# SUE - System-code Uncertainty Evaluation
# Version 3.00, November 2024

## Program Description
## User's Guide
## Test Problems

Under the contract of **PIONEER**

Public

| | | | |
|---|---|---|---|
| Author(s): | M.M. Stempniewicz | Reviewed: | E.A.R. de Geus |
| | | | D.C. Visser |
| | | Approved: | I.J.V. de Kock |
| Reference: | 26315/24.285017 Rev. 2 | Status: | **Final** |
| 154 pages | 2024-11-30 | | |

# Abstract

System-code Uncertainty Evaluation (SUE) is a simple and user-friendly program to perform uncertainty analysis with system thermal-hydraulic (STH) and computational fluid dynamics (CFD) codes. The current version of the program is specifically intended for:

- SPECTRA, RELAP5, MELCOR, and FLUENT (CFD).

For other codes post processing is possible if the quantities of interest (QoI) may be written to a simple text file or CSV file.

- Chapter 2 provides the Program Description (theory manual). The following methodologies are available:
  - Random Sampling (RS) methodology,
  - DS-Standard methodology, based on Deterministic Sampling (DS),
  - DS-Hadamard methodology, based on Deterministic Sampling,
  - DS-Simplex methodology, based on Deterministic Sampling,
  - Engineering Hot-Spot Factor (EHSF) methodology,
  - User defined matrix of uncertain parameters.
- Chapter 3 provides the User's Guide, including the following parts.
  - Description of SUE input file,
  - Description of code inputs required,
  - Description of SUE output files.
- Chapter 4 provides the description of the test problems.
  - Analysis of PBF Test LOC-11C with the system code SPECTRA,
  - Analysis of PBF Test LOC-11C with the system code RELAP5,
  - Comparison of SPECTRA and RELAP5 results,
  - Analysis of PBF Test LOC-11C with the system code MELCOR.

The main conclusions from the test case calculations performed are as follows.

- The Deterministic Sampling methodologies give very similar results as the Random Sampling methodologies. The DS methodologies allow to significantly reduce the number of runs when the number of uncertain parameters is small. In the present case the DS methodologies required 6 - 10 runs, while the RS methodologies needed hundreds of calculations.
- Verification of SUE was performed using SPECTRA, RELAP5, and MELCOR. Calculations are described in this report. Further verification was performed by comparing SUE / RELAP5 results with RAVEN / RELAP5 results.

NRG Petten
Westerduinweg 3
P.O. Box 25
1755 ZG Petten
The Netherlands

NRG Arnhem
Utrechtseweg 310 - B50-West
P.O. Box 9034
6800 ES Arnhem
The Netherlands

## List of Contents

# 1 Introduction

System-code Uncertainty Evaluation (SUE) is a simple and user-friendly program to perform uncertainty analysis with system thermal-hydraulic (STH) and computational fluid dynamics (CFD) codes. The current version of the program is specifically intended for three STH codes and one CFD code:

- SPECTRA,
- RELAP5,
- MELCOR,
- FLUENT (CFD).

For other codes post processing is possible if the quantities of interest (QoI) may be written to a simple text file or CSV file.

- Chapter 2 provides the Program Description (theory manual).
- Chapter 3 provides the User's Guide (input requirements).
- Chapter 4 provides the description of the test problems.
- Finally, Chapter 5 provides the summary and conclusions.

# 2 Program Description

## 2.1 Introduction

This chapter provides the theory description, including:

- General description of what the code does - section 2.2.
- Discussion of uncertain parameters, how to define them, what types of uncertain parameters are available - section 2.3.
- Available methodologies - section 2.4.
- Output parameters - section 2.5.

## 2.2 General Description

SUE is an integrated software (Fortran program) to perform UQ analyses. The program performs the following tasks:

1. Based on the selected methodology and uncertain parameters, SUE first determines the number of runs required, N.
2. Next, it prepares input files for all N runs.
3. Next, it executes the program (SPECTRA, RELAP5, MELCOR, FLUENT, or other) N times.
4. Finally, it performs post processing, including calculation of minimum/maximum values of selected parameters, mean value and standard deviation, Pearson's correlation coefficients, Spearman's rank correlation coefficient, engineering hot spot factors.

The steps 1 through 3 may be performed with any STH or CFD code. There is no need to manipulate in any way with the STH/CFD codes that are being used. SUE takes care of everything; prepares all input files and starts all calculations. Therefore the use of SUE is very simple and user-friendly.

The step 4, post-processing is performed only for the selected programs (STH codes: SPECTRA, RELAP5, MELCOR, CFD code: FLUENT) because SUE can read output/plot files only for these programs. SUE may also be used with other codes, if these codes can output of the quantities of interest in a simple text file.

## 2.3 Uncertain Parameters

The uncertain parameters are defined in the SUE input file. Three types of uncertain parameters are distinguished.

- Independent parameters. These are discussed in section 2.3.1.
- Parameters that are directly related to a single independent parameters, either as being proportional to the independent parameter, i.e. multiplied by a constant factor, or differing by a constant added value. These are referred to here as "parameters dependent on a single uncertain parameter" or shortly "dependent parameters". These parameters are discussed in section 2.3.2.
- Parameters that are functions of several independent parameters. These are referred to here as Functions of independent parameters. The functions are discussed in section 2.3.3.

### 2.3.1 Independent Parameters

The independent uncertain parameters need to be defined by the user in the SUE input deck (section 3.1.9), including:

- distribution: normal or uniform,
- mean value,
- standard deviation,
- minimum value,
- maximum value.

Not all parameters need to be defined; default values exist (see 3.1.9).

Each uncertain parameter defined in the SUE input, must be present in the code input as **$XXX**, where XXX is the uncertain parameter number. For example:

```
*         dx [m]     Mat  Power  T [K]   N  N-start
310100  $001          901   0.0   569.0   1  7   *  GAP SIZE
```

During the execution, the current values of uncertain parameters are determined using the applied methodology (see section 2.4), the values of $XXX are replaced by the current values, and the code is executed.

### 2.3.2 Parameters Dependent on a Single Uncertain Parameter

These are parameters that are directly related to a single independent parameters, either as being proportional to the independent parameter, i.e. multiplied by a constant factor, or differing by a constant added value.

- Type: "MULTIPLY":

$$y = \mu_y \cdot x / \mu_x$$

- Type: "ADD":

$$y = \mu_y + x - \mu_x$$

Here $\mu_x$ mean value of independent parameter *x*,
$\mu_y$ mean value of dependent parameter *y*,
*x* actual value of independent parameter *x*,
*y* actual value of dependent parameter *y*,

The dependent parameters are defined in the code input as **$XXX@VALUE**. Here $XXX is the independent parameter and VALUE is the numerical value of the dependent parameter.

These parameters are used to change several input parameters simultaneously. For example, suppose that the user wishes to increase the thermal conductivity of a certain material, that is defined by a table as a function of temperature. For each temperature, the value of thermal conductivity need to be increased by a certain factor. An example of how this is done is shown in section 3.2.2.

### 2.3.3 Functions of Multiple Uncertain Parameters

Functions of several (up to 100) uncertain parameters may be defined. Two types of functions are available:

- Addition:

$$F = \sum_i \left( \left( A_i \times x_i + B_i \right)^{C_i} \right)$$

- Multiplication:

$$F = \prod_i \left( \left( A_i \times x_i + B_i \right)^{C_i} \right)$$

Here: $A_i$ multiplicative constant for the uncertain parameter number *i*,
$B_i$ additive constant for the uncertain parameter number *i*,
$C_i$ exponent for the uncertain parameter number *i*,

Each function defined in the SUE input, must be present in the code input as **#XXX**, where XXX is the function number. For example:

```
*  #001   *   FN-001
```

Functions may be useful in a variety of situations. For example, suppose that the power is measured by a device that is calibrated using flow measurement and temperature measurement. The power is equal to:

$$Q = W \times c_p \times (T_1 - T_2)$$

Suppose the measurement of the flow, $W$, and the temperatures, $T_1$, $T_2$, have uncertainties. We need to define the initial reactor power consistently with these values. If we treat $W$, $T_1$, $T_2$, as independent uncertain parameters, and $c_p$ as constant, we may use the following functions to define power:

$$F_1 = (T_1 - T_2)$$

$$F_2 = c_p \times W \times F_1$$

## 2.4 Methodologies

An overview of methodologies may be found in literature, [5], [6], [7], [8], [9], [10], [11], [14]. The following methodologies are currently available within SUE:

- Random Sampling (RS) methodology - section 2.4.1.
- Deterministic Sampling, DS-Standard methodology - section 2.4.2.
- Deterministic Sampling, DS-Hadamard methodology - section 2.4.3.
- Deterministic Sampling, DS-Simplex methodology - section 2.4.4.
- Engineering Hot-Spot Factor (EHSF) methodology - section 2.4.5.
- User defined matrix of uncertain parameters - section 2.4.6.

These methodologies were selected for the current version of SUE. Other methodologies may be easily added in the future. The methodology is selected by the user in the SUE input deck - see Chapter 3. section 3.1.1.

### 2.4.1 Random Sampling (RS) Methodology

Among others, the GRS method [6] has been developed for the determination of uncertainties. The state of knowledge about all uncertain parameters is described by ranges and probability distributions - Figure 1. In order to get information about the uncertainty of the computer code results, a number of code runs have to be performed. For each of these calculation runs, all identified uncertain parameters are varied simultaneously.

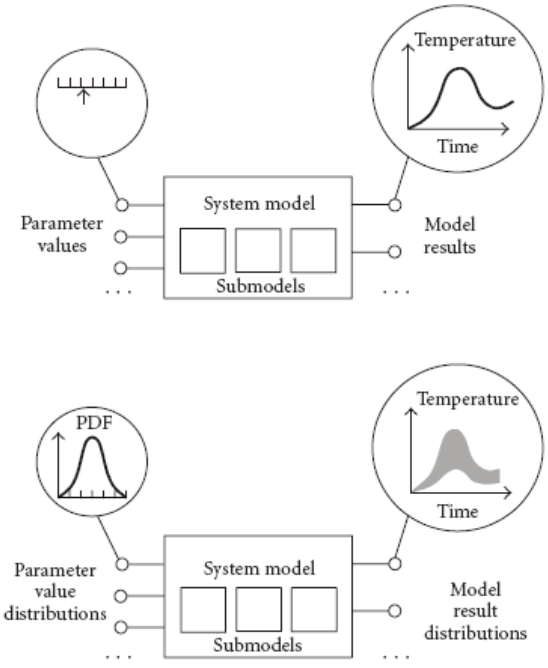



*Figure 1: Consideration of input parameter value ranges instead of discrete values [6]*

Uncertain parameters are uncertain input values, models, initial and boundary conditions, numerical values like convergence criteria and maximum time step size, and so forth. Model uncertainties are expressed by adding on or multiplying correlations by corrective terms, or by a set of alternative model formulations. Uncertainties in nodalization, to describe the important phenomena, are to be taken into account in the code validation process. However, alternative nodalization schemes can be included in the uncertainty analysis. Code validation results are a fundamental basis to quantify parameter uncertainties.

The selection of parameter values according to their specified probability distributions, their combination, and the evaluation of the calculation results requires a method. Following a proposal by GRS [6], the central part of the method is a set of statistical techniques. The advantage of using these techniques is that the number of code runs needed is independent of the number of uncertain parameters. In each code run, all uncertain parameters are varied simultaneously. In order to quantify the effect of these variations on the result, statistical tools are used. Because the number of runs is independent of the number of uncertain parameters, no a priori ranking of input parameters is necessary to reduce their number in order to cut computation cost.

The number of code runs depends on the user-defined probability content and confidence level of the statistical tolerance limits used in the uncertainty statements of the results. The required minimum number of these runs is given by Wilks' formula [7], [15], [16]. The correlations between number of code runs, confidence level, and probability of Wilks' formula are defined below:

- One-side tolerance limit:

$$1 - \alpha^N \geq \beta$$

- Two-side tolerance limit:

$$1 - \alpha^N - N \cdot (1 - \alpha) \cdot \alpha^{N-1} \geq \beta$$

Here $\alpha$ is probability, $\beta$ is the confidence level that the maximum code result will not be exceeded with the probability of $\alpha$, and $N$ denotes the number of code runs. The minimum number of code runs is tabulated in Table 1 [5].

*Table 1: Minimum number of runs for one-sided and two-sided tolerance limits*

| | One-side tolerance limits | | | Two-side tolerance limits | | |
|---|---|---|---|---|---|---|
| β \ α | 0.90 | 0.95 | 0.99 | 0.90 | 0.95 | 0.99 |
| 0.90 | 22 | 45 | 230 | 38 | 77 | 388 |
| 0.95 | 29 | 59 | 299 | 46 | 93 | 473 |
| 0.99 | 44 | 90 | 459 | 64 | 130 | 662 |

The sampling is performed by dividing the distribution function into non-overlapping intervals of equal length except for the first and last intervals (which are half-size), followed by the random selection of a value within each interval. The number of intervals is a user-defined parameter, with a minimum of 3 and a maximum of 10001 (section 3.1.8). Figure 2 and Figure 3 show the uniform and normal distribution functions for number of intervals equal to 11. A more detailed discussion about the scheme is provided in Appendix A.

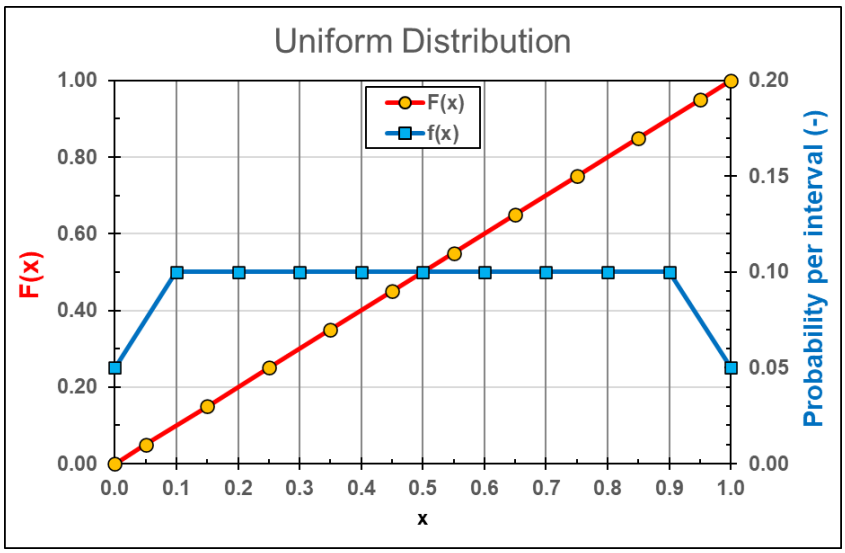



*Figure 2: Sampling, uniform distribution, NINTDF=11 - Appendix A*

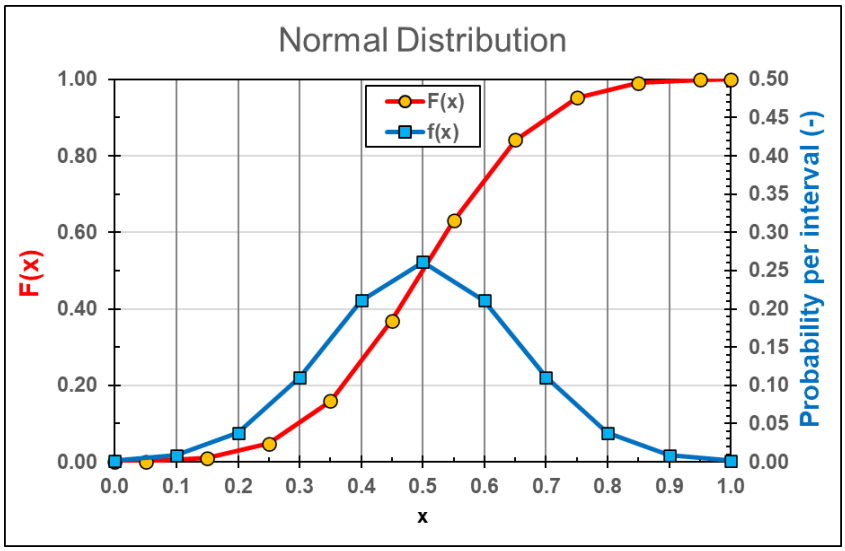



*Figure 3: Sampling, normal distribution, NINTDF=11 - Appendix A*

### 2.4.2 DS-Standard Methodology

The Deterministic Sampling DS-Standard methodology is described for example in [9], [10]. The main idea of this method is to characterize a continuous probability distribution function with a set of samples, called sigma points, which represent the moments of that distribution function. Since the sigma points are few in number, the use of DS can drastically reduce the number of samples compared to Random Sampling methodologies (RS). Therefore, it represents a considerable decrease in the number of computations required for UQ. Moreover, compared to stochastic methods, DS does not rely on random number generators, which means that random sampling errors (i.e., statistical noise) are not present in using this methodology [10]. Therefore, the accuracy of the represented PDFs through DS methods are independent of the amount of samples of the ensemble.

The DS-Standard ensemble makes use of the simplest excitation matrix [10]. The number of runs, *N*, in the DS-Standard ensemble is equal to:

$$N = 2n$$

Here *n* is the number of uncertain input parameters. As an example, for three input parameters (*n* = 3), the DS-Standard ensemble consists of 6 samples (*N* = 6) given by:

$$\begin{vmatrix} \mu_1+\sqrt{n}\sigma_1 & \mu_1 & \mu_1 & \mu_1-\sqrt{n}\sigma_1 & \mu_1 & \mu_1 \\ \mu_2 & \mu_2+\sqrt{n}\sigma_2 & \mu_2 & \mu_2 & \mu_2-\sqrt{n}\sigma_2 & \mu_2 \\ \mu_3 & \mu_3 & \mu_3+\sqrt{n}\sigma_3 & \mu_3 & \mu_3 & \mu_3-\sqrt{n}\sigma_3 \end{vmatrix}$$

Here $\mu_i$ is the mean value and $\sigma_i$ is the standard deviation of the uncertain parameter $x_i$. In a simpler notation, this can be represented as:

$$\sqrt{n}\cdot\begin{vmatrix} +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \end{vmatrix}$$

For each row, the sum is zero. This means that for each uncertain parameter the value averaged over all runs is equal to the mean value. The main advantage of DS-Standard is its simplicity, whereas its downside is its strong dependence to the number of input parameters.

In DS-Standard method, the factor $\sqrt{n}$ is present. For larger number of n, this may lead to unrealistic values of parameters. In SUE, the values of: $\mu_i + \sqrt{n}\cdot\sigma_i$ and $\mu_i - \sqrt{n}\cdot\sigma_i$ are limited by the (user-defined) minimum and maximum values, which is defined by the user for each parameter - see Chapter 3, section 3.1.9. Thus the following checks are made:

$$\mu_i - \sqrt{n}\sigma_i \geq x_{\min,i} \qquad \mu_i + \sqrt{n}\sigma_i \leq x_{\max,i}$$

A warning message is written to the diagnostics file every time the limit is applied (see section 3.3.3). Such warnings indicate that a different methodology should be used.

### 2.4.3 DS-Hadamard Methodology

The DS-Hadamard methodology is described in [9], [10]. The methodology is based on Hadamard excitation matrix. Construction of the Hadamard matrix is described in [12]:

Examples of Hadamard matrices were actually first constructed by James Joseph Sylvester in 1867. Let $H$ be a Hadamard matrix of order $n$. Then the partitioned matrix

$$\begin{bmatrix} H & H \\ H & -H \end{bmatrix}$$

is a Hadamard matrix of order $2n$. This observation can be applied repeatedly and leads to the following sequence of matrices, also called Walsh matrices.

$$H_1 = [1],$$
$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$
$$H_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix},$$

and

$$H_{2^k} = \begin{bmatrix} H_{2^{k-1}} & H_{2^{k-1}} \\ H_{2^{k-1}} & -H_{2^{k-1}} \end{bmatrix} = H_2 \otimes H_{2^{k-1}},$$

for $2 \leq k \in N$, where $\otimes$ denotes the Kronecker product.

In this manner, Sylvester constructed Hadamard matrices of order $2^k$ for every non-negative integer $k$.[2]

Sylvester's matrices have a number of special properties. They are symmetric and, when $k \geq 1$ ($2^k > 1$), have trace zero. The elements in the first column and the first row are all positive. The elements in all the other rows and columns are evenly divided between positive and negative. Sylvester matrices are closely connected with Walsh functions.

The first row contains only positive numbers. Other rows contain the same amount of positive and negative numbers. Therefore, when these rows are used, then for each uncertain parameter the value averaged over all runs is equal to the mean value. With the DS-Hadamard ensemble, the number of runs, $N$, is equal to:

$$N = 2^{ceil\left(\frac{n+5}{4}\right)}$$

Here $n$ is the number of uncertain input parameters. For example, for five input parameters ($n$ = 5), the ensemble consists of 8 samples ($N$ = 8). The matrix construction is as follows:

- The full Hadamard matrix of order of 8 is constructed - see section 3.3.1.
- The reduced Hadamard matrix is created by skipping the first row and using the next five ($N$=5). (The first five rows are chosen arbitrarily; any rows other than the first one may be used. Use of different rows is equivalent to changing the order of uncertain parameters). The reduced matrix looks as follows.

```
REDUCED HADAMARD MATRIX

 \ RUN:
  \   1  2  3  4  5  6  7  8
PAR\ -- -- -- -- -- -- -- --
  1   1 -1  1 -1  1 -1  1 -1
  2   1  1 -1 -1  1  1 -1 -1
  3   1 -1 -1  1  1 -1 -1  1
  4   1  1  1  1 -1 -1 -1 -1
  5   1 -1  1 -1 -1  1 -1  1
```

The uncertain parameters are then given by $x_i = \mu_i + \sigma_i \times$ matrix.

### 2.4.4 DS-Simplex Methodology

The DS-Simplex methodology is described in [9], [10], [24], [25]. The minimal simplex ensemble was introduced in [25]. A simplex ensemble can be generated from half the standard ensemble, complemented by one "cancellation unit sample" $1^{n\times1}$ to cancel the first moments, The DS-Simplex ensemble points in the direction of a drastic reduction of samples. Hence, it represents the minimal sized ensemble and the most efficient replacement to the DS-standard. The number of runs, *N*, in the DS-Simplex ensemble is equal to:

$$N = n + 1$$

Here *n* is the number of uncertain input parameters. The DS-Simplex ensemble can be generated from half the standard ensemble, complemented by one "cancellation unit sample", $1^{n\times1}$, to cancel the first moments [10]:

$$\sqrt{n+1} \bullet \perp\{|I^{n\times n} \quad - 1^{n\times1}|\}, \;\; m = n + 1$$

The operator: $\perp$ is performing classical Gram-Schmidt orthogonalization and normalization of rows. This procedure is described in [26]. A copy is provided below:

The Gram–Schmidt process [ edit ]

The vector projection of a vector $\mathbf{v}$ on a nonzero vector $\mathbf{u}$ is defined as

$$\operatorname{proj}_{\mathbf{u}}(\mathbf{v}) = \frac{\langle \mathbf{v}, \mathbf{u} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle} \mathbf{u},$$

where $\langle \mathbf{v}, \mathbf{u} \rangle$ denotes the inner product of the vectors $\mathbf{u}$ and $\mathbf{v}$. This means that $\operatorname{proj}_{\mathbf{u}}(\mathbf{v})$ is the orthogonal projection of $\mathbf{v}$ onto the line spanned by $\mathbf{u}$. If $\mathbf{u}$ is the zero vector, then $\operatorname{proj}_{\mathbf{u}}(\mathbf{v})$ is defined as the zero vector.

Given $k$ vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ the Gram–Schmidt process defines the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ as follows:

$$\begin{aligned}
\mathbf{u}_1 &= \mathbf{v}_1, & \mathbf{e}_1 &= \frac{\mathbf{u}_1}{\|\mathbf{u}_1\|} \\
\mathbf{u}_2 &= \mathbf{v}_2 - \operatorname{proj}_{\mathbf{u}_1}(\mathbf{v}_2), & \mathbf{e}_2 &= \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \\
\mathbf{u}_3 &= \mathbf{v}_3 - \operatorname{proj}_{\mathbf{u}_1}(\mathbf{v}_3) - \operatorname{proj}_{\mathbf{u}_2}(\mathbf{v}_3), & \mathbf{e}_3 &= \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \\
\mathbf{u}_4 &= \mathbf{v}_4 - \operatorname{proj}_{\mathbf{u}_1}(\mathbf{v}_4) - \operatorname{proj}_{\mathbf{u}_2}(\mathbf{v}_4) - \operatorname{proj}_{\mathbf{u}_3}(\mathbf{v}_4), & \mathbf{e}_4 &= \frac{\mathbf{u}_4}{\|\mathbf{u}_4\|} \\
&\vdots & &\vdots \\
\mathbf{u}_k &= \mathbf{v}_k - \sum_{j=1}^{k-1} \operatorname{proj}_{\mathbf{u}_j}(\mathbf{v}_k), & \mathbf{e}_k &= \frac{\mathbf{u}_k}{\|\mathbf{u}_k\|}.
\end{aligned}$$

The procedure is illustrated below, using an example for $n$ = 2. For such case, the matrix:

$$\{|I^{n\times n} \quad - 1^{n\times 1}|\}$$

consists of:

```
SOURCE MATRIX

 \ RUN:
  \   1  2  3
PAR\ -- -- --
  1   1  0 -1
  2   0  1 -1
```

Such source matrix is printed in the SUE output file. Next, we construct the final matrix using the Gram-Schmidt process, as follows:

- $\mathbf{v_1}$ = (1, 0, –1)
- $\mathbf{u_1}$ = $\mathbf{v_1}$ = (1, 0, –1)
- $||\mathbf{u_1}||$ = $(1^2 + 0^2 +(-1)^2 )^{1/2} = \sqrt{2}$
- $\mathbf{e_1}$ = $\mathbf{u_1}/||\mathbf{u_1}||$ = $1/\sqrt{2}$ (1, 0, –1) = ( $1/\sqrt{2}$ , 0, $-\sqrt{2}$)
- $\mathbf{u_2}$ = $\mathbf{v_2}$ – $\text{proj}_{\mathbf{u1}}(\mathbf{v_2})$

since $\mathbf{v_2}$ = (0, 1, –1), we have :

- $\text{proj}_{\mathbf{u1}}(\mathbf{v_2})$ = $\langle \mathbf{v_2},\mathbf{u_1} \rangle$ / $\langle \mathbf{u_1},\mathbf{u_1} \rangle$ $\mathbf{u_1}$ =
  = [ 0×1 + 1×0 + (–1)×(–1) ] / [ 1×1 + 0×0 + (–1)×(–1) ] = ½ $\mathbf{u_1}$ =
  = ½ (1, 0, –1)

Therefore:

- $\mathbf{u_2}$ = (0,1,–1) – ½ (1, 0, –1) = ( –½, 1, –½ )
- $||\mathbf{u_2}||$ = $( ½^2 +1^2 + ½^2 )^{1/2} = \sqrt{3}/\sqrt{2}$
- $\mathbf{e_2}$ = $\mathbf{u_2}/||\mathbf{u_2}||$ = $\sqrt{2}/\sqrt{3}$ ( –½, 1, –½ ) = ($1/\sqrt{6}$, $\sqrt{2}/\sqrt{3}$, $-1/\sqrt{6}$)

Now, we recall that the matrix is multiplied by square root of $n$+1:

$$\sqrt{n+1} \bullet \perp \{|I^{n\times n} \quad - 1^{n\times 1}|\}$$

Since $n$+1=3, the rows are given by:

- $\sqrt{3}$ $\mathbf{e_1}$ = $\sqrt{3}$ ( $1/\sqrt{2}$ , 0, $-1/\sqrt{2}$) = ( $\sqrt{3}/\sqrt{2}$, 0, $-\sqrt{3}/\sqrt{2}$)
- $\sqrt{3}$ $\mathbf{e_2}$ = $\sqrt{3}$ ( $1/\sqrt{6}$, $\sqrt{2}/\sqrt{3}$, $-1/\sqrt{6}$) = ( $-1/\sqrt{2}$, $\sqrt{2}$, $-1/\sqrt{2}$)

Finally, we arrive at the following elements of the DS-Simplex matrix:

- $\sqrt{3}/\sqrt{2}$ 0 $-\sqrt{3}/\sqrt{2}$
- $-1/\sqrt{2}$ $\sqrt{2}$ $-1/\sqrt{2}$

or:

- 1.225 0.000 –1.225
- –0.707 1.414 –0.707

The final DS-Simplex matrix is printed in the see SUE output file:

```
DS-SIMPLEX MATRIX

 \ RUN:
  \       1      2      3
PAR\ ------ ------ ------
  1   1.225  0.000 -1.225
  2  -0.707  1.414 -0.707
```

The uncertain parameters are then given by $x_i = \mu_i + \sigma_i \times$ matrix. Therefore, the DS-simplex ensemble is given by: (see [10]):

$$\begin{vmatrix} \mu_1 + 1.225\sigma_1 & \mu_1 & \mu_1 - 1.225\sigma_1 \\ \mu_2 - 0.707\sigma_2 & \mu_2 + 1.414\sigma_2 & \mu_2 - 0.707\sigma_2 \end{vmatrix}$$

For higher number of variables, next rows of the matrix are easily constructed from the previous rows, using the following relation [26]:

$$\mathbf{u}_k = \mathbf{v}_k - \sum_{j=1}^{k-1} \mathrm{proj}_{\mathbf{u}_j}(\mathbf{v}_k)$$

As in DS Standard and DS Hadamard methodologies, also for DS-Simplex it holds that for each uncertain parameter the value averaged over all runs is equal to the mean value.

### 2.4.5 EHSF Methodology

The Engineering Hot Spot Factor (ESHF) methodology is described e.g. in [22] (chapter 8). In developing the thermal design of a nuclear reactor, it is customary to consider first the nominal performance of the reactor with each of the primary design variables at a completely specified nominal value and then to evaluate the effect on reactor performance of possible variations in each of the primary design variables from its nominal value. Hot spot and hot channel factors are used to express the extent to which actual reactor performance may deviate from its nominal performance owing to the cumulative effect of variations of all primary design variables from their nominal values.

In this methodology, all uncertain input parameters are varied individually to their maximum and minimum value (defined by the user, e.g. as mean value ±2$\sigma$). If we vary the parameter $x_j$ to its extreme value ($x_j + \Delta x_j$), keeping all other parameters at their nominal value, then the subfactor relative to parameter $x_j$ affecting the property $y$. is given by $f_{j,y}$ ([22], eq. 8-23):

$$f_{j,y} = \frac{y(0, ..., \Delta x_j, ..., 0)}{y(0, ..., 0, ..., 0)}$$

Since we vary all uncertain input parameters subsequently to their maximum and the minimum value, the number of runs, $N$, is equal to:

$$N = 2n$$

Here n is the number of uncertain input parameters. For example, for three input parameters ($n$ = 3), the ensemble consists of 6 samples ($N$ = 6), and the matrix defining the parameter values is given by:

$$\begin{vmatrix} +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \end{vmatrix}$$

The overall hot spot factor, $F_y$, is obtained from ([22], eq. 8-50, statistical approach):

$$F_y = 1 + \sqrt{\sum_{j=1}^{n} (f_{j,y} - 1)^2}$$

The statistical approach is usually applied because the probability of the most unfavorable value of all uncertainties occurring at the same position at the same time is very small [22]):

Alternatively, hot spot factor may be obtained from ([22], eq. 8-34, deterministic approach):

$$F_y = \prod_{j=1}^{n} f_{j,y}$$

The deterministic approach takes each parameter that affects the property of interest as having the most unfavorable value. In this way worst values are taken to occur at the same location at the same time [22]. This method is very conservative and pessimistic.

