 has the same maps, except that the exponents a , b , c have fixed values, and cannot be affected by the user.

A.1 Approach

The basic approach in the SPECTRA code is quite different than in codes such as RELAP, TRAC, etc. These codes require the user to provide data tables specifying maps for all possible conditions (four quadrant curves - see (Dimenna, 1988)). Alternatively, they offer built-in curves for typical pumps (Bingham Westinghouse pump curves are available in RELAP).

In general, it is quite difficult to find sufficient data to determine the four quadrant curves; specifically the data for reverse speed and reverse flow are typically not available from the manufacturer. The required input data is extensive; the user must provide a sufficient amount of data to cover all possible conditions, even if some conditions are never expected to occur. Consequently users of RELAP or TRAC typically prefer to use the built-in maps. Thus the modelling is either tedious or not flexible.

The pump/compressor model in SPECTRA was designed to provide flexible modelling, while simultaneously limiting the amount of effort in input data preparation. The pump/compressor maps are approximated by a standard equation, which is built into the code. The coefficients in this equation are defined by the user. The user has therefore to define only a few input parameters that will provide the full pump/compressor map.

Pump/compressor map is approximated in SPECTRA by a parabolic equation. The shape of map depends on the user-defined parameters, such as V_0 , C_{RS} , C_{RF} , C_{DS} , C_{VS} and exponents a , b , c . The user-defined parameters and their effect on the pressure head are illustrated in Figure 4-6.

Pump/Compressor Model - Test MAP

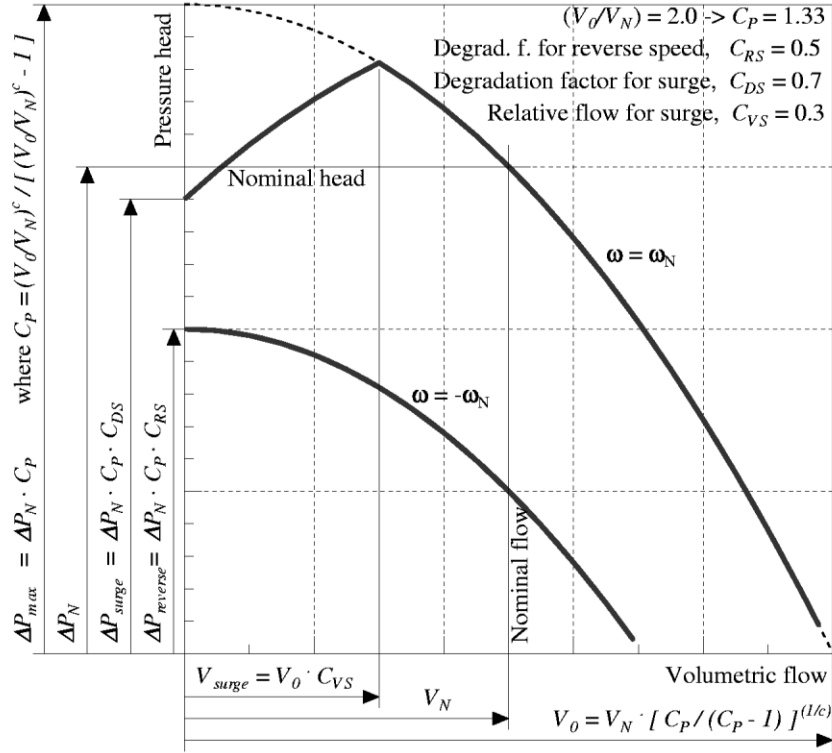


Figure 4-6 Influence of input parameters: C_P , C_{RS} , C_{DS} , C_{VS} , on the pump map.

Note that in the previous code versions C_P was the pump/compressor input parameter, instead of V_0 . This was changed in order to make the pump/compressor input parameters the same as the turbine input parameters. There is a simple relation between C_P and V_0 . The relation is shown in the section describing the input parameters (section 2.2.8), so the user can easily convert his old input decks.

The user must in each case check his maps. This is done quite simply. A test run is set up, with a pump being between two volumes with time dependent conditions. The conditions should be selected in such way as to force the pump to operate in the range that needs to be plotted to create a full map. Several identical pumps may be set, each operating with different speed. The resulting flow and pressure head (or pressure ratio) of each pump are then plotted. Instead of plotting them against time ($V=f(t)$, $\Delta P=f(t)$), they are plotted against each other ($\Delta P=f(V)$). In this way maps with curves for several different pump/compressor speeds are obtained. Such maps are discussed in sections A.2.2 and A.2.3. Examples of input files for creating such maps are given in Volume 3.

A.2 Pump/Compressor Maps

Section A.2.1 shows definitions of reduced (dimensionless) parameters, which are being used with the pump/compressor maps. The discussion of the pump/compressor maps is provided in two parts. In the first part (section A.2.2) an "ideal" map is described, that is a map based on parabolic equation, in which surge does not appear (surge degradation factor, $C_{DS} = 1.0$). The second part (section A.2.3) describes how the surge is modelled.

A.2.1 Reduced Parameters

The reduced (dimensionless) parameters, which are being used with the pump/compressor maps, are:

- Reduced speed, ω_R ,
- Reduced flow, V_R .
- Reduced pressure head P_R , or reduced pressure ratio, Π_R .

The user has several options as to how these parameters are defined. The available definitions are discussed below.

Reduced speed, ω_R

The reduced speed ω_R , is calculated based on the user defined nominal speed, ω_N , (s^{-1}), and eventually the nominal temperature T_N , (K). If the nominal temperature, T_N , is not specified, then the reduced speed is defined as:

$$\omega_R = \left(\frac{\omega}{\omega_N} \right) \quad (1)$$

If a positive nominal temperature, T_N , is specified, then the reduced speed is defined as:

$$\omega_R = \frac{\left(\frac{\omega}{\omega_N} \right)}{\sqrt{\frac{T}{T_N}}} \quad (2)$$

In the above definitions ω is the pump speed and T is the temperature at the inlet to the pump/compressor. The first definition is appropriate for typical pumps (see for example (Featherstone, 1982)), while the second is appropriate for typical gas compressors (see for example (Logan, 1995)).

Reduced flow, V_R

The reduced flow V_R , is calculated based on the user defined nominal volumetric flow, V_N , (m^3/s) and eventually the nominal temperature T_N , the nominal fluid velocity, v_N , the nominal gas constant, R_N . If only the nominal flow, V_N , is entered, then the reduced flow is defined as:

$$V_R = \left(\frac{V}{V_N} \right) \quad (3)$$

If a positive nominal temperature, T_N , is specified, then the reduced flow is defined as:

$$V_R = \frac{\left(\frac{V}{V_N} \right)}{\sqrt{\frac{T}{T_N}}} \quad (4)$$

If a positive nominal fluid velocity, v_N , is specified, then the reduced flow is defined as:

$$V_R = \frac{\left(\frac{V}{V_N} \right)}{\sqrt{\frac{T}{T_N}}} \frac{\sqrt{\frac{1 + v^2 / 2c_p T}{1 + v_N^2 / 2c_p T_N}}}{\left(\frac{1 + v^2 / 2RT}{1 + v_N^2 / 2RT_N} \right)} \quad (5)$$

Finally, if a positive nominal gas constant, R_N , is specified, then the reduced flow is defined as:

$$V_R = \frac{\left(\frac{V}{V_N} \right)}{\left(\frac{R}{R_N} \right) \sqrt{\frac{T}{T_N}}} \frac{\sqrt{\frac{1 + v^2 / 2c_p T}{1 + v_N^2 / 2c_p T_N}}}{\left(\frac{1 + v^2 / 2RT}{1 + v_N^2 / 2RT_N} \right)} \quad (6)$$

In the above definitions V is the pump volumetric flow, T is the gas temperature at the inlet to the pump, v is the fluid velocity in the pump/compressor. R and c_p are the perfect gas constant and the specific heat at constant pressure for the gas mixture flowing through the pump/compressor.

The first definition (equation (3)) is appropriate for typical pumps (see for example (Featherstone, 1982)). The last definition (equation (6)) is appropriate for typical gas compressors, as will be shown below. The intermediate definitions are approximations of the exact formula for compressors.

In case of gas compressors, the maps are frequently defined using so called, “corrected flow”, W_{corr} , defined as (see for example (Logan, 1995)):

$$W_{corr} = W \frac{\sqrt{T_{tot}}}{p_{tot}} \quad (7)$$

Where W is the mass flow, T_{tot} is the total temperature (based on the enthalpy, $h=c_p T$, and the kinetic energy, $v^2/2$), and p_{tot} is the total pressure (static, p , and dynamic, $\rho v^2/2$). The above formula can be transformed as follows:

$$\begin{aligned}
 W \frac{\sqrt{T_{tot}}}{p_{tot}} &= W \frac{\sqrt{T + v^2 / 2c_p}}{p + \rho v^2 / 2} = W \frac{\sqrt{T}}{p} \frac{\sqrt{1 + v^2 / 2c_p T}}{1 + \rho v^2 / 2p} = \\
 &= \rho V \frac{\sqrt{T}}{p} \frac{\sqrt{1 + v^2 / 2c_p T}}{1 + \rho v^2 / 2p} = \frac{V}{R\sqrt{T}} \frac{\sqrt{1 + v^2 / 2c_p T}}{1 + v^2 / 2RT}
 \end{aligned} \tag{8}$$

In the above transformation use was made of the perfect gas law: $p = \rho RT$, and the relation $W = \rho V$. The above formula is written in SPECTRA in a dimensionless form, by replacing each dimensional parameter by the ratio of the parameter and its nominal value. The result is:

$$\frac{\left(\frac{V}{V_N} \right)}{\left(\frac{R}{R_N} \right) \sqrt{\frac{T}{T_N}}} \frac{\sqrt{\frac{1 + v^2 / 2c_p T}{1 + v_N^2 / 2c_p T_N}}}{\left(\frac{1 + v^2 / 2RT}{1 + v_N^2 / 2RT_N} \right)} \tag{9}$$

The above formula is identical to the last formula for V_R , (equation (6) shown above). Therefore the equation (6) gives a dimensionless form of the corrected flow, W_{corr} .

If the gas composition does not change during calculations, then the gas constant R is always equal to the R_N , and the gas constant ratio can be removed from the formula. Therefore equation (5) is exact as long as the gas composition does not change. If additionally the dynamic terms can be neglected compared to the static terms, then the terms with velocity squared disappear from the formula (9), and it becomes identical with the equation (4). Summarising, the following options may be used to calculate the reduced flow:

1. Equation (3), appropriate for pumps,
2. Equation (4), appropriate for compressors with no gas composition changes and dynamic terms neglected.
3. Equation (5), appropriate for compressors with no gas composition changes.
4. Equation (6), appropriate for compressors without any restrictions and simplifications.

Reduced pressure head P_R , or reduced pressure ratio, Π_R

The user can define either the nominal pressure head (Pa), or the nominal pressure ratio, (-). If the nominal pressure head, ΔP_N , is specified, then the pump/compressor map uses the reduced pressure head, ΔP_R , defined as:

$$\Delta P_R = \left(\frac{\Delta P}{\Delta P_N} \right) \tag{10}$$

If the nominal pressure ratio, Π_N is specified, then the pump/compressor map uses the reduced pressure ratio, Π_R , defined as:

$$\Pi_R = \left(\frac{\Pi}{\Pi_N} \right) \tag{11}$$

In the above definitions ΔP and Π are the pressure head and the pressure ratio respectively. If the pressure ratio is used, then the reduced pressure head, ΔP_R , is replaced by $(\Pi - 1) / (\Pi_R - 1)$.

A.2.2 Pump/Compressor Maps - Ideal Map with no Surge

Definitions and detailed descriptions of all parameters are provided in the User's Guide section 2.2.8. Below a short description is provided how each parameter affects the shape of the pump/compressor pressure head.

The pump/compressor model is based on the map, which is approximated by the following equation:

$$\Delta P_R = C_{RS} C_P \omega_R^a \mp C_{RF} (C_P - 1) \omega_R^b V_R^c \quad (12)$$

where: ΔP_R - Reduced pressure head, (-). If the nominal pressure ratio, Π_N , is specified, the pressure head is equal to: $\Delta P_N(t) = (\Pi_N - 1) \cdot P_0(t)$, where $P_0(t)$ is the current pressure upstream the pump. In this case the reduced pressure head, ΔP_R , in the above formula is replaced by $(\Pi - 1) / (\Pi_N - 1)$, where $\Pi = (\Delta P / P_0 + 1)$, ΔP is the actual pressure head in (Pa), and Π_N is the nominal pressure ratio (input parameter) that is related to the nominal pressure head, $\Delta P_N(t)$ (time-dependent) by $\Pi_N = \Delta P_N(t) / P_0(t) + 1$.

V_R - Reduced pump flow, (-).

ω_R - Reduced pump speed, (-).

C_P - Constant defining the shape of pressure head in pump map, (-), $C_P > 1.0$. The value of C_P is related to the input parameters V_N (VFNPJN), and V_0 (VF0PJN), as:
 $C_P = (V_0 / V_N)^c / ((V_0 / V_N)^c - 1)$

C_{RS} - Degradation factor for reverse speed, (-),

$\omega > 0.0$: $C_{RS} = 1.0$

$\omega < 0.0$: C_{RS} is given by the user-defined parameters CRSPJN.

C_{RF} - Degradation factor for reverse flow, (-),

$V > 0.0$: $C_{RF} = 1.0$

$V < 0.0$: C_{RF} is given by the user-defined parameters CRFPJN.

a - First exponent (default value of 2.0).

b - Second exponent (default value of 1.0).

c - Third exponent (default value of 2.0).

In the above equation the sign is – in case of positive flow, and + in case of negative flow. The parameters V_0 , C_{RS} , C_{RF} , a , b , c , are user-defined. The influence of these parameters on the shape of pump map is discussed below.