The selection of method is based on the user-defined input parameter IHSDEF (input record 100004, section 3.1.3).

In the implementation in SUE, two hot spot factors are calculated.

- The positive factor $F_{y,p}$, is calculated by selecting the largest value of $f_{j,y}$ for every uncertain parameter:

  $$f_{j,y} = \text{Max} ( f_{j,y+} , f_{j,y-} , 1.0 )$$

  Here $f_{j,y+}$ is the value of the quantity of interest obtained for the uncertain parameter $x_j$ varied to its extreme positive value ($x_j + \Delta x_j$), while $f_{j,y-}$ is the value of the quantity of interest obtained for the uncertain parameter $x_j$ varied to its extreme negative value ($x_j - \Delta x_j$) - see Figure 4.

- The negative factor $F_{y,n}$, is calculated by selecting the smallest value of $f_{j,y}$ for every uncertain parameter:

  $$f_{j,y} = \text{Min} ( f_{j,y+} , f_{j,y-} , 1.0 )$$

Two remarks can be made here:

- The hot spot factors are calculated for the extreme values (minimum/maximum) of the quantities of interest, including local and global extremes (see below, discussion around Figure 5). The user needs to pick the value that is relevant. For example, in the case of maximum fuel temperature the interesting value is, of course, the value multiplied by $F_{y,p}$. However, in the case of other parameters, such as for example gap conductance, the interesting value is equal to the value divided by $F_{y,n}$.
- The method is strictly correct if all uncertain parameters have monotonic behavior (section 3.3.1). If this is not the case, a warning message is printed to the diagnostics file, for example:

```
 * * *  =SUE= WARNING IN SOLVSU
              EHSF METHODOLOGY, PLOT PARAMETER:   1
              UNCERTAIN PARAMETER   j =  8
              GLOBAL MAXIMUM IN THE TIME RANGE t >  2.00000E+03
              EFFECT OF THE U.P. SHOWS NON-MONOTONIC BEHAVIOR

                y( x0 )     y( x0+dx(j) )  y( x0-dx(j) )
              4.72040E+02    4.72060E+02    4.72100E+02
   AT T =     3.00072E+03    3.00073E+03    3.00072E+03

              FOR  x = x0+dx(j) :   fy(j)=  1.00004E+00
              FOR  x = x0-dx(j) :   fy(j)=  1.00013E+00

              BOTH VALUES ARE > 1.0 OR BOTH < 1.0
              MINIMUM OR MAXIMUM VALUE MAY LIE WITHIN THE CONSIDERED RANGE
```

Physically it means that the value of the quantity of interest has non-monotonic behavior, which indicates that there may be a local minimum/maximum within the considered range, as shown in Figure 4 (c). Possibly a local maximum may be found somewhere in the range between ($x_j$ – $\Delta x_j$) and ($x_j$ + $\Delta x_j$), so the calculations should be re-done trying different $\Delta x_j$. However, it has to be remembered that SUE provides statistical analysis for two cases:

- Local minimum (and maximum), for the time value that the minimum (or maximum) is reached in the reference run)
- Global minimum (and maximum), taken for each run for the time value when the minimum (or maximum) is reached in this run.

The warning messages from the local extremum may be encountered more often and typically can be ignored. The warnings from the global extremum are quite rare and usually the values of $f_{j,y+}$ and $f_{j,y-}$ are very close to 1.0. This is illustrated in Figure 5. Suppose that the quantity of interest here is the maximum cladding temperature, which increases during the accident until the reactor is shutdown and decreases afterwards. The local maximum values are shown in the Figure 5 (a). Both $f_{j,y+}$ and $f_{j,y-}$ are < 1.0, which may happen quite often (for many uncertain parameters) and therefore the warnings can be ignored. The global maximum values are shown in the Figure 5 (b). In this case having both $f_{j,y+}$ and $f_{j,y-}$ are < 1.0 is rather unlikely and if happens both values are typically very close to 1.0, in which case the warnings can also be ignored. Only if the values are significantly different then 1.0 the results should be investigated carefully and different values of $\Delta x_j$ should be considered. More details on this methodology are provided in the example case, shown in section 4.2.6.

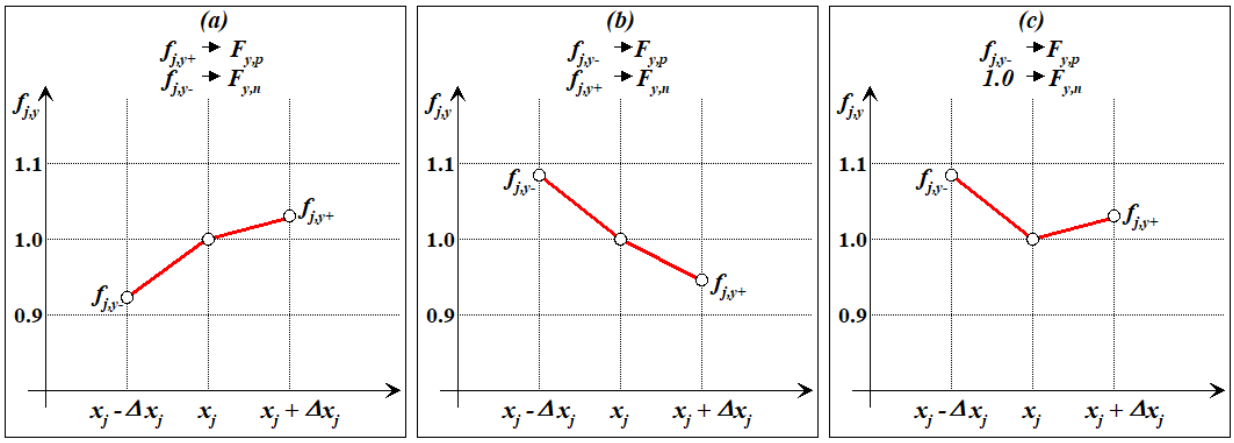



*Figure 4: Calculation of hot-spot factors, EHSF methodology*

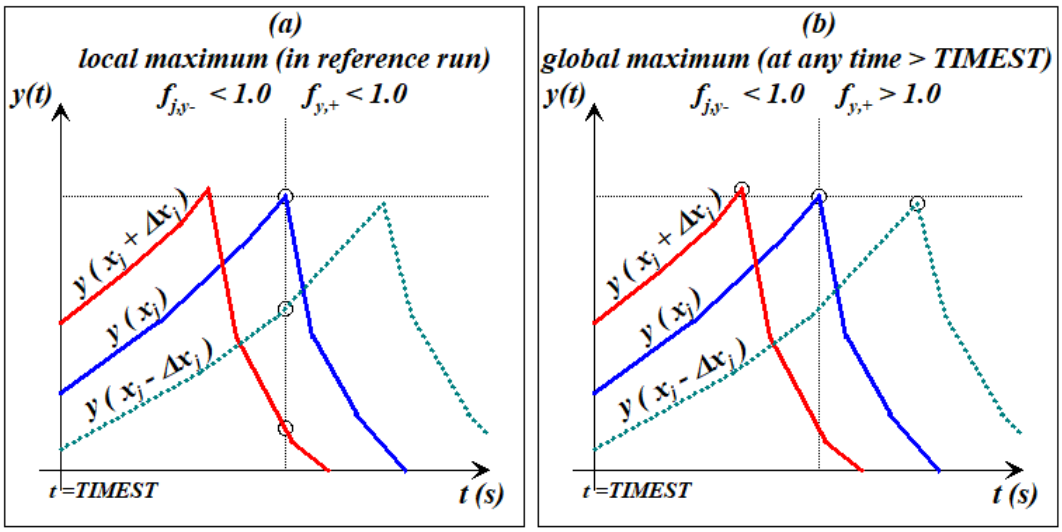



*Figure 5: Example of local and global maximum*

### 2.4.6 User-Defined Matrix

In the case of the user-defined matrix methodology, the user has to provide the matrix containing values of uncertain parameters. The matrix must be supplied in the input file with fixed name:

- **PAR-VAL.CSV**

The input format may be comma separated variables (CSV) but also other formats, e.g., values separated by spaces. This method is illustrated in the example case, shown in section 4.2.7.

In this case the hot spot factor parameters, described in the previous section are also calculated.

## 2.5 Output Parameters

SUE provides the following output parameters. For each plot parameter (selected by the user - section 3.1.13), the output files give:

- Minimum peak value, including:
  - The time, $t_{min}$, at which the minimum value was obtained,
  - The values of given plot parameters obtained in all runs at this time point: ($y_i(t_{min})$, $i$ = 1, ..., $N$)
  - The mean value at this time point
  - The standard deviation at this time point
  - The smallest value at this time and the run number in which it is obtained
  - The largest value at this time and the run number in which it is obtained
  - The Pearson's correlation coefficients for each uncertain parameters and the current plot parameter.
  - The Spearman's rank correlation coefficients for each uncertain parameters and the current plot parameter.
  - Finally a block is printed where the plot parameter values are ordered as Y(1)<Y(2)<...<Y(n). This allows to make graphs such as e.g., Figure 35, Figure 36, etc. The number of intervals n is selected automatically by the code as: n = 2×ceil($N$/10)+1, where $N$ is the number of runs. This block is not printed if the standard deviation is zero at this point.
- Maximum peak value, including:
  - The time, $t_{min}$, at which the maximum value was obtained,
  - The values of given plot parameters obtained in all runs at this time point: ($y_i(t_{min})$, $i$ = 1, ..., $N$)
  - The mean value at this time point
  - The standard deviation at this time point
  - The smallest value at this time and the run number in which it is obtained
  - The largest value at this time and the run number in which it is obtained
  - The Pearson's correlation coefficients for each uncertain parameters and the current plot parameter.
  - The Spearman's rank correlation coefficients for each uncertain parameters and the current plot parameter.
  - Finally a block is printed where the plot parameter values are ordered as Y(1)<Y(2)<...<Y(n). This allows to make graphs such as e.g., Figure 35, Figure 36, etc. The number of intervals n is selected automatically by the code as: n = 2×ceil($N$/10)+1, where $N$ is the number of runs. This block is not printed if the standard deviation is zero at this point.

The definition of each of these parameters is provided below.

### 2.5.1 Mean Value

The mean value at time *t* is obtained as:

$$\mu_y(t) = \frac{\sum_{i=1}^{N} y_i(t)}{N}$$

Here:

| | |
|---|---|
| $y_i(t)$ | value of the parameter *y*, at the time *t*, obtained in the run number *i*, |
| $\mu_y(t)$ | mean value of the parameter *y*, at the time *t*, |
| *N* | total number of runs. |

### 2.5.2 Standard Deviation

The standard deviation at time *t* is obtained as:

$$\sigma_y(t) = \sqrt{\frac{\sum_{i=1}^{N} \left[\mu_y(t) - y_i(t)\right]^2}{N}}$$

Here:

| | |
|---|---|
| $y_i(t)$ | value of the parameter *y*, at the time *t*, obtained in the run number *i*, |
| $\mu_y(t)$ | mean value of the parameter *y*, at the time *t*, |
| $\sigma_y(t)$ | standard deviation of the parameter *y*, at the time *t*, |
| *N* | total number of runs. |

### 2.5.3 Smallest Value

The smallest value at time *t* is obtained as:

$$y_{min}(t) = \mathrm{Min}[\, y_i(t)\, ]_{i=1,\ldots,N}$$

Here:

| | |
|---|---|
| $y_i(t)$ | value of the parameter *y*, at the time *t*, obtained in the run number *i*, |
| $y_{min}(t)$ | the smallest value of the parameter *y*, at the time *t*, |
| *N* | total number of runs. |

### 2.5.4 Largest Value

The largest value at time *t* is obtained as:

$$y_{max}(t) = \mathrm{Max}[\, y_i(t) \,]_{i=1,\ldots,N}$$

Here:

| | |
|---|---|
| $y_i(t)$ | value of the parameter *y*, at the time *t*, obtained in the run number *i*, |
| $y_{min}(t)$ | the smallest value of the parameter *y*, at the time *t*, |
| *N* | total number of runs. |

### 2.5.5 Pearson's Correlation Coefficient

The Pearson's correlation coefficient at time *t* is obtained as:

$$P_{xy}(t) = \frac{\sum_{i=1}^{N}\left(x_i - \mu_x\right)\cdot\left(y_i(t) - \mu_y(t)\right)}{\sqrt{\sum_{i=1}^{N}\left(x_i - \mu_x\right)^2}\cdot\sqrt{\sum_{i=1}^{N}\left(y_i(t) - \mu_y(t)\right)^2}}$$

Here:

| | |
|---|---|
| $x_i$ | value of the uncertain parameter *x*, in the run number *i*, |
| $\mu_x$ | mean value of the parameter *x*, |
| $y_i(t)$ | value of the parameter *y*, at the time *t*, obtained in the run number *i*, |
| $\mu_y(t)$ | mean value of the parameter *y*, at the time *t*, |
| *N* | total number of runs. |

The Pearson's correlation coefficient is a measure of linear correlation between two data sets [19]. The value is always between –1 and 1. If there is a clear correlation between x and y, the value of $P_{xy}$ is close to –1 or 1. An absolute value of 1 implies that a linear equation describes the relationship between X and Y perfectly, with all data points lying on a line.

- If the value is positive, an increase in the uncertain parameter *x* causes an increase of the quantity of interest *y* (in other words both tend to be simultaneously greater than, or simultaneously less than, their respective mean values).
- If the value is negative, an increase in the uncertain parameter *x* causes a decrease of the quantity of interest *y* (both tend to lie on opposite sides of their respective mean values).

The Pearson correlation coefficient is a good choice when all of the following are true [21]:

- Both variables are quantitative.
- The variables are normally distributed.
- The data have no outliers.
- The relationship is linear.

### 2.5.6 Spearman's Rank Correlation Coefficient

The Spearman's rank correlation coefficient is defined as [20]:

$$r_s = \rho[\, R[X], R[Y]\,] = \frac{cov[\, R[X],\ R[Y]\,]}{\sigma_{R[X]}\ \sigma_{R[Y]}}$$

where $\rho$ denotes the conventional Pearson correlation coefficient operator, but applied to the rank variables, $cov[\, R[X], R[Y]\,]$ is the covariance of the rank variables, $\sigma_{R[X]}$, $\sigma_{R[Y]}$. are the standard deviations of the rank variables.

When all ranks are distinct integers (no ties), Spearman's rank correlation coefficient can be computed using the simple formula [20]:

$$r_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)}$$

where $d_i = R[X_i] - R[Y_i]$ is the difference between the two ranks, the uncertain parameter and the quantity of interest.

While Pearson's correlation assesses linear relationships, Spearman's correlation assesses monotonic relationships. Spearman's rank correlation coefficient is a better choice than the Pearson correlation coefficient when one or more of the following is true [21]:

- The variables are ordinal.
- The variables aren't normally distributed.
- The data includes outliers.
- The relationship between the variables is non-linear and monotonic.

In SUE, the Spearman's rank is computed from the simple formula. Therefore can be used in the random sampling, which provides distinct ranks, and not the deterministic samplings. Therefore Spearman's rank correlation coefficient is not printed for DS methodologies (IMTSEL = 2 through 5). The use of Spearman's rank correlation coefficient is recommended in the case of uniform distribution of the uncertain parameters. Pearson's correlation coefficient is recommended in the case of normal distribution of the uncertain parameters.

### 2.5.7 Hot Spot Factors

The parameters described in sections 2.5.1 through 2.5.5 are meaningless for the EHSF methodology and therefore should not be used. In the case of EHSF methodology, the hot spot factors (see section 2.4.5) are printed in the output file (section 3.3.1).

# 3 User's Guide

This chapter provides the SUE User's Guide. The full description of the input data needed to run the program as well as the output data is given.

- Section 3.1 gives a detailed description of SUE input data file (*.SUE). Examples of inputs are shown.
- Section 3.2 presents description of the input requirements for the input files of the system code (SPECTRA, RELAP5, etc.)
- Section 3.3 presents a description of the output files, including:
    - Main output file (*.OUT). The variables printed in the main SUE output data file are shown and shortly described. Examples of output are presented.
    - Time-dependent plot files in text (*.ASC) or excel (*.CSV) formats.
    - Diagnostics file (*.DIA).

## 3.1 SUE Input File

SUE input file must have an extension ".SUE". 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.

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. The title must not be longer than 80 characters.

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.

### 3.1.1 Record: 100000, Methodology Selection

This record is required.

W-1 (I) IMTSEL Methodology selection:
=1: Random sampling, (RS) methodology,
=2: Deterministic sampling, standard (DS-Standard),
=3: Deterministic sampling, Hadamard (DS-Hadamard),
=4: Deterministic sampling, Simplex (DS-Simplex)
=5: Deterministic sampling, EHSF,
=6: User-defined, all UP values are defined by the user.
*Acceptable range*: 1, 2, 3, 4, 5, 6
*Default value*: 1

W-2 (I) NBINS Number of bins for generating frequency graphs (e.g. .Figure 8)
*Acceptable range*: ≥ 0
*Default value*: based on the number of runs, N: ceiling(N/10)×2 + 1

W-3 (I) IOPTN Option:
=0: full run
=1: analyze only, no code runs are performed
With IOPTN=1 the user may re-analyze existing calculations, for example using different values of NBINS, IHSDEF, IFORMT, TIMEST. The methodology and uncertain parameters cannot of course be changed without re-doing the code runs.
*Acceptable range*: 0, 1
*Default value*: 0

*Example:*

```
*         IMTSEL    NBINS  IOPTN
100000      1         0      0      *    1=RS
```

### 3.1.2 Record: 100001, Random Sampling (RS) Methodology Parameters

This record is required if the RS methodology is selected (IMTSEL=1).

W-1 (I) ISIDED One-sided or two-sided tolerance limits:
=1: one-sided
=2: two-sided
*Acceptable range*: 1, 2
*Default value*: 2

W-2 (I) IPROBA Probability, α (%).
*Acceptable range*: 90, 95, 99
*Default value*: 95

W-3 (I) ICONFB Confidence level, β (%).
*Acceptable range*: 90, 95, 99
*Default value*: 95

W-4 (I) IREPRS(1) Random series indicator
=0: random series (not repeatable)
>0: pseudo-random series (repeatable).
Starting point for the pseudorandom number generator.
The same value of IREPRS will give the same results.
*Acceptable range*: any integer
*Default value*: 0

W-5 (I) NADDRN Number of additional runs (above the minimum, Table 2).
*Acceptable range*: ≥ 0
*Default value*: 0

*Example:*

```
*          ISIDED    IPROBA    ICONFB    IREPRS    NADDRN
100001     2         95        95        123456    0
```

The number of code runs, as a function of ISIDED, IPROBA, ICONFB are shown in Table 2.

*Table 2: Minimum number of runs for one-sided and two-sided tolerance limits*

| | One-side tolerance limits | | | Two-side tolerance limits | | |
|---|---|---|---|---|---|---|
| β \ α | 0.90 | 0.95 | 0.99 | 0.90 | 0.95 | 0.99 |
| 0.90 | 22 | 45 | 230 | 38 | 77 | 388 |
| 0.95 | 29 | 59 | 299 | 46 | 93 | 473 |
| 0.99 | 44 | 90 | 459 | 64 | 130 | 662 |

### 3.1.3 Record: 100004, EHSF Parameters

This record is required if EHSF methodology is selected (IMTSEL=5).

W-1 (I) IHSDEF Method to calculate overall hot spot factor:

=1: $F_y = 1 + \sqrt{\sum_{j=1}^{N} (f_{j,y} - 1)^2}$ (statistical approach)

=2: $F_y = \prod_{j=1}^{N} f_{j,y}$ (deterministic approach)

*Acceptable range*: 1, 2
*Default value*: 1

*Example:*

```
*          IHSDEF
100004     2
```

### 3.1.4 Record: 105000, Input File Name

This record is required. This record defines the input file for the system code (SPECTRA, RELAP5, etc.).

| | | |
|---|---|---|
| W-1 (A) | INFILE | Name of the file containing the input for the code.<br>The name may optionally be enclosed in quotes.<br>*Acceptable range*: any string, up to 512 characters<br>*Default value*: none |

*Example:*

```
105000   'GAP-PBF-LOC-11C.SPE'                    *  BASE INPUT FILE
```

**Note:**

In the case of SPECTRA synchronized runs, a full simulation consists of several input decks with a three-digit suffix to indicate the run number within the set of synchronized runs. This is usually done for liquid metal reactors and molten salt reactors, where the primary system and the secondary system may be modeled in different runs that are coupled using synchronized EDF. For example, suppose that we have two inputs, representing as follows:

| | |
|---|---|
| JOB-001.SPE | primary system, |
| JOB-002.SPE | secondary system. |

Such naming scheme of the synchronized runs is needed for the graphical post-processor (Visor) to work properly.

In such case the name that needs to be defined as the INFILE, is: "JOB.SPE". SUE automatically detects the presence of a synchronized run and proceeds accordingly. First, SUE checks if the file JOB.SPE is present. If not, it checks for the presence of a file JOB-001.SPE. If the file is present, then SUE continues checking for the presence of JOB-002, JOB-003, etc. and thus determines the number of synchronized runs. Next, it proceeds with the UQ analysis. In the considered example, the runs will be executed in separate subdirectories named using a three-digit number (as is the case of RELAP5 runs) and the run number is not added to the input files. For example, in the case of two runs (consisting of the primary and the secondary system models), the file names will be:

| | | |
|---|---|---|
| \001\ | | Run 1 |
| | JOB-001.SPE | primary system, |
| | JOB-002.SPE | secondary system, |

This is done in order to be in agreement with the Visor requirements.

The synchronized runs are of course started simultaneously. The maximum number of simultaneous runs (NSRMAX, section 3.1.7) is in this case the number of simultaneous sets of runs, so in the current example, if NRSMAX=6, a total of twelve runs will be started simultaneously. For the post-processing, SUE first searches for the quantities of interest (section 3.1.12) in the first file (JOB-001). If it doesn't find it there, it searches the subsequent file (or files).

In conclusion, the UQ analysis of synchronized runs is transparent to the user. The code automatically detects the presence of such runs (multiple input files) and proceeds accordingly.

### 3.1.5 Record: 115000, Input File Containing Uncertain Parameters

This record is required. If the uncertain parameters are defined directly in the input file (INFILE, record 105000), then the same name must be provided in this record. In some codes, the model files are included in the input file using certain keyword, for example, in SPECTRA: ATTACH keyword, in MELCOR: INCLUDE keyword (in the 2.x versions, R*I*F in version 1.8.6 or earlier). Example of defining uncertain parameters in a separate file in SPECTRA is shown in section 4.2.

| | | |
|---|---|---|
| W-1 (A) | UPFILE | Name of the file containing the uncertain parameters.<br>The name may optionally be enclosed in quotes.<br>*Acceptable range*: any string, up to 512 characters<br>*Default value*: none |

*Example:*

```
115000  'UNPAR' *  FILE CONTAINING UNCERTAIN PARAMETERS
```

### 3.1.6 Record: 125000, Code To Run

This record is required. It defines the full path to the system code (SPECTRA, RELAP5, etc.) executable.

| | | |
|---|---|---|
| W-1 (A) | PROGNM | Full path to a code to run<br>The name may be enclosed in quotes.<br>Version with forward slashes enclosed in quotes works in both Windows and Linux systems (see examples below).<br>*Acceptable range*: any string, up to 512 characters<br>*Default value*: none |

*Examples:*
*(a) Windows system only:*

```
125000    C:\SPECTRA.361\Z-EXE\SPECTRA-3-61.EXE  *  PROGRAM TO RUN (WIN)
```

*(b) Windows and Linux systems:*

```
125000   'C:/SPECTRA.361/Z-EXE/SPECTRA-3-61.EXE' *  PROGRAM TO RUN (WIN)
125000   '~/SPECTRA/Z-EXE/SPECTRA.X'             *  PROGRAM TO RUN (LIN)
```

### 3.1.7 Record: 130000, Maximum Number of Simultaneous Runs

This record is required. It defines how many runs of the system code (SPECTRA, RELAP5, etc.) may be started simultaneously. SUE will start NSRMAX runs at a time. When the runs

are finished, SUE will start another set of NSRMAX runs, and will proceed in this manner until all runs are finished.

The number of runs that can be run simultaneously depends on the computer being used. In general, the number of simultaneous runs should not exceed the number of processors available. In some cases, there may be other limitations; for example code license may limit the number of runs that can be started simultaneously.

W-1 (I) NSRMAX Maximum number of simultaneous runs.
*Acceptable range*: $1 \leq NSRMAX \leq 100$
*Default value*: none

*Example:*
```
130000    4    *  MAX. NUMBER OF SIMULTANEOUS RUNS
```

### 3.1.8 Record: 200000, Uncertain Parameters - General Data

This record is optional.

W-1 (I) INPOPT Option determining how the input is entered:
=1: records 200XXX define relative values of $\sigma$, $X_{min}$, $X_{max}$, .
=2: records 200XXX define absolute values of $\sigma$, $X_{min}$, $X_{max}$
*Acceptable range*: 1, 2
*Default value*: 1

W-2 (I) NINTDF Number of intervals applied for random sampling.
*Acceptable range*: $3 \leq NINTDF \leq 1{,}000{,}000{,}001$
*Default value*: 1,000,001

W-3 (I) IUPERR Handling of errors in uncertain parameters
.
=1: warn if UP is outside the range XMINUP - XMAXUP.
=2: reset UP to the range XMINUP - XMAXUP.
*Acceptable range*: 1, 2
*Default value*: 1

*Example:*
```
*        INPOPT  NINTDF  IUPERR
200000     1       0       1
```

The parameter NINTDF is used with the RS methodology (IMTSEL=1) to sample the value of the uncertain parameter. The total range is divided into NINTDF equal parts.

$$\Delta x = \frac{x_{\max} - x_{\min}}{NINTDF - 1}$$

The random sampling method and the use of this parameter is provided in Appendix A.

### 3.1.9 Records: 200XXX, Uncertain Parameters Data

These records are required. XXX is the number of the uncertain parameter. The maximum number of uncertain parameters is 500.

W-1 (I) IDISTR — Distribution of the uncertain parameter XXX:
=1: normal distribution
=2: uniform distribution
*Acceptable range*: 1, 2
*Default value*: none

W-2 (R) XMEAUP — Mean (reference) value, $\mu$, of the uncertain parameter XXX.
*Acceptable range*: XMINUP ≤ XMEAUP ≤ XMAXUP
*Default value*: none

W-3 (R) SIGMUP — Standard deviation, $\sigma$, of the uncertain parameter XXX.
if INPOPT=1: relative value
if INPOPT=2: absolute value
*Acceptable range*: $0.0 \le \text{SIGMUP} \le 10^{10}$
*Default values*: uniform: $\sigma = \sqrt{(x_{max} - x_{min})/12}$ [18]
normal: $\sigma = (x_{max} - \mu)/3 = (\mu - x_{min})/3$ if both are equal

W-4 (R) XMINUP — Minimum value, $x_{min}$, of the uncertain parameter XXX:
if INPOPT=1: relative value
if INPOPT=2: absolute value
*Acceptable range*: $-10^{10} \le \text{XMINUP} \le \text{XMEAUP}$ if IMTSEL=1 or,6
$-10^{10} \le \text{XMINUP} < \text{XMEAUP}$ if IMTSEL=2 - 5
*Default values*: uniform distr. : none
normal distr.: $\mu - 3\sigma$

W-5 (R) XMAXUP — Maximum value, $x_{max}$, of the uncertain parameter XXX:
if INPOPT=1: relative value
if INPOPT=2: absolute value
*Acceptable range*: $\text{XMEAUP} \le \text{XMAXUP} \le 10^{10}$ if IMTSEL=1 or 6
$\text{XMEAUP} < \text{XMAXUP} \le 10^{10}$ if IMTSEL=2 - 5
*Default values*: uniform distr. : none
normal distr.: $\mu + 3\sigma$

W-6 (I) IDPTYP — Type of eventual dependent parameters associated with the uncertain parameter XXX:
=1: 'add' type
=2: 'multiply' type
*Acceptable range*: 1, 2
*Default values*: 1 if XMEAUP = 0.0
2 if XMEAUP ≠ 0.0

If IDPTYP=1, then the relation between the dependent parameter *y* and the independent parameter *x* is:

$$y - \mu_y = x - \mu_x$$

If IDPTYP=2, then the relation between the dependent parameter *y* and the independent parameter *x* is:

$$y / \mu_y = x / \mu_x$$

Here $\mu_x$ and $\mu_y$ are the mean values, *x* and *y*. are the actual values of the parameters *x* and *y*.

The dependent parameters are explained in section 3.2. The input of absolute versus relative values (effect of INPOPT) is illustrated in Appendix A.

*Examples:*

*(a) relative input:*

```
*        INPOPT  NINTDF
200000     1       0
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL COND.
```

*(b) absolute input:*

```
*        INPOPT  NINTDF
200000     2       0
*        IDISTR    MEAN     SIGMA   MIN       MAX
200001      2    0.100E-3   0.0     0.088E-3  0.112E-3  *  INITIAL GAP SIZE
200002      1    3.300E-6   9.90E-7 0.0       0.0       *  FUEL SURFACE R.
200003      1    1.780E-6   5.34E-7 0.0       0.0       *  CLAD SURFACE R.
200004      1    0.90       0.09    0.0       0.999990  *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0       0.0       *  FUEL THERMAL C.
```

Note: Default values of minimum/maximum exist for normal distribution therefore these values may be omitted or entered as zero (which is done here for parameters 2, 3, and 5). Similarly, default values of mean and sigma exist for uniform distribution therefore these values may be omitted or entered as zero (which is done here for sigma in parameter 1).

### 3.1.10 Records: 210XXX, Functions of UP - Function Type

These records are optional. The records define functions of uncertain parameters. XXX is the function number. The maximum number of functions is 500.

W-1 (I) IFUNCT Function type:

=1: addition function $F = \sum_i \left[ \left( A_i \times x_i + B_i \right)^{C_i} \right]$

=2: multiplication function $F = \prod_i \left[ \left( A_i \times x_i + B_i \right)^{C_i} \right]$

*Acceptable range*: 1, 2
*Default value*: 2

Here:

$A_i$ multiplicative constant for the uncertain parameter number *i*,
$B_i$ additive constant for the uncertain parameter number *i*,
$C_i$ exponent for the uncertain parameter number *i*,

The values of $A_i$, $B_i$, $C_i$, are defined in the records 211XXX.

W-2 (R) RFUNCT Reference value. If a non-zero value is entered, then this value is used in the reference run (000). If 0.0 or no value is entered, then the value for reference run is calculated as for other runs.
*Acceptable range*: any real
*Default value*: none

### 3.1.11 Records: 211XXX, Functions of UP - Argument Data

These records are optional. XXX is the function number. The records define functions of uncertain parameters. The maximum number of functions is 500.

Each record 211XXX defines data for one uncertain parameter affecting the function XXX. The number of uncertain parameters is equal to the number of records with this number. The ordering of parameters is irrelevant, since both types, addition and multiplication, are independent of the argument order. The maximum number of arguments is 100.