Influence of $C_P (V_0/V_N)$ on the pump map is shown in Figure 4-7. The following nominal parameters were assumed to make the plot.

$$\Delta P_N = 1.0 \times 10^5 \text{ Pa,}$$

$$V_N = 1.0 \text{ m}^3/\text{s,}$$

$$\omega_N = 50.0 \text{ s}^{-1}.$$

Figure 4-7 shows pressure heads made for values of V_0/V_N between 10.0 (corresponding C_P of 1.01) and 1.01 (corresponding C_P of 50.8). The corresponding values of C_P , calculated for the default value of the exponent c ($c=2.0$) are shown below:

$$V_0/V_N = 10.0 \quad C_P = 1.01$$

$$V_0/V_N = 3.3 \quad C_P = 1.10$$

$$V_0/V_N = 2.0 \quad C_P = 1.33$$

$$V_0/V_N = 1.2 \quad C_P = 3.27$$

$$V_0/V_N = 1.01 \quad C_P = 50.8$$

(typical water pump)

(typical gas compressor)

(piston pump)

Pump/Compressor Model - Test MAPCP

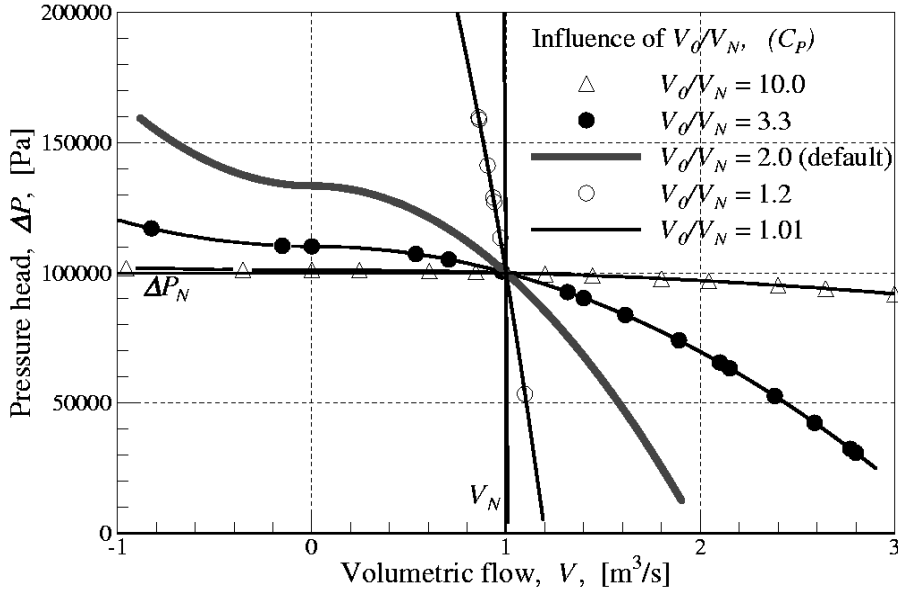


Figure 4-7 Influence of the parameter V_0 , on the pump maps.
 V_0/V_N between 10.0 ($C_P = 1.01$) and 1.01 ($C_P = 50.8$).

It is seen that when V_0/V_N is very small ($V_0/V_N=1.01$) then the pressure head makes a nearly vertical line. This means that the pump flow is nearly constant, independently of the pressure head. This shape is typical for the piston pumps. When V_0/V_N is very large, the pressure head line becomes flat. (If the Type 1 pump is used, then very large values of V_0/V_N may also cause numerical solution problems - the flow is quite sensitive to any pressure changes.).

The influence of the degradation factor for reverse flow, C_{RF} , on the pump map is illustrated in Figure 4-8. The value of C_{RF} affects the pump map only in the reverse flow range. If the default value is used ($C_{RF} = 1.0$) then the pressure head lines in the negative flow range are symmetrical to the lines in the positive flow range. If $C_{RF} < 1.0$ then the pressure head lines in the negative flow are flatter than in the positive flow. If $C_{RF} > 1.0$ then the pressure head lines in the negative flow are steeper than in the positive flow. Comparison with the pump map from RELAP-5 (Dimenna, 1988), shown in Volume 3, shows that the latter value is appropriate to represent the pump map from RELAP-5.

The influence of the degradation factor for reverse speed, C_{RS} , on the pump map is illustrated in Figure 4-9 through Figure 4-12. The figures show pump maps on the ω - V diagram for several different pressure heads, ranging from -1.0 bar to $+1.0$ bar. The pump nominal values assumed to plot the maps shown in these figures are:

$$\begin{aligned} \Delta P_N &= 1.0 \times 10^5 \text{ Pa,} \\ V_N &= 1.0 \text{ m}^3/\text{s,} \\ \omega_N &= 50.0 \text{ s}^{-1}. \end{aligned}$$

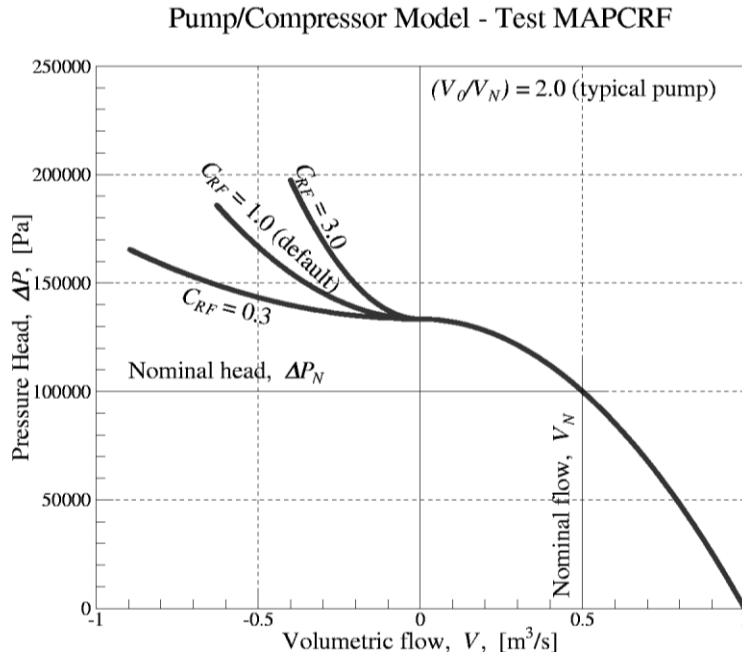


Figure 4-8 Influence of the parameter C_{RF} , on the pump maps. C_{RF} between 0.3 and 3.0.

Figure 4-9 shows the pump map for $C_{RS} = 0.1$. This is the map of a typical centrifugal pump (such as built-in RELAP code - compare (Dimenna, 1988), figure 8-1, constant head lines). It is seen that when the pump speed is reversed the lines bend to the right, which means the flow tends to be in the positive direction, although it is smaller than in case of the positive pump speed.

To illustrate the influence of C_{RS} , the pump map for $C_{RS} = 1.0$ is shown in Figure 4-10. The lines are symmetrical with respect to the horizontal axis, which means the pump behaves exactly the same when it turns forward or reverse. Such pumps do not exist in practice. Theoretically one could build such a pump if the blades were made flat, and several outlet collectors were placed symmetrically around the pump. The pump would have to look something like the one shown in Figure 4-10. Such a pump would of course be very inefficient, and the example is shown here only to illustrate the influence of C_{RS} on the shape of the pump map.

The above two examples show that for the centrifugal machines (pumps, centrifugal compressors or centrifugal fans) an appropriate value of C_{RS} is positive and less than 1.0:

$$\text{centrifugal pumps : } 0.0 < C_{RS} < 1.0$$

It is observed that with decreasing C_{RS} the lines of the pump map become more vertical in the negative pump speed range.

Figure 4-11 shows the pump map for $C_{RS} = -0.1$. This is a map of an axial pump/compressor. When the pump speed is reversed, the flow also reverses.

Figure 4-12 shows the pump map for $C_{RS} = -1.0$. For this value the lines are symmetrical with respect to the coordinate center. That means when the pump speed is reversed the behavior is the same as if it

was placed in the opposite direction and running forward. An example of such pump is a simple, low efficiency axial fan, with flat blades.

The above two examples show that for the axial machines (typical compressors, fans) an appropriate value of C_{RS} is negative, and not smaller than -1.0 :

$$\text{axial pumps : } -1.0 < C_{RS} < 0.0$$

It is observed that with decreasing absolute value of C_{RS} the lines of the pump map become more vertical in the negative pump speed range.

The maps discussed above were produced using the value of exponents: $a=2.0$, $b=0.0$ (default settings for the Type 1 pump). Comparisons with typical pump and compressors maps show that a better value for the exponent b is $0.5 - 1.0$. Below, Figure 4-13 and Figure 4-14 show two maps for $a=2.0$, $b=0.5$. The first map (Figure 4-13) is a “centrifugal pump” map, with $C_{RS} = +0.1$. The second map (Figure 4-14) is an “axial pump” map, with $C_{RS} = -0.1$. The value of $b=0.5$ is a default setting for the Type 2 pump (the pump type recommended for general use). When $b > 0.0$ the pressure head is equal to zero when the pump/compressor speed is zero. This is more realistic than having a non-zero head with zero speed, which is the case when $b = 0.0$.

The influence of the exponents a , b , c , on the pump maps is shown in Figure 4-15 through Figure 4-20. The Type 1 pump settings ($a=2.0$, $b=0.0$) are shown in Figure 4-15. With these values of exponents the pressure head lines run approximately parallel, and never cross. See also the turbine map with the same a , b , appendix B, Figure 4-32. Note that compared to the pump/compressor maps, the turbine maps are “upside-down” because of different definition of the turbine pressure ratio (inverse).

Figure 4-16 shows the pressure head lines for ($a=2.0$, $b=1.0$). The lines cross each other in negative head range, which is not visible here, but will be clearly visible in the turbine maps - see appendix B, Figure 4-33. Note that compared to the pump/compressor maps, the turbine maps are “upside-down”.

Figure 4-17 shows the pressure head lines for ($a=2.0$, $b=2.0$). The lines cross each other in the same point, at the value of pressure head equal to zero. This is not visible here, but will be clearly visible in the turbine maps (see appendix B, Figure 4-34 - note that compared to the pump/compressor maps, the turbine maps are “upside-down”).

Figure 4-18 shows the pressure head lines for ($a=3.0$, $b=1.0$). Comparison of Figure 4-16 and Figure 4-18 shows that increasing the value of a one obtains a pump that is more sensitive to the speed changes, i.e. a certain (say 10%) change of speed running at nominal conditions results in larger change of the pressure head.

The influence of the exponent c on the pump/compressor map is shown in Figure 4-19 and Figure 4-20. These figures show the maps obtained with the exponent c equal to 3.0 (default value is 2.0), and all other parameters being the same as shown in Figure 4-15 and Figure 4-16. Thus the influence of the exponent c is seen by comparing Figure 4-19 with Figure 4-15, and Figure 4-20 with Figure 4-16.

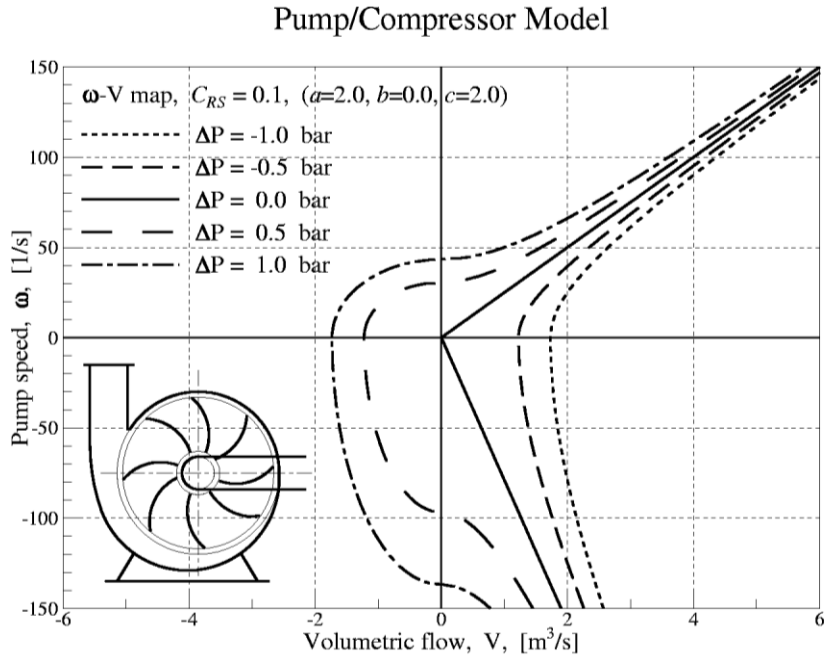


Figure 4-9 Influence of the parameter C_{RS} on the pump maps.
 $C_{RS} = 0.1$ (typical centrifugal pump).

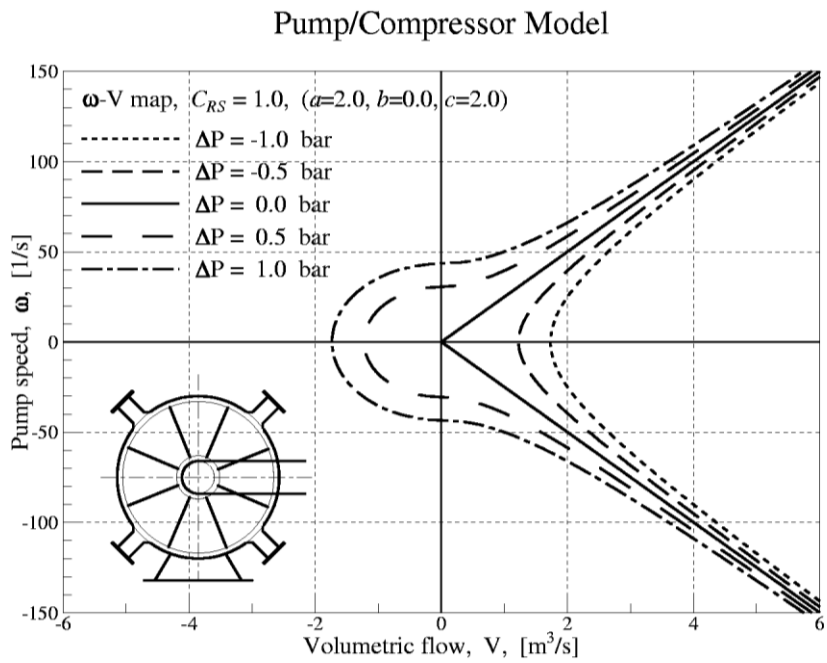


Figure 4-10 Influence of the parameter C_{RS} , on the pump maps.
 $C_{RS} = 1.0$ (theoretical centrifugal "pump").

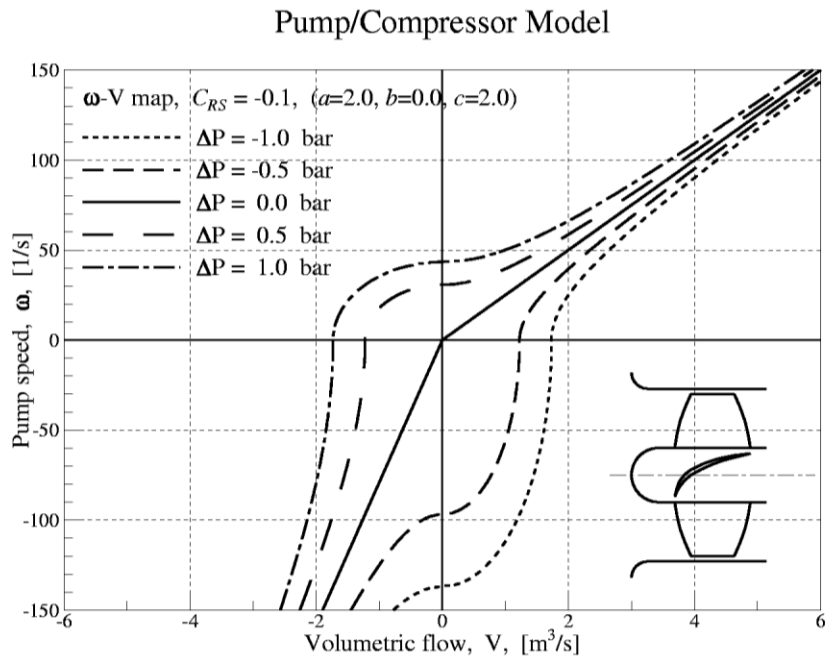


Figure 4-11 Influence of the parameter C_{RS} , on the pump maps.
 $C_{RS} = -0.1$ (typical axial pump).

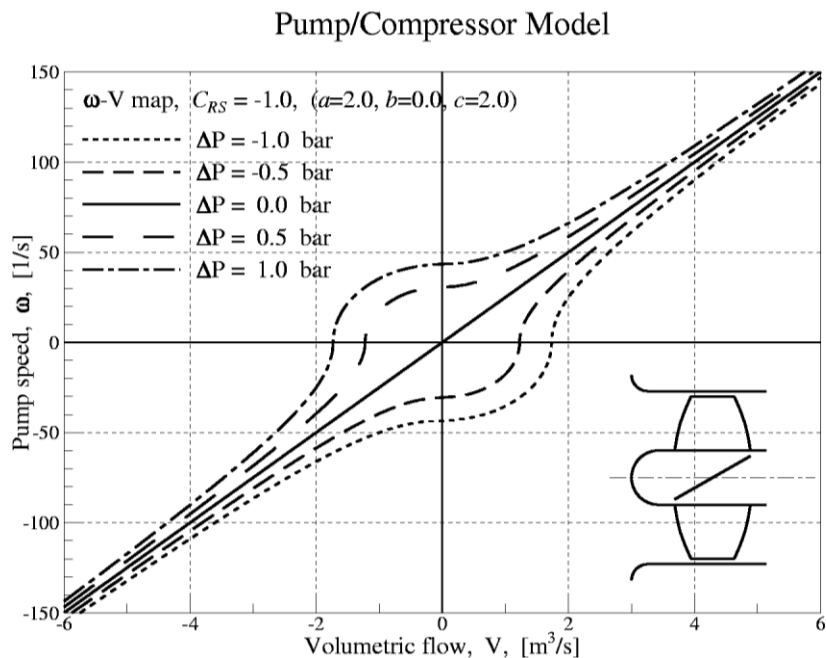


Figure 4-12 Influence of the parameter C_{RS} , on the pump maps.
 $C_{RS} = -1.0$ (theoretical axial "pump").

Pump/Compressor Model

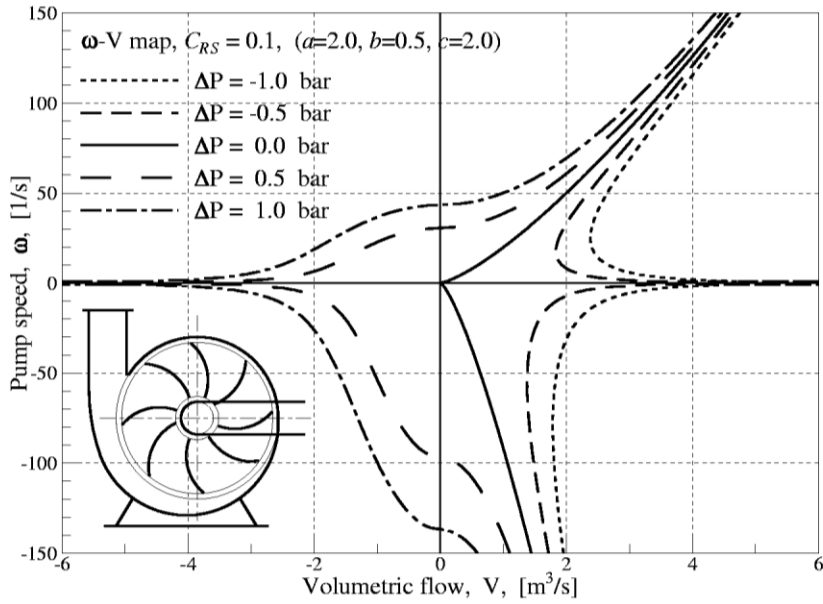


Figure 4-13 Influence of the parameter C_{RS} , on the pump maps.
 $C_{RS} = 0.1$ ($a=2.0, b=0.5, c=2.0$).

Pump/Compressor Model

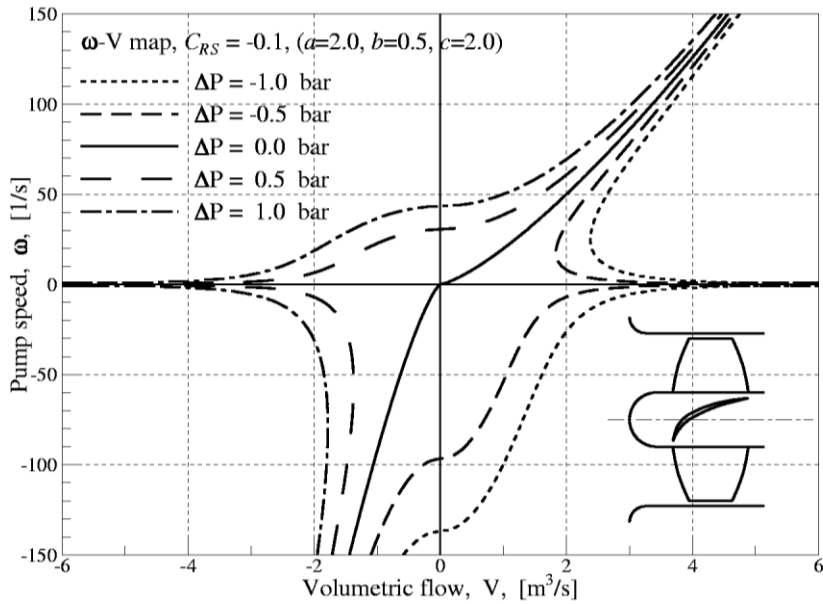


Figure 4-14 Influence of the parameter C_{RS} , on the pump maps.
 $C_{RS} = -0.1$ ($a=2.0, b=0.5, c=2.0$).

Pump/Compressor Model - Test MAP20

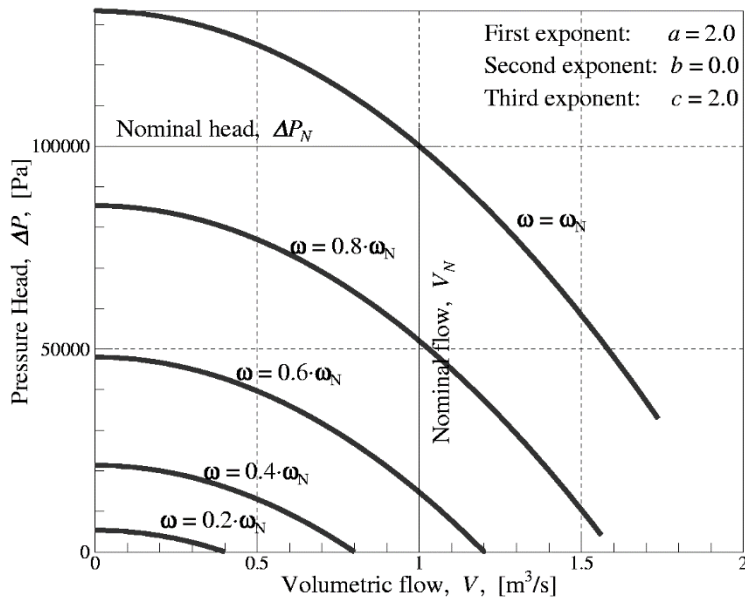


Figure 4-15 Influence of exponents on map, $a=2.0$, $b=0.0$, $c=2.0$ (Type 1 pump).

Pump/Compressor Model - Test MAP21

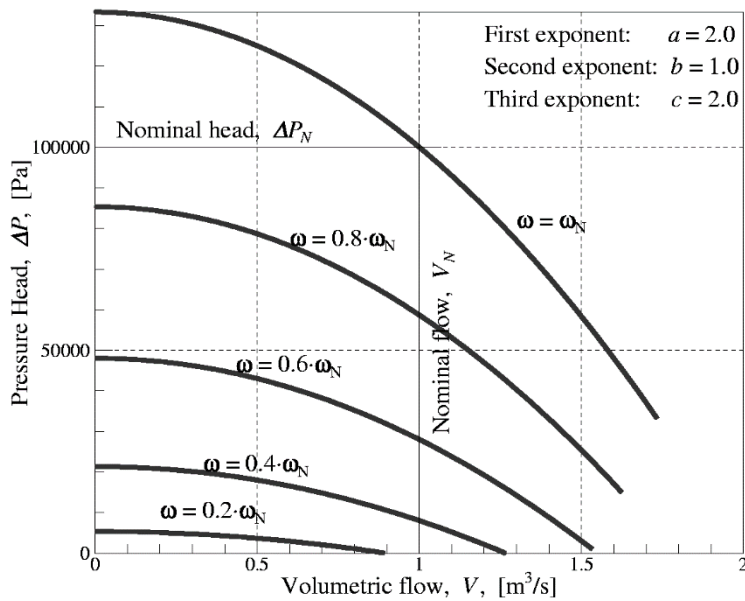


Figure 4-16 Influence of exponents on map, $a=2.0$, $b=1.0$, $c=2.0$ (default for Type 2 pump).

Pump/Compressor Model - Test MAP22

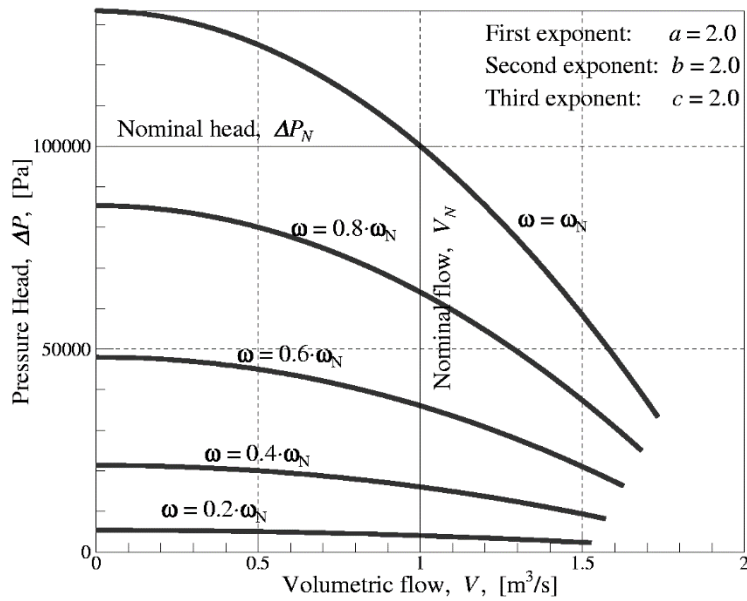


Figure 4-17 Influence of exponents on map, $a=2.0$, $b=2.0$, $c=2.0$.

Pump/Compressor Model - Test MAP31

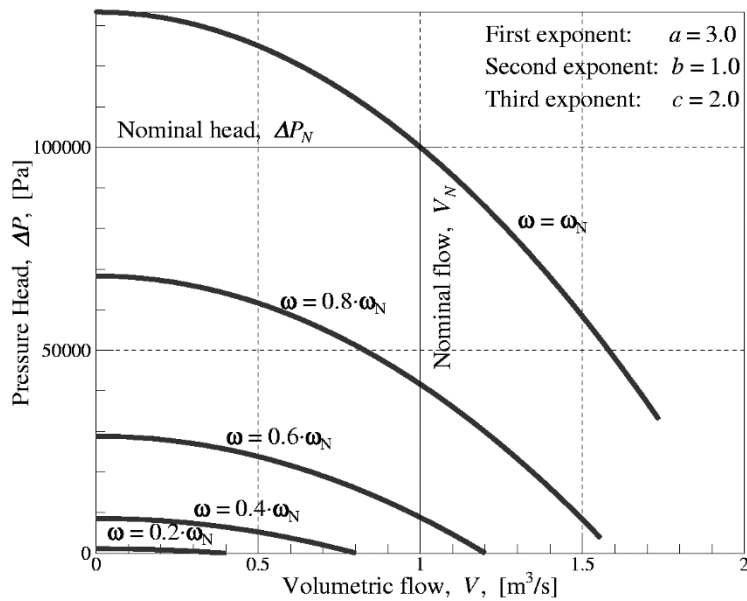


Figure 4-18 Influence of exponents on map, $a=3.0$, $b=1.0$, $c=2.0$.

Pump/Compressor Model - Test MAP203

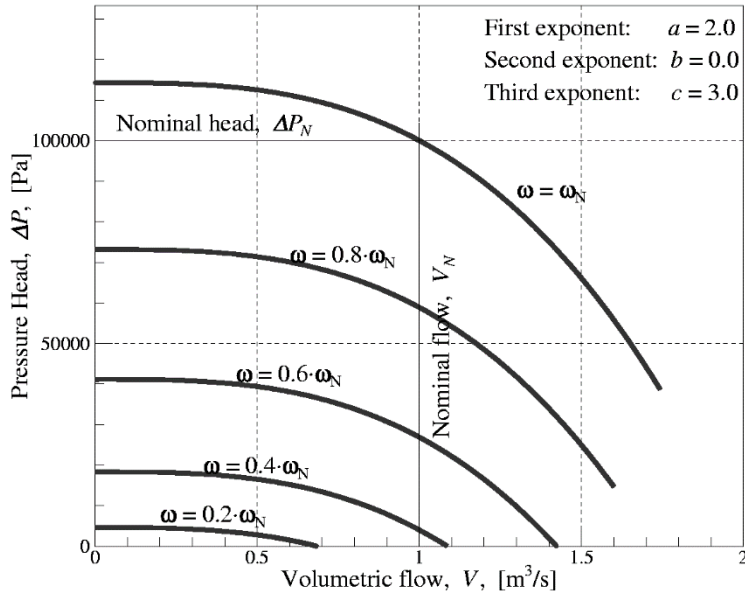


Figure 4-19 Influence of exponents on map, $a=2.0$, $b=0.0$, $c=3.0$ (compare Figure 4-15).

Pump/Compressor Model - Test MAP213

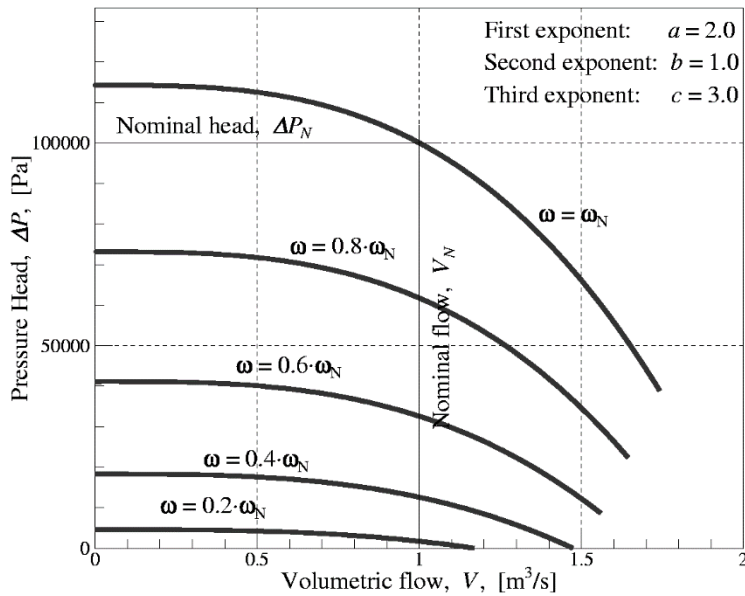


Figure 4-20 Influence of exponents on map, $a=2.0$, $b=1.0$, $c=3.0$ (compare Figure 4-16).