W-1 (I) KFUNCT Uncertain parameter number or
–(function number) when negative.
*Acceptable range*: reference to u.p. defined in 200XXX or function, defined earlier.
*Default value*: none

W-2 (R) AFUNCT Multiplicative constant, $A_i$.
*Acceptable range*: $-10^{10} \le$ AFUNCT $\le 10^{10}$
*Default value*: 1.0

W-3 (R) BFUNCT Additive constant, $B_i$.
*Acceptable range*: $-10^{10} \le$ BFUNCT $\le 10^{10}$
*Default value*: 0.0

W-4 (R) CFUNCT Exponent, $C_i$.
Note: if $C_i < 0.0$, then $A_i x_i + B_i$ must be positive.
*Acceptable range*: $-10^{10} \le$ CFUNCT $\le 10^{10}$
*Default value*: 1.0

*Examples:*

*(a)*

```
210001   2    0.0   *  Multiplication, reference value to be calculated
*      KFUNCT AFUNCT BFUNCT CFUNCT
211001   1      1.0    0.0    1.0  *  uncertain par. 1: (1.0*X1+0.0)^1.0
211001   2      1.0    0.0    1.0  *  uncertain par. 2: (1.0*X2+0.0)^1.0
211001   3      1.0    0.0    1.0  *  uncertain par. 3: (1.0*X3+0.0)^1.0
```

The example above defines following function: $F_1 = x_1 \times x_2 \times x_3$

*(b)*

```
210002   2   0.5   *  Multiplication, reference value = 0.5
*      KFUNCT AFUNCT BFUNCT CFUNCT
211002   1      1.0    1.0    1.0  *  uncertain par. 1: (1.0*X1+1.0)^1.0
211002  -1      1.0    1.0   -2.0  *  function 1:       (1.0*F1+1.0)^-2.0
```

The example above defines following function: $F_2 = \dfrac{x_1 + 1}{(F_1 + 1)^2}$

### 3.1.12 Record: 300000, Plot Parameters (Quantities of Interest)

This record is optional.

W-1 (I) IOUTPT Option for reading plot parameters:
=1: SPECTRA plot file *.PLT,
=2: RELAP5 output file, minor edits,
=3: MELCOR output file, EDF,
=4: FLUENT output file,
≥5: Other code, no post-processing is performed.
*Acceptable range*: IOUTPT > 0
*Default value*: 1

W-2 (I) IFORMT Format of the outputs, time-dependent values are given as:
=1: text files, *.ASC
=2: comma separated values (readable for excel), *.CSV
*Acceptable range*: 1 or 2
*Default value*: 1

W-3 (R) TIMEST Time to start analysis (s). The user may wish to analyze only a part of calculations, for example to eliminate the initial period, when the model is approaching steady state. The values shown in section 3.3.1, including the local and the global minimum / maximum peak values, the Pearson correlation coefficient, the hot spot factors, etc., are provided for times > TIMEST.
*Acceptable range*: $-10^{10} \le$ TIMEST$\le 10^{10}$
*Default value*: $-10^{10}$

*Example:*

```
*       IOUTPT  IFORMT  TIMEST
300000  2       2       1000.0 * processing of RELAP5 output, into *.CSV
*                              * files, starting from t = 1000.0 s
```

### 3.1.13 Records: 305XXX, Plot Parameters (Quantities of Interest) Data

These records are required for IOUTPT = 1, 2, 3, 4 (SPECTRA, RELAP5, MELCOR, FLUENT). For those codes the post-processing of the quantities of interest is possible. For other codes post processing is possible only if the quantities of interest (QoI) can be provided in a simple text file, consisting of columns: time, QoI1, QoI2, QoI3, ... (see QOIFIL).

SPECTRA and RELAP5 codes (IOUTPT = 1 or 2)

XXX is the number of the plot parameter. The maximum number of the plot parameters is 100. The plot parameters requested in this record must be present in the SPECTRA plot file or in the RELAP5 minor edits. In the case of RELAP5, all variables in the minor edits are processed and in the order appearing in the minor edits; the number of plot parameters in the records 300XXX must be equal to the number of minor edit parameters in the RELAP5 output file.

W-1 (A) PLVNAM Name of the plot parameter number XXX:
*Acceptable range*: any string, up to 64 characters
*Default value*: none

When the calculations are finished, tabulated time dependent data are available in the files: *-XXX.ASC or *-XXX.CSV, depending on the input parameter IOUTPT. The content of the files is discussed in section 3.3.2. XXX is the parameter number. The number of files is equal to the number of records 300XXX.

MELCOR and FLUENT codes (IOUTPT = 3 or 4)

W-1 (A) FILENM Name of the output file containing plot parameters.
In MELCOR, this is the name of the External Data File
*Acceptable range*: any string, up to 64 characters
*Default value*: none

W-2 (I) N Number of plot parameters present in the output file FILENM.
The number of columns in FILENM must be equal to N+1
*Acceptable range*: any string, up to 64 characters
*Default value*: none

When the calculations are finished, time dependent graphs are available in the files: *-XXX.ASC or *-XXX.CSV, depending on the input parameter IOUTPT. The content of the files is discussed in section 3.3.2. XXX is the parameter number. The number of files is equal to the value of N, entered in the record 300002.

*Examples:*

*(a) SPECTRA:*

```
305001   SC-100-Tcel-0001  *  Cell  1, centerline
305002   SC-100-Tcel-0010  *  Cell 10, clad surface
305003   SC-100-hGap-0000  *  Gap conductance
```

*(b) RELAP5:*

```
305001   httemp         100100101 *  Cell  1, centerline
305002   httemp         100100111 *  Cell 10, clad surface
305003   hgap             1001001 *  Gap conductance
```

*(c) MELCOR:*

```
305001   GAP-EDF.DAT  *  Name of MELCOR External Data File (EDF)
305002   2            *  Number of plot parameters in the MELCOR EDF
```

*(d) FLUENT:*

```
305001   molfhe-z14.out  *  Name of FLUENT output file
305002   1               *  Number of plot parameters in the output file
```

### 3.1.14 Record: 305000, File Containing Quantities of Interest

For codes other than SPECTRA, RELAP5, MELCOR, FLUENT, post processing is possible only if the quantities of interest QoI may be written to a simple text file or CSV file, consisting of columns: time, QoI1, QoI2, QoI3, ..., with headers in the first row.

W-1 (A) QOIFIL Name of the file containing quantities of interest.
The name may optionally be enclosed in quotes.
*Acceptable range*: any string, up to 64 characters
*Default value*: none

## 3.2 Code Inputs

### 3.2.1 Independent Parameters

All independent uncertain parameters, defined in the SUE input (records 200XXX - section 3.1.9), must appear in the code input as $XXX, where XXX is the parameter number. The examples below show parts of SPECTRA, RELAP5, and MELCOR inputs where the uncertain parameter number 1 is shown.

- SPECTRA

```
*          dx [m]      Mat  Power  T [K]   N  N-start
310100   $001          901   0.0   569.0   1  7   *  GAP SIZE
```

- RELAP5

```
*           x(Node) [m]      Node
11001101    7.75000e-04        1  *  HS-100 C:  1
11001102    7.75000e-04        2  *  - Cell  :  2
11001103    7.75000e-04        3  *  - Cell  :  3
11001104    7.75000e-04        4  *  - Cell  :  4
11001105    7.75000e-04        5  *  - Cell  :  5
11001106    7.75000e-04        6  *  - Cell  :  6
11001107    $001               7  *  - Cell  :  7
```

- MELCOR

```
TF03100   'TC-Gap filling  '    1  1.0E-4  0.0
*              T [K]        k [W/m-K]
TF03111     3.73000E+02    $001
```

The presence of all parameters defined in SUE input and in the code input is checked and printed in the output file for each parameter, including its presence in the SUE input and the exact (line number) location in the code input, for example (see section 3.3.1):

```
  INDEPENDENT PARAMETERS ($)

           SUE  INPUT      CODE INPUT
  No.    (0=NO,1=YES)      LINE No.
  ---    ------------     ----------
   1           1               3
```

### 3.2.2 Dependent Parameters

All dependent parameters appear in the code input following $XXX@, where XXX is the independent parameter number. The mean value of the dependent parameter is written directly behind @. The examples below show parts of SPECTRA and RELAP5 inputs where the uncertain parameter number 1 is shown.

- SPECTRA

```
*       k    [W/m/K]
801101  300.0    $005@9.01
801101  400.0    $005@7.37
[...]
```

- RELAP5

```
*              T [K]        k [W/m/K]
20110101    3.00000e+02    $005@9.01
20110102    4.00000e+02    $005@7.37
[...]
```

- MELCOR

```
TF01100    'TC-Fuel, UO2 - R'    28  1.0  0.0
*               T [K]        k [W/m-K]        T [K]        k [W/m-K]
TF01111      3.00000E+02    $002@9.0100    4.00000E+02    $002@7.3700
```

All dependent parameters are printed in the output file for each parameter, including the corresponding independent parameter and the exact (line number) location in the code input, for example (see section 3.3.1):

```
  DEPENDENT PARAMETERS (@)

         INDEP.PARAM.     CODE INPUT      MEAN
  No.       NUMBER         LINE No.       VALUE
  ---    ------------     ----------  -----------
   1           5              16      9.01000E+00
```

The relationship between the independent and all its dependent parameters is printed in the SUE output file for, for example (see section 3.3.1):

```
  INDEPENDENT PARAMETERS ($)

         RELATION TO
  No.    DEPENDENT P.
  ---    ------------
   1       MULTIPL
```

The 'MULTIPLY' type means that

$$y = \mu_y \cdot x / \mu_x$$

Here $\mu_x$ mean value of independent parameter $x$,
$\mu_y$ mean value of dependent parameter $y$,
$x$ actual value of independent parameter $x$,
$y$ actual value of dependent parameter $y$,

Another possible type is 'ADD'. In this case the relationship between the independent and the dependent parameters is:

$$y = \mu_y + x - \mu_x$$

### 3.2.3 Functions

A function of a number (maximum of 100) of independent parameters may be defined. In the following example, two functions are defined:

- Function 001:

$$F_1 = x_4 \times x_5$$

  This function defines a product of independent parameters 4 and 5.

- Function 002:

$$F_2 = F_1 + x_5$$

  This function defines a sum of the function 1 and the independent parameter 5.

The input records defining these functions are:

```
*
*       FUNCTION F-001
210001  2   *  Type, 2=MULTIPLY
*       U.P.    A     B     C
211001   4     1.0   0.0   1.0
211001   5     1.0   0.0   1.0
*
*       FUNCTION F-002
210002  1   *  Type, 1=ADD
*       U.P.    A     B     C
211002  -1     1.0   0.0   1.0
211002   5     1.0   0.0   1.0
```

If a function uses another function as an argument, it must have a higher number, because the functions are evaluated sequentially.

Each defined function must be present in the input deck, marked as **#XXX**, where XXX is the function number. Dependent parameters may follow a function in the same way as it is done for uncertain parameters, e.g. **#XXX@1.0**. Dependent parameter is either added to the function value or multiplied by the function value, depending on the function type, IFUNCT.

An example presented above is provided in \GAP-SPE-3-DEP\. The function F-001 is set equal to the U.P. 001. The initial gap size is defined as:

```
*         dx [m]      Mat  Power  T [K]    N  N-start
310100  #001@1.0      901   0.0   569.0    1  7    *  GAP SIZE*
```

The function F-001 is defined as 'multiply' (IFUNCT=2), therefore in this example the initial gap size is equal to the value of F-001, so the value of U.P. 001. With the following definition the gap size would be twice larger:

```
*         dx [m]      Mat  Power  T [K]    N  N-start
310100  #001@2.0      901   0.0   569.0    1  7    *  GAP SIZE*
```

## 3.3 SUE Output Files

The SUE output files consist of:

- Main output file (*.OUT) - section 3.3.1.
- Time-dependent graphs (*.ASC or *.CSV) - section 3.3.2.
- Diagnostics file (*.DIA) - section 3.3.3.

### 3.3.1 Main Output File (*.OUT)

- Output of main input data parameters

```
================================================================================
 =SUE=  SUE Version 3.00, Nov. 2024, Windows

 System-code
   Uncertainty
     Evaluation

--------------------------------------------------------------------------------
 Validity:  unlimited
--------------------------------------------------------------------------------

================================================================================
 INPUT DATA DIAGNOSTICS
================================================================================

================================================================================
 =IN=  MAIN DATA
================================================================================

  METHODOLOGY:  DS-SIMPLEX  (IMTSEL = 4)

  No. OF BINS:  NBINS =    0
  RUN OPTION :  IOPTN =    0

  FILE NAMES
  - CODE INPUT FILE NAME: GAP-PBF-LOC-11C.SPE
  - INPUT FILE WITH U.P.: UNPAR
  - PROGRAM TO RUN      : C:/SPECTRA/Z-EXE/SPECTRA.EXE
  - SIMULTANEOUS RUNS   : NSRMAX = 4

  SEPARATE FILE WITH U.P. PRESENT
```

- Output of uncertain parameter data and functions data

```
================================================================================
 =IN=  UNCERTAIN PARAMETERS DATA
================================================================================

  INPUT OPTION                                : INPOPT = 1
  No. OF INTERVALS IN DISTRIBUTION FUNCTION : NINTDF = 201

--------------------------------------------------------------------------------

  INDEPENDENT PARAMETERS - DISTRIBUTIONS, RELATIVE VALUES

  No.    DISTRIBUTION      MEAN       SIG.(REL)    MIN.(REL)    MAX.(REL)
  ---    ------------   -----------  -----------  -----------  -----------
   1       Uniform      1.00000E-04  6.92820E-02  8.80000E-01  1.12000E+00
   2       Normal       3.30000E-06  3.00000E-01  1.00000E-01  1.90000E+00
   3       Normal       1.78000E-06  3.00000E-01  1.00000E-01  1.90000E+00
   4       Normal       9.00000E-01  1.00000E-01  7.00000E-01  1.11110E+00
   5       Normal       1.00000E+00  1.00000E-01  7.00000E-01  1.30000E+00

  INDEPENDENT PARAMETERS - DISTRIBUTIONS, ABSOLUTE VALUES

  No.    DISTRIBUTION      MEAN       SIG.(ABS)    MIN.(ABS)    MAX.(ABS)
  ---    ------------   -----------  -----------  -----------  -----------
   1       Uniform      1.00000E-04  6.92820E-06  8.80000E-05  1.12000E-04
   2       Normal       3.30000E-06  9.90000E-07  3.30000E-07  6.27000E-06
   3       Normal       1.78000E-06  5.34000E-07  1.78000E-07  3.38200E-06
   4       Normal       9.00000E-01  9.00000E-02  6.30000E-01  9.99990E-01
   5       Normal       1.00000E+00  1.00000E-01  7.00000E-01  1.30000E+00


  INDEPENDENT PARAMETERS ($)

          SUE  INPUT     CODE INPUT
  No.    (0=NO,1=YES)     LINE No.
  ---    ------------    ----------
   1           1              3
   2           1              8
   3           1              8
   4           1             12
   5           1             43

  INDEPENDENT PARAMETERS ($)

         RELATION TO
  No.    DEPENDENT P.
  ---    ------------
   1       MULTIPL
   2       MULTIPL
   3       MULTIPL
   4       MULTIPL
   5       MULTIPL

--------------------------------------------------------------------------------

  DEPENDENT PARAMETERS (@)

         INDEP.PARAM.    CODE INPUT      MEAN
  No.       NUMBER        LINE No.       VALUE
  ---    ------------    ----------  -----------
   1           5             16      9.01000E+00
   2           5             17      7.37000E+00
   3           5             18      6.23000E+00
   4           5             19      5.40000E+00
   5           5             20      4.78000E+00
   6           5             21      4.29000E+00
   7           5             22      3.90000E+00
   8           5             23      3.59000E+00
   9           5             24      3.34000E+00
  10           5             25      3.14000E+00
  11           5             26      2.97000E+00
```

```
 12           5             27      2.84000E+00
 13           5             28      2.74000E+00
 14           5             29      2.66000E+00
 15           5             30      2.61000E+00
 16           5             31      2.58000E+00
 17           5             32      2.57000E+00
 18           5             33      2.58000E+00
 19           5             34      2.61000E+00
 20           5             35      2.65000E+00
 21           5             36      2.72000E+00
 22           5             37      2.80000E+00
 23           5             38      2.90000E+00
 24           5             39      3.02000E+00
 25           5             40      3.15000E+00
 26           5             41      3.30000E+00
 27           5             42      3.47000E+00
 28           5             43      3.66000E+00

--------------------------------------------------------------------------------

 FUNCTIONS OF INDEPENDENT UNCERTAIN PARAMETERS (#)


 FUNCTION:   1 IFUNCT =  2

      U.P./FUN
  i    NUMBER      AFUNCT(i)     BFUNCT(i)     CFUNCT(i)
 ---    ----     ------------  ------------  ------------
  1       4       1.00000E+00   0.00000E+00   1.00000E+00
  2       5       1.00000E+00   0.00000E+00   1.00000E+00

 FUNCTION:   2 IFUNCT =  1

      U.P./FUN
  i    NUMBER      AFUNCT(i)     BFUNCT(i)     CFUNCT(i)
 ---    ----     ------------  ------------  ------------
  1      -1       1.00000E+00   0.00000E+00   1.00000E+00
  2       5       1.00000E+00   0.00000E+00   1.00000E+00


 FUNCTIONS OF INDEPENDENT UNCERTAIN PARAMETERS (#)

         SUE  INPUT     CODE INPUT
 No.    (0=NO,1=YES)     LINE No.
 ---    ------------    ----------
  1           1             51
  2           1             51

--------------------------------------------------------------------------------
```

In this case two functions have been defined (for testing and demonstration purposes only) as follows:

$$F_1 = x_4 \times x_5$$

$$F_2 = F_1 + x_5$$

- Number of runs and methodology-related data - the example below shows output for the Hadamard matrix (IMTSEL=4)

```
--------------------------------------------------------------------------------

 =IN=  TOTAL NO. OF RUNS AND DETERMINATION OF UNCERTAIN PARAMETERS

 =IN=  TOTAL NO. OF RUNS  : NRUNST = 8

 =IN=  DETERMINATION OF UNCERTAIN PARAMETERS
       DETERMINISTIC SAMPLING - HADAMARD MATRIX

FULL HADAMARD MATRIX

 \  J:
  \   1  2  3  4  5  6  7  8
 I \ -- -- -- -- -- -- -- --
  1   1  1  1  1  1  1  1  1
  2   1 -1  1 -1  1 -1  1 -1
  3   1  1 -1 -1  1  1 -1 -1
  4   1 -1 -1  1  1 -1 -1  1
  5   1  1  1  1 -1 -1 -1 -1
  6   1 -1  1 -1 -1  1 -1  1
  7   1  1 -1 -1 -1 -1  1  1
  8   1 -1 -1  1 -1  1  1 -1

REDUCED HADAMARD MATRIX

 \ RUN:
  \   1  2  3  4  5  6  7  8
PAR\ -- -- -- -- -- -- -- --
  1   1 -1  1 -1  1 -1  1 -1
  2   1  1 -1 -1  1  1 -1 -1
  3   1 -1 -1  1  1 -1 -1  1
  4   1  1  1  1 -1 -1 -1 -1
  5   1 -1  1 -1 -1  1 -1  1

TRANSPOSED REDUCED HADAMARD MATRIX

 \ PAR:
  \   1  2  3  4  5
RUN\ -- -- -- -- --
  1   1  1  1  1  1
  2  -1  1 -1  1 -1
  3   1 -1 -1  1  1
  4  -1 -1  1  1 -1
  5   1  1  1 -1 -1
  6  -1  1 -1 -1  1
  7   1 -1 -1 -1 -1
  8  -1 -1  1 -1  1

================================================================================
 =IN=  END OF UNCERTAIN PARAMETERS DATA
================================================================================
```

- Plot parameters for the post-processing

```
================================================================================
 =IN=  PLOT PARAMETERS DATA
================================================================================

  RESULT FILE:  SPECTRA PLOT FILE (IOUTPT = 1)

  OUTPUT FORMAT:  *.CSV, EXCEL FILES (IFORMT = 2)

  LIST OF PLOT PARAMETERS

  No.    NAME
  ---    ----------------
   1     SC-100-Tcel-0001
   2     SC-100-Tcel-0010
   3     SC-100-hGap-0000

================================================================================
 =IN=  END OF PLOT PARAMETERS DATA
================================================================================
```

- Results of calculations - values of uncertain parameters in different runs

```
================================================================================
 =SL=  VALUES OF UNCERTAIN PARAMETERS IN ALL RUNS
================================================================================

     VALUES OF UNCERTAIN PARAMETERS (UP) AND FUNCTIONS (FN) IF PRESENT

         UP/FN NUMBER
     RUN            1            2            3            4            5
     --- ------------ ------------ ------------ ------------ ------------

 UP: 001  1.06928E-04  4.29000E-06  2.31400E-06  9.90000E-01  1.10000E+00
 FN: 001  1.08900E+00  2.18900E+00

 UP: 002  9.30718E-05  4.29000E-06  1.24600E-06  9.90000E-01  9.00000E-01
 FN: 002  8.91000E-01  1.79100E+00

 UP: 003  1.06928E-04  2.31000E-06  1.24600E-06  9.90000E-01  1.10000E+00
 FN: 003  1.08900E+00  2.18900E+00

 UP: 004  9.30718E-05  2.31000E-06  2.31400E-06  9.90000E-01  9.00000E-01
 FN: 004  8.91000E-01  1.79100E+00

 UP: 005  1.06928E-04  4.29000E-06  2.31400E-06  8.10000E-01  9.00000E-01
 FN: 005  7.29000E-01  1.62900E+00

 UP: 006  9.30718E-05  4.29000E-06  1.24600E-06  8.10000E-01  1.10000E+00
 FN: 006  8.91000E-01  1.99100E+00

 UP: 007  1.06928E-04  2.31000E-06  1.24600E-06  8.10000E-01  9.00000E-01
 FN: 007  7.29000E-01  1.62900E+00

 UP: 008  9.30718E-05  2.31000E-06  2.31400E-06  8.10000E-01  1.10000E+00
 FN: 008  8.91000E-01  1.99100E+00

 UP: 000  1.00000E-04  3.30000E-06  1.78000E-06  9.00000E-01  1.00000E+00
 FN: 000  9.00000E-01  1.90000E+00
```

The code runs are given a suffix -nnn, where nnn is the run number. In the present example the input file name is GAP-PBF-LOC-11C.SPE. The run number 1 gets the name GAP-PBF-LOC-11C-001.SPE. After performing all runs that are required by the selected methodology, SUE performs one run with all parameters are given the mean (reference) value - section 3.1.9. This is referred to here as the reference run and it gets the suffix -000. The run -000 and all the values of parameters are seen in the last row of the output above.

If functions of uncertain parameters are present, then the printout gives the values of both uncertain parameters (UP) and the functions (FN). In the reference run, the functions 001 and 002 are equal to:

$$F_1 = x_4 \times x_5 = 0.9 \times 1.0 = 0.9$$

$$F_2 = F_1 + x_5 = 0.9 + 1.0 = 1.9$$

The functions are used only for demonstration purposes and not needed for calculations. Nonetheless they must be defined in the input file. It was defined in the comment record:

```
*
*  #001  #002   *   F-001, F-002
```

- Results of calculations - values of parameters selected for post-processing. Below the output is presented for the first parameter only (SC-100-Tcel-0001, fuel centerline temperature, output for SPECTRA, DS-Hadamard (Case 3) run (section 4.2.3).
    - The first block indicates the data file (*.CSV) containing the mean value, the standard deviation, the minimum and the maximum value for every time point in the reference run. Such file may be used to generate graphs, e.g. Figure 6, Figure 7.
    - The next blocks contain data for the time point when the given parameter reaches minimum and maximum in the reference run (local minimum / maximum).

```
================================================================================
 =SL=  OUTPUT OF CALCULATED RESULTS
================================================================================

 =SL=  OUTPUT FOR    3 PLOT PARAMETERS

 =SL=  PLOT PARAMETER NO.   1   ---------------------------------------------

       FILE:> GAP-SPE-001.CSV
       CONTAINS: MEAN, SIGMA, MINIMUM, MAXIMUM, FOR EACH TIME POINT

       MINIMUM PEAK VALUE AT GIVEN TIME (MIN. IN REFERENCE RUN)
       ========================================================
       TIME = 0.00000E+00

        RUN      VALUE        TIME, (s)
       -----  ------------  ------------  VALUE-VALUE0  VALUE/VALUE0
          0    5.69000E+02   0.00000E+00  ------------  ------------
          1    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00
          2    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00
          3    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00
          4    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00
          5    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00
```

```
   6    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00
   7    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00
   8    5.69000E+02   0.00000E+00   0.00000E+00   1.00000E+00

          VALUE      RUN
       ------------  -----
MEAN :  5.69000E+02
SIGMA:  0.00000E+00
MIN. :  5.69000E+02     1
MAX. :  5.69000E+02     1

PEARSON CORRELATION COEFFICIENTS
UNCERT.
 PAR.     VALUE
-----  ------------
   1    0.00000E+00
   2    0.00000E+00
   3    0.00000E+00
   4    0.00000E+00
   5    0.00000E+00

MAXIMUM PEAK VALUE AT GIVEN TIME (MAX. IN REFERENCE RUN)
========================================================
TIME = 1.00000E+04

 RUN      VALUE       TIME, (s)
-----  ------------  ------------  VALUE-VALUE0  VALUE/VALUE0
   0    2.76359E+03   1.00000E+04  ------------  ------------
   1    2.67105E+03   1.00000E+04  -9.25400E+01   9.66515E-01
   2    2.91216E+03   1.00000E+04   1.48570E+02   1.05376E+00
   3    2.63332E+03   1.00000E+04  -1.30270E+02   9.52862E-01
   4    2.90232E+03   1.00000E+04   1.38730E+02   1.05020E+00
   5    2.94617E+03   1.00000E+04   1.82580E+02   1.06607E+00
   6    2.61553E+03   1.00000E+04  -1.48060E+02   9.46425E-01
   7    2.92235E+03   1.00000E+04   1.58760E+02   1.05745E+00
   8    2.60716E+03   1.00000E+04  -1.56430E+02   9.43396E-01

          VALUE      RUN
       ------------  -----
MEAN :  2.77626E+03
SIGMA:  1.45989E+02
MIN. :  2.60716E+03     8
MAX. :  2.94617E+03     5

PEARSON CORRELATION COEFFICIENTS
UNCERT.
 PAR.     VALUE
-----  ------------
   1    1.16208E-01
   2    6.82928E-02
   3    3.71089E-02
   4    2.36663E-02
   5   -9.89751E-01

     PARAMETER RANGE        No. OF    RELATIVE
  MINIMUM       MAXIMUM      RUNS     FREQUENCY
------------  ------------  ------  ------------
 2.60716E+03   2.72016E+03      4    1.50000E+00
 2.72016E+03   2.83317E+03      0    0.00000E+00
 2.83317E+03   2.94617E+03      4    1.50000E+00
```

- Next, the program searches for minimum and maximum value for all time points (global minimum / maximum). The next blocks contain the minimum and the maximum values of the given parameters and the timing when the value is reached (in general the timing may be different in each run, although in the present example the maximum is reached in all runs at the same time, 10,000 s).

MINIMUM PEAK VALUE AT ANY TIME
==========

| RUN | VALUE | TIME, (s) | VALUE-VALUE0 | VALUE/VALUE0 |
|---|---|---|---|---|
| 0 | 5.69000E+02 | 0.00000E+00 | | |
| 1 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |
| 2 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |
| 3 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |
| 4 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |
| 5 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |
| 6 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |
| 7 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |
| 8 | 5.69000E+02 | 0.00000E+00 | 0.00000E+00 | 1.00000E+00 |

| | VALUE | RUN |
|---|---|---|
| MEAN : | 5.69000E+02 | |
| SIGMA: | 0.00000E+00 | |
| MIN. : | 5.69000E+02 | 1 |
| MAX. : | 5.69000E+02 | 1 |

PEARSON CORRELATION COEFFICIENTS
UNCERT.

| PAR. | VALUE |
|---|---|
| 1 | 0.00000E+00 |
| 2 | 0.00000E+00 |
| 3 | 0.00000E+00 |
| 4 | 0.00000E+00 |
| 5 | 0.00000E+00 |

MAXIMUM PEAK VALUE AT ANY TIME
==========

| RUN | VALUE | TIME, (s) | VALUE-VALUE0 | VALUE/VALUE0 |
|---|---|---|---|---|
| 0 | 2.76359E+03 | 1.00000E+04 | | |
| 1 | 2.67105E+03 | 1.00000E+04 | -9.25400E+01 | 9.66515E-01 |
| 2 | 2.91216E+03 | 1.00000E+04 | 1.48570E+02 | 1.05376E+00 |
| 3 | 2.63332E+03 | 1.00000E+04 | -1.30270E+02 | 9.52862E-01 |
| 4 | 2.90232E+03 | 1.00000E+04 | 1.38730E+02 | 1.05020E+00 |
| 5 | 2.94617E+03 | 1.00000E+04 | 1.82580E+02 | 1.06607E+00 |
| 6 | 2.61553E+03 | 1.00000E+04 | -1.48060E+02 | 9.46425E-01 |
| 7 | 2.92235E+03 | 1.00000E+04 | 1.58760E+02 | 1.05745E+00 |
| 8 | 2.60716E+03 | 1.00000E+04 | -1.56430E+02 | 9.43396E-01 |

| | VALUE | RUN |
|---|---|---|
| MEAN : | 2.77626E+03 | |
| SIGMA: | 1.45989E+02 | |
| MIN. : | 2.60716E+03 | 8 |
| MAX. : | 2.94617E+03 | 5 |

PEARSON CORRELATION COEFFICIENTS
UNCERT.

| PAR. | VALUE |
|---|---|
| 1 | 1.16208E-01 |
| 2 | 6.82928E-02 |
| 3 | 3.71089E-02 |
| 4 | 2.36663E-02 |
| 5 | -9.89751E-01 |

| PARAMETER RANGE MINIMUM | MAXIMUM | No. OF RUNS | RELATIVE FREQUENCY |
|---|---|---|---|
| 2.60716E+03 | 2.72016E+03 | 4 | 1.50000E+00 |
| 2.72016E+03 | 2.83317E+03 | 0 | 0.00000E+00 |
| 2.83317E+03 | 2.94617E+03 | 4 | 1.50000E+00 |

Note: If the random sampling methodology is selected, then the Spearman's rank correlation coefficient is printed below the Pearson's correlation coefficient.. For example, SPECTRA, random sampling methodology (Case 1-99-1) run (section 4.2.1). gives the following fuel centerline temperature, output:

```
            VALUE      RUN
          ------------  -----
MEAN :   2.84036E+03
SIGMA:   1.53088E+02
MIN. :   2.48810E+03    595
MAX. :   3.49140E+03    257

PEARSON CORRELATION COEFFICIENTS
UNCERT.
 PAR.      VALUE
-----  ------------
   1     1.48602E-01
   2     1.76985E-01
   3     1.19318E-01
   4     4.37677E-02
   5    -9.70540E-01

SPEARMAN RANK CORRELATION COEFFICIENTS
UNCERT.
 PAR.      VALUE
-----  ------------
   1     1.63440E-01
   2     1.58596E-01
   3     1.32745E-01
   4     4.41067E-02
   5    -9.77590E-01
```

**EHSF (IMTSEL = 5)**

In the case of the EHSF methodology, an additional block is printed, showing the hot spot factors and the values of the variables (quantities of interest). The printout is somewhat different for different methods of calculating the overall hot spot factor. This is the file for SPECTRA of the EHSF runs (Case 4-1 and 4-2) (section 4.2.6).