Negative values of the exponent b , although generally not recommended, was found useful for matching some compressor map data. If $b < 0.0$, then the term with ω_R^b is becoming large when the speed is small, giving unrealistically large pump head or compressor pressure ratio for a slowly turning machine. To prevent this a limit is imposed on ω_R^b : $\omega_R^b < \omega_{lim}^b$. For lower speeds the term is linearly interpolated to give zero for zero speed (see Figure 4-21). Default value of ω_{lim}^b is equal to 10.0 (input parameter BLMPJN, Word 27, records 231XXX and 233XXX). The data in Figure 4-21 is shown for the limit equal to 2.0. The pump/compressor map for the parameter b equal to -1.0 is shown in Figure 4-22. Comparison with Figure 4-20 shows how the map changes when the value of b is changed from $+1.0$ to -1.0 .

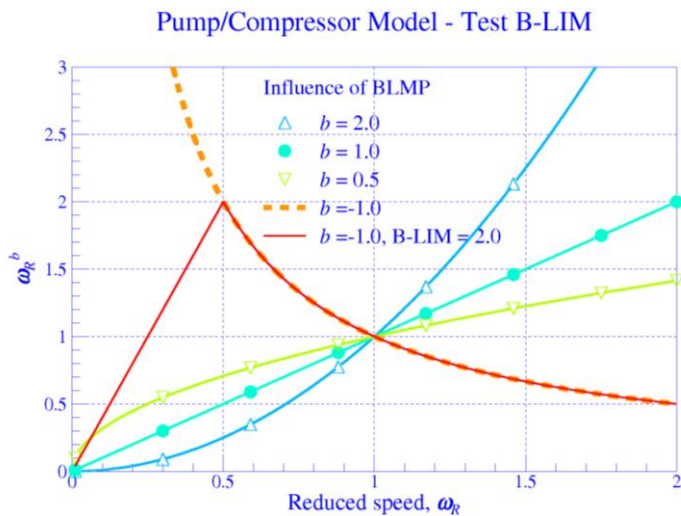


Figure 4-21 Influence of the limit B-LIM in case of negative b .

Pump/Compressor Model - Test MAP2X3

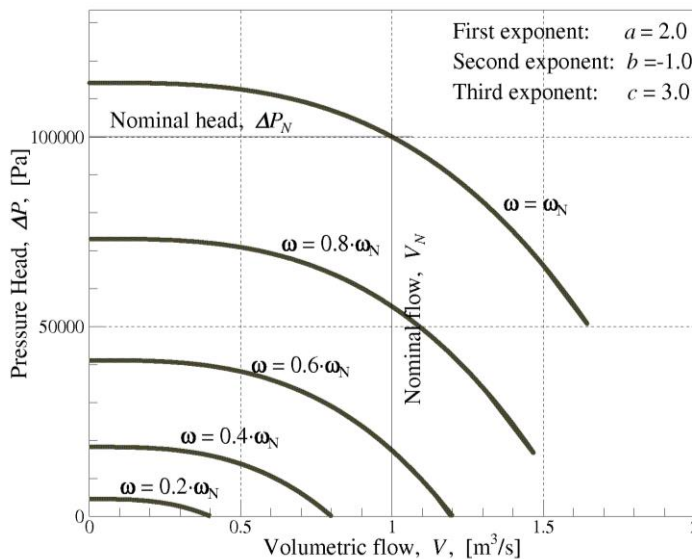


Figure 4-22 Influence of exponents on map, $a=2.0$, $b=-1.0$, $c=3.0$ (compare Figure 4-20).

A.2.3 Pump/Compressor Maps - Degradation of Head (Surge Model)

In the low flow range the machines such as compressors typically lose their capability to provide head. This is called “surge”. In case of pumps the maps are close to the ideal maps, shown above. However, even in case of pumps a small decrease of head in low flow range is typically observed - see Volume 3 - comparison with pump model from RELAP-5.

In SPECTRA three input parameters are introduced in order to model the pump/compressor behavior in the low flow range. These are:

- C_{VS} relative volumetric flow at which degradation begins, defined as a ratio of the flow at which surge starts to the flow at zero pressure head at nominal speed (see Figure 4-6).
- C_{DS} degradation factor, defined as the ratio of the degraded pressure head at zero flow to the un-degraded pressure head at zero flow (resulting from the un-degraded pump/compressor model equation - see Figure 4-6).
- s exponent in surge region interpolation.

The low flow region (the surge region) is defined as a region where the volumetric flow is:

$$V < V_{surge} = C_{VS} \cdot V_0(\omega) = C_{VS} \cdot V_N \cdot \left(\frac{C_P}{C_P - 1} \right)^{1/c} \cdot \left(\frac{\omega_R^a}{\omega_R^b} \right)^{1/c}$$

In the low flow range the pump head is decreased by introducing an effective speed, ω' , defined as:

$$\omega' = \omega \cdot [C_{DS}^{1/a} + (1 - C_{DS}^{1/a}) \cdot (V / V_{surge})^{1/s}]$$

Substituting the above formula into the pump/compressor model equation, shown in section A.2.2, one obtains the formula applied in the low flow (surge) region:

$$\Delta P_R = C_P \cdot \omega_R^a \cdot [C_{DS}^{1/a} + (1 - C_{DS}^{1/a}) \cdot (V / V_{surge})^{1/s}]^a \mp$$

$$\mp (C_P - 1) \cdot \omega_R^b \cdot [C_{DS}^{1/a} + (1 - C_{DS}^{1/a}) \cdot (V / V_{surge})^{1/s}]^b \cdot V_R^c$$

The influence of the surge parameters C_{VS} and C_{DS} is discussed first for a typical compressor. Next, examples of a typical pump are shown and the influence of the exponent s on the stability of the pump is discussed.

For the next case a very small degradation factor was assumed:

$$\begin{array}{ll} \text{relative flow:} & C_{VS} = 0.7, \\ \text{degradation factor} & C_{DS} = 0.01. \end{array}$$

Such a small value of C_{DS} is appropriate for gas compressors. The value of the constant C_P has been chosen as 3.0 (typical compressor). With this value of C_P the lines are relatively steep ($C_P \sim 1.3$ for typical pump maps - see discussion below), and the relative flow for surge, C_{VS} , is large (0.7) compared to a typical pump (~ 0.3 - see discussion below). The resulting pressure head map is shown in Figure 4-23.

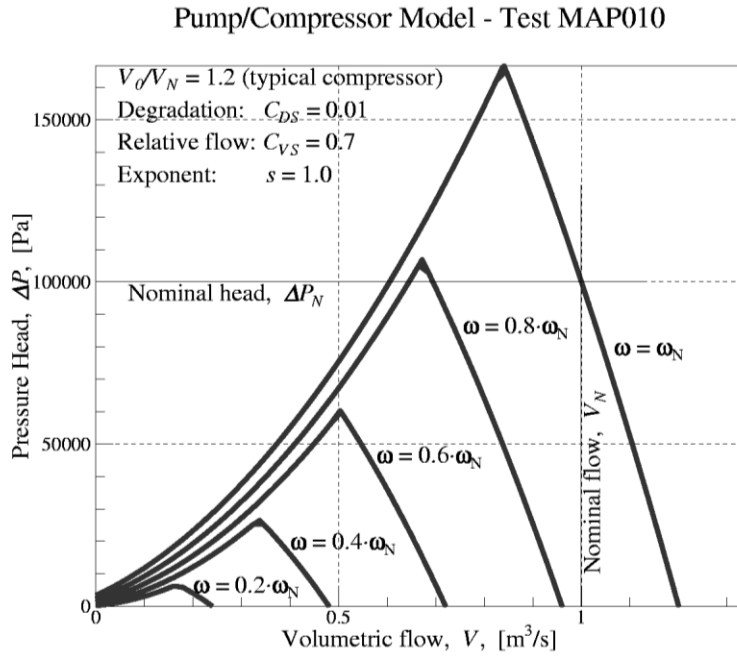


Figure 4-23 Influence of surge parameters on map, $C_{DS}=0.01$, $C_{VS}=0.7$ ($V_0/V_N=1.2$ - typical compressor).

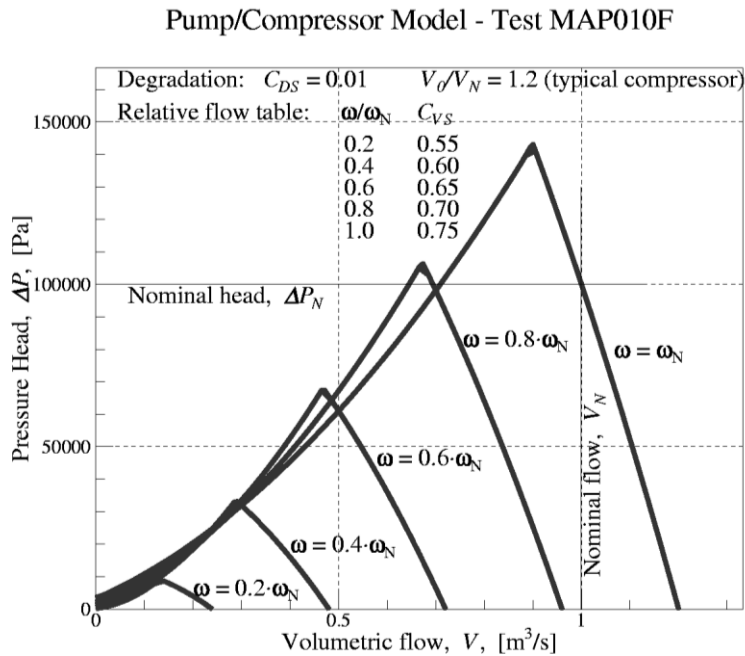


Figure 4-24 Influence of surge parameters on map, $C_{DS}=0.01$, $C_{VS}=f(\omega)$ ($V_0/V_N=1.2$ - typical compressor).

SPECTRA Code Manuals - Volume 2: User's Guide

The equation determining the pump/compressor map implies that at the nominal speed ($\omega_R=1.0$), V_N , is related to V_0 by (see Figure 4-6):

$$\frac{V_N}{V_0} = \left(\frac{C_P - 1}{C_P} \right)^{1/c}$$

The relative flow for surge is typically smaller than the nominal flow, thus:

$$C_{VS} = \frac{V_{surge}}{V_0} < \frac{V_N}{V_0} = \left(\frac{C_P - 1}{C_P} \right)^{1/c}$$

Therefore: for $C_P = 1.3$, $C_{VS} < 0.480$,
 for $C_P = 3.0$, $C_{VS} < 0.816$.

If C_{VS} is greater than the limit defined by the above formula, the code issues a warning message.

The next example is presented to illustrate the ability of the user to specify a variable surge limit: $C_{VS} = f(\omega)$. All the parameters are the same as above, except for the C_{VS} . In the present case the value is tabulated, as shown in the table below.

Table 4-1 Example of volumetric flow limit for surge as a function of speed.

ω/ω_N	0.20	0.40	0.60	0.80	1.00
C_{VS}	0.55	0.60	0.65	0.70	0.75

The results are shown in Figure 4-24. The pressure head lines are very similar to those observed in Figure 4-27. The only difference is the location of the surge limit. In Figure 4-24 the surge limit varies from 0.55 to 0.75, depending on the speed, while in Figure 4-23 it is constant and equal to 0.7.

The next examples show maps with low values of the degradation factor. Such maps are appropriate for typical water pumps. Before the pump examples are shown, a short discussion is presented on the stability of pump characteristics. The pump map has locally unstable characteristics if there is a region where the pressure head decreases with decreasing fluid flow. In this region stable operation of the pump is impossible; the fluid flow will oscillate between the two points bounding the unstable part of the map.

In order to obtain conditions for stable pump characteristics, it is important to find out what is the pressure head at zero flow, compared to the pressure head at the surge point. The pump/compressor pressure head at zero flow is equal to:

$$\Delta P_R|_{V=0.0} = C_P \cdot \omega_R^a \cdot C_{DS}$$

The surge point flow is equal to:

$$\frac{V_{surge}}{V_0} = C_{VS}$$

Using the relation between V_N and V_0 :

$$\frac{V_0}{V_N} = \left(\frac{C_P}{C_P - 1} \right)^{1/c} \cdot \left(\frac{\omega_R^a}{\omega_R^b} \right)^{1/c}$$

the relative flow at surge can be expressed as:

$$\left(\frac{V_{surge}}{V_N} \right) = \left(\frac{V_{surge}}{V_0} \right) \cdot \left(\frac{V_0}{V_N} \right) = C_{VS} \cdot \left(\frac{\omega_R^a}{\omega_R^b} \right)^{1/c} \cdot \left(\frac{C_P}{C_P - 1} \right)^{1/c}$$

The pressure head at the surge point is therefore equal to:

$$\Delta P_R|_{V=surge} = C_P \cdot \omega_R^a - (C_P - 1) \cdot \omega_R^b \cdot \left(\frac{\omega_R^a}{\omega_R^b} \right) \cdot \left(\frac{C_P}{C_P - 1} \right) \cdot C_{VS}^c$$

or:

$$\Delta P_R|_{V=surge} = C_P \cdot \omega_R^a \cdot (1 - C_{VS}^c)$$

The pressure head at zero flow is equal to the pressure head at the surge point if:

$$C_P \cdot \omega_R^a \cdot C_{DS} = C_P \cdot \omega_R^a \cdot (1 - C_{VS}^c)$$

or:

$$C_{DS} = 1 - C_{VS}^c$$

If the head at zero flow is smaller than the pressure head at the surge point, then there will certainly be an unstable region in the pump map. The necessary condition to obtain a stable pump is therefore: $C_{DS} \geq 1 - C_{VS}^c$. As will be shown below, this condition is not sufficient to obtain a stable pump. A proper value of the exponent s is needed to ensure a fully stable pump map.

The example cases presented below were calculated using the default value of $V_0/V_N = 2.0$ (typical centrifugal pump). In the first case the value of C_{VS} was set to 0.3 (This value is still somewhat too high compared to a typical pump - see Volume 3 - but it gives a more clearly visible unstable region.)

relative flow: $C_{VS} = 0.3,$

To obtain a stable map, the value of C_{DS} must be greater than or equal to $1 - 0.3^2 = 0.91$. The first example was run with this value:

degradation factor $C_{DS} = 0.91.$

The resulting pressure head map is shown in Figure 4-25. It is seen that although the pressure head at the surge point and at the zero flow are the same, there is an unstable region in the pump map. The unstable region is marked in the figure.

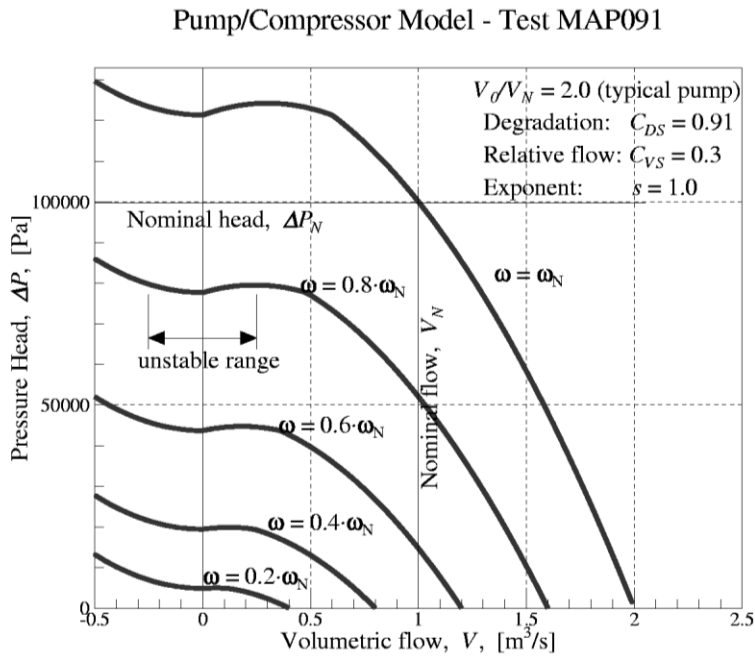


Figure 4-25 Influence of surge parameters on map, $C_{DS}=0.91$, $C_{VS}=0.3$, $s=1.0$ ($V_0/V_N=2.0$ - typical pump).

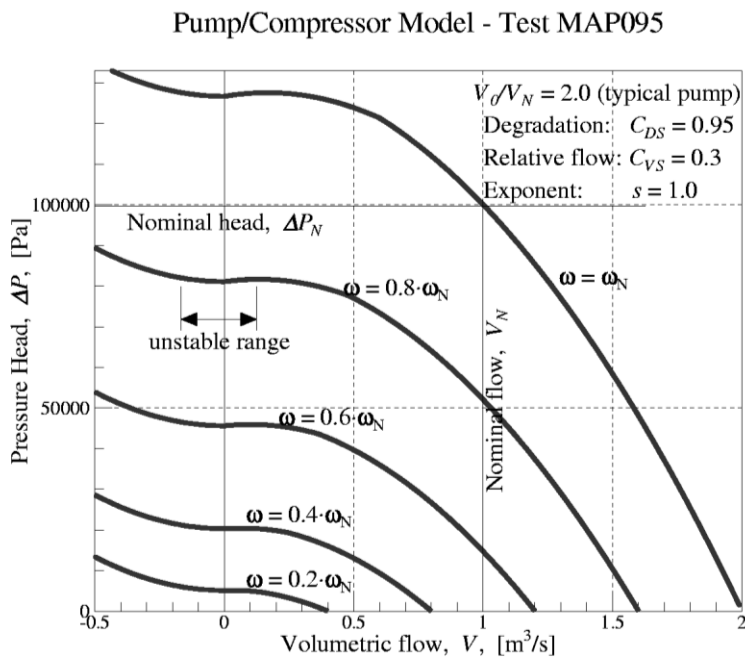


Figure 4-26 Influence of surge parameters on map, $C_{DS}=0.95$, $C_{VS}=0.3$, $s=1.0$ ($V_0/V_N=2.0$ - typical pump).

Pump/Compressor Model - Test MAP091S

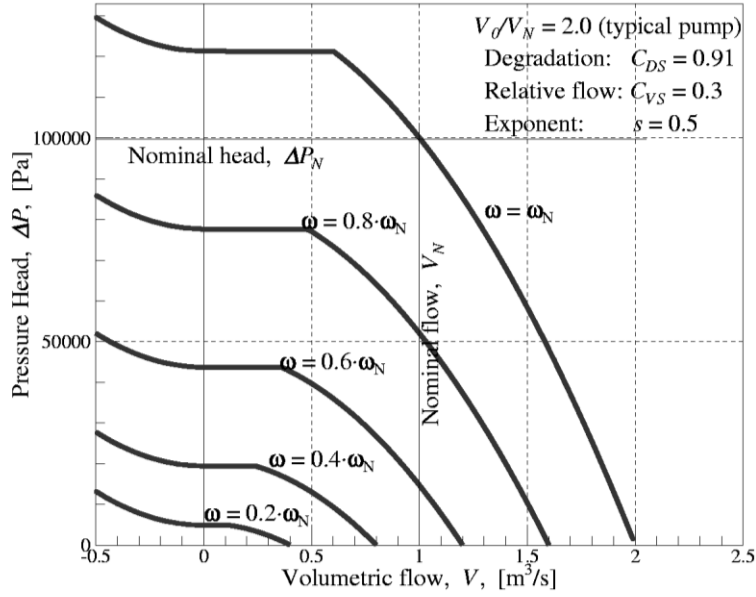


Figure 4-27 Influence of surge parameters on map, $C_{DS}=0.91$, $C_{VS}=0.3$, $s=0.5$ ($V_0/V_N=2.0$ - typical pump).

Pump/Compressor Model - Test MAP095S

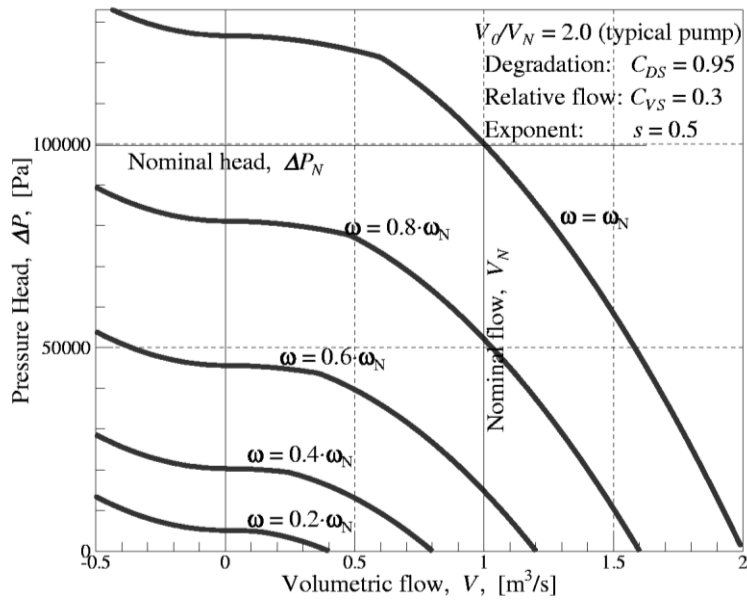


Figure 4-28 Influence of surge parameters on map, $C_{DS}=0.95$, $C_{VS}=0.3$, $s=0.5$ ($V_0/V_N=2.0$ - typical pump).

In the next example the degradation factor was set to a higher value:

$$\text{degradation factor} \quad C_{DS} = 0.95.$$

The resulting pressure head map is shown in Figure 4-26. It is seen that the unstable region still exists, although it is smaller than in the previous case.

The next two cases were run with the same degradation factors, namely 0.91 and 0.95 respectively, but with the exponent s decreased from 1.0 (the default value) to 0.5. The results are shown in Figure 4-27 and Figure 4-28. It is seen that there is no unstable region in both maps.

It is interesting to note that the map shown in Figure 4-27 is similar to the pump map applied in the MELCOR code (see (Summers, 1997), Reference Manual, CVH/FL Package). MELCOR however does not take into account a change of the pressure head with the pump speed; the pump is simply on (nominal speed) or off (zero pressure head). Moreover in MELCOR the pump head does not change in negative speed range, so the MELCOR model and the model shown in Figure 4-27 are identical provided that a check valve is present, prohibiting backflow through the pump.

The above examples show that in order to obtain a stable map the exponent s should be set to 0.5. The default value of s (1.0) was selected because this is most appropriate for gas compressors, and the surge model is of primary importance for gas compressors. If $s = 0.5$ is used for the example shown in Figure 4-23, then the pressure head will become negative in the low flow range - see the example case shown in Figure 4-29.

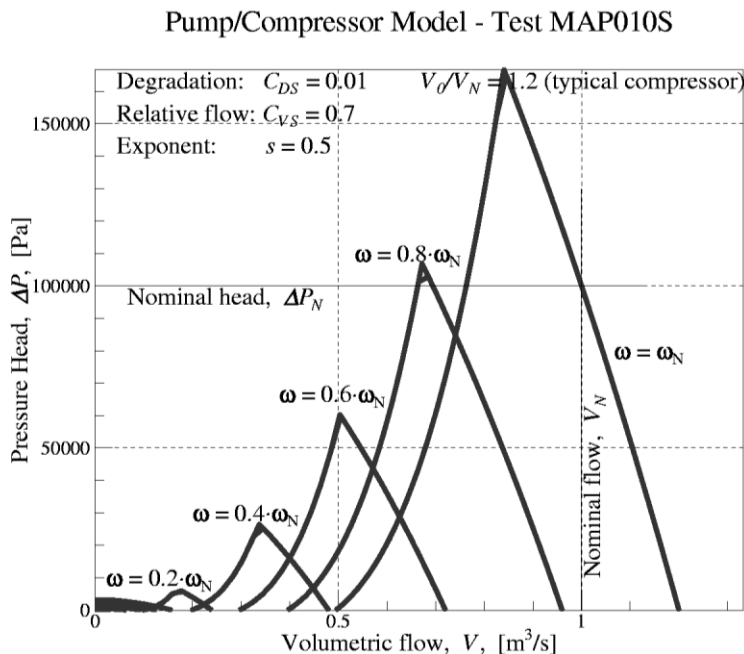


Figure 4-29 Influence of surge parameters on map, $C_{DS}=0.01$, $C_{VS}=0.7$, $s=0.5$ ($V_0/V_N=2.0$ - typical compressor).

SPECTRA Code Manuals - Volume 2: User's Guide

Use of the exponent s in order to provide a stable map may be important in analyses involving typical pumps. For example, the pump model applied in RELAP-5 (Dimenna, 1988) is best approximated using a stable map, with $s = 0.5$ - see Volume 3.

References of Appendix A

Dimenna, 1988

R.A. Dimenna, J.R. Larson, R.W. Johnson, T.K. Larson, C.S. Miller, J.E. Streit, R.G. Hanson, D.M. Kiser, "RELAP5/MOD2 Models and Correlations", NUREG/CR-5194, EGG-2531, August 1988.

Featherstone, 1982

R.E. Featherstone, C. Nalluri, "Civil Engineering Hydraulics - Essential Theory with Worked Examples", ISBN-13: 978-0632038633, Granada Publishing Limited, London, 1982.

Logan, 1995

E. Logan, "Handbook of Turbomachinery", Marcel Dekker Inc., New York, ISBN: 0-8247-9263-7, 1994, ISBN 0-8247-0995-0, 1995.

Summers, 1997

R.M. Summers, et.al., "MELCOR Computer Code Manuals, Reference Manuals, Version 1.8.4, July 1997", NUREG/CR-6119, Vol. 2, Rev. 1, SAND97-2398, published: May 1998.

appendix B Turbine Maps

The turbine model is based on the same approach as the turbine Type 2 model (see appendix A). In fact the turbine model uses exactly the same subroutine as the Type 2 turbine/compressor. Only the input procedures are slightly different. All input parameters are the same as in case of the Type 2 pump. The turbine nominal parameters, such as nominal flow and pressure ratio or head, are internally converted by the code into nominal parameters of an “equivalent pump”, as shown in Figure 4-30. The equivalent pump is defined as a pump/compressor that has exactly the same map as the turbine, if the map is plotted in terms of the pump pressure ratio (outlet divided by inlet pressure) rather than the turbine pressure ratio (inlet divided by outlet pressure).

The “equivalent pump” approach allows to perform calculations using the same subroutines that are calculating pumps/compressors. The equation defining turbine behavior is therefore exactly the same as the equation defining the pump/compressor map (see appendix A), and is therefore not discussed here. Only the conversion to the “Equivalent Pump” is shown below.

Using the equation defining the pump map (appendix A), it may be shown that nominal parameters of the equivalent pump are related to the turbine parameters as follows:

- nominal volumetric flow:

$$V_{E.P.} = V_0 \cdot [(C_P - 1) / C_P]^{(1/c)}$$

- nominal pressure ratio (if the pressure ratio is entered):

$$\Pi_{E.P.} = 1 + \frac{1 - 1/\Pi_N}{(C_P - 1) (V_N / V_{E.P.})^c - C_P}$$

- nominal pressure head (if the pressure head is entered):

$$\Delta P_{E.P.} = \frac{\Delta P_N}{(C_P - 1) (V_N / V_{E.P.})^c - C_P}$$

- where:
- Π_N - nominal turbine pressure ratio, (-), (user defined),
 - ΔP_N - nominal turbine pressure head, (Pa), (alternatively user defined),
 - V_N - nominal turbine flow, (m³/s), (user defined),
 - V_0 - flow at zero-head $\Delta P = 0.0$ (or $\Pi=1.0$), (m³/s), (user defined),
 - $\Pi_{E.P.}$ - nominal pressure ratio of the “equivalent pump”, (-),
 - $\Delta P_{E.P.}$ - nominal pressure head of the “equivalent pump”, (Pa),
 - C_P - constant in pump map (see appendix A). Note that the value of this constant affects the nominal parameters of the “equivalent pump”, but does not influence the turbine map, which is fully defined by V_N , V_0 , and Π_N or ΔP_N .
 - c - third exponent in turbine map definition, (-) (user defined).

The conversion to the “equivalent pump” is done automatically within the code; it is “transparent” for the user, i.e. the user works only with the turbine parameters (V_N , V_0 , Π_N or ΔP_N) while internally calculations are performed using the equivalent pump parameters ($V_{E.P.}$, $\Pi_{E.P.}$ or $\Delta P_{E.P.}$).

Turbine Model - Test MAP

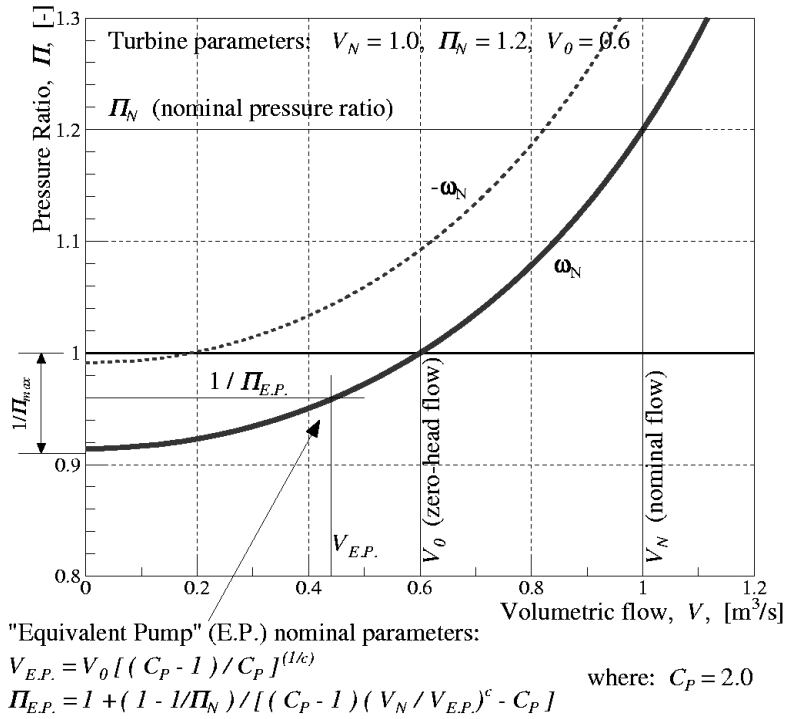


Figure 4-30 Turbine map - conversion of the turbine parameters into the “Equivalent Pump” parameters, performed internally by the code.