- IHSDEF = 1 (statistical approach)

In this case the overall hot spot factor is defined as follows.

$$F_y = 1 + \sqrt{\sum_{j=1}^{N} (f_{j,y} - 1)^2}$$

Two values are calculated:

- $F_{y,p}$ is calculated by using all $f_{j,y}$ values that are >1
- $F_{y,n}$ is calculated by using all $f_{j,y}$ values that are <1

Both $F_{y,p}$ and $F_{y,n}$ are > 1. The output file provides the following data:

- Columns of data values of arranged by run and by uncertain parameters, including:
  - dx(j) = variation of uncertain parameter
  - dy(j) = change in the calculated quantity of interest (same as VALUE–VALUE0, see previous page. Since the example case shown on previous page is different than shown here, the values are not the same. For full output see \GAP-SPE-4-1\GAP-SPE.OUT)

- Ratio [dy(j)/y(j) / [dx(j)/x(i)], showing the relative effect of the change of x(j).
- fy(i) = ratio of the calculated quantity of interest (same as VALUE/VALUE0, see previous page). This is the parameter described in 2.4.5, noted as $f_{j,y}$ .
- fy(i) – 1.0

- The values of overall hot spot factors, $F_{y,p}$ and $F_{y,n}$.
- The value of the quantity of interest multiplied by $F_{y,p}$ and divided by $F_{y,n}$.

ENGINEERING HOT SPOT FACTORS (EHSF) DATA - BY RUN

| RUN | j | dx(j) | dy(j) | (dy/y)/(dx/x) | fy(j) | fy(j) - 1.0 |
|---|---|---|---|---|---|---|
| 1 | 1 | 1.20000E-05 | 4.29915E+01 | 1.29637E-01 | 1.01556E+00 | 1.55564E-02 |
| 2 | 2 | 2.97000E-06 | 2.51892E+01 | 1.01274E-02 | 1.00911E+00 | 9.11468E-03 |
| 3 | 3 | 1.60200E-06 | 1.38760E+01 | 5.57889E-03 | 1.00502E+00 | 5.02100E-03 |
| 4 | 4 | 9.99900E-02 | -1.26709E+00 | -4.12687E-03 | 9.99542E-01 | -4.58495E-04 |
| 5 | 5 | 1.00000E-01 | -1.26985E+02 | -4.59494E-01 | 9.54051E-01 | -4.59494E-02 |
| 6 | 1 | -1.20000E-05 | -3.60073E+01 | 1.08577E-01 | 9.86971E-01 | -1.30292E-02 |
| 7 | 2 | -2.97000E-06 | -2.92136E+01 | 1.17455E-02 | 9.89429E-01 | -1.05709E-02 |
| 8 | 3 | -1.60200E-06 | -1.49143E+01 | 5.99636E-03 | 9.94603E-01 | -5.39672E-03 |
| 9 | 4 | -2.70000E-01 | 2.46851E+00 | -2.97742E-03 | 1.00089E+00 | 8.93226E-04 |
| 10 | 5 | -1.00000E-01 | 1.44384E+02 | -5.22452E-01 | 1.05225E+00 | 5.22452E-02 |

ENGINEERING HOT SPOT FACTORS (EHSF) DATA - BY U.P.

| RUN | j | dx(j) | dy(j) | (dy/y)/(dx/x) | fy(j) | fy(j) - 1.0 |
|---|---|---|---|---|---|---|
| 1 | 1 | 1.20000E-05 | 4.29915E+01 | 1.29637E-01 | 1.01556E+00 | 1.55564E-02 |
| 6 | 1 | -1.20000E-05 | -3.60073E+01 | 1.08577E-01 | 9.86971E-01 | -1.30292E-02 |
| 2 | 2 | 2.97000E-06 | 2.51892E+01 | 1.01274E-02 | 1.00911E+00 | 9.11468E-03 |
| 7 | 2 | -2.97000E-06 | -2.92136E+01 | 1.17455E-02 | 9.89429E-01 | -1.05709E-02 |
| 3 | 3 | 1.60200E-06 | 1.38760E+01 | 5.57889E-03 | 1.00502E+00 | 5.02100E-03 |
| 8 | 3 | -1.60200E-06 | -1.49143E+01 | 5.99636E-03 | 9.94603E-01 | -5.39672E-03 |
| 4 | 4 | 9.99900E-02 | -1.26709E+00 | -4.12687E-03 | 9.99542E-01 | -4.58495E-04 |
| 9 | 4 | -2.70000E-01 | 2.46851E+00 | -2.97742E-03 | 1.00089E+00 | 8.93226E-04 |
| 5 | 5 | 1.00000E-01 | -1.26985E+02 | -4.59494E-01 | 9.54051E-01 | -4.59494E-02 |
| 10 | 5 | -1.00000E-01 | 1.44384E+02 | -5.22452E-01 | 1.05225E+00 | 5.22452E-02 |

HOT SPOT FACTORS, Fy-p = 1.05550E+00
Fy-n = 1.04922E+00

| | VALUE | VALUE * Fy-p | VALUE / Fy-n |
|---|---|---|---|
| RUN (000) | 2.76359E+03 | 2.91698E+03 | 2.63395E+03 |

In the case of maximum fuel temperature the interesting value is, of course, the value multiplied by $F_{y,p}$. However, in the case of other parameters, such as for example gap conductance, the interesting value is equal to the value divided by $F_{y,n}$. The implementation is strictly correct if all uncertain parameters have monotonic behavior; in other words if the column dy(j) has the same amount of pluses and minuses. If this is not the case, a warning message is printed to the diagnostics file.

- IHSDEF = 2 (deterministic approach, conservative)

In this case the overall hot spot factor is defined as follows.

$$F_y = \prod_{j=1}^{N} f_{j,y}$$

In this case $F_{y,p} > 1$ while $F_{y,n} < 1$. The output file provides the value of the quantity of interest multiplied by $F_{y,p}$ and by $F_{y,n}$.

```
ENGINEERING HOT SPOT FACTORS (EHSF) DATA - BY RUN

 RUN    j       dx(j)         dy(j)      (dy/y)/(dx/x)     fy(j)      fy(j) - 1.0
----- ----- ------------  ------------  ------------  ------------  ------------
   1    1    1.20000E-05   4.29915E+01   1.29637E-01   1.01556E+00   1.55564E-02
   2    2    2.97000E-06   2.51892E+01   1.01274E-02   1.00911E+00   9.11468E-03
   3    3    1.60200E-06   1.38760E+01   5.57889E-03   1.00502E+00   5.02100E-03
   4    4    9.99900E-02  -1.26709E+00  -4.12687E-03   9.99542E-01  -4.58495E-04
   5    5    1.00000E-01  -1.26985E+02  -4.59494E-01   9.54051E-01  -4.59494E-02

   6    1   -1.20000E-05  -3.60073E+01   1.08577E-01   9.86971E-01  -1.30292E-02
   7    2   -2.97000E-06  -2.92136E+01   1.17455E-02   9.89429E-01  -1.05709E-02
   8    3   -1.60200E-06  -1.49143E+01   5.99636E-03   9.94603E-01  -5.39672E-03
   9    4   -2.70000E-01   2.46851E+00  -2.97742E-03   1.00089E+00   8.93226E-04
  10    5   -1.00000E-01   1.44384E+02  -5.22452E-01   1.05225E+00   5.22452E-02

ENGINEERING HOT SPOT FACTORS (EHSF) DATA - BY U.P.

 RUN    j       dx(j)         dy(j)      (dy/y)/(dx/x)     fy(j)      fy(j) - 1.0
----- ----- ------------  ------------  ------------  ------------  ------------
   1    1    1.20000E-05   4.29915E+01   1.29637E-01   1.01556E+00   1.55564E-02
   6    1   -1.20000E-05  -3.60073E+01   1.08577E-01   9.86971E-01  -1.30292E-02
   2    2    2.97000E-06   2.51892E+01   1.01274E-02   1.00911E+00   9.11468E-03
   7    2   -2.97000E-06  -2.92136E+01   1.17455E-02   9.89429E-01  -1.05709E-02
   3    3    1.60200E-06   1.38760E+01   5.57889E-03   1.00502E+00   5.02100E-03
   8    3   -1.60200E-06  -1.49143E+01   5.99636E-03   9.94603E-01  -5.39672E-03
   4    4    9.99900E-02  -1.26709E+00  -4.12687E-03   9.99542E-01  -4.58495E-04
   9    4   -2.70000E-01   2.46851E+00  -2.97742E-03   1.00089E+00   8.93226E-04
   5    5    1.00000E-01  -1.26985E+02  -4.59494E-01   9.54051E-01  -4.59494E-02
  10    5   -1.00000E-01   1.44384E+02  -5.22452E-01   1.05225E+00   5.22452E-02

HOT SPOT FACTORS, Fy-p = 1.08474E+00
                  Fy-n = 9.26214E-01

               VALUE     VALUE * Fy-p  VALUE * Fy-n
----------- ------------  ------------  ------------
RUN (000)    2.76359E+03   2.99776E+03   2.55967E+03
```

This definition gives somewhat larger values of the hot spot factors, compared to the previous case.

### User-defined matrix (IMTSEL = 6)

In this case the hot spot factors are also printed. Compared to the methodology 4, the values of $\Delta x_j$ and $(\Delta y_j/y_j)$ / $(\Delta x_j/x_j)$ are not printed. An example printout is shown below.

```
ENGINEERING HOT SPOT FACTORS (EHSF) DATA - BY RUN

 RUN    j       dy(j)         fy(j)
----- ----- ------------  ------------
   1    0   -9.25400E+01   9.66515E-01
   2    0    1.48570E+02   1.05376E+00
   3    0   -1.30270E+02   9.52862E-01
   4    0    1.38730E+02   1.05020E+00
   5    0    1.82580E+02   1.06607E+00
   6    0   -1.48060E+02   9.46425E-01
   7    0    1.58760E+02   1.05745E+00
   8    0   -1.56430E+02   9.43396E-01

HOT SPOT FACTORS, Fy-p = 1.11435E+00
                  Fy-n = 1.09704E+00

               VALUE     VALUE * Fy-p  VALUE / Fy-n
----------- ------------  ------------  ------------
RUN (000)    2.76359E+03   3.07960E+03   2.51912E+03
```

### 3.3.2 Time-Dependent Graphs (*.ASC or *.CSV)

For each time point, SUE calculates the following values for each of the plot parameters defined in records 300XXX (section 3.1.13):

- Mean value: $\mu_y(t) = \dfrac{\sum_{i=1}^{N} y_i(t)}{N}$
- Standard deviation: $\sigma_y(t) = \sqrt{\dfrac{\sum_{i=1}^{N} \left[\mu_y(t) - y_i(t)\right]^2}{N}}$
- Minimum value: $y_{min}(t) = \text{Min}[\, y_i(t) \,]_{i=1,\ldots,N}$
- Maximum value: $y_{max}(t) = \text{Max}[\, y_i(t) \,]_{i=1,\ldots,N}$
- The run number, with: $y_{min}(t)$
- The run number, with: $y_{max}(t)$

Here $t$ is the current time, $y_i(t)$ is the value of plot parameter $y$ obtain in the run number $i$ at the time $t$, and $N$ is the total number of runs performed (depending on the selected methodology). The value of $t$ printed is equal to the average of all runs.

SUE checks if the time points are in agreement in all runs with the assumed tolerance. If a discrepancy is detected and error message is generated. In such case the user should decrease the maximum time step. The recommended value of the maximum time step should be smaller than $\Delta t_{max} < 0.1 \times \Delta t_{plt}$. Here $\Delta t_{max}$ is the maximum time step for the code advancements and $\Delta t_{plt}$ is the time interval for plotting.

An example of the contents of the file GAP-SPE-001.CSV (sec. 4.2.3) is shown below.

```
TIME,MEAN,SIGMA,MINIMUM,MAXIMUM,RUN-MIN,RUN-MAX
0.00000E+00, 5.69000E+02, 0.00000E+00, 5.69000E+02, 5.69000E+02,001,001
1.00000E+03, 1.03180E+03, 4.48929E+01, 9.65661E+02, 1.10607E+03,003,005
2.00010E+03, 1.29261E+03, 7.02885E+01, 1.19292E+03, 1.40410E+03,003,005
3.00010E+03, 1.53463E+03, 9.23374E+01, 1.40766E+03, 1.67434E+03,003,005
4.00010E+03, 1.65806E+03, 1.02550E+02, 1.52057E+03, 1.80965E+03,003,005
5.00000E+03, 1.87833E+03, 1.18316E+02, 1.72594E+03, 2.04553E+03,003,005
6.00000E+03, 1.97419E+03, 1.23885E+02, 1.81810E+03, 2.14532E+03,003,005
7.00000E+03, 2.24636E+03, 1.35523E+02, 2.08759E+03, 2.42518E+03,003,005
8.00000E+03, 2.47157E+03, 1.40207E+02, 2.31840E+03, 2.65071E+03,003,005
9.00000E+03, 2.54688E+03, 1.40668E+02, 2.39245E+03, 2.72594E+03,008,005
1.00000E+04, 2.77626E+03, 1.45989E+02, 2.60716E+03, 2.94617E+03,008,005
```

Such a file may be used to generate graph, e.g. Figure 6 and Figure 7. Similar figures are presented in sections 4.2.3 and 4.2.1 but with power rather than time on the $x$-axis (sections 4.2.3 Figure 27, section 4.2 Figure 9).

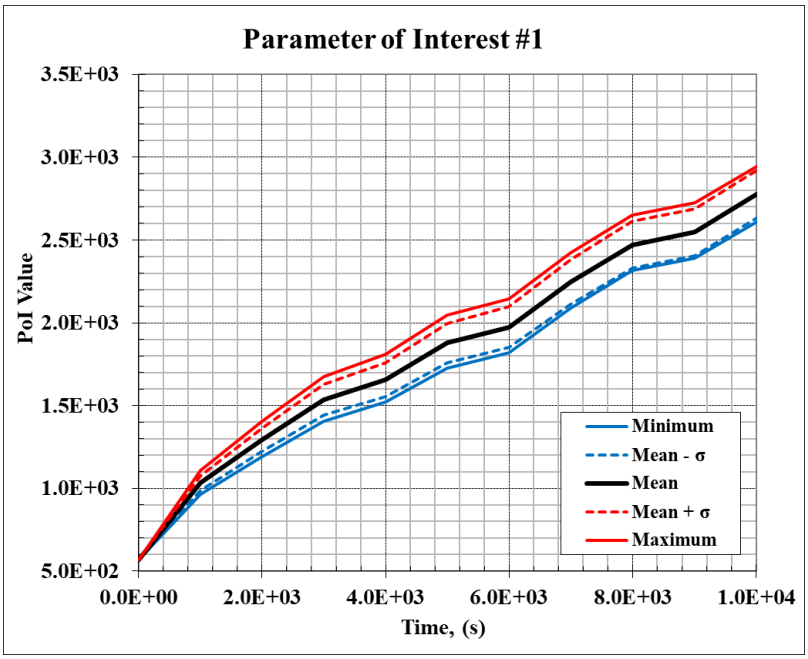



*Figure 6: Centerline temperatures, SPECTRA, RS (Case 3, sec. 4.2.3)*

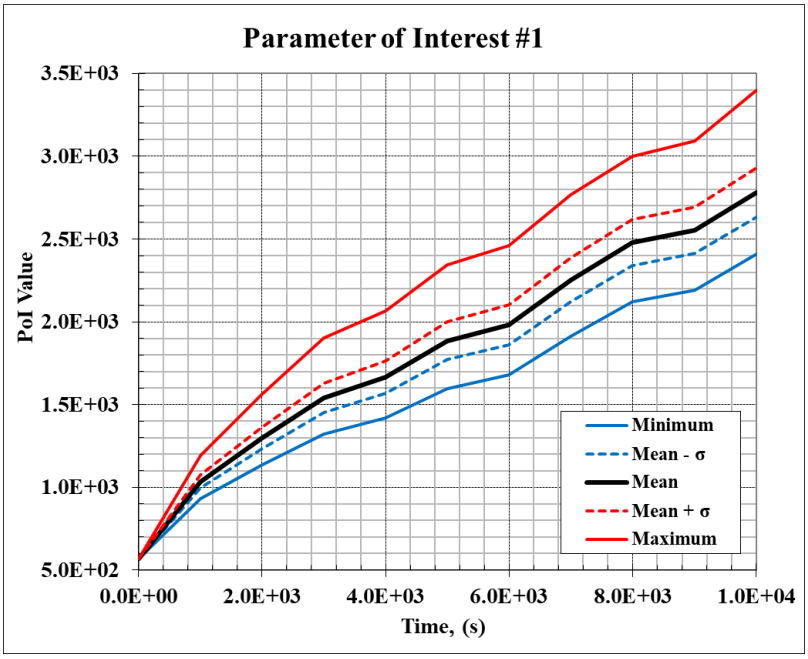



*Figure 7: Centerline temperatures, SPECTRA, DS-H (Case 1-99-1, sec. 4.2.1)*

### 3.3.3 Diagnostics File (*.DIA)

The diagnostics file contains:

- the list of all command lines executed,
- the diagnostics of all plot parameters (quantities of interest) read from the code output/plot files, including the number of points read,
- diagnostics from the search from global/minimum/maximum, including the identification if each calculations is completed successfully, giving the following outputs in case of run completed and failed, respectively:

```
> RUN:  18, OK
> RUN:  19, HAS FAILED. ELIMINATED
```

An example of diagnostics file is given below. This is the file for SPECTRA of the DS-Hadamard (Case 3) run (section 4.2.3).

```
================================================================================
 =SUE=  SUE Version 3.00, Nov. 2024, Windows

 System-code
   Uncertainty
     Evaluation

--------------------------------------------------------------------------------
 Validity:  unlimited
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
 Run executed on :    1/06/2024,  14:24:55.96
--------------------------------------------------------------------------------
 Input data diagnostics
================================================================================


 * * *  =IN=  WARNING: NORMAL DISTRIBURTION, MAX. VALUE
              INPUT VALUE DIFFERENT THAN DEFAULT
              VARIABLE NUMBER:      I  =  4
              INPUT   VALUE: XMAXUP(I) = 1.11110E+00
              DEFAULT VALUE:   XMAX(I) = 1.30000E+00

  CALCULATIONS OF:   8 RUNS

  COMMAND LINES EXECUTED:

 >start C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-001
 >start C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-002
 >start C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-003
 >call  C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-004
 >start C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-005
 >start C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-006
 >start C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-007
 >call  C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-008
 >call  C:/SPECTRA/Z-EXE/SPECTRA.EXE GAP-PBF-LOC-11C-000

 > ANALYSIS OF RESULTS

 > PLOT PARAMETER (QUANTITY OF INTEREST):   1
 > RUN:   0, READ POINTS:     11
 > RUN:   1, READ POINTS:     11
```

```
> RUN:   2, READ POINTS:     11
> RUN:   3, READ POINTS:     11
> RUN:   4, READ POINTS:     11
> RUN:   5, READ POINTS:     11
> RUN:   6, READ POINTS:     11
> RUN:   7, READ POINTS:     11
> RUN:   8, READ POINTS:     11

> SEARCH FOR GLOBAL MIN / MAX
> RUN:   1, OK
> RUN:   2, OK
> RUN:   3, OK
> RUN:   4, OK
> RUN:   5, OK
> RUN:   6, OK
> RUN:   7, OK
> RUN:   8, OK
> RUN:   0, OK

> TOTAL NUMBER OF RUNS:   8
> NUMBER OF RUNS OK   :   8

> PLOT PARAMETER (QUANTITY OF INTEREST):   2
> RUN:   0, READ POINTS:     11
> RUN:   1, READ POINTS:     11
> RUN:   2, READ POINTS:     11
> RUN:   3, READ POINTS:     11
> RUN:   4, READ POINTS:     11
> RUN:   5, READ POINTS:     11
> RUN:   6, READ POINTS:     11
> RUN:   7, READ POINTS:     11
> RUN:   8, READ POINTS:     11

> SEARCH FOR GLOBAL MIN / MAX
> RUN:   1, OK
> RUN:   2, OK
> RUN:   3, OK
> RUN:   4, OK
> RUN:   5, OK
> RUN:   6, OK
> RUN:   7, OK
> RUN:   8, OK
> RUN:   0, OK

> TOTAL NUMBER OF RUNS:   8
> NUMBER OF RUNS OK   :   8

> PLOT PARAMETER (QUANTITY OF INTEREST):   3
> RUN:   0, READ POINTS:     11
> RUN:   1, READ POINTS:     11
> RUN:   2, READ POINTS:     11
> RUN:   3, READ POINTS:     11
> RUN:   4, READ POINTS:     11
> RUN:   5, READ POINTS:     11
> RUN:   6, READ POINTS:     11
> RUN:   7, READ POINTS:     11
> RUN:   8, READ POINTS:     11

> SEARCH FOR GLOBAL MIN / MAX
> RUN:   1, OK
> RUN:   2, OK
> RUN:   3, OK
> RUN:   4, OK
> RUN:   5, OK
> RUN:   6, OK
> RUN:   7, OK
> RUN:   8, OK
> RUN:   0, OK

> TOTAL NUMBER OF RUNS:   8
> NUMBER OF RUNS OK   :   8

 ->  RUN STATISTICS
     ------------------------------------------------------------------------
     Analyzed runs           :     8
```

```
     Processor time (CPU) [s]:  0.219       ( 0.608E-04 [hrs] )
     Clock time     (RUN) [s]:   253.       ( 0.704E-01 [hrs] )
     ------------------------------------------------------------------------

 ->  =SUE=  SUE Version 3.00, Nov. 2024, Windows
     FILES CLOSED ON :  1/06/2024,  14:29:09.34
     LOGGED IN AS    : STEMPNIEWICZ
```

In the case of DS-S methodology, warning messages are printed every time the minimum-maximum limits are activated (see section 2.4.2). An example of such warning message (generated for the Case 2) is given below:

```
 * * *  =SUE= WARNING IN DSSMET
              PERFORMING DETERMINISTIC SAMPLING
              FOR THE DS-S METHODOLOGY
              UNCERTAIN PARAMETER NUMBER,   I =  1
              RUN NUMBER,                IRUN =  1
              SQRT(n) * SIGMA =  1.54919E-05
              XMAXUP - MEAN V.=  1.20000E-05
              XMAXUP LIMIT ACTIVATED. UNCERTAIN PARAMETER VALUE:
              FROM METHODOLOGY=  1.15492E-04
              ACTUAL USED     =  1.12000E-04
              SUCH MESSAGES INDICATE THAT
              A DIFFERENT METHODOLOGY SHOULD BE USED
```

The message says that instead of the value $1.54919\times10^{-5}$, which is given by the methodology, the value of $1.12\times10^{-5}$ is used, as the maximum defined by the user for this value.

# 4 Test Problem

## 4.1 PBF Test LOC-11C

### 4.1.1 Test Description

The test problem considered is the steady-state average centerline temperature data from the Power Burst Facility (PBF) Test LOC-11C [17]. The test was primarily used to evaluate the dynamic gap conductance model in RELAP 5 [3] (Volume IV), as well as SPECTRA [1] (Volume 3).

The test consists of LWR fuel rod. The test data and the models of RELAP5 and SPECTRA are described in references [1] and [3]. The calculations are performed with the power increased in steps. After each power increase, calculations are run for a sufficient time (1000 s) to obtain stationary state. The full run consists of 10 steps; the total run time is 10,000 seconds. Since only the stationary-state values are interesting for this test, the plot points were made every 1000 s, which means that each plot point represents the values for different power level. (Of course, it had been earlier assessed using frequent plot points that the 1000 second periods were sufficiently long to obtain stable results.)

### 4.1.2 Sources of Uncertainties Considered

The effects of uncertainties on the most important input parameters, such as material properties, initial and boundary conditions related to the system description and physical models are considered as part of this analysis. Uncertainty ranges and distributions assumed in this study for the different variables (quantities of interest) under consideration were assumed based the LMFR analysis performed at PSI [13]. The values are given in Table 3 as multipliers for the corresponding values.

*Table 3: Input uncertainty ranges and distributions of the parameters considered*

| Variable | Distribution | Mean | Std dev | Min | Max |
|---|---|---|---|---|---|
| Initial gap width | Uniform | $0.10\times10^{-3}$ m | - | 0.88 | 1.12 |
| Fuel roughness | Normal | $3.30\times10^{-6}$ m | 0.30 | - | - |
| Clad roughness | Normal | $1.78\times10^{-6}$ m | 0.30 | - | - |
| Centerline shift | Normal | 0.90 | 0.10 | | |
| Fuel thermal conductivity | Normal | 1.00 | 0.10 | - | - |

## 4.2 PBF Test LOC-11C, SPECTRA Analysis

Calculations were performed using the following methodologies:

- RS methodology - section 4.2.1.
  - Case 1-99-1: α=99%, β=99% (pseudo-random series 1).
  - Case 1-99-2: α=99%, β=99% (pseudo-random series 2).
  - Case 1-95: α=95%, β=95% (pseudo-random series 1).
- DS-Standard methodology - section 4.2.2.
- DS-Hadamard methodology - section 4.2.3.
- DS-Simplex methodology - section 4.2.4.
- EHSF methodology - section 4.2.6.
- User-defined matrix of uncertain parameters - section 4.2.7.

### 4.2.1 RS Methodology

The RS methodology is used with 2-sided tolerance limits, probability α = 99%, and confidence level, β = 99%. The SUE input deck is provided below:

```
= SUE INPUT FOR: GAP-PBF-LOC-11C, SPECTRA
* ========================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      1    *    RS
*
*         RS METHODOLOGY DATA
*         ISIDED   IPROBA    ICONFB    IREPRS
100001    2        99        99        123456
*
*
105000   'GAP-PBF-LOC-11C.SPE'                  *  BASE INPUT FILE
115000   'UNPAR'                                *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'C:/SPECTRA.361/Z-EXE/SPECTRA-3-61.EXE' *  PROGRAM TO RUN
130000    6                                     *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
```

```
300000   1          2
*
305001   SC-100-Tcel-0001  *  Cell  1, centerline
305002   SC-100-Tcel-0010  *  Cell 10, clad surface
305003   SC-100-hGap-0000  *  Gap conductance
```

The data for uncertain parameters were entered using relative values for $\sigma$, $x_{min}$, $x_{max}$, (INPOPT=1), which means the absolute values are obtained by multiplying the entered values by the mean values. It was checked that identical results are obtained when absolute values are defined in input (INPOPT=2). The input for this case is:

```
*        INPOPT  NINTDF
200000     2       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN       MAX
200001      2    0.100E-3   0.0     0.088E-3  0.112E-3  *  INITIAL GAP SIZE
200002      1    3.300E-6   9.90E-7 0.0       0.0       *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   5.34E-7 0.0       0.0       *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.09    0.0       0.999990  *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0       0.0       *  FUEL THERMAL CONDUCTIVITY
```

The values of centerline shift are difficult to estimate. It is believed that the most likely position of the fuel pellet is when it touches the cladding on one side (shift = 1.0). For the current test it was assumed that the centerline shift is 0.9 ±0.1, thus $\mu$=0.9, $\sigma$=0.1. The maximum value is set to 1.1111 relative or 0.99999 absolute (=0.9×1.1111).

The uncertain parameters were defined in a separate file, where all data are defined as the replacement records. The SPECTRA input file (GAP-PBF-LOC-11C.SPE), is as follows:

```
*
* ================================================================================
= Gap model, UQ
* ================================================================================
*
ATTACH './GAP-PBF-LOC-11C'  * Model
ATTACH './MPD'              * Material properties data
*
* ========================  SL - Solver (Time Step) Data  ======================
*
900000   0.0                                        **  Start time
*         DTMAX    DTMIN  DTPRT   DTPLT   TEND
900001    0.100   1.0E-8  1000.   1000. 10000.0   **  Time steps
*
*
* ========================  Scenario specific input data  ======================
*
*
ATTACH 'UNPAR'   *  ATTACH THE UNCERTAIN PARAMETER REPLACEMENT FILE
*
*
* ======================  End of Input  ======================================
```

The file GAP-PBF-LOC-11C contains the input model of the facility. The file MPD contains the thermo-physical properties of all solid materials (fuel, cladding). The time step data defines the total run time (10,000 s) with output and plot points being written every 1000 s (to get values at the end of each power step). The file UNPAR contains all the parameters with uncertainties, written as replacement records. The file is shown below:

```
*         dx [m]      Mat  Power  T [K]   N  N-start
310100  $001          901   0.0   569.0   1  7   *  GAP SIZE
*
*      GAP 1
```

```
*      Radiation        Gas conduction                            Solid conduction
*       Ef      Ec      Cd      Rf          Rc        Cj        C-s   Pa      Hc      n
341001  0.0     0.0     0.0   $002         $003         0.0       0.0   0       009   0.0
*
*      Dynamic expansion model
*      Gap [m] swell creep  shift       strain-f strain-c Young
340001  0.0    0.0   0.0   $004         005      006      007    *   CENTERLINE SHIFT
*
*
*       k             rgo Cp
800101 $005           1.0 1.0   *   Fuel, UO2 property multipliers
*
* ======================================================================
*                    End of Input
* ======================================================================
*
*
```

The uncertain parameters are marked in red. In this input the fuel thermal conductivity multiplier is defined in the record 800101, containing constant multipliers for thermal conductivity, density, and specific heat for the material 101 ($UO_2$). An alternative way of defining the thermal conductivity is by using the dependent uncertain parameters. The input is as follows:

```
*         dx [m]     Mat  Power  T [K]   N  N-start
310100  $001         901   0.0   569.0   1  7   *  GAP SIZE
*
*      GAP 1
*      Radiation        Gas conduction                            Solid conduction
*       Ef      Ec      Cd      Rf          Rc        Cj        C-s   Pa      Hc      n
341001  0.0     0.0     0.0   $002         $003         0.0       0.0   0       009   0.0
*
*      Dynamic expansion model
*      Gap [m] swell creep  shift       strain-f strain-c Young
340001  0.0    0.0   0.0   $004         005      006      007    *   CENTERLINE SHIFT
*
*
801101  0.0  *  start replacement data
*       k   [W/m/K]
801101  300.0   $005@9.01
801101  400.0   $005@7.37
801101  500.0   $005@6.23
801101  600.0   $005@5.40
801101  700.0   $005@4.78
801101  800.0   $005@4.29
801101  900.0   $005@3.90
801101 1000.0   $005@3.59
801101 1100.0   $005@3.34
801101 1200.0   $005@3.14
801101 1300.0   $005@2.97
801101 1400.0   $005@2.84
801101 1500.0   $005@2.74
801101 1600.0   $005@2.66
801101 1700.0   $005@2.61
801101 1800.0   $005@2.58
801101 1900.0   $005@2.57
801101 2000.0   $005@2.58
801101 2100.0   $005@2.61
801101 2200.0   $005@2.65
801101 2300.0   $005@2.72
801101 2400.0   $005@2.80
801101 2500.0   $005@2.90
801101 2600.0   $005@3.02
801101 2700.0   $005@3.15
801101 2800.0   $005@3.30
801101 2900.0   $005@3.47
801101 3000.0   $005@3.66
*
* ======================================================================
*                    End of Input
* ======================================================================
```

The thermal conductivity data for the material 101 is defined following $005@. The sign $005 means the uncertain parameter 5. The dependent parameter type must be defined as "multiply" (IDPTYP=2). The sign @ precedes the value of the dependent parameter. During the calculations, the value of the independent parameter is sampled using its data (μ=1.0, σ=0.1) and then the value of the dependent parameter is obtained from (section 3.2.2):

$$y = \mu_y \cdot x / \mu_x$$

Suppose the sampled value of the parameter $005 is 0.9. The value of conductivity for the first point (T=300 K) is 9.01. This means that SUR will replace $005@9.01 by

$$y = 9.01 \cdot 0.9 / 1.0 = 8.109$$

It was checked that identical results are obtained with both inputs, the one with the conductivity multiplier defined in the record 800101 and the one with the conductivity tabulated versus temperature, defined in the records 801101.