The parameters available to tune the turbine map are: V_0 , the exponents a , b , c , and the constant C_{RS} , determining the turbine behavior in case of negative speed. The influence of these parameters on the turbine map is discussed below.

The influence of the parameter V_0 on the turbine maps is quite obvious from the definition of the parameter. It is illustrated below, in Figure 4-31. The lines shown in this figure were obtained for a turbine with $\Pi_N = 1.5$, $V_N = 1.0 \text{ m}^3/\text{s}$, $\omega_N = 50.0 \text{ s}^{-1}$, $a = 2.0$, $b = 1.0$, $c = 1.0$, running at nominal speed.

The influence of the exponents a , b , c , on the turbine maps is shown in Figure 4-32 through Figure 4-37. The following values were used to produce maps shown in these figures:

$$\begin{aligned} \Pi_N &= 1.5, \\ V_N &= 1.0 \text{ m}^3/\text{s}, \\ V_0 &= 0.5 \text{ m}^3/\text{s}, \\ \omega_N &= 50.0 \text{ s}^{-1}. \end{aligned}$$

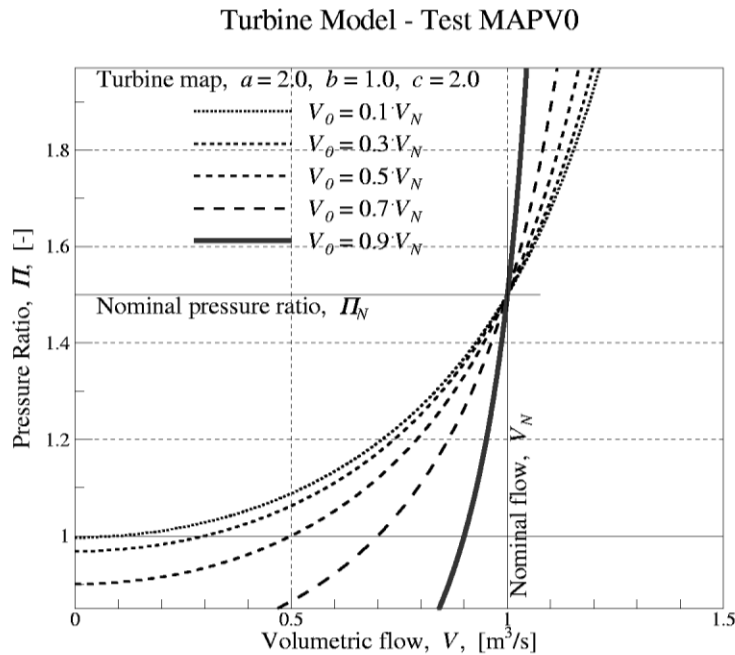


Figure 4-31 Influence of V_0 on turbine map ($a=2.0$, $b=1.0$, $c=2.0$),

The map obtained for ($a=2.0$, $b=0.0$, $c=2.0$) is shown in Figure 4-32. With these values of the exponents the pressure ratio lines run approximately parallel, and never cross. See also the pump/compressor map with the same a , b , c , - appendix A, Figure 4-15. Note that compared to the turbine maps, the pump/compressor maps are “upside-down” because of a different definition of the pressure ratio (inverse).

Figure 4-33 shows the pressure ratio lines for ($a=2.0$, $b=1.0$, $c=2.0$). The lines cross each other at flow $V > V_0$. (See also the pump/compressor maps with the same a , b , c , - appendix A, Figure 4-16. Note that compared to the turbine maps, the pump/compressor maps are “upside-down”.)

Figure 4-34 shows the pressure ratio lines for ($a=2.0$, $b=2.0$, $c=2.0$). The lines cross each other in the same point; the point where the pressure head is equal to zero (or the pressure ratio equal to one, or the volumetric flow equal to: $V=V_0$). With this set of constants the turbine becomes more sensitive to changes of speed; the pressure ratio is small for small turbine velocity and large for large velocity. (See also the pump/compressor map with the same a , b , c , - see appendix A, Figure 4-17. Note that compared to the turbine maps, the pump/compressor maps are “upside-down”).

Figure 4-35 shows the pressure ratio lines for ($a=3.0$, $b=1.0$, $c=2.0$). Comparison of Figure 4-33 and Figure 4-35 shows that increasing the value of a , the lines cross at higher value of flow. (See also the pump/compressor map with the same a , b , c , - see appendix A, Figure 4-18. Note that compared to the turbine maps, the pump/compressor maps are “upside-down”).

Note that in the case of a turbine, a machine more sensitive to speed changes is obtained by increasing the exponent b , while in case of pumps/compressors the same is achieved by increasing the exponent a .

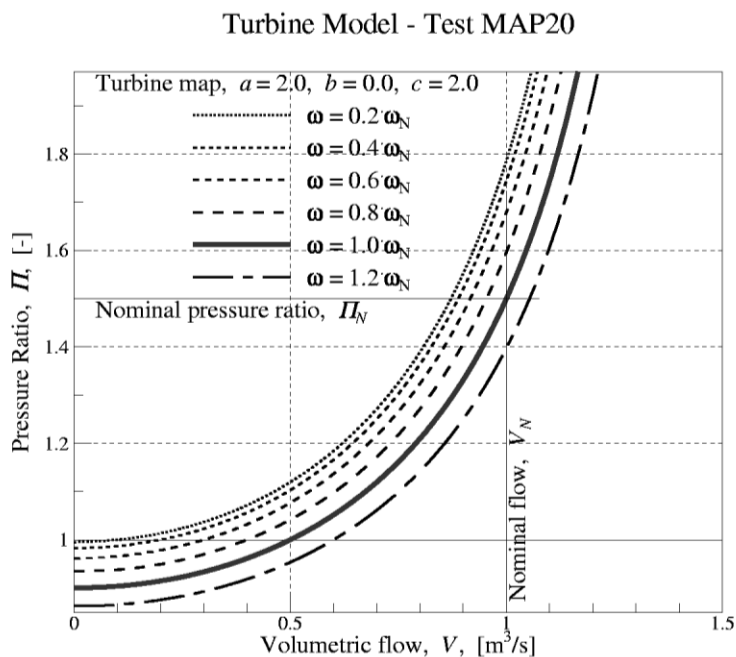


Figure 4-32 Influence of exponents on turbine map, $a=2.0$, $b=0.0$, $c=2.0$.

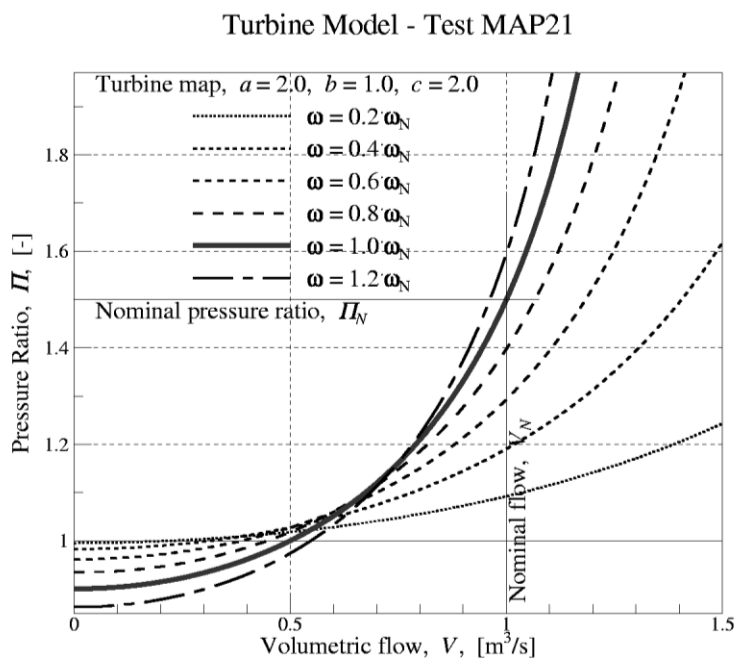


Figure 4-33 Influence of exponents on turbine map, $a=2.0$, $b=1.0$, $c=2.0$.

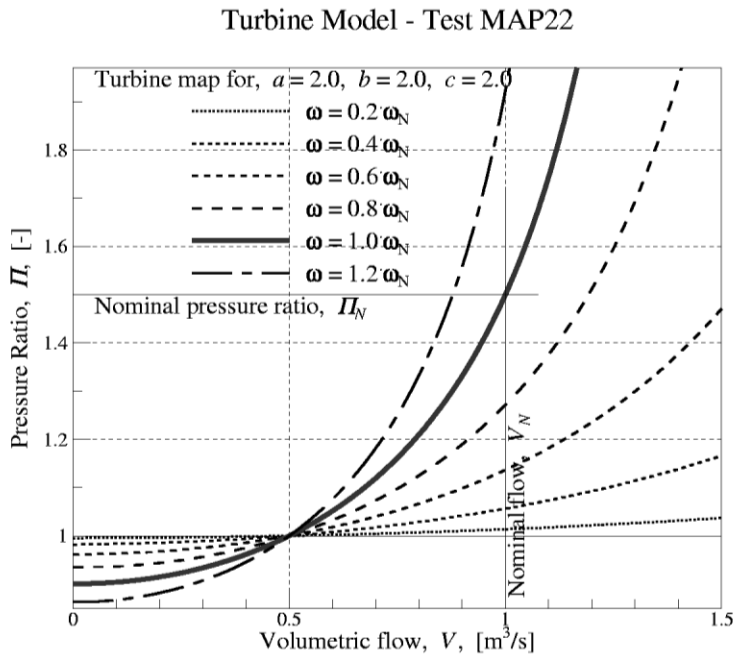


Figure 4-34 Influence of exponents on turbine map, $a=2.0, b=2.0, c=2.0$.

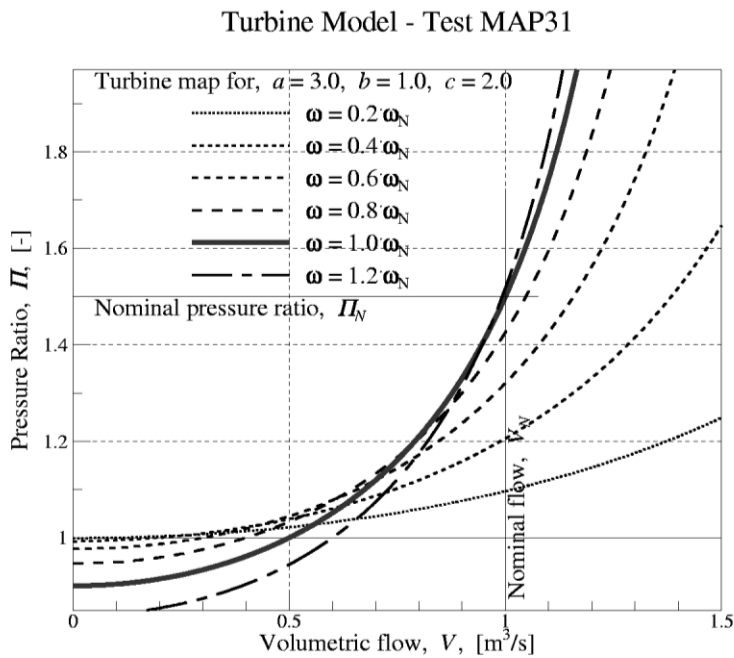


Figure 4-35 Influence of exponents on turbine map, $a=3.0, b=1.0, c=2.0$.

Turbine Model - Test MAP213

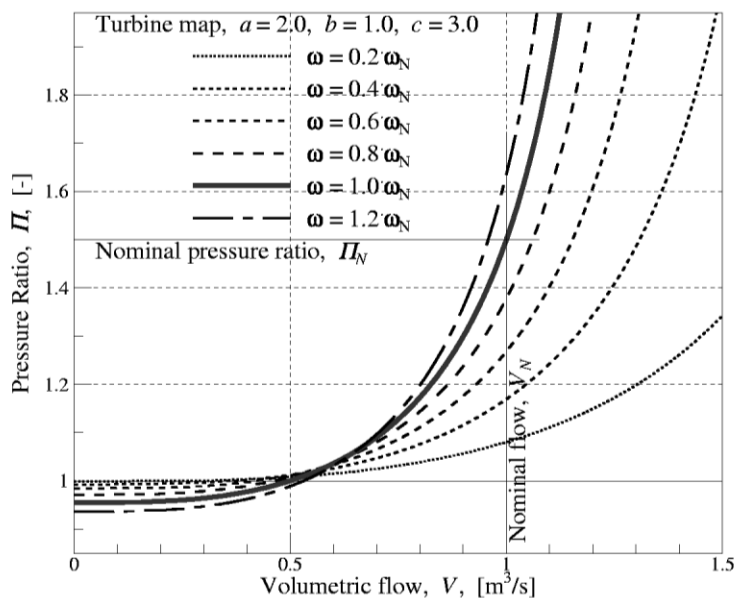


Figure 4-36 Influence of exponents on turbine map, $a=2.0$, $b=1.0$, $c=3.0$.

Turbine Model - Test MAP214

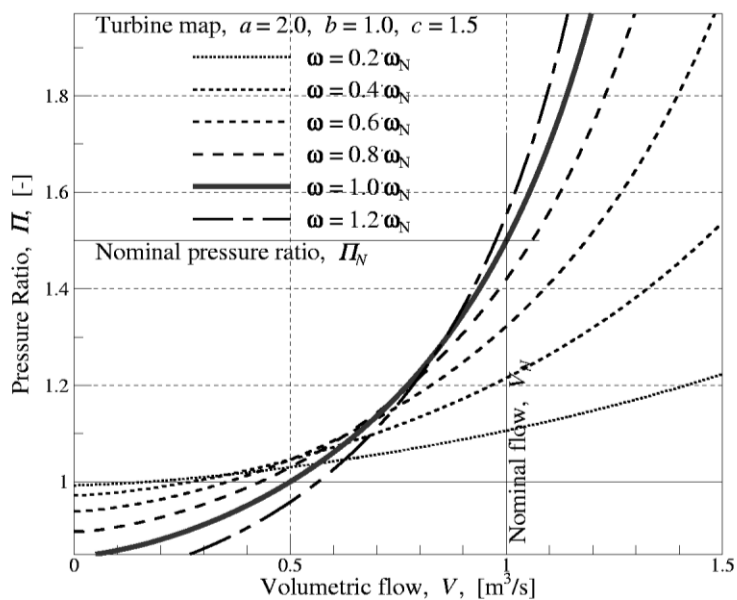


Figure 4-37 Influence of exponents on turbine map, $a=2.0$, $b=1.0$, $c=1.5$.

The influence of the third exponent, c , is illustrated in Figure 4-36 and Figure 4-37. The maps shown in these figures should be compared to the map shown in Figure 4-33, to see how the map changes when c is increased from the default value of 2.0 (Figure 4-33) to 3.0 (Figure 4-36), and decreased to 1.5 (Figure 4-37).

The influence of the reverse speed degradation factor, C_{RS} , on the turbine maps is shown in Figure 4-38, Figure 4-39 and Figure 4-40. The following values were used to produce maps shown in these figures:

$$\begin{aligned}\Pi_N &= 1.5, \\ V_N &= 1.0 \text{ m}^3/\text{s}, \\ V_0 &= 0.5 \text{ m}^3/\text{s}, \\ \omega_N &= 50.0 \text{ s}^{-1}, \\ a &= 2.0, \\ b &= 1.0, \\ c &= 2.0.\end{aligned}$$

Figure 4-38 shows turbine maps for $C_{RS} = 0.1$ for the turbine speed, ω , between +100% and -100%. It is seen that in case of negative (reverse) speed the pressure ratio is larger than for a corresponding positive speed. The difference is small for small $|\omega|$, and increases with increasing $|\omega|$.

Figure 4-39 shows turbine maps for $C_{RS} = 2.0$ for the turbine speed, ω , between +100% and -100%. In contrast to the previous case, the negative (reverse) speed gives smaller pressure ratio than that for a corresponding positive speed. Again, the difference is small for small $|\omega|$, and increases with increasing $|\omega|$.

Generally, it may be observed that for $C_{RS} < 1.0$ the lines at reverse speed are above those at the corresponding normal speed, while for $C_{RS} > 1.0$ the lines at reverse speed are below those at the corresponding normal speed.

Finally, Figure 4-40 shows turbine maps for $C_{RS} = -1.0$ for the turbine speed, ω , between +100% and -100%. With decreasing the value of C_{RS} , the pressure lines are higher in negative (reverse) speed range.

The influence of the parameter C_{RS} may be shortly described by looking at the maps for the (nearly) zero fluid flow and $\omega = +100\%$ and $\omega = -100\%$. If C_{RS} is positive, then at nearly zero flow the turbine acts as compressor, i.e. it provides pressure head in the normal flow direction, for both forward and reverse speeds. On the other hand, if C_{RS} is negative, then at zero flow and $\omega = +100\%$ the turbine acts as compressor, providing (a small) pressure head in the normal flow direction, while at zero flow and $\omega = -100\%$ it acts as a compressor providing (a small) head in the reversed flow direction. It should be noted that for large fluid flows and $\omega = -100\%$ it acts as a compressor providing a large pressure head in the reversed flow direction.

The default value of C_{RS} is -1.5. The value was chosen based on comparisons with four-quadrant turbine data, shown in (Bemmert, 1980). In the previous SPECTRA versions the default value of C_{RS} was equal to 0.1.

Turbine Model - Test MAP01

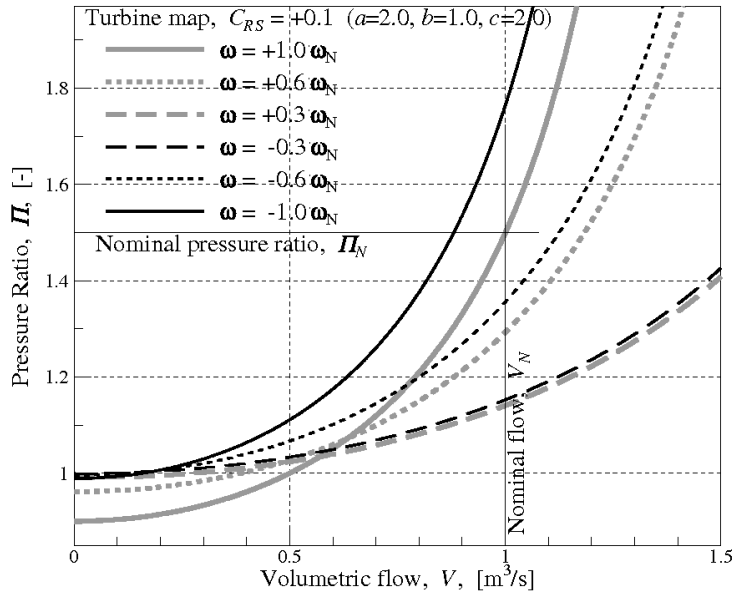


Figure 4-38 Influence of C_{RS} on turbine map, $C_{RS}=0.1$.

Turbine Model - Test MAP2

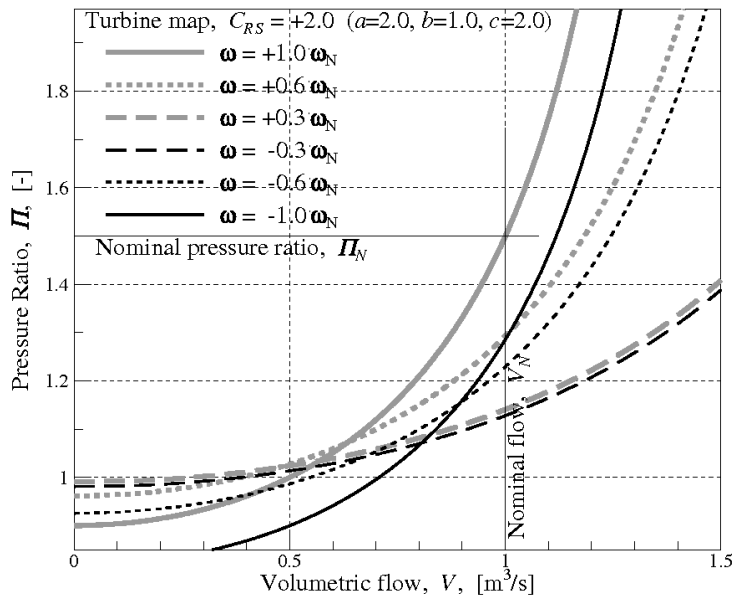


Figure 4-39 Influence of C_{RS} on turbine map, $C_{RS}=2.0$.

Turbine Model - Test MAP1

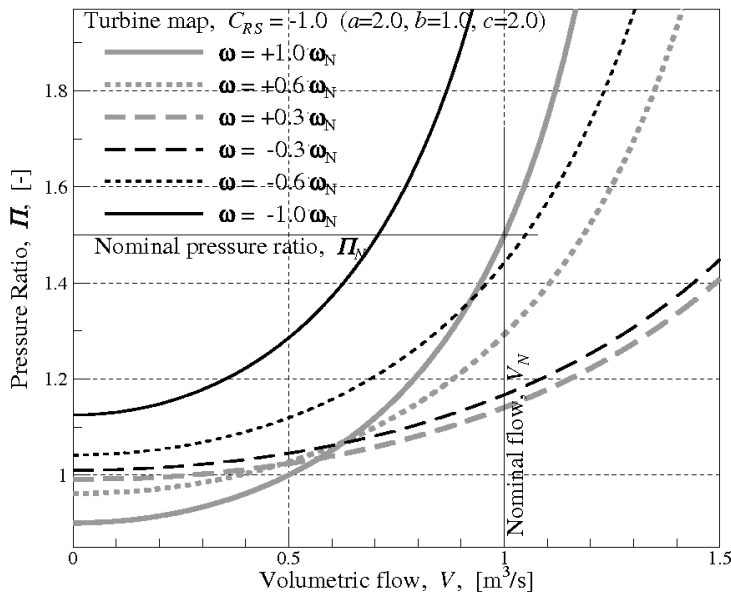


Figure 4-40 Influence of C_{RS} on turbine map, $C_{RS}=-1.0$.

The influence of the reverse flow degradation factor, C_{RF} , on the turbine maps is shown in Figure 4-41 and Figure 4-42. The following values were used to produce the maps shown in these figures:

$$\begin{aligned}
 \Pi_N &= 1.5, \\
 V_N &= 1.0 \text{ m}^3/\text{s}, \\
 V_0 &= 0.5 \text{ m}^3/\text{s}, \\
 \omega_N &= 50.0 \text{ s}^{-1}, \\
 a &= 2.0, \\
 b &= 1.0, \\
 c &= 2.0, \\
 C_{RS} &= -1.5.
 \end{aligned}$$

The default value of value of C_{RS} was used in both figures. Comparison of Figure 4-41 and Figure 4-42 gives an indication of the influence of the reverse flow degradation factor, C_{RF} . The default value of C_{RF} is 0.05. The value was chosen based on comparisons with four-quadrant turbine data, shown in (Bemmer, 1980). In the previous SPECTRA versions the reverse speed factor was not used, which means that C_{RF} was by definition equal to 1.0.

Comparison of the maps obtained with different values of C_{RS} and C_{RF} with measurement data from (Bemmer, 1980), is shown in Figure 4-43 and Figure 4-44. The turbine nominal data were assumed following the data in (Bemmer, 1980):

$$\begin{aligned}
 \Pi_N &= 3.91, \\
 V_N &= 3.0 \text{ m}^3/\text{s}, \\
 \omega_N &= 116.7 \text{ s}^{-1}, (7000 \text{ rev}/\text{min}).
 \end{aligned}$$

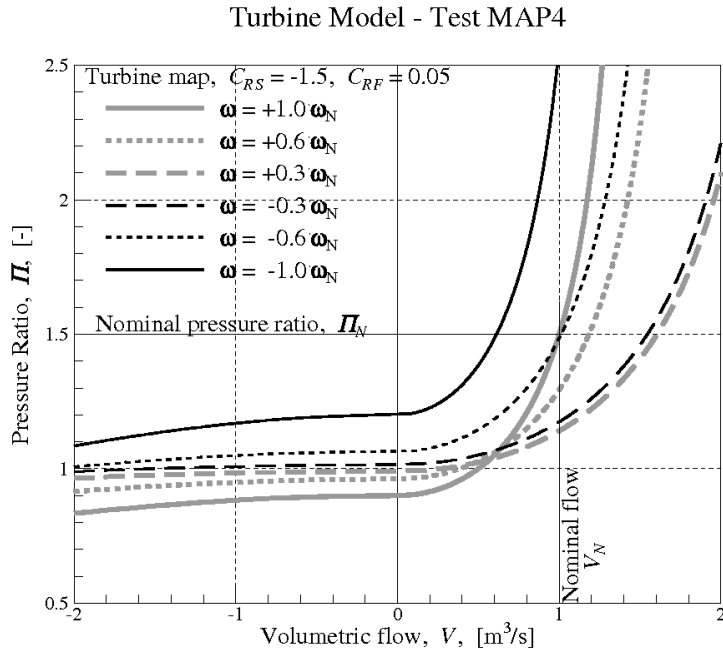


Figure 4-41 Influence of C_{RF} on turbine map, $C_{RF}=0.2$, $C_{RS}=-1.5$.

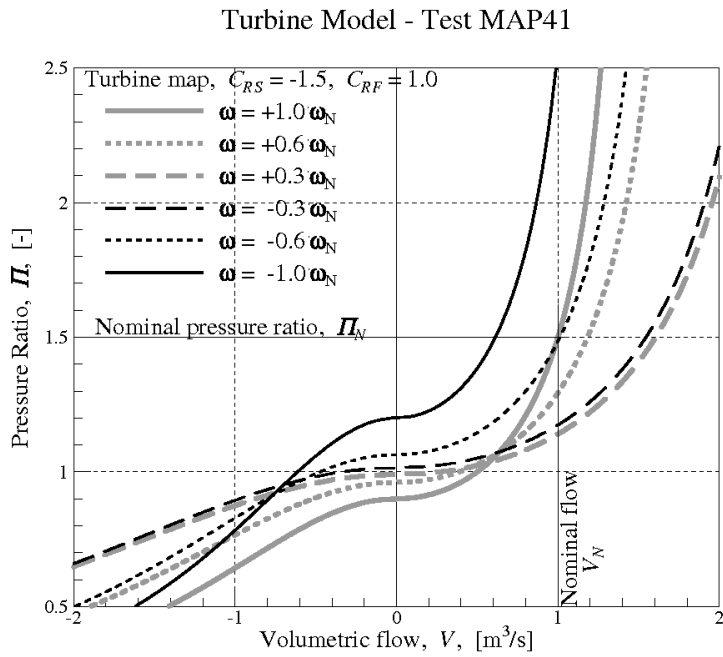


Figure 4-42 Influence of C_{RF} on turbine map, $C_{RF}=1.0$, $C_{RS}=-1.5$.

The values of V_0 and the exponents, suitable to represent reasonably well the turbine behavior in the normal operating conditions (positive speed, positive flow) were selected in a few trials as:

$$\begin{aligned}V_0 &= 1.0 \text{ m}^3/\text{s}, \\a &= 2.0, \\b &= 0.5, \\c &= 2.0.\end{aligned}$$

The parameters determining the turbine behavior in the reverse speed and reverse flow conditions were selected to be:

$$\begin{aligned}C_{RS} &= -1.5, \\C_{RF} &= 0.05.\end{aligned}$$

Figure 4-43 shows the measured power for positive (normal) and negative (reversed) flows and speeds. The positive speed values are plotted using solid lines and empty markers, while the negative speed values are plotted using dashed lines and filled markers.

Figure 4-44 shows the calculated values. The positive speed values are plotted using grey lines and empty markers, while the negative speed values are plotted using dark lines and filled markers. The left graph in Figure 4-44 shows values obtained with a constant efficiency of 1.0. In case of reversed speed and normal (positive) flow the fluid decompression is very similar to the decompression occurring in normal speed. Therefore the power calculated with the efficiency of 1.0 is negative (meaning the power is obtained from the machine – watch the scale in Figure 4-44). Based on the measured data it is clear that the power should be positive (the power is consumed by the turbine turning on backwards). This may be best explained using a h - s (enthalpy-entropy) graph, shown in Figure 4-45.

In case of an ideal isentropic expansion from a given pressure p_1 to another pressure p_2 , one obtains maximum power – this is the line 1-2a. This is an ideal process and it does not occur in practice. A practical process in a turbine at its normal operating conditions is shown by the line 1-2b. In such case some energy is dissipated as heat and the energy that is obtained from the turbine is smaller. The isentropic efficiency is in this case equal to:

$$\eta = \frac{\Delta h_1}{\Delta h_0}$$

A typical turbine has the efficiency of 0.7 - 0.9 in the typical operating conditions. The case of turbine turning on reverse (Figure 4-43 dashed lines), the fluid decompression is shown by the line 1-2c in Figure 4-45. The amount of energy dissipated as heat is so large that the exit enthalpy is higher than the inlet enthalpy. Consequently one has to put energy into the turbine to keep it running. In this case the turbine efficiency is negative, as shown in Figure 4-45.

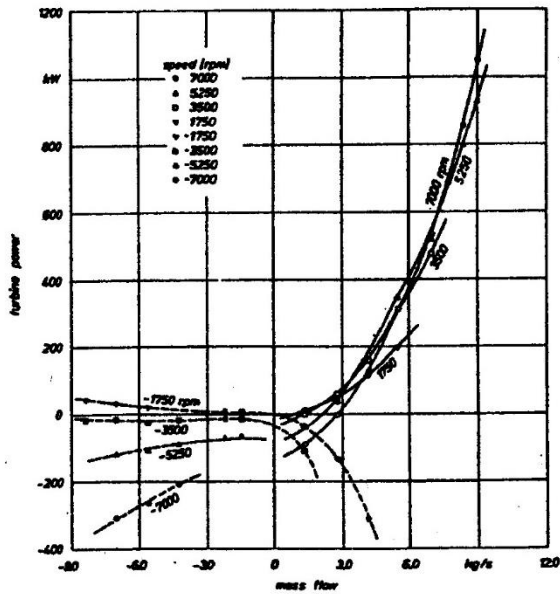


Figure 4-43 Power – reference (Bemert, 1980).