When SUE is executed, it creates the files:
UNPAR-001, UNPAR-002, ...
where all the parameters preceded by $ are replaced by their actual values. Furthermore, it creates the input decks, and the input decks:
GAP-PBF-LOC-11C-001.SPE, GAP-PBF-LOC-11C-002.SPE, ...
where the statement ATTACH UNPAR is replaced by
ATTACH UNPAR-001, ATTACH UNPAR-002, ...
and executes the SPECTRA runs. The commands that are being executed are written to the SUE diagnostics file (section 3.3.3).

For the selected parameters, 2-sided tolerance limits, probability α = 99%, and confidence level, β = 99%, the number of runs is 662 (Table 1). Repeatable series were chosen, to be able to reproduce the results. Two cases were considered with different pseudo-random series:

- Case 1-99-1: Starting point for the pseudo-random series, IREPRS = 123456.
- Case 1-99-2: Starting point for the pseudo-random series, IREPRS = 654321.

Additionally, a run was performed for α=95%, β=95%: Case 1-95. The number of runs is 93 (Table 1).

The results obtained for the Case 1-99-1 are shown in Figure 8, Figure 9, Figure 10, and Figure 11. Figure 8 and Figure 9 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range"). The last value (3398 K - Figure 8) is the upper tolerance limit.

Figure 10 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

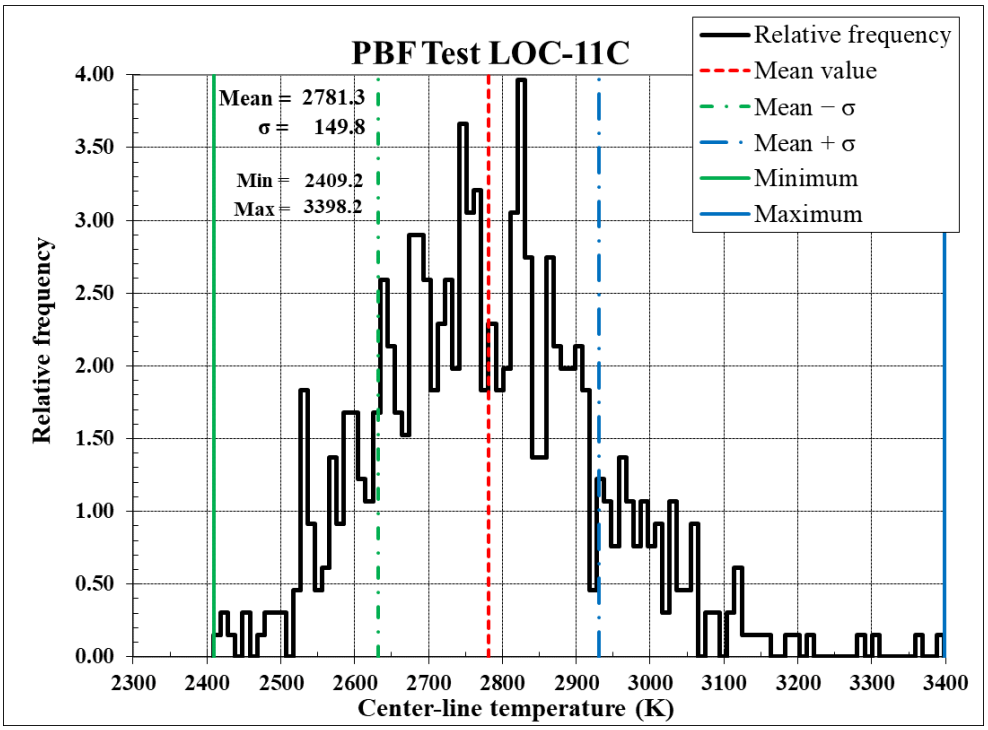



*Figure 8: Centerline temperature at t=10,000 s, SPECTRA, RS (Case 1-99-1)*

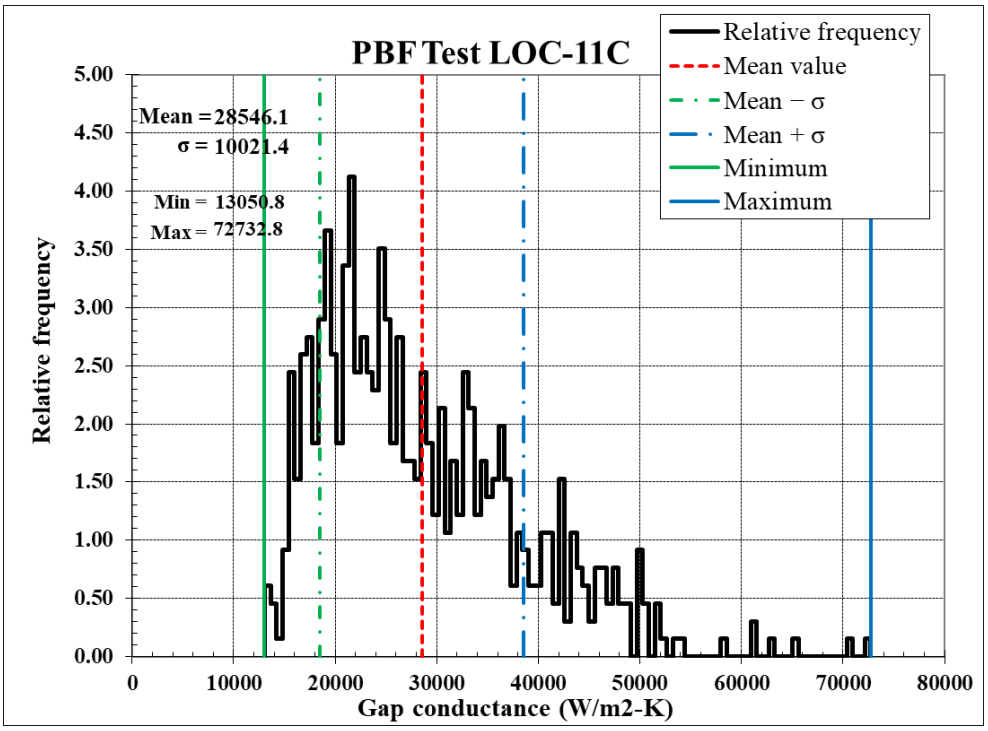
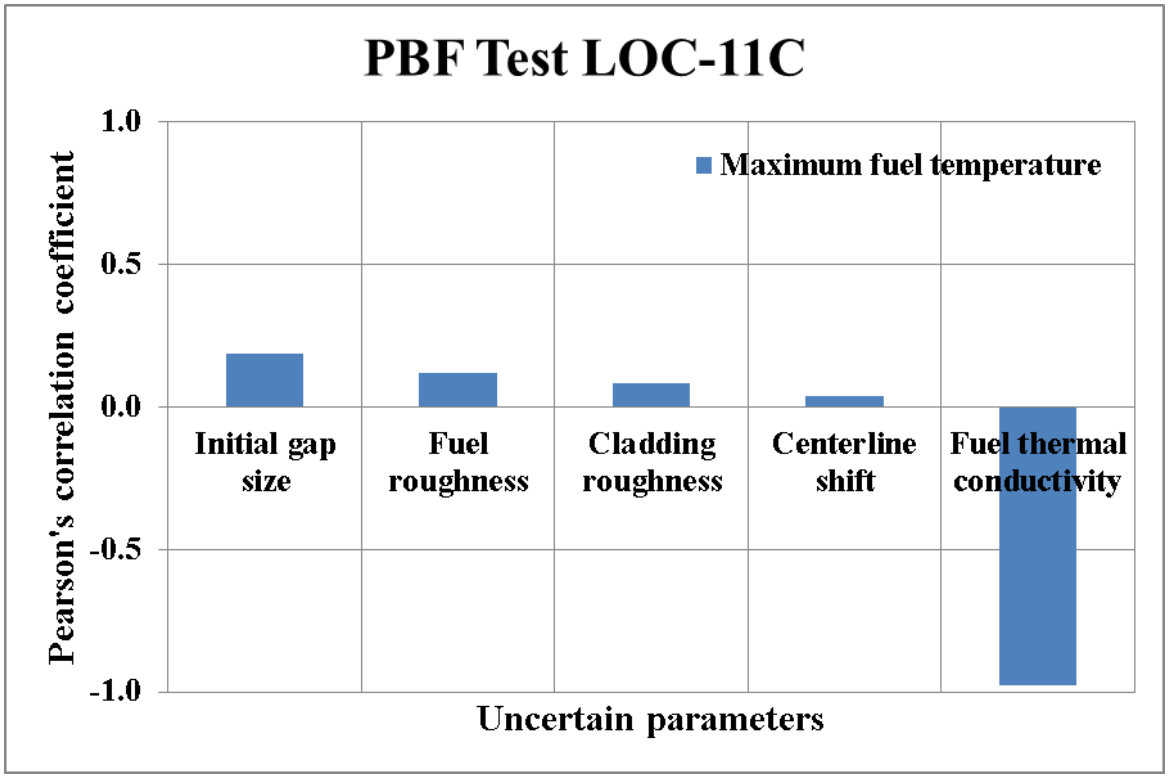



*Figure 9: Gap conductance at t=10,000 s, SPECTRA, RS (Case 1-99-1)*



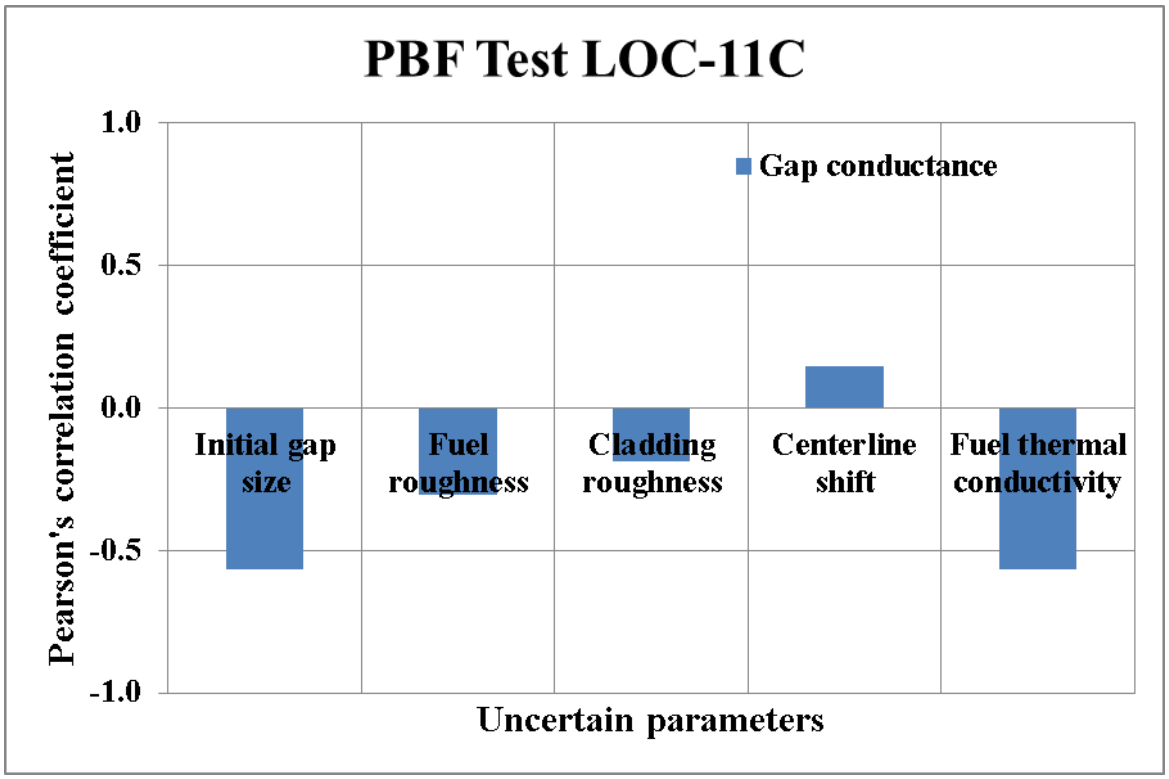




*Figure 10: Pearson's correlation coefficients, SPECTRA, RS (Case 1-99-1)*

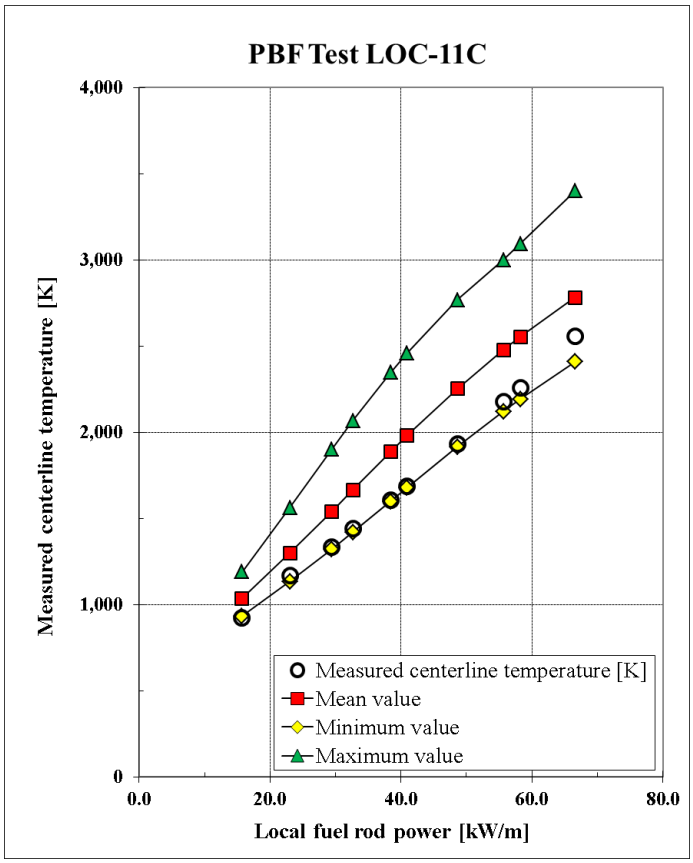



*Figure 11: Centerline temperatures, SPECTRA, RS (Case 1-99-1)*

The results obtained for the Case 1-99-2 are shown in Figure 12, Figure 13, Figure 14, and Figure 15. Figure 12 and Figure 13 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range"). The last value (3374 K - Figure 12) is the upper tolerance limit.

Figure 14 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

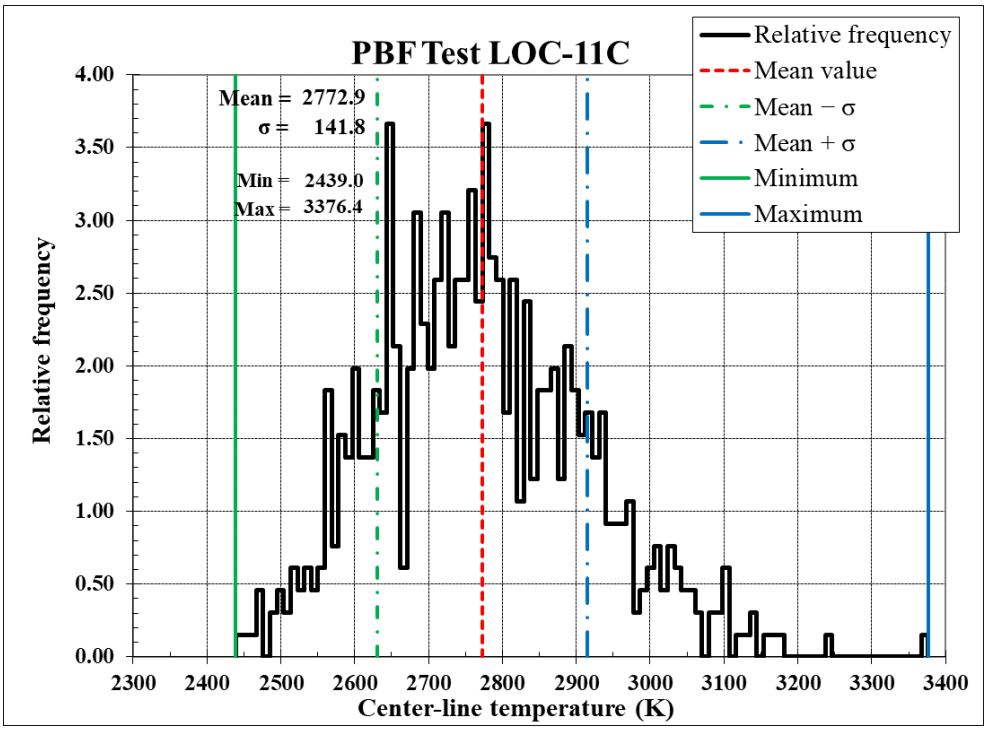



*Figure 12: Centerline temperature at t=10,000 s, SPECTRA, RS (Case 1-99-2)*

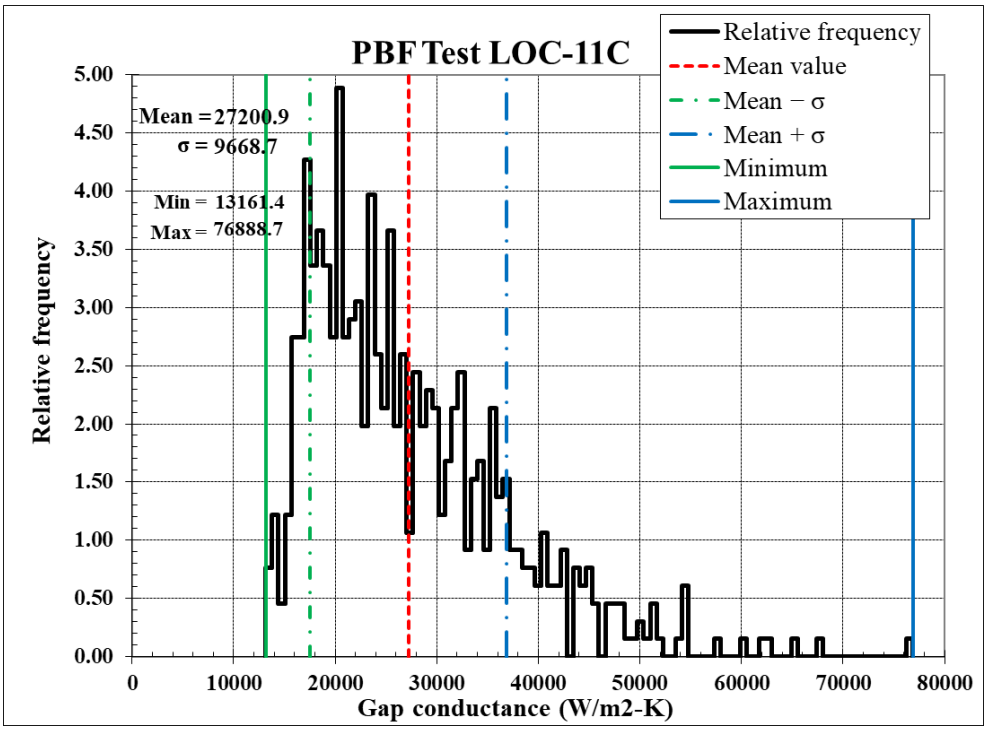



*Figure 13: Gap conductance at t=10,000 s, SPECTRA, RS (Case 1-99-2)*

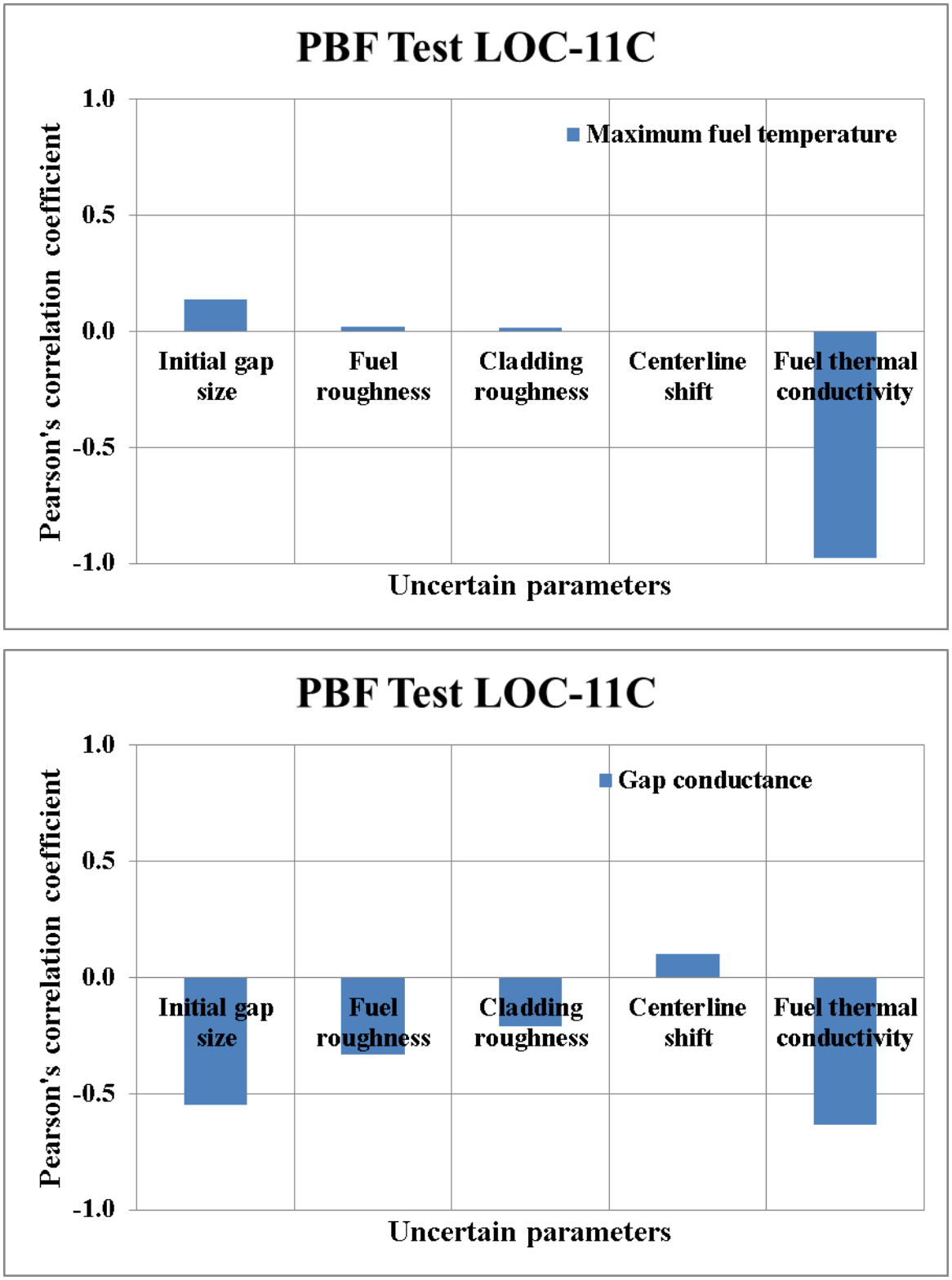



*Figure 14: Pearson's correlation coefficients, SPECTRA, RS (Case 1-99-2)*

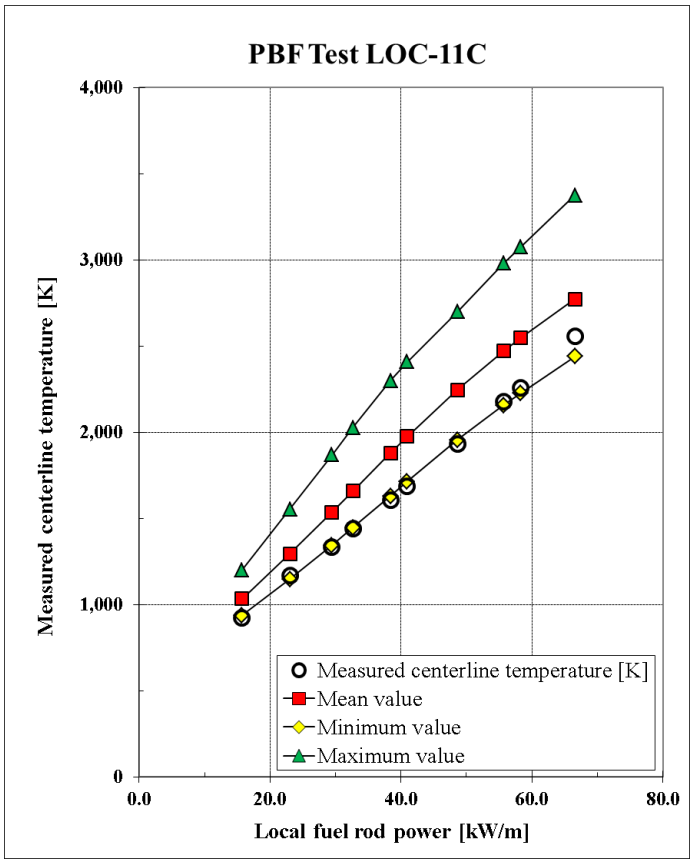



*Figure 15: Centerline temperatures, SPECTRA, RS (Case 1-99-2)*

The results obtained for the Case 1-95 are shown in Figure 16, Figure 17, Figure 18, and Figure 19. Figure 16 and Figure 17 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range"). The last value (3219 K - Figure 16) is the upper tolerance limit.

Figure 18 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

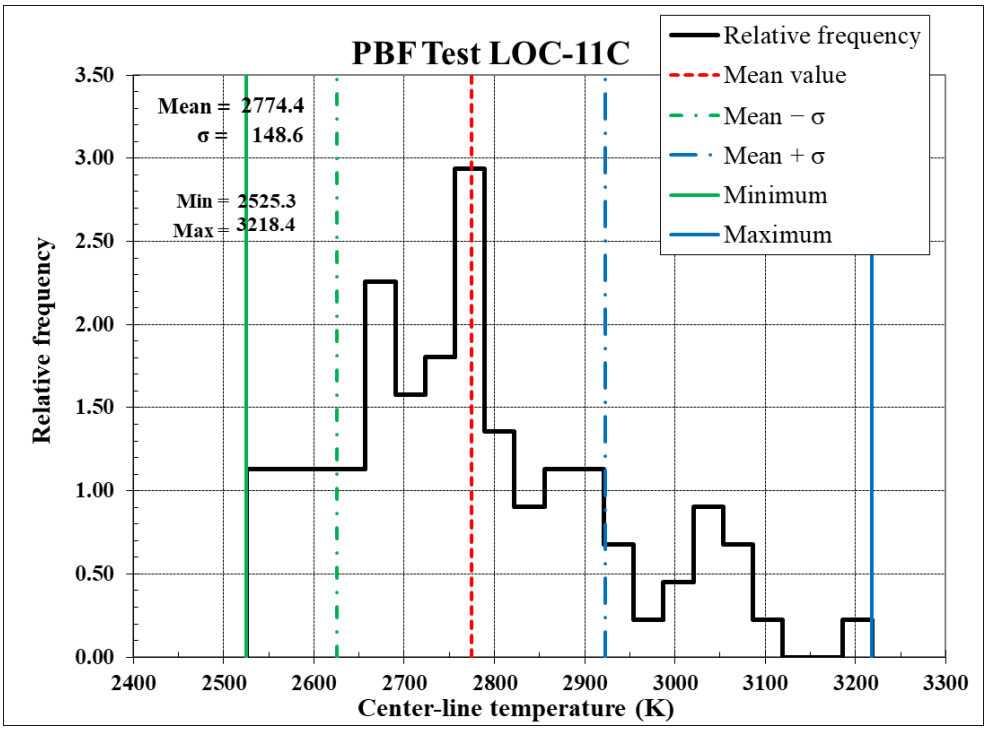



*Figure 16: Centerline temperature at t=10,000 s, SPECTRA, RS (Case 1-95)*

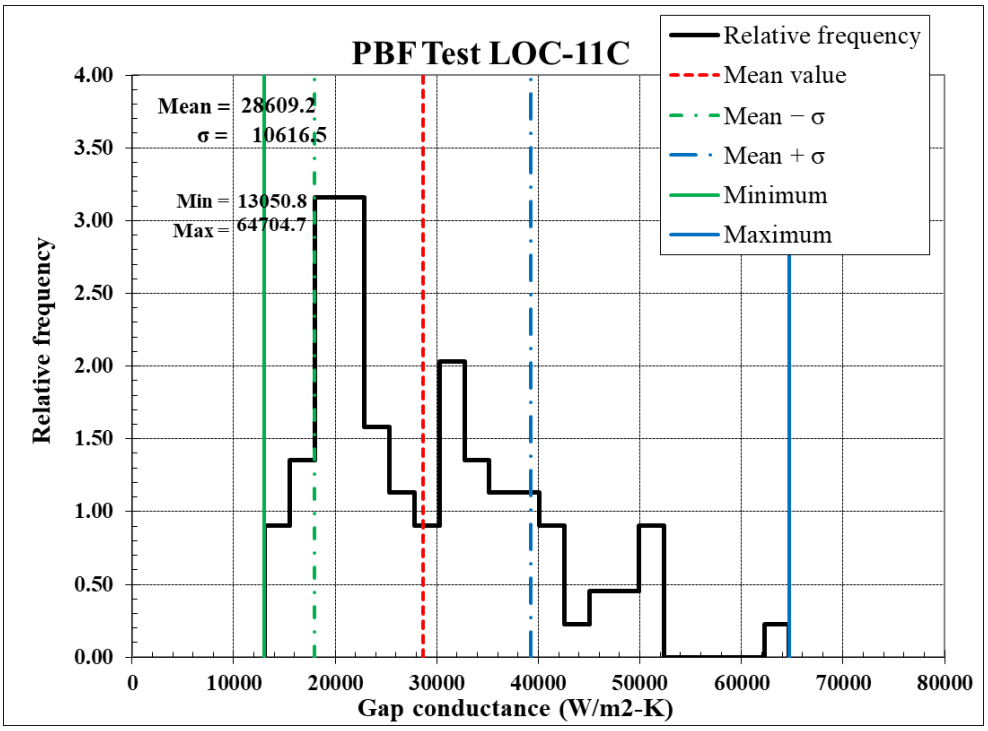
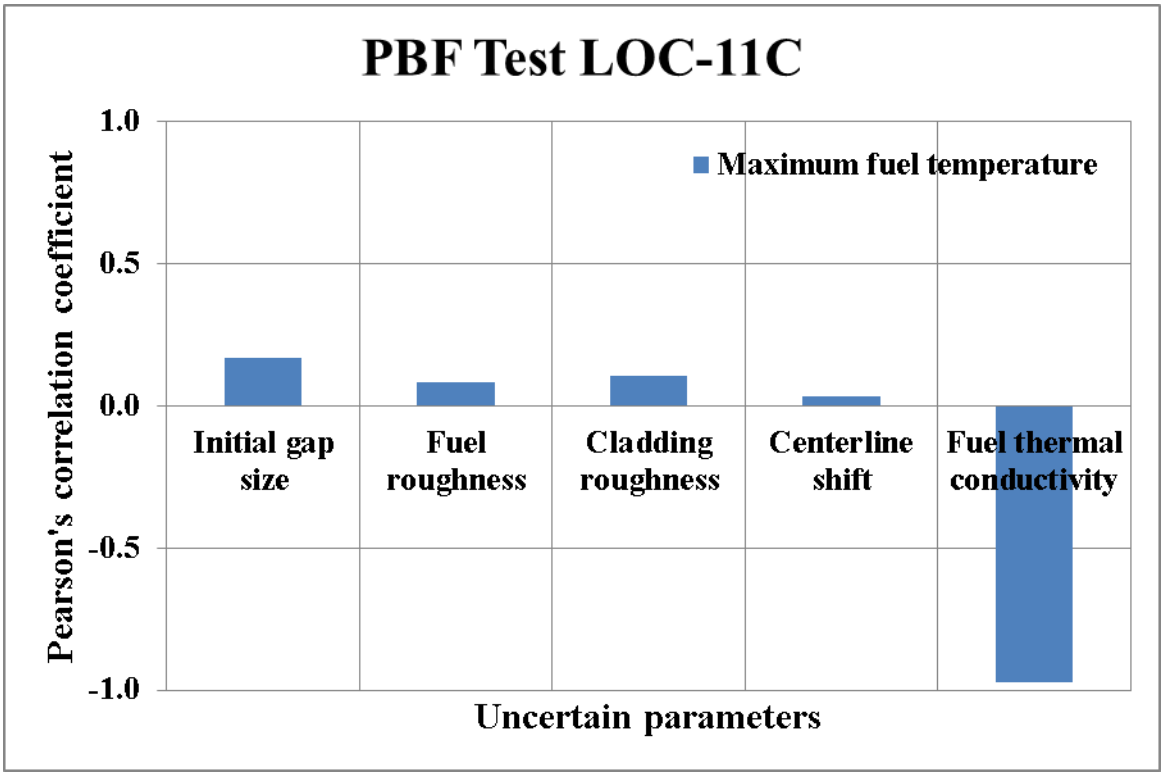