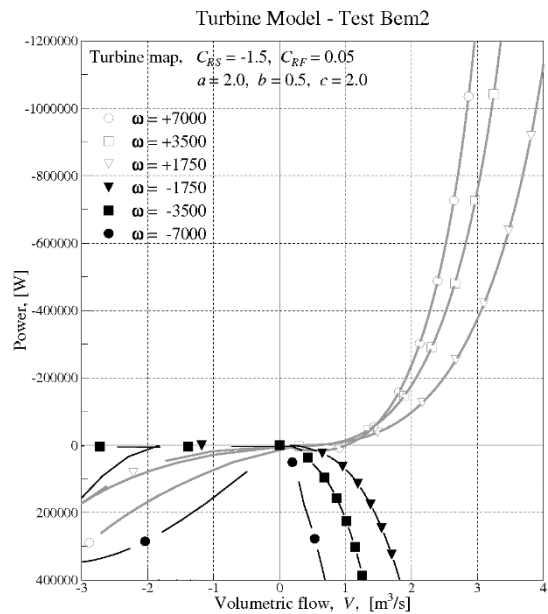
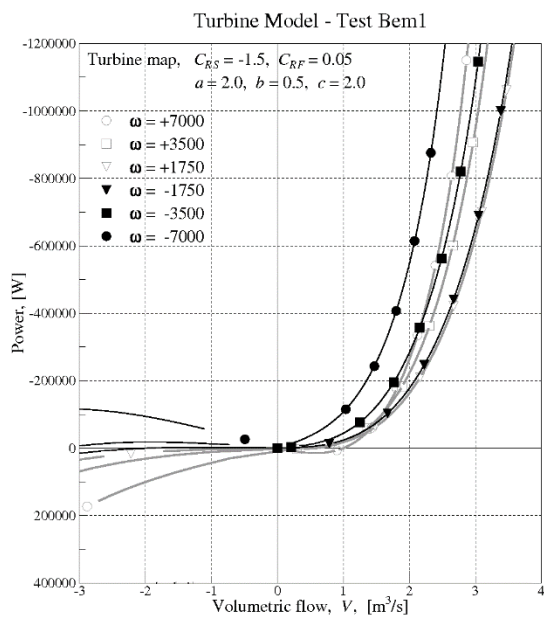


Figure 4-44 Turbine power $C_{RS} = -1.5$ $C_{RF} = 0.05$ (default in V. 2.10)
left: only positive efficiency, right: negative efficiency in reverse speed.

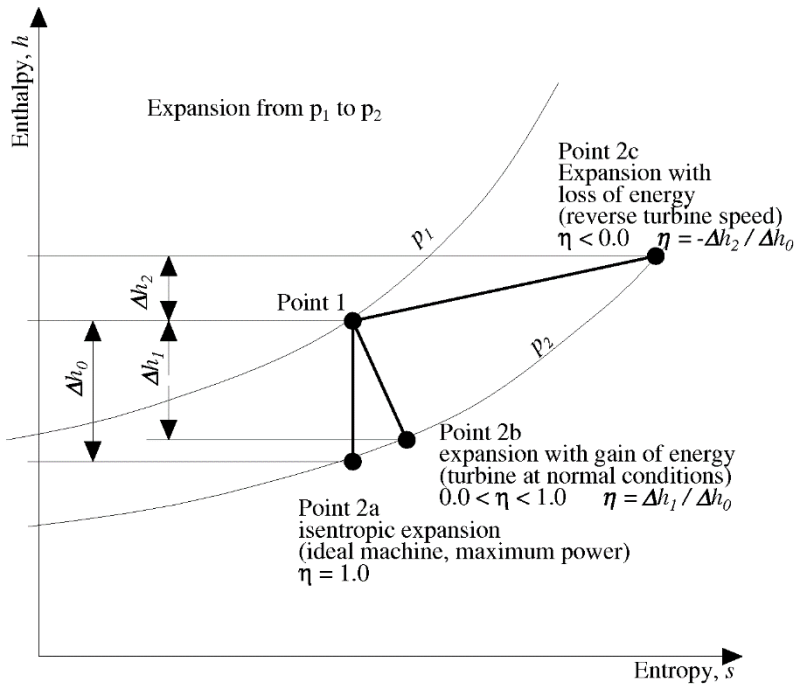


Figure 4-45 Illustration of the gas expansion in a turbine on the h - s diagram.

Looking at Figure 4-43 it is clear that the efficiency is negative in all cases with reverse speed (except maybe the lowest negative speed case, in the negative flow range). For the calculations shown in the right graph in Figure 4-44 the following efficiencies were used:

	Positive flow	Negative (reverse) flow
• $N = +7000$ rev/min:	$\eta = +0.9$	$\eta = +0.6$
• $N = +3500$ rev/min:	$\eta = +0.8$	$\eta = +0.4$
• $N = +1750$ rev/min:	$\eta = +0.6$	$\eta = +0.2$
• $N = -1750$ rev/min:	$\eta = -3.0$	$\eta = -0.1$
• $N = -3500$ rev/min:	$\eta = -5.0$	$\eta = -0.3$
• $N = -7000$ rev/min:	$\eta = -7.0$	$\eta = -3.0$

The values of efficiencies were obtained in few trials, in order to provide a reasonably good match to the measured data, shown in Figure 4-43. For simplicity a constant efficiency was defined for each speed, thus the efficiency was in fact only a function of speed: $\eta = \eta(N)$. The efficiency could be made as a function of both flow and speed, $\eta = \eta(V, N)$ and in this way a better match could be obtained.

References of Appendix B

- Bemmert 1980 K. Bemmert, P. Zehner, "Measurements of the Four-Quadrant Characteristics on a Multi-Stage Turbine", *Journal of Engineering for Power, Transactions of ASME*, Vol. **102**, pp. 316-321, April 1980.

appendix C Pressure Loss Coefficients for Valves

In general the pressure loss coefficient of a valve changes with the valve open fraction. Sometimes the change is so significant that it is important to include a variable loss coefficient in the computational model.

- The following expression may be used to calculate the loss factors (forward and reverse):

$$K_V = K_0 \cdot \left[C_V + (1 - C_V) \frac{A_V}{A_0} \right]$$

- Tabular Function may be used. The TF value is calculated by the program using the open fraction as an argument. The loss factors (forward and reverse) are calculated from:

$$K_V = K_0 \cdot TF(A_V / A_0)$$

These two methods are described in the following subsections.

C.1 Pressure Loss Coefficient Given by an Analytical Expression

SPECTRA uses two values to define valve characteristics: K_0 and C_V . The actual loss coefficient is calculated from:

$$K_V = K_0 \left[C_V + (1 - C_V) \frac{A_V}{A_0} \right]$$

K_V	current valve loss coefficient, (-)
K_0	loss coefficient for fully open valve, (-) (FLCFJN or FLCRJN, record 210XXX)
C_V	valve resistance increase coefficient, (-) (CVVLJN, record 220XXX)
A_V	current valve open area, (m ²)
A_0	area for fully open valve, (m ²) (AMAXJN, record 200XXX)

The values of K_0 and C_V may be estimated, using the following relations:

$$C_V = \frac{K_V / K_0 - A_V / A_0}{1 - A_V / A_0}$$
$$K_V \rightarrow K_0 \quad \text{when } A_V \rightarrow A_0$$
$$K_V \rightarrow K_0 \cdot C_V \quad \text{when } A_V \rightarrow 0.0$$

Data can easily be obtained from appropriate handbooks. Below a calculation procedure is shown, to obtain the coefficients for two valve types: a butterfly valve and a rectangular gate valve.

- Butterfly Valve

Reference (Idel, 1986) gives loss coefficients for a butterfly valve in a tube of a circular cross section (Diagram 9-16 in (Idel, 1986)). In case of a thin plane disk (Curve 2 in Diagram 9-16) the values are:

θ°	0	10	20	30	40	50	60	70
K_{Idel}	0.30	0.52	1.54	4.50	11.0	29.0	108.0	625.0

It must be remembered that the loss factors given in (Idel, 1986), K_{Idel} , are related to the velocity in a fully open channel. To obtain values related to the actual valve flow area one must multiply these values by the area ratio squared: $(A/A_0)^2$. For a given angle, θ , the open area is given by: $A=A_0 \cdot (1-\sin\theta)$. Therefore the loss factors related to the actual flow area are equal to: $K=K_{Idel} \times (1-\sin\theta)^2$. The values of K , as well as K_{Idel} , are shown in Figure 4-46.

The value of K_0 , needed for SPECTRA input, is equal to the loss factor for the fully open valve, thus 0.30. It has been found using a trial and error procedure, that a value of $C_V=7.0$ represents well the K values in Figure 4-46. Thus, for the butterfly valve considered here the appropriate values are:

$$K_0 = 0.30,$$

$$C_V = 7.0.$$

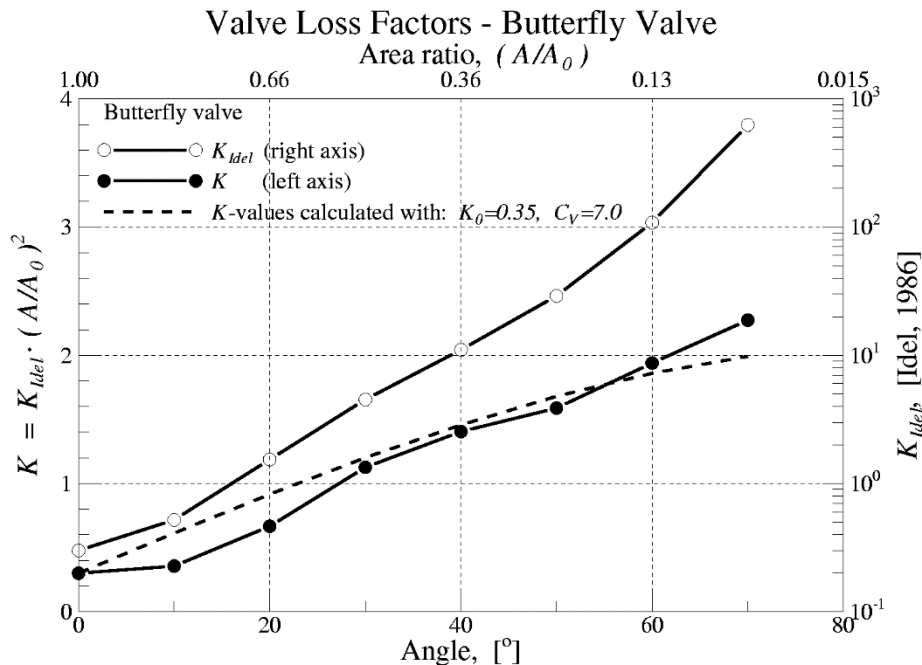


Figure 4-46 Loss factors, butterfly valve.

- Gate Valve

For a rectangular, single disk, gate valve the loss coefficients are given as a function of the ratio of the disk position (h), to the channel width (a) (Idel, 1986), Diagram 9-5). The values are:

h/a	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
K_{Idel}	193	44.5	17.8	8.12	4.02	2.08	0.95	0.39	0.09

Again the values of K_{Idel} are related to the velocity in a fully open channel. The values are therefore multiplied by the area ratio squared: $(A/A_0)^2$. For a rectangular valve $(A/A_0)^2$ is simply equal to $(h/a)^2$. The values of K , as well as K_{Idel} , are shown in Figure 4-47.

The value of K_0 , needed for SPECTRA input, is equal to the loss factor for the fully open valve, thus 0.09. It has been found using a trial and error procedure, that a value of $C_v=25.0$ represents well the K values in Figure 4-47. Thus, for the rectangular gate valve considered here the appropriate values are:

$$K_0 = 0.09,$$

$$C_v = 25.0.$$

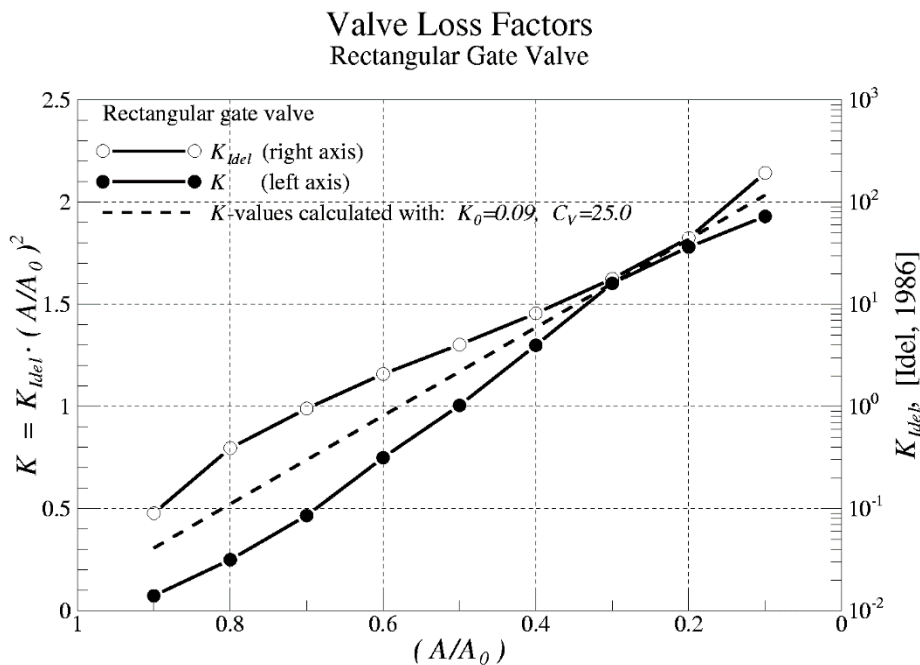


Figure 4-47 Loss factors, gate valve.

C.2 Pressure Loss Coefficient Given by a Table

With this option the pressure loss factors (forward and reverse) are calculated from:

$$K_v = K_0 \cdot TF(A_v / A_0)$$

K_0 constant multiplier on the pressure loss coefficient (forward and reverse)

TF Tabular Function evaluated for the current valve open fraction, A_v/A_0 , (-) (the TF number is indicated by negative value of CVVLJN, record 220XXX)

For example, in case of a butterfly valve the values are:

θ°	0	10	20	30	40	50	60	70
A/A_0	1.00	0.826	0.658	0.500	0.357	0.234	0.134	0.0603
K_{Idel}	0.30	0.52	1.54	4.50	11.0	29.0	108.0	625.0
K	0.30	0.355	0.667	1.13	1.40	1.59	1.94	2.27

The input deck defining such valve is discussed in Volume 3.

References of Appendix C

Idel, 1986 I.E. Idelchik, "Handbook of Hydraulic Resistance", Second Edition, ISBN 3-540-15962-2, Hemisphere Publishing Corporation, 1986.