*Figure 17: Gap conductance at t=10,000 s, SPECTRA, RS (Case 1-95)*



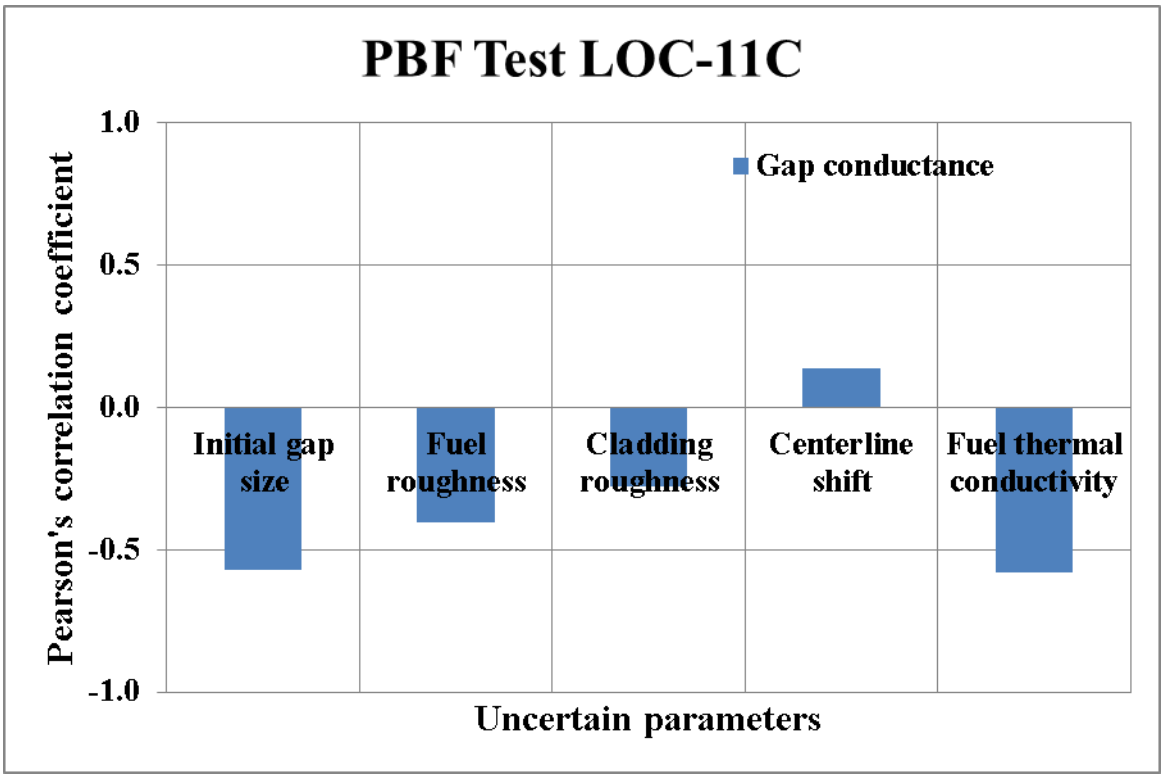




*Figure 18: Pearson's correlation coefficients, SPECTRA, RS (Case 1-95)*

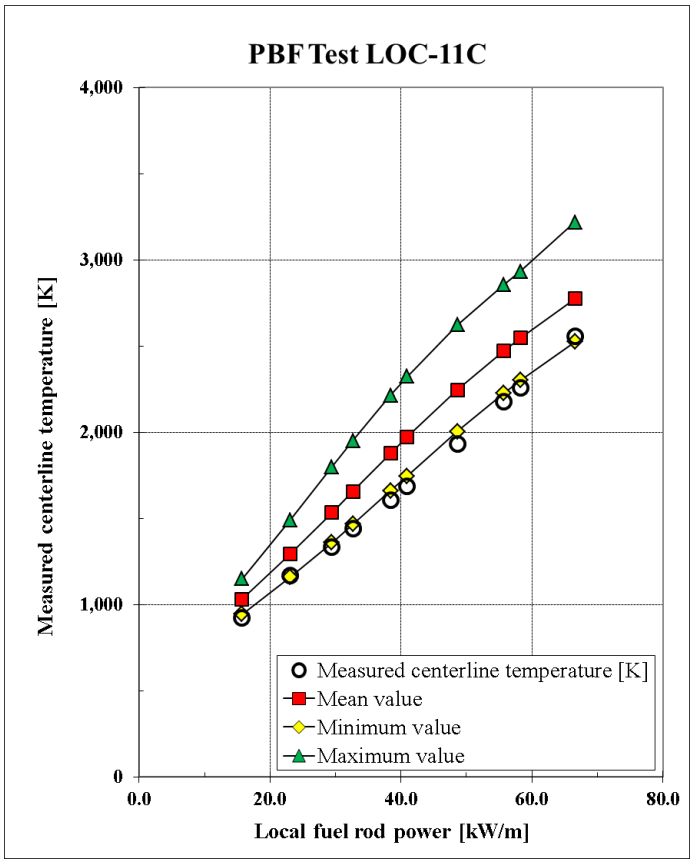



*Figure 19: Centerline temperatures, SPECTRA, RS (Case 1-95)*

Table 4 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 4: Main parameters, SPECTRA, Cases 1*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2781 | 150 | 28.5 | 10.0 |
| Case 1-99-2 | 662 | 2773 | 142 | 27.2 | 9.7 |
| Case 1-95 | 93 | 2774 | 149 | 28.6 | 10.6 |

### 4.2.2 DS Standard Methodology

The SUE input data file for the DS-Standard methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, SPECTRA
* ======================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      2    *    DS-STANDARD
*
*
105000   'GAP-PBF-LOC-11C.SPE'                    *  BASE INPUT FILE
115000   'UNPAR'                                  *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'C:/SPECTRA.361/Z-EXE/SPECTRA-3-61.EXE' *  PROGRAM TO RUN
130000    4                                       *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   1          2
*
305001   SC-100-Tcel-0001  *  Cell  1, centerline
305002   SC-100-Tcel-0010  *  Cell 10, clad surface
305003   SC-100-hGap-0000  *  Gap conductance
*
*
* ========================================================================
*  END OF INPUT FILE
* ========================================================================
*
```

The SPECTRA input files (GAP-PBF-LOC-11C.SPE, UNPAR) are the same as described in the previous section.

The results obtained for the DS-S methodology, referred to here as Case 2, are shown in Figure 20, Figure 21, Figure 22, and Figure 23. Figure 20 and Figure 21 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: “relative frequency” versus “parameter range”).

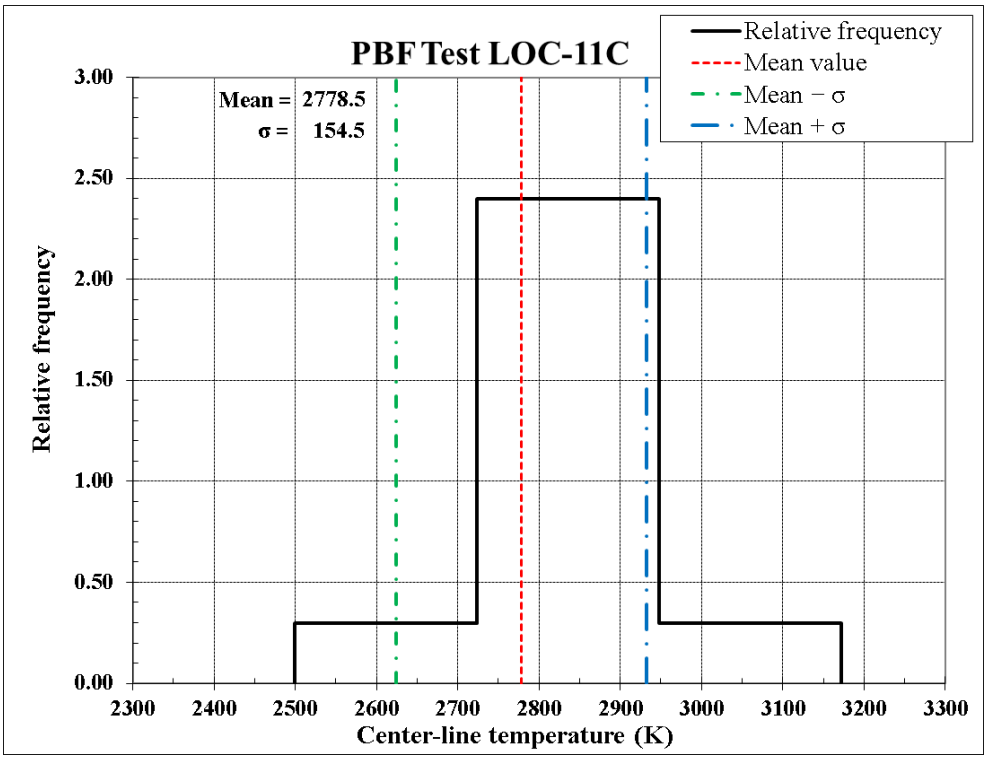



*Figure 20: Centerline temperature at t=10,000 s, SPECTRA, DS-Standard (Case 2)*

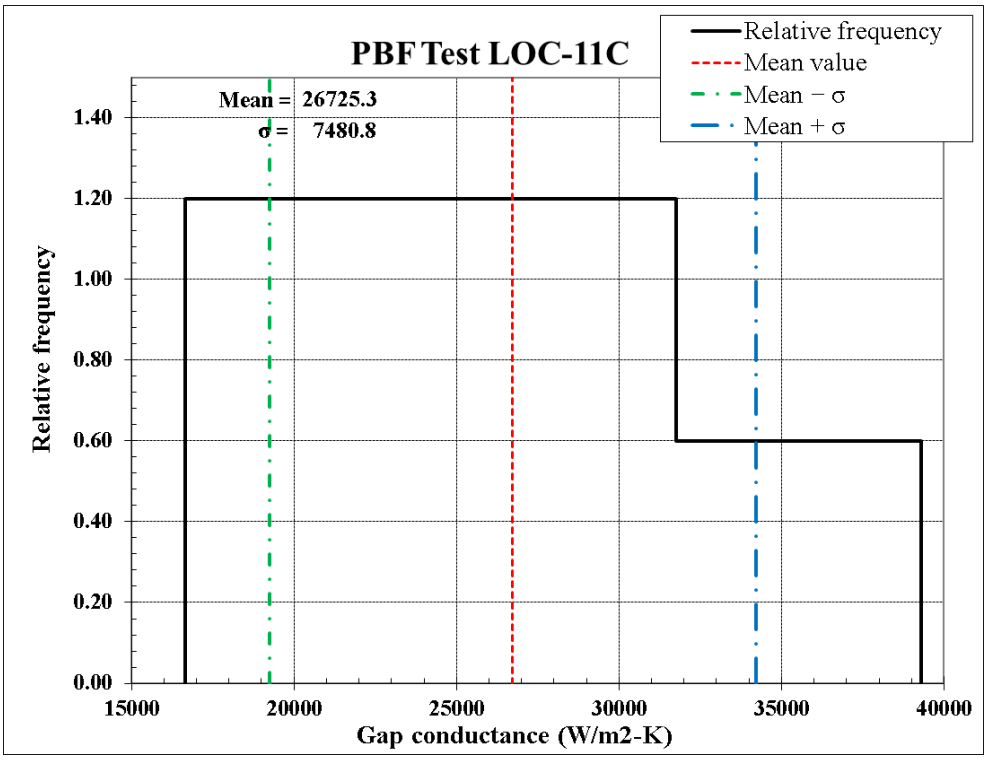



*Figure 21: Gap conductance at t=10,000 s, SPECTRA, DS-Standard (Case 2)*

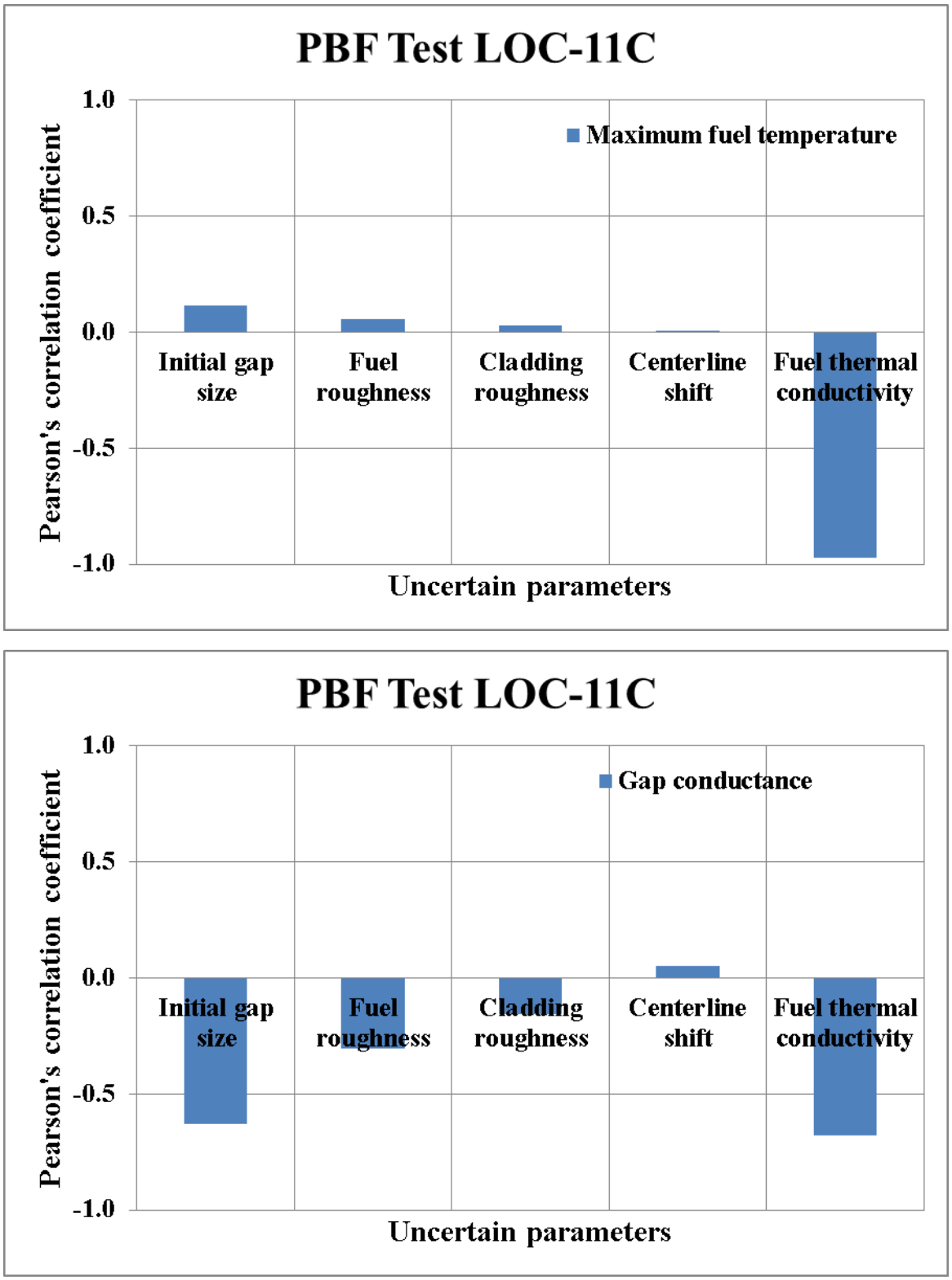



*Figure 22: Pearson's correlation coefficients, SPECTRA, DS-Standard (Case 2)*

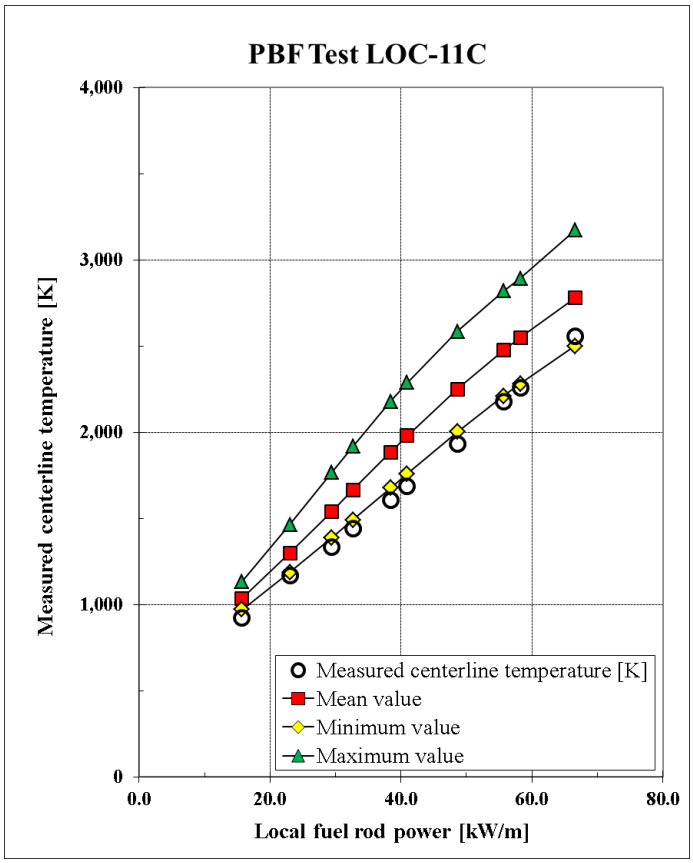



*Figure 23: Centerline temperatures, SPECTRA, DS-Standard (Case 2)*

Figure 22 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

Table 5 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 5: Main parameters, SPECTRA, Cases 1 and 2*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2781 | 150 | 28.5 | 10.0 |
| Case 1-99-2 | 662 | 2773 | 142 | 27.2 | 9.7 |
| Case 1-95 | 95 | 2774 | 149 | 28.6 | 10.6 |
| Case 2 | 10 | 2779 | 155 | 26.7 | 7.5 |

### 4.2.3 DS Hadamard Methodology

The SUE input data file for the DS-Hadamard methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, SPECTRA
* ======================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      4    *    DS-HADAMARD
*
*
105000   'GAP-PBF-LOC-11C.SPE'                    *  BASE INPUT FILE
115000   'UNPAR'                                  *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'C:/SPECTRA.361/Z-EXE/SPECTRA-3-61.EXE' *  PROGRAM TO RUN
130000    4                                       *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   1          2
*
305001   SC-100-Tcel-0001  *  Cell  1, centerline
305002   SC-100-Tcel-0010  *  Cell 10, clad surface
305003   SC-100-hGap-0000  *  Gap conductance
*
*
* ========================================================================
*  END OF INPUT FILE
* ========================================================================
*
```

The SPECTRA input files (GAP-PBF-LOC-11C.SPE, UNPAR) are the same as described in the previous section.

The results obtained for the DS-H methodology, referred to here as Case 3, are shown in Figure 24, Figure 25, Figure 26, and Figure 27. Figure 24 and Figure 25 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: “relative frequency” versus “parameter range”).

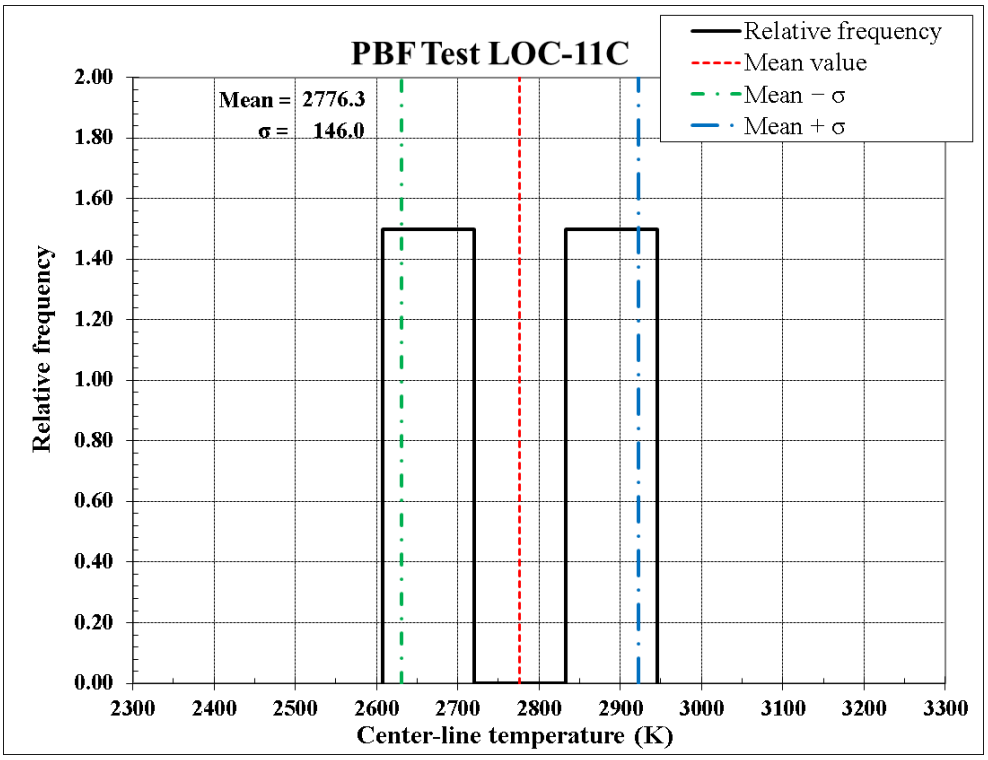



*Figure 24: Centerline temperature at t=10,000 s, SPECTRA, DS-H (Case 3)*

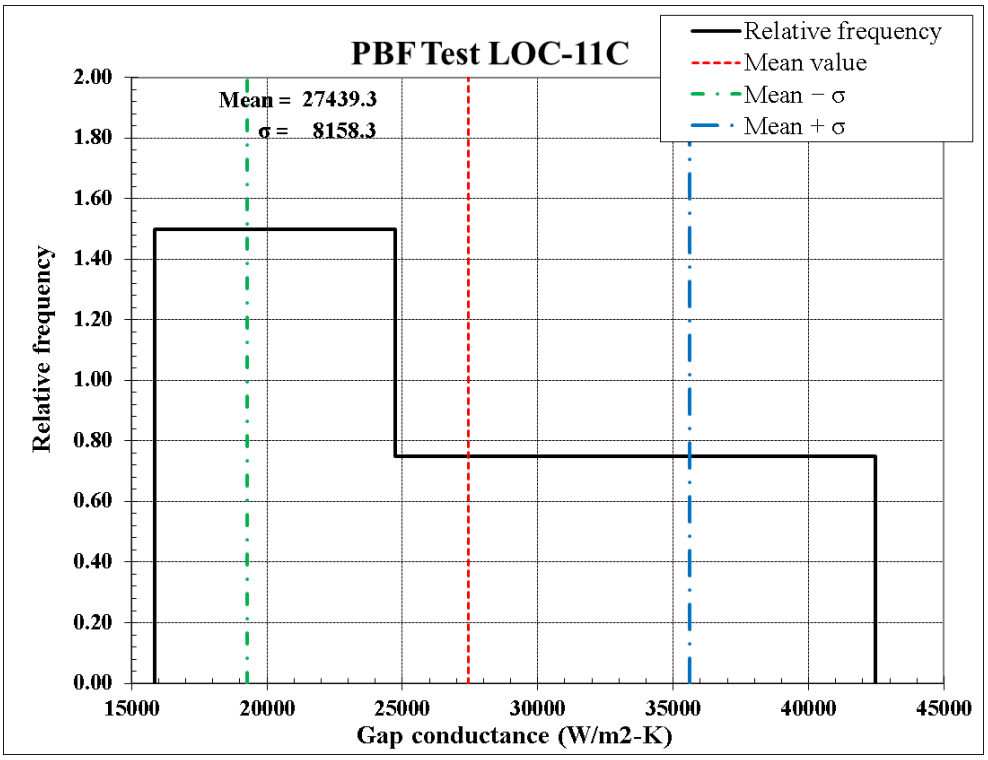



*Figure 25: Gap conductance at t=10,000 s, SPECTRA, DS-H (Case 3)*

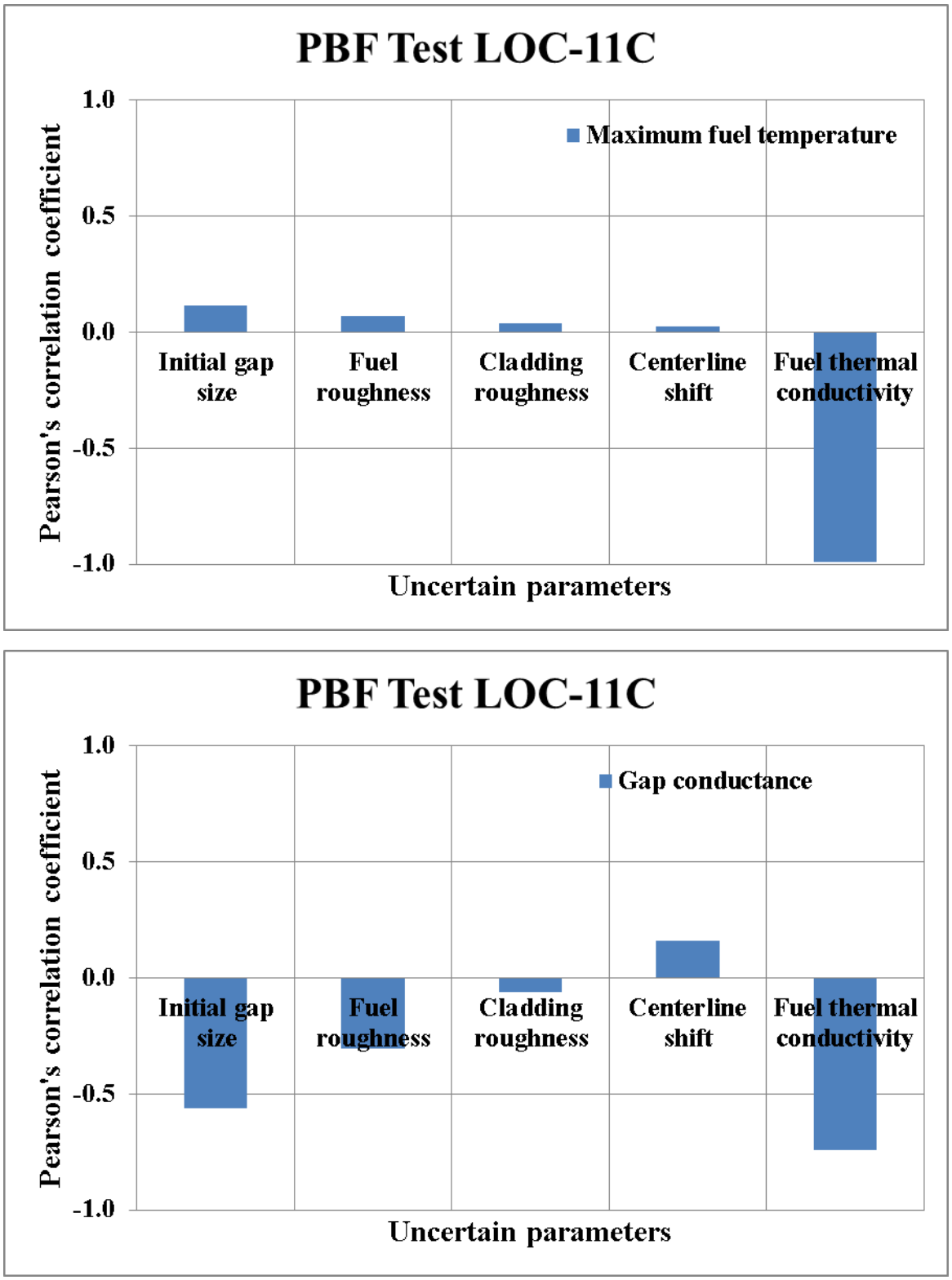



*Figure 26: Pearson's correlation coefficients, SPECTRA, DS-H (Case 3)*

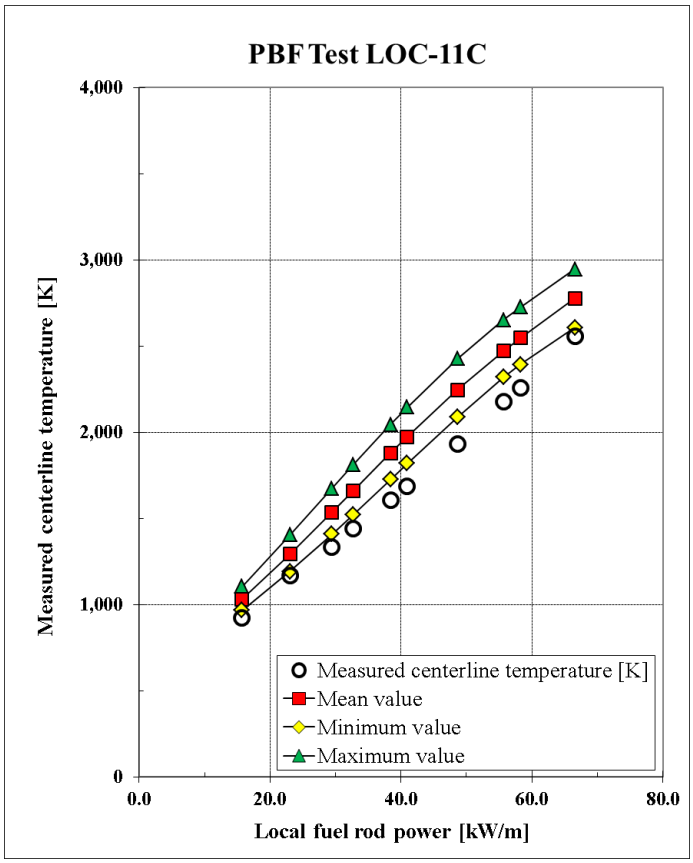



*Figure 27: Centerline temperatures, SPECTRA, DS-H (Case 3)*

Figure 26 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

Table 6 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 6: Main parameters, SPECTRA, Cases 1, 2, and 3*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2781 | 150 | 28.5 | 10.0 |
| Case 1-99-2 | 662 | 2773 | 142 | 27.2 | 9.7 |
| Case 1-95 | 95 | 2774 | 149 | 28.6 | 10.6 |
| Case 2 | 10 | 2779 | 155 | 26.7 | 7.5 |
| Case 3 | 8 | 2776 | 146 | 27.4 | 8.2 |

### 4.2.4 DS Simplex Methodology

The SUE input data file for the DS-Simplex methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, SPECTRA
* ======================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      4    *    4=DS-SIMPLEX
*
*
105000   'GAP-PBF-LOC-11C.SPE'                    *  BASE INPUT FILE
115000   'UNPAR'                                  *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'C:/SPECTRA.361/Z-EXE/SPECTRA-3-61.EXE' *  PROGRAM TO RUN
130000    4                                       *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF  IUPERR
200000     1       0       2
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   1          2
*
305001   SC-100-Tcel-0001  *  Cell  1, centerline
305002   SC-100-Tcel-0010  *  Cell 10, clad surface
305003   SC-100-hGap-0000  *  Gap conductance
*
*
* ========================================================================
*  END OF INPUT FILE
* ========================================================================
*
```

The SPECTRA input files (GAP-PBF-LOC-11C.SPE, UNPAR) are the same as described in the previous section.

In the present case, the input parameter IUPERR (see section 3.1.8) is set to 2 in order to reset the uncertain parameters if the value is beyond the minimum / maximum limits (XMINUP / XMAXUP). This is done for the following reason.

The DS-Simplex matrix (see section 2.4.4) for n = 5 is as follows (SUE output file):

```
 =IN=  DETERMINATION OF UNCERTAIN PARAMETERS
       DETERMINISTIC SAMPLING - SIMPLEX METHOD

[...]
```

```
DS-SIMPLEX MATRIX

 \ RUN:
  \       1       2       3       4       5       6
PAR\ ------ ------ ------ ------ ------ ------
  1   1.732  0.000  0.000  0.000  0.000 -1.732
  2  -1.000  2.000  0.000  0.000  0.000 -1.000
  3  -0.707 -0.707  2.121  0.000  0.000 -0.707
  4  -0.548 -0.548 -0.548  2.191  0.000 -0.548
  5  -0.447 -0.447 -0.447 -0.447  2.236 -0.447
```

The value of parameter 4 (centerline shift) in the run number four is equal to $\mu + 2.191\ \sigma$, which is 1.097 (SUE output file for IUPERR=1):

```
     VALUES OF UNCERTAIN PARAMETERS (UP) AND FUNCTIONS (FN) IF PRESENT

         UP/FN NUMBER
     RUN              1              2              3              4              5
     --- -------------- -------------- -------------- -------------- --------------
 UP: 001  1.1200000E-04  2.3100000E-06  1.4024050E-06  8.5070497E-01  9.5527864E-01
 UP: 002  1.0000000E-04  5.2800000E-06  1.4024050E-06  8.5070497E-01  9.5527864E-01
 UP: 003  1.0000000E-04  3.3000000E-06  2.9127851E-06  8.5070497E-01  9.5527864E-01
 UP: 004  1.0000000E-04  3.3000000E-06  1.7800000E-06  1.0971801E+00  9.5527864E-01
 UP: 005  1.0000000E-04  3.3000000E-06  1.7800000E-06  9.0000000E-01  1.2236068E+00
 UP: 006  8.8000001E-05  2.3100000E-06  1.4024050E-06  8.5070497E-01  9.5527864E-01
 UP: 000  1.0000000E-04  3.3000000E-06  1.7800000E-06  9.0000000E-01  1.0000000E+00
```

Such value (centerline shift > 1.0) will not be accepted by SPECTRA and the run would fail. The option IUPERR=2 resets the value to the maximum, which is defined in the input as 0.9×1.1111 and is equal to 0.99999 ≤ 1.0 (SUE output file for IUPERR=1):

```
     VALUES OF UNCERTAIN PARAMETERS (UP) AND FUNCTIONS (FN) IF PRESENT

         UP/FN NUMBER
     RUN              1              2              3              4              5
     --- -------------- -------------- -------------- -------------- --------------
 UP: 001  1.1200000E-04  2.3100000E-06  1.4024050E-06  8.5070497E-01  9.5527864E-01
 UP: 002  1.0000000E-04  5.2800000E-06  1.4024050E-06  8.5070497E-01  9.5527864E-01
 UP: 003  1.0000000E-04  3.3000000E-06  2.9127851E-06  8.5070497E-01  9.5527864E-01
 UP: 004  1.0000000E-04  3.3000000E-06  1.7800000E-06  9.9999000E-01  9.5527864E-01
 UP: 005  1.0000000E-04  3.3000000E-06  1.7800000E-06  9.0000000E-01  1.2236068E+00
 UP: 006  8.8000001E-05  2.3100000E-06  1.4024050E-06  8.5070497E-01  9.5527864E-01
 UP: 000  1.0000000E-04  3.3000000E-06  1.7800000E-06  9.0000000E-01  1.0000000E+00
```

Note that in the case of RELAP5 calculations (section 4.3.4) this was not needed because RELAP5 automatically sets the centerline shift to 1.0 if the value is outside the valid range. In both cases the necessary correction leads to violation of the methodology property that "for each uncertain parameter the value averaged over all runs is equal to the mean value" (section 2.4.4). A possible solution to this problem would be to reduce the value of $\sigma$. However, for the sake of consistency with other inputs, this has not been done.

Correctness of the DS Simplex matrix obtained for this case by SUE was verified by independent calculations [27]. The results obtained for the DS-Simplex methodology, referred to here as Case 4, are shown in Figure 28, Figure 29, Figure 30, and Figure 31. Figure 28 and Figure 29 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range").

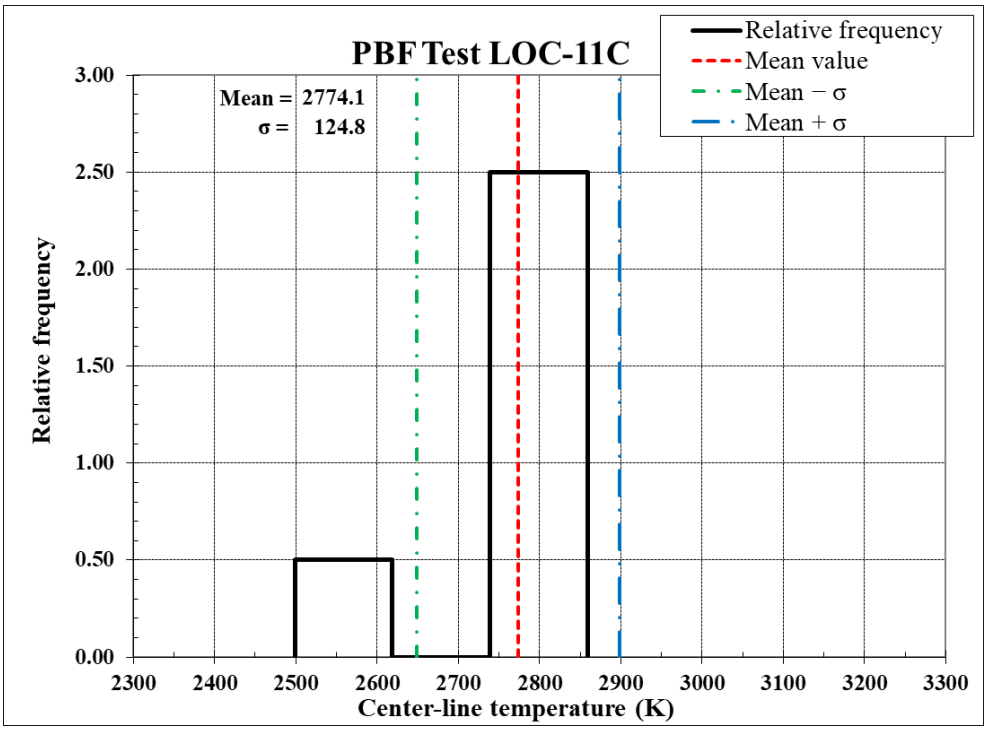



*Figure 28: Centerline temperature at t=10,000 s, SPECTRA, DS-Simplex (Case 4)*

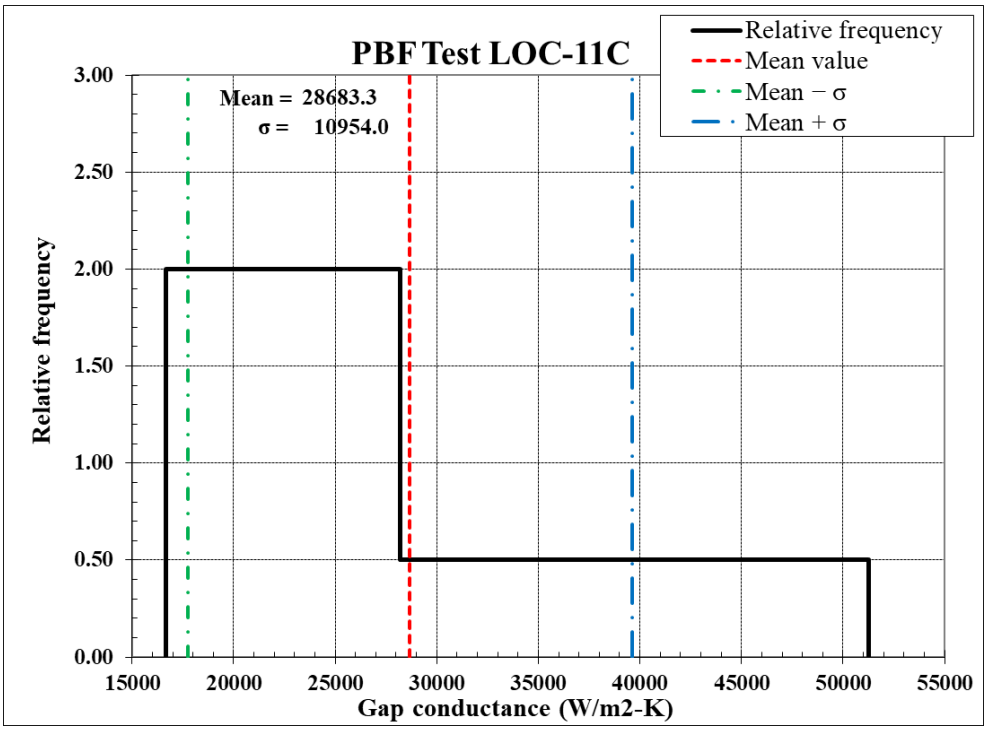



*Figure 29: Gap conductance at t=10,000 s, SPECTRA, DS-Simplex (Case 4)*

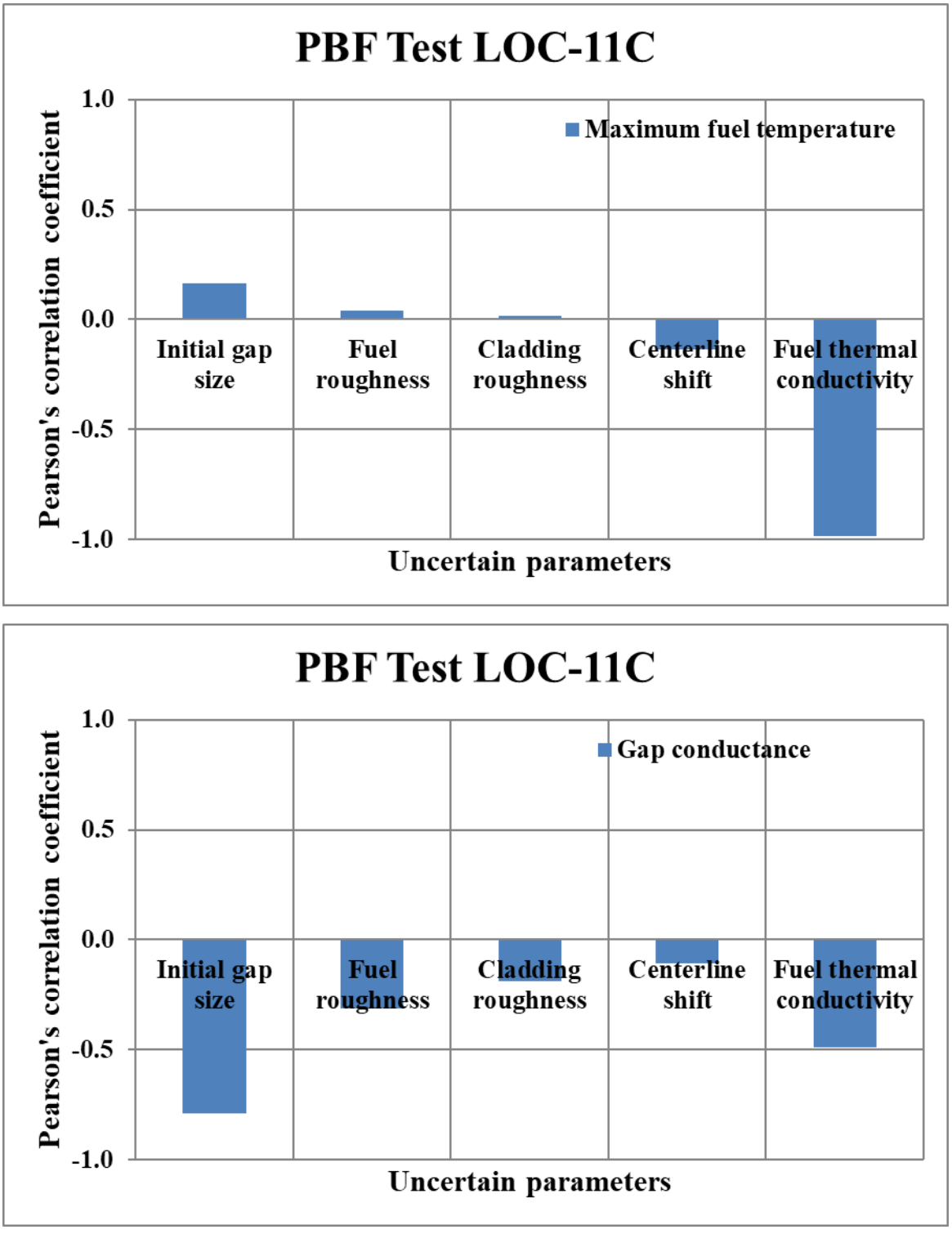



*Figure 30: Pearson's correlation coefficients, SPECTRA, DS-Simplex (Case 4)*

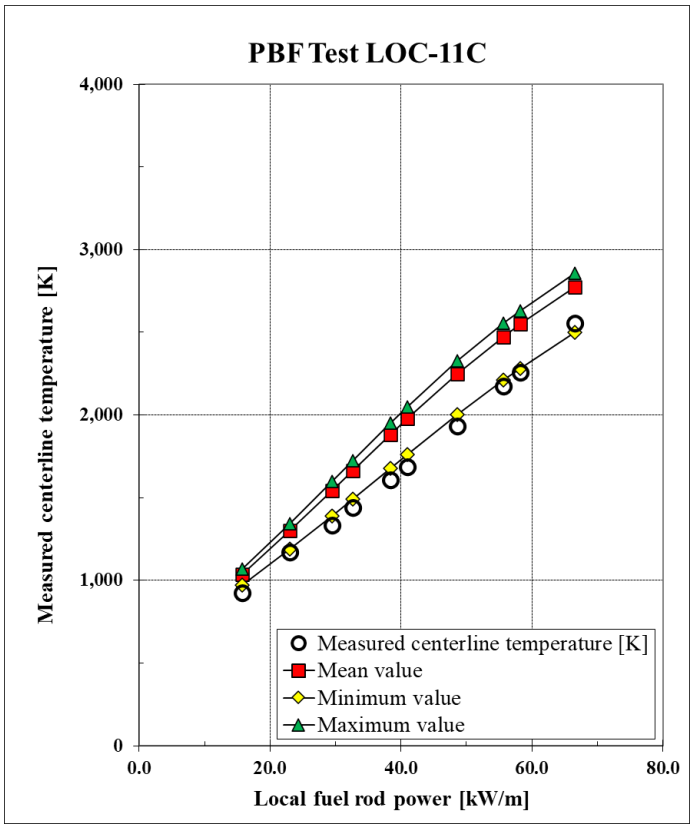



*Figure 31: Centerline temperatures, SPECTRA, DS-Simplex (Case 4)*

Figure 30 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

Table 7 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 7: Main parameters, SPECTRA, Cases 1, 2, 3, and 4*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2781 | 150 | 28.5 | 10.0 |
| Case 1-99-2 | 662 | 2773 | 142 | 27.2 | 9.7 |
| Case 1-95 | 95 | 2774 | 149 | 28.6 | 10.6 |
| Case 2 | 10 | 2779 | 155 | 26.7 | 7.5 |
| Case 3 | 8 | 2776 | 146 | 27.4 | 8.2 |
| Case 4 | 6 | 2774 | 125 | 28.7 | 10.9 |

### 4.2.5 RS versus DS Methodologies

Comparison of the results obtained with the Deterministic Sampling (DS) and the Random Sampling (RS) methodologies is shown in Table 8 and Table 9. It is seen that both methodology types give very similar results. The DS methodologies allow to significantly reduce the number of runs in the case when the number of uncertain parameters is small. In the present case the DS methodologies required 6 - 10 runs, while the RS methodology requires hundreds of calculations.

*Table 8: Center-line temperatures, RS versus DS methodologies*

| **Methodology Type** | **Center-line T (K)** | |
|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| Random Sampling | 2773 - 2781 | 142 - 150 |
| Deterministic Sampling | 2774 - 2779 | 125 - 155 |

*Table 9: Gap conductance, RS versus DS methodologies*

| **Methodology Type** | **Center-line T (K)** | |
|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| Random Sampling | 27.2 - 28.6 | 9.7 - 10.6 |
| Deterministic Sampling | 26.7 - 28.7 | 7.5 - 10.9 |

This is also seen in Figure 6 and Figure 7. While the minimum and maximum values show much wider spread in the Case 1-99-1, the values of $\mu \pm \sigma$ are practically the same in both Figure 6 and Figure 7.

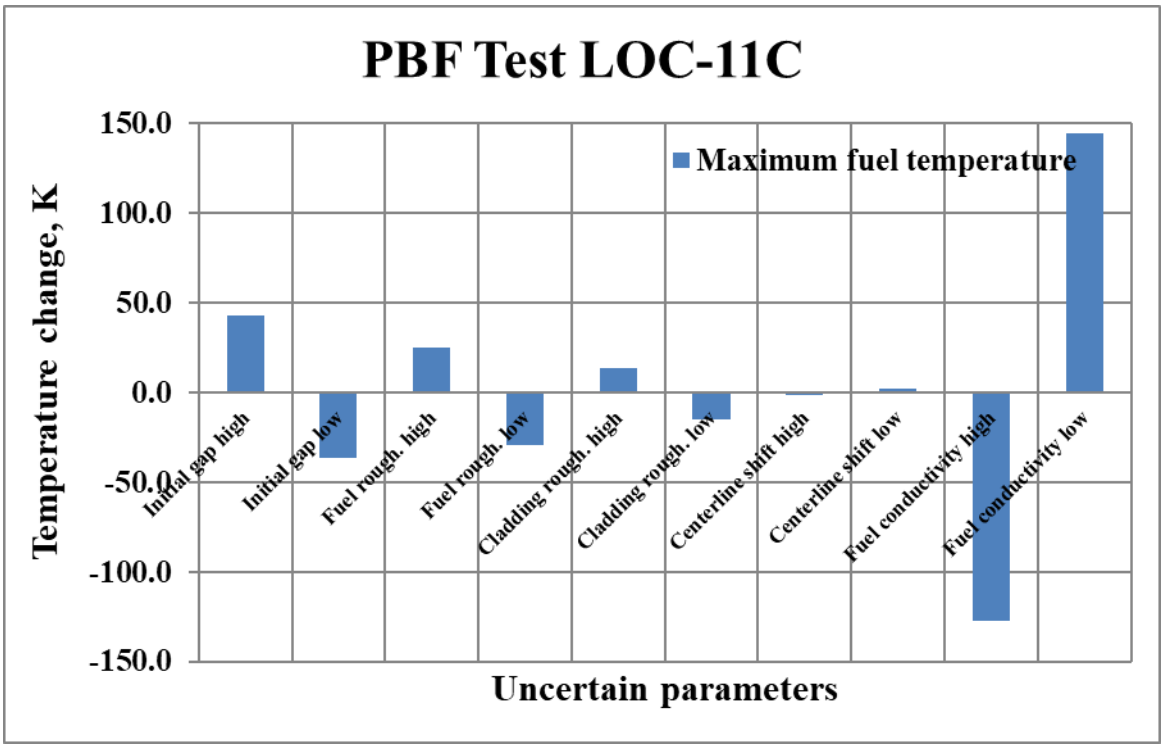
### 4.2.6 EHSF Methodology

The SUE input data file for the EHSF methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, SPECTRA
* ======================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      5    *    EHSF
100004      1    *    HOT SPOT DEFINITION
*
*
105000   'GAP-PBF-LOC-11C.SPE'                  *  BASE INPUT FILE
115000   'UNPAR'                                *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'C:/SPECTRA/Z-EXE/SPECTRA.EXE'         *  PROGRAM TO RUN
130000    4                                     *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.9    1.1    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   1          2
*
305001   SC-100-Tcel-0001  *  Cell  1, centerline
305002   SC-100-Tcel-0010  *  Cell 10, clad surface
305003   SC-100-hGap-0000  *  Gap conductance
*
*
* ====================================================================
*  END OF INPUT FILE
* ====================================================================
*
```

Two versions are analyzed with the two alternative hot spot definitions:

- Test GAP-SPE-4-1: IHSDEF=1, $F_y = 1 + \sqrt{\sum_{j=1}^{N} (f_{j,y} - 1)^2}$
- Test GAP-SPE-4-2: IHSDEF=2, $F_y = \prod_{j=1}^{N} f_{j,y}$



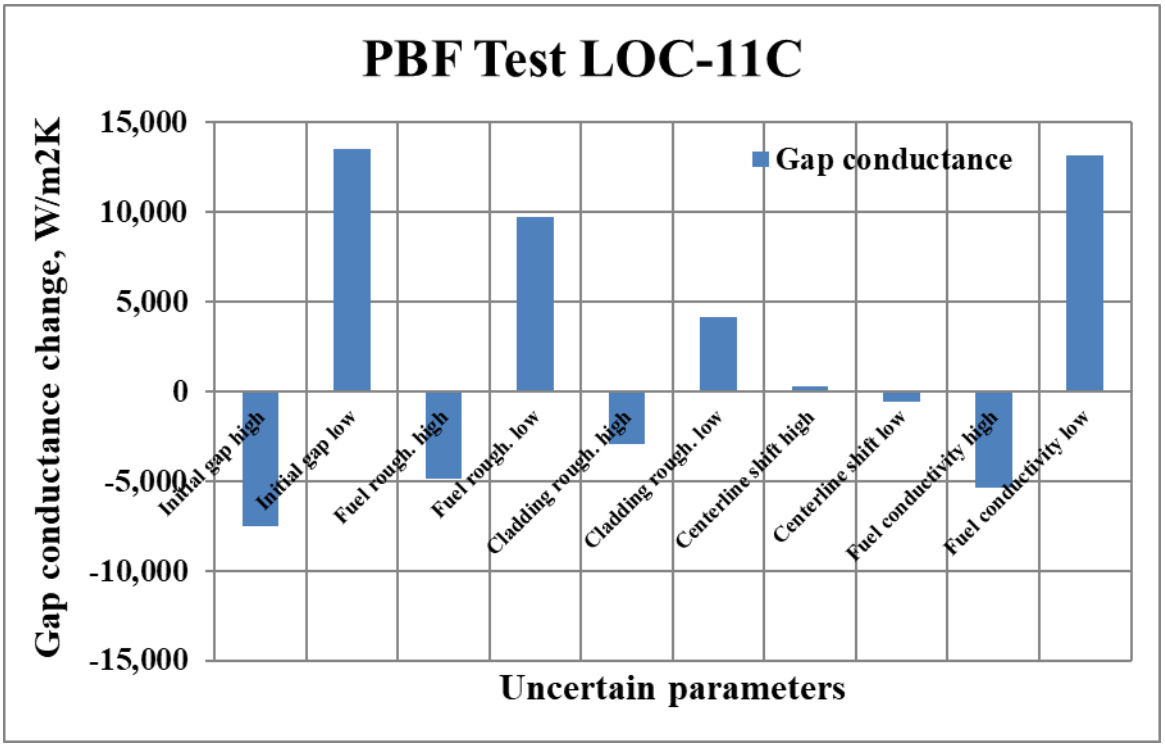




*Figure 32: Effect of u.p. on fuel T and gap cond., SPECTRA, EHSF (Case 5)*

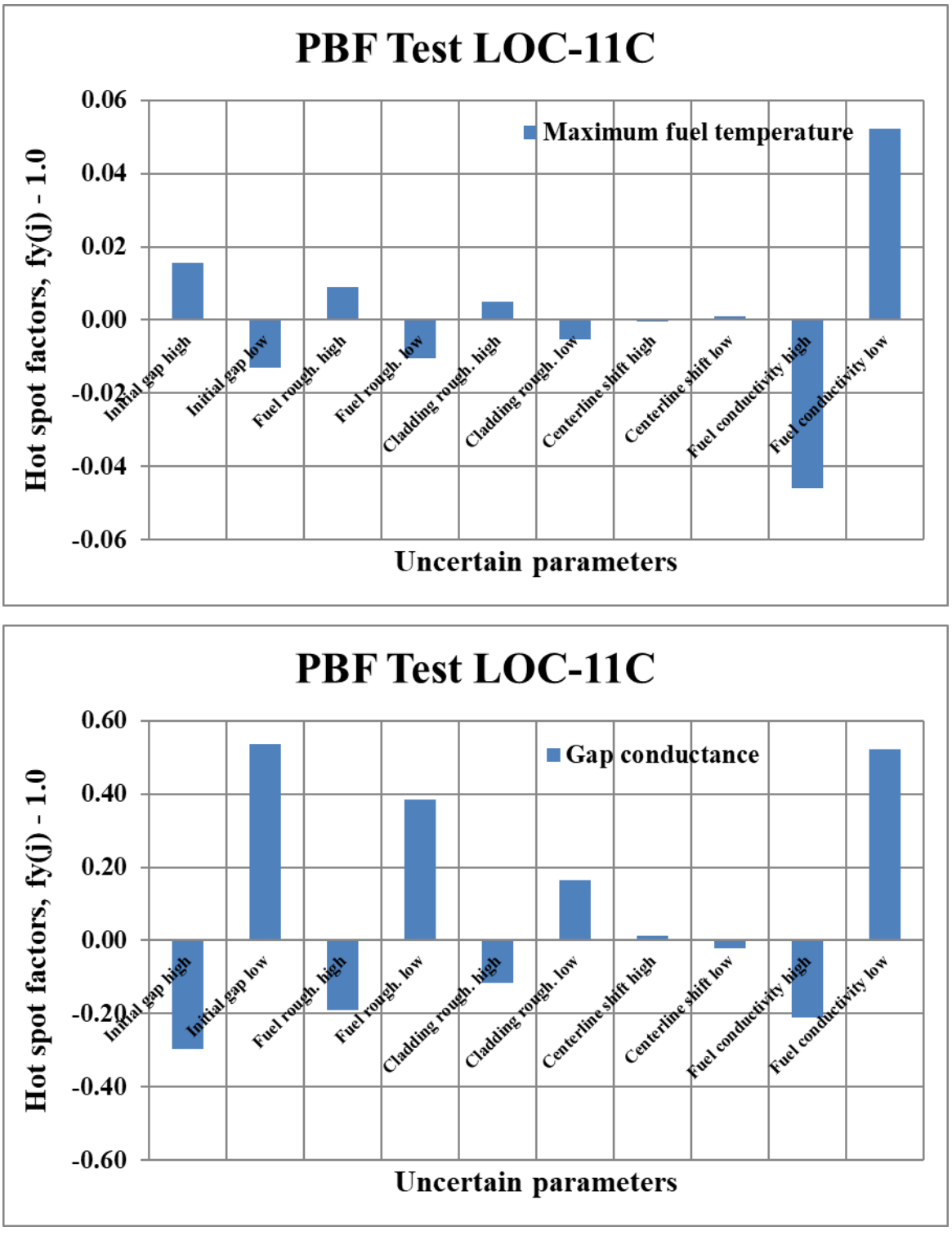



*Figure 33: Hot spot factors, fy(j), SPECTRA, EHSF (Case 5)*

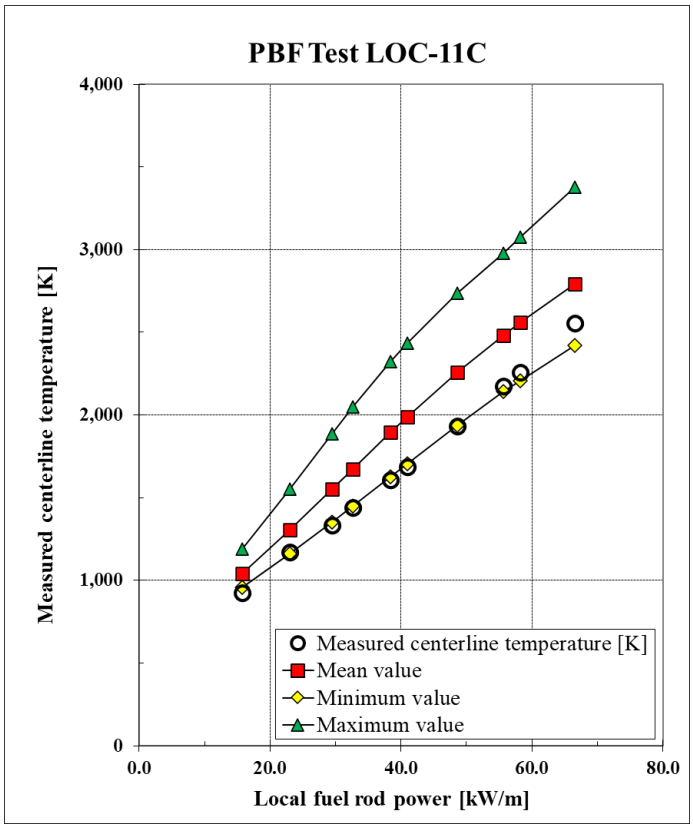



*Figure 34: Centerline temperatures, SPECTRA, EHSF (Case 5)*

The results obtained for the EHSF methodology, referred to here as Case 4, are shown in Figure 32, Figure 33, and Figure 34. Figure 32 shows the influence of each parameter on the maximum fuel temperature and the gap conductance. It is seen that the fuel conductivity has the most profound effect on the maximum temperature. The centerline shift has the smallest effect. Figure 33 shows the hot individual spot factors, $f_y(j)$, for the maximum fuel temperature and the gap conductance. The overall hot spot factors, $F_y(j)$ are equal to:

- Maximum fuel temperature
  - Test GAP-SPE-4-1: IHSDEF=1:

```
HOT SPOT FACTORS, Fy-p = 1.05550E+00
                  Fy-n = 1.04922E+00

                VALUE     VALUE * Fy-p  VALUE / Fy-n
----------- ------------  ------------  ------------
RUN (000)    2.76359E+03   2.91697E+03   2.63395E+03
```

  - Test GAP-SPE-4-2: IHSDEF=2:

```
HOT SPOT FACTORS, Fy-p = 1.08473E+00
                  Fy-n = 9.26206E-01

                VALUE     VALUE * Fy-p  VALUE * Fy-n
----------- ------------  ------------  ------------
RUN (000)    2.76359E+03   2.99775E+03   2.55965E+03
```

- Gap conductance
  - Test GAP-SPE-4-1: IHSDEF=1:

```
HOT SPOT FACTORS, Fy-p = 1.85757E+00
                  Fy-n = 1.42815E+00

                VALUE     VALUE * Fy-p  VALUE / Fy-n
----------- ------------  ------------  ------------
RUN (000)    2.52749E+04   4.69500E+04   1.76977E+04
```

  - Test GAP-SPE-4-2: IHSDEF=2:

```
HOT SPOT FACTORS, Fy-p = 3.81875E+00
                  Fy-n = 3.87413E-01

                VALUE     VALUE * Fy-p  VALUE * Fy-n
----------- ------------  ------------  ------------
RUN (000)    2.52749E+04   9.65185E+04   9.79182E+03
```

### 4.2.7 User-Defined Matrix

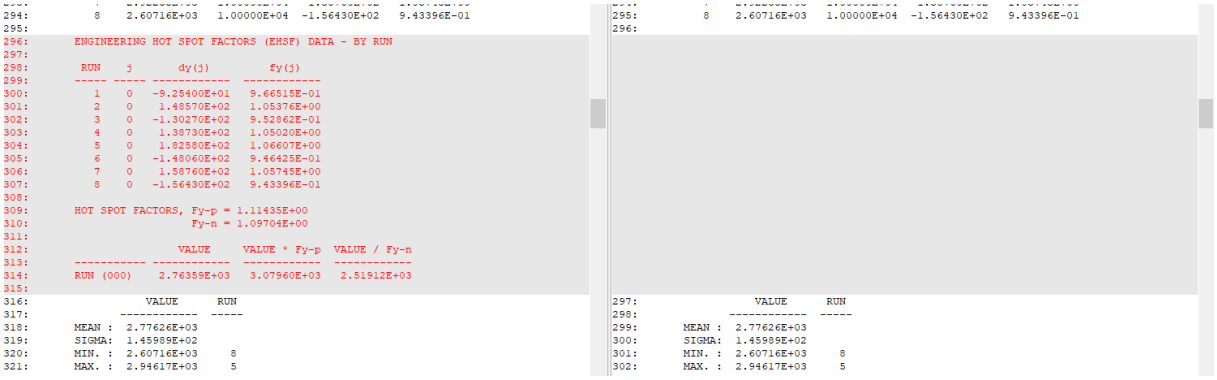
For this test the values of uncertain parameters (defined in the file PAR-VAL.CSV) were specified the same as for the case DS-H, described in section 4.2.3. It was checked that the results of the current test, referred to here as Case 5, were the same as the results of the DS-H, (Case 3) by comparing the SUE output files. The only difference in the output is related to the part of input diagnostics, where the methodology is printed. The listing of differences is provided below.

```
135: =IN=  TOTAL NO. OF RUNS  : NRUNST = 8
136:
137: =IN=  DETERMINATION OF UNCERTAIN PARAMETERS
138:       DETERMINISTIC SAMPLING - USER-DEFINED
139:
140:       THE VALUES MUST BE PROVIDED IN THE FILE:
141:       PAR-VAL.CSV
142:
143:       THE FILE HAS THE FOLLOWING STRUCTURE:
144:
145:       M,N
146:       header0,   header1 ,   header2 , ...,   headerN
147:             1, value(1,1), value(1,2), ..., value(1,N)
148:             2, value(2,1), value(2,2), ..., value(2,N)
149:             ...
150:             M, value(M,1), value(M,2), ..., value(1,N)
151:
152:       HERE: M = NRUNST, NUMBER OF RUNS
153:             N = NUNPAR, NUMBER OF UNCERTAIN PARAMETERS
154:
155:=============================================================================
```

```
135: =IN=  TOTAL NO. OF RUNS  : NRUNST = 8
136:
137: =IN=  DETERMINATION OF UNCERTAIN PARAMETERS
138:       DETERMINISTIC SAMPLING - HADAMARD MATRIX
139:
140:FULL HADAMARD MATRIX
141:
142: \  J:
143:  \   1  2  3  4  5  6  7  8
144: I \ -- -- -- -- -- -- -- --
145:  1   1  1  1  1  1  1  1  1
146:  2   1 -1  1 -1  1 -1  1 -1
147:  3   1  1 -1 -1  1  1 -1 -1
148:  4   1 -1 -1  1  1 -1 -1  1
149:  5   1  1  1  1 -1 -1 -1 -1
150:  6   1 -1  1 -1 -1  1 -1  1
151:  7   1  1 -1 -1 -1 -1  1  1
152:  8   1 -1 -1  1 -1  1  1 -1
153:
154:REDUCED HADAMARD MATRIX
155:
156: \ RUN:
157:  \   1  2  3  4  5  6  7  8
158:PAR\ -- -- -- -- -- -- -- --
159:  1   1 -1  1 -1  1 -1  1 -1
160:  2   1  1 -1 -1  1  1 -1 -1
161:  3   1 -1 -1  1  1 -1 -1  1
162:  4   1  1  1  1 -1 -1 -1 -1
163:  5   1 -1  1 -1 -1  1 -1  1
164:
165:TRANSPOSED REDUCED HADAMARD MATRIX
166:
167: \ PAR:
168:  \   1  2  3  4  5
169:RUN\ -- -- -- -- --
170:  1   1  1  1  1  1
171:  2  -1  1 -1  1 -1
172:  3   1 -1 -1  1  1
173:  4  -1 -1  1  1 -1
174:  5   1  1  1 -1 -1
175:  6  -1  1 -1 -1  1
176:  7   1 -1 -1 -1 -1
177:  8  -1 -1  1 -1  1
178:
179:=============================================================================
```

[...]

Additional blocks of the hot spot data, e.g.:



```
294:         8    2.60716E+03   1.00000E+04  -1.56430E+02   9.43396E-01
295:
296:       ENGINEERING HOT SPOT FACTORS (EHSF) DATA - BY RUN
297:
298:        RUN    j       dy(j)          fy(j)
299:       ----- ----- ------------  ------------
300:          1     0   -9.25400E+01   9.66515E-01
301:          2     0    1.48570E+02   1.05376E+00
302:          3     0   -1.30270E+02   9.52862E-01
303:          4     0    1.38730E+02   1.05020E+00
304:          5     0    1.82580E+02   1.06607E+00
305:          6     0   -1.48060E+02   9.46425E-01
306:          7     0    1.58760E+02   1.05745E+00
307:          8     0   -1.56430E+02   9.43396E-01
308:
309:       HOT SPOT FACTORS, Fy-p = 1.11435E+00
310:                         Fy-n = 1.09704E+00
311:
312:                         VALUE     VALUE * Fy-p  VALUE / Fy-n
313:       ---------- ------------  ------------  ------------
314:       RUN (000)    2.76359E+03   3.07960E+03   2.51912E+03
315:
316:                    VALUE       RUN
317:                ------------  -----
318:       MEAN :   2.77626E+03
319:       SIGMA:   1.45989E+02
320:       MIN. :   2.60716E+03      8
321:       MAX. :   2.94617E+03      5
```

```
295:         8    2.60716E+03   1.00000E+04  -1.56430E+02   9.43396E-01
296:
297:                    VALUE       RUN
298:                ------------  -----
299:       MEAN :   2.77626E+03
300:       SIGMA:   1.45989E+02
301:       MIN. :   2.60716E+03      8
302:       MAX. :   2.94617E+03      5
```

## 4.3 PBF Test LOC-11C, RELAP5 Analysis

Calculations were performed using three methodologies:

- RS methodology - section 4.3.1
  - Case 1-99-1: α=99%, β=99%, pseudo-random series 1.
  - Case 1-99-2: α=99%, β=99%, pseudo-random series 2.
  - Case 1-95: α=95%, β=95%.
- DS-Standard methodology - section 4.3.2.
- DS-Hadamard methodology - section 4.3.3.
- DS Simplex methodology - section 4.3.4.

### 4.3.1 RS Methodology

The RS methodology is used with 2-sided tolerance limits, probability α = 99%, and confidence level, β = 99%. The SUE input deck is provided below:

```
= SUE INPUT FOR: GAP-PBF-LOC-11C, RELAP5
* ======================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      1    *    RS
*
*         RS METHODOLOGY DATA
*         ISIDED   IPROBA    ICONFB    IREPRS
100001    2        99        99        123456
*
*
105000   'GAP-PBF-LOC-11C.INP'              *  BASE INPUT FILE
115000   'GAP-PBF-LOC-11C.INP'              *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'c:\relap5-mod33jz\exe\relap5.exe' *  PROGRAM TO RUN
130000    1                                 *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   2          2
*
305001   httemp         100100101 *  Cell  1, centerline
305002   httemp         100100111 *  Cell 10, clad surface
305003   hgap             1001001 *  Gap conductance
```

The data for uncertain parameters were entered using relative values for $\sigma$, $x_{min}$, $x_{max}$, (INPOPT=1), which means the absolute values are obtained by multiplying the entered values by the mean values. It was checked that identical results are obtained when absolute values are defined in input (INPOPT=2). The input for this case is:

```
*        INPOPT  NINTDF
200000     2       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN       MAX
200001      2    0.100E-3   0.0     0.088E-3  0.112E-3  *  INITIAL GAP SIZE
200002      1    3.300E-6   9.90E-7 0.0       0.0       *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   5.34E-7 0.0       0.0       *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.09    0.0       0.999990  *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0       0.0       *  FUEL THERMAL CONDUCTIVITY
```

The values of centerline shift are difficult to estimate. It is believed that the most likely position of the fuel pellet is when it touches the cladding on one side (shift = 1.0). For the current test it was assumed that the centerline shift is 0.9 ±0.1, thus $\mu$=0.9, $\sigma$=0.1. The maximum value is set to 1.1111 relative or 0.99999 absolute (=0.9×1.1111).

The uncertain parameters were defined in the RELAP5 input file. The relevant parts of the RELAP5 model file input file (GAP-PBF-LOC-11C.INP), are presented below:

```
[...]
*
*          x(Node) [m]     Node
*
11001101   7.75000e-04       1  *  HS-100 C:  1
11001102   7.75000e-04       2  *  - Cell  :  2
11001103   7.75000e-04       3  *  - Cell  :  3
11001104   7.75000e-04       4  *  - Cell  :  4
11001105   7.75000e-04       5  *  - Cell  :  5
11001106   7.75000e-04       6  *  - Cell  :  6
*1001107   1.00000e-04       7  *  - Cell  :  7
11001107   $001              7  *  - Cell  :  7
11001108   2.03300e-04       8  *  - Cell  :  8
11001109   2.03300e-04       9  *  - Cell  :  9
11001110   2.03300e-04      10  *  - Cell  : 10

[...]

*   Gap:   Fuel rough.  Clad rough.    swell       creep        shift      axial
11001011  $002         $003         0.00000e+00  0.00000e+00  $004          1

[...]

*
*             T [K]       k [W/m/K]
20110101   1.00000e+00   $005@9.01000e+00
20110102   3.00000e+02   $005@9.01000e+00
20110103   4.00000e+02   $005@7.37000e+00
20110104   5.00000e+02   $005@6.23000e+00
20110105   6.00000e+02   $005@5.40000e+00
20110106   7.00000e+02   $005@4.78000e+00
20110107   8.00000e+02   $005@4.29000e+00
20110108   9.00000e+02   $005@3.90000e+00
20110109   1.00000e+03   $005@3.59000e+00
20110110   1.10000e+03   $005@3.34000e+00
20110111   1.20000e+03   $005@3.14000e+00
```

```
20110112   1.30000e+03   $005@2.97000e+00
20110113   1.40000e+03   $005@2.84000e+00
20110114   1.50000e+03   $005@2.74000e+00
20110115   1.60000e+03   $005@2.66000e+00
20110116   1.70000e+03   $005@2.61000e+00
20110117   1.80000e+03   $005@2.58000e+00
20110118   1.90000e+03   $005@2.57000e+00
20110119   2.00000e+03   $005@2.58000e+00
20110120   2.10000e+03   $005@2.61000e+00
20110121   2.20000e+03   $005@2.65000e+00
20110122   2.30000e+03   $005@2.72000e+00
20110123   2.40000e+03   $005@2.80000e+00
20110124   2.50000e+03   $005@2.90000e+00
20110125   2.60000e+03   $005@3.02000e+00
20110126   2.70000e+03   $005@3.15000e+00
20110127   2.80000e+03   $005@3.30000e+00
20110128   2.90000e+03   $005@3.47000e+00
20110129   3.00000e+03   $005@3.66000e+00
20110130   9.99900e+03   $005@3.66000e+00
```

The thermal conductivity data for the material 101 is defined following $005@. The sign $005 means the uncertain parameter 5. The dependent parameter type must be defined as "multiply" (IDPTYP=2). The sign @ precedes the value of the dependent parameter. During the calculations, the value of the independent parameter is sampled using its data (μ=1.0, σ=0.1) and then the value of the dependent parameter is obtained from (section 3.2.2):

$$y = \mu_y \cdot x / \mu_x$$

Suppose the sampled value of the parameter $005 is 0.9. The value of conductivity for the first point (T=300 K) is 9.01. This means that SUR will replace $005@9.01 by

$$y = 9.01 \cdot 0.9 / 1.0 = 8.109$$

When SUE is executed, it creates the RELAP5 input files:
GAP-PBF-LOC-11C-001.INP, GAP-PBF-LOC-11C-002.INP, ...
and executes the RELAP5 runs. The commands that are being executed are written to the SUE diagnostics file (section 3.3.3).

For the selected parameters, 2-sided tolerance limits, probability α = 99%, and confidence level, β = 99%, the number of runs is 662 (Table 1). Repeatable series were chosen, to be able to reproduce the results. Two cases were considered with different pseudo-random series:

- Case 1-99-1: Starting point for the pseudo-random series, IREPRS = 123456.
- Case 1-99-2: Starting point for the pseudo-random series, IREPRS = 654321.

Additionally, a run was performed for α=95%, β=95%: Case 1-95. The number of runs is 93 (Table 1).

The results obtained for the Case 1-99-1 are shown in Figure 35, Figure 36, Figure 37, and Figure 38. Figure 35 and Figure 36 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range"). The last value (3491 K - Figure 35) is the upper tolerance limit.

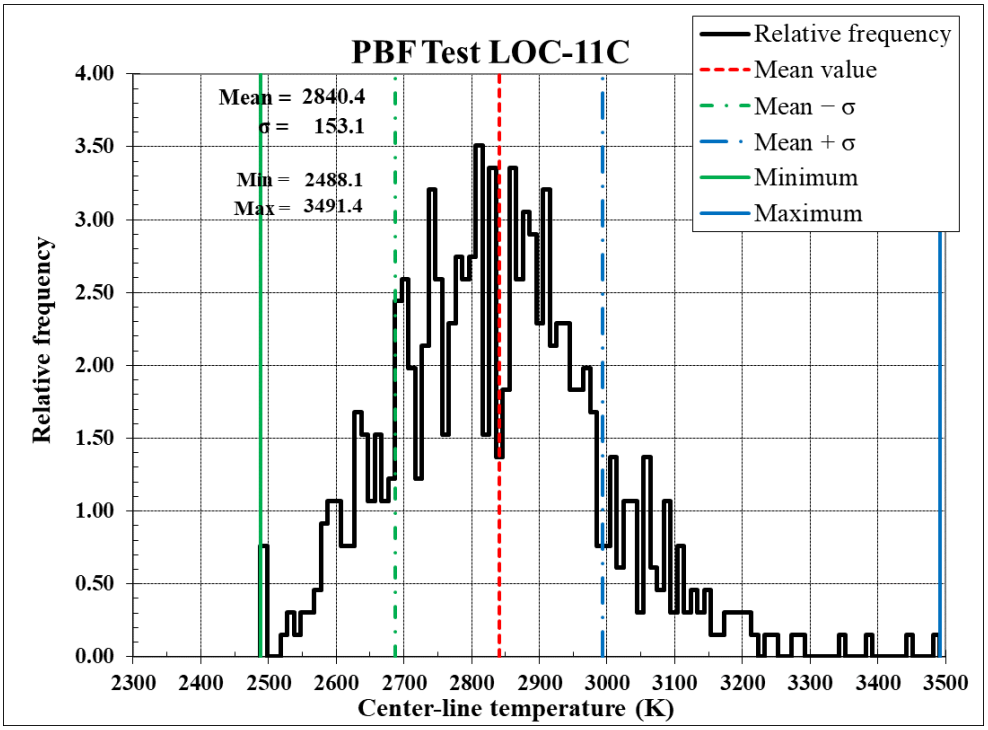



*Figure 35: Centerline temperature at t=10,000 s, RELAP5, RS (Case 1-99-1)*

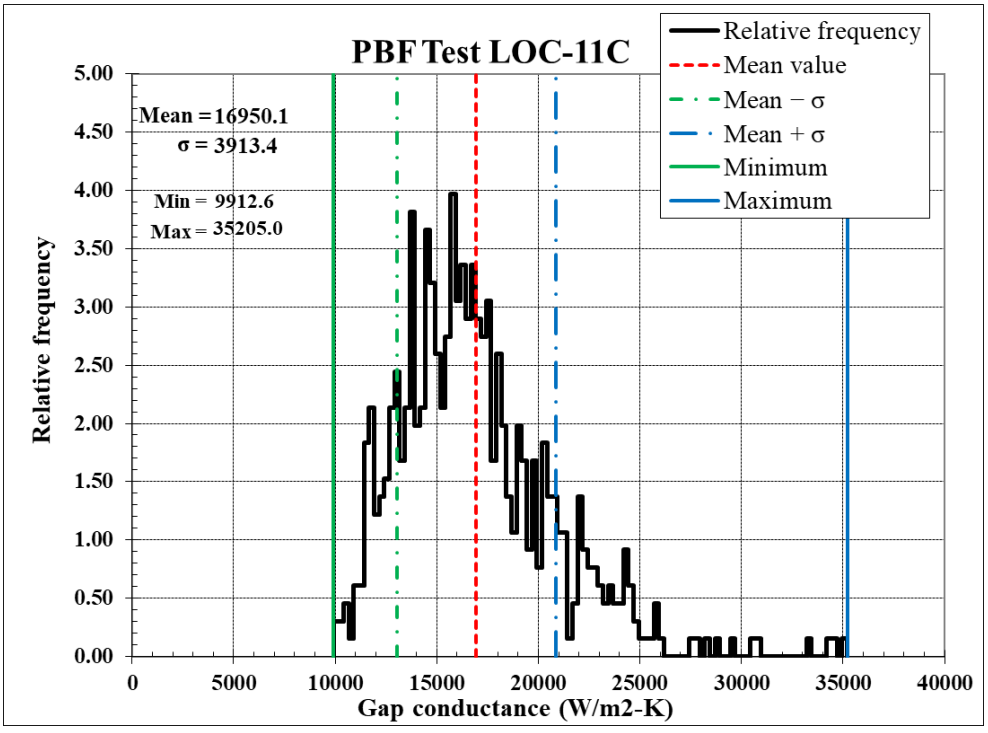



*Figure 36: Gap conductance at t=10,000 s, RELAP5, RS (Case 1-99-1)*

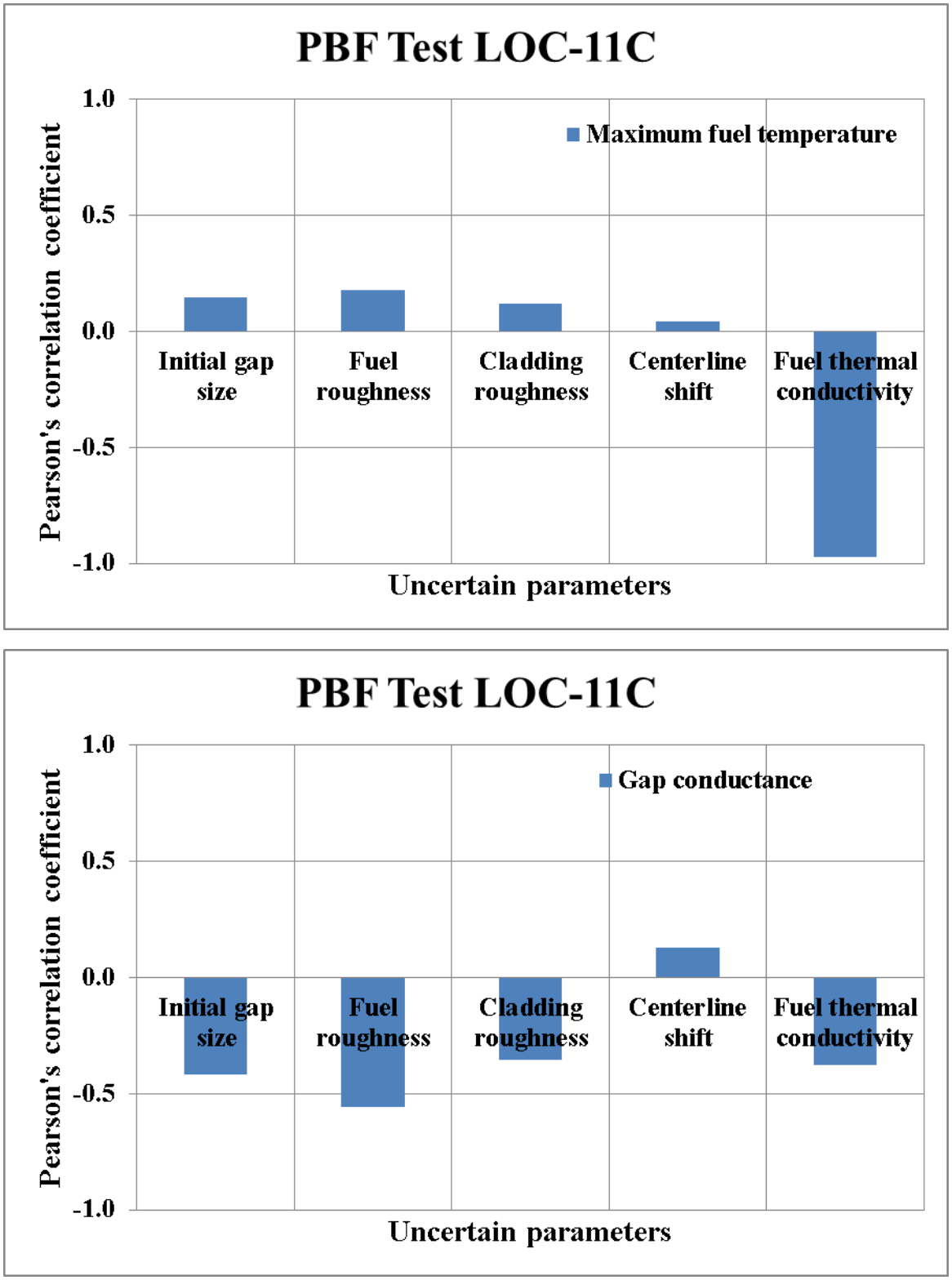



*Figure 37: Pearson's correlation coefficients, RELAP5, RS (Case 1-99-1)*

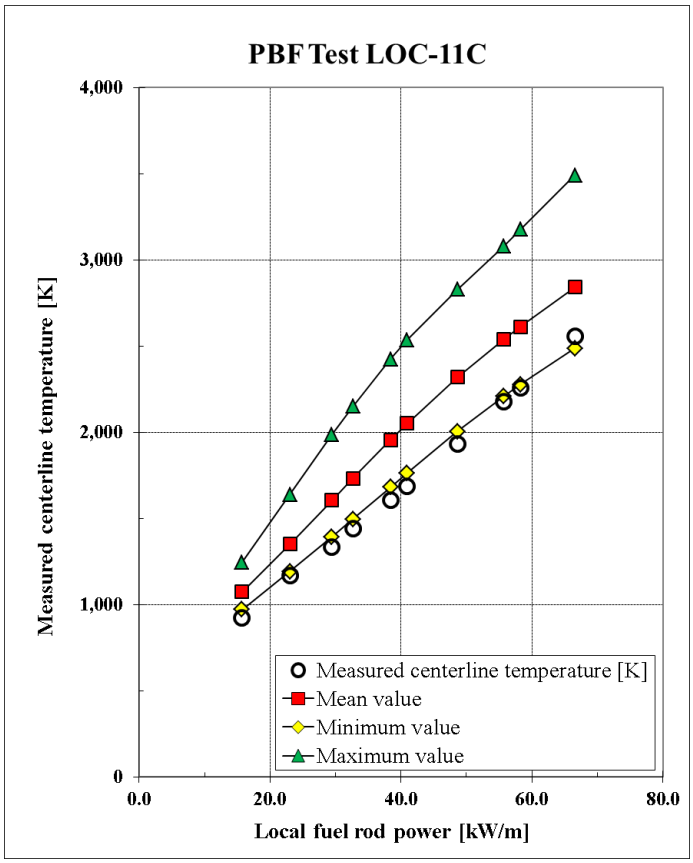



*Figure 38: Centerline temperatures, RELAP5, RS (Case 1-99-1)*

Figure 37 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

The results obtained for the Case 1-99-2 are shown in Figure 39, Figure 40, Figure 41, and Figure 42. Figure 39 and Figure 40 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range"). The last value (3457 K - Figure 39) is the upper tolerance limit.

Figure 41 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

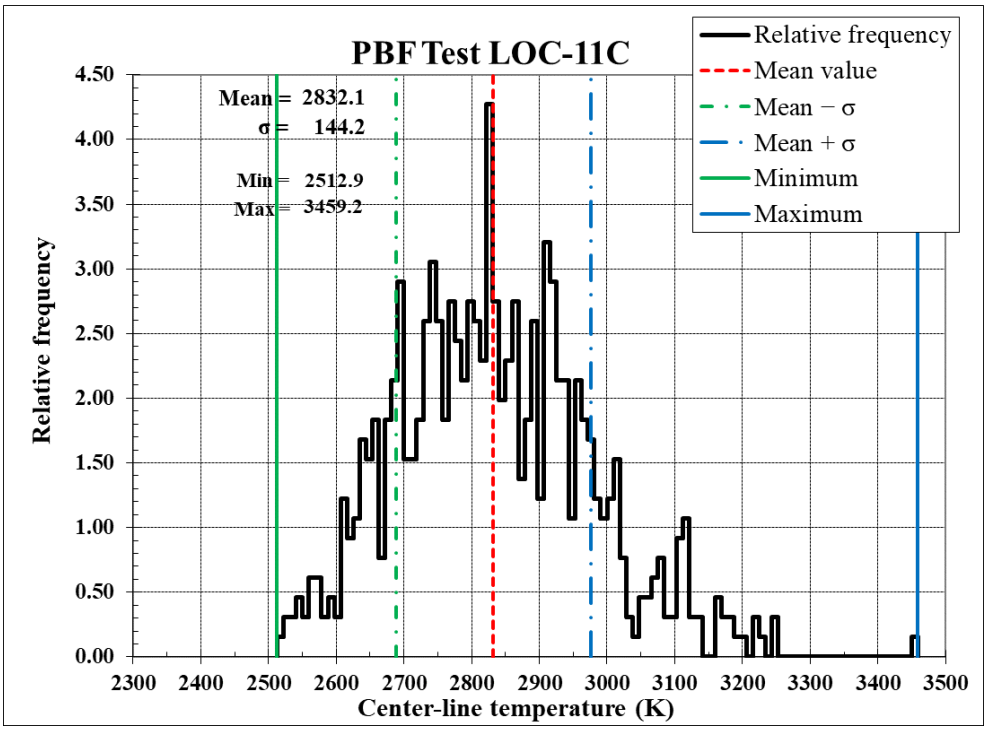



*Figure 39: Centerline temperature at t=10,000 s, RELAP5, RS (Case 1-99-2)*

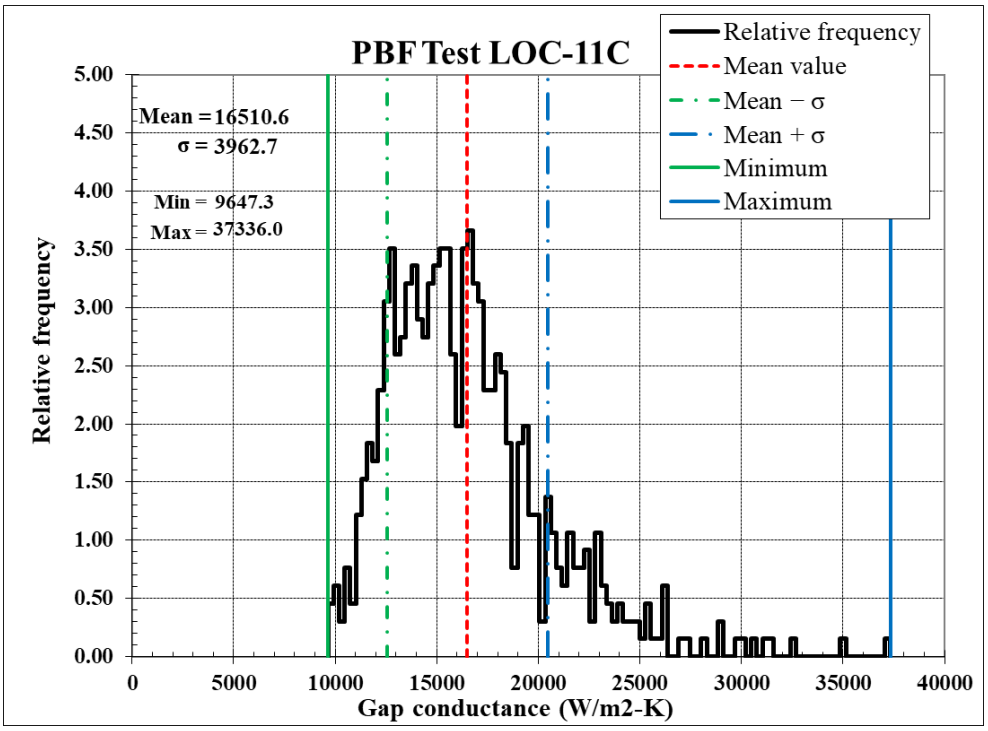



*Figure 40: Gap conductance at t=10,000 s, RELAP5, RS (Case 1-99-2)*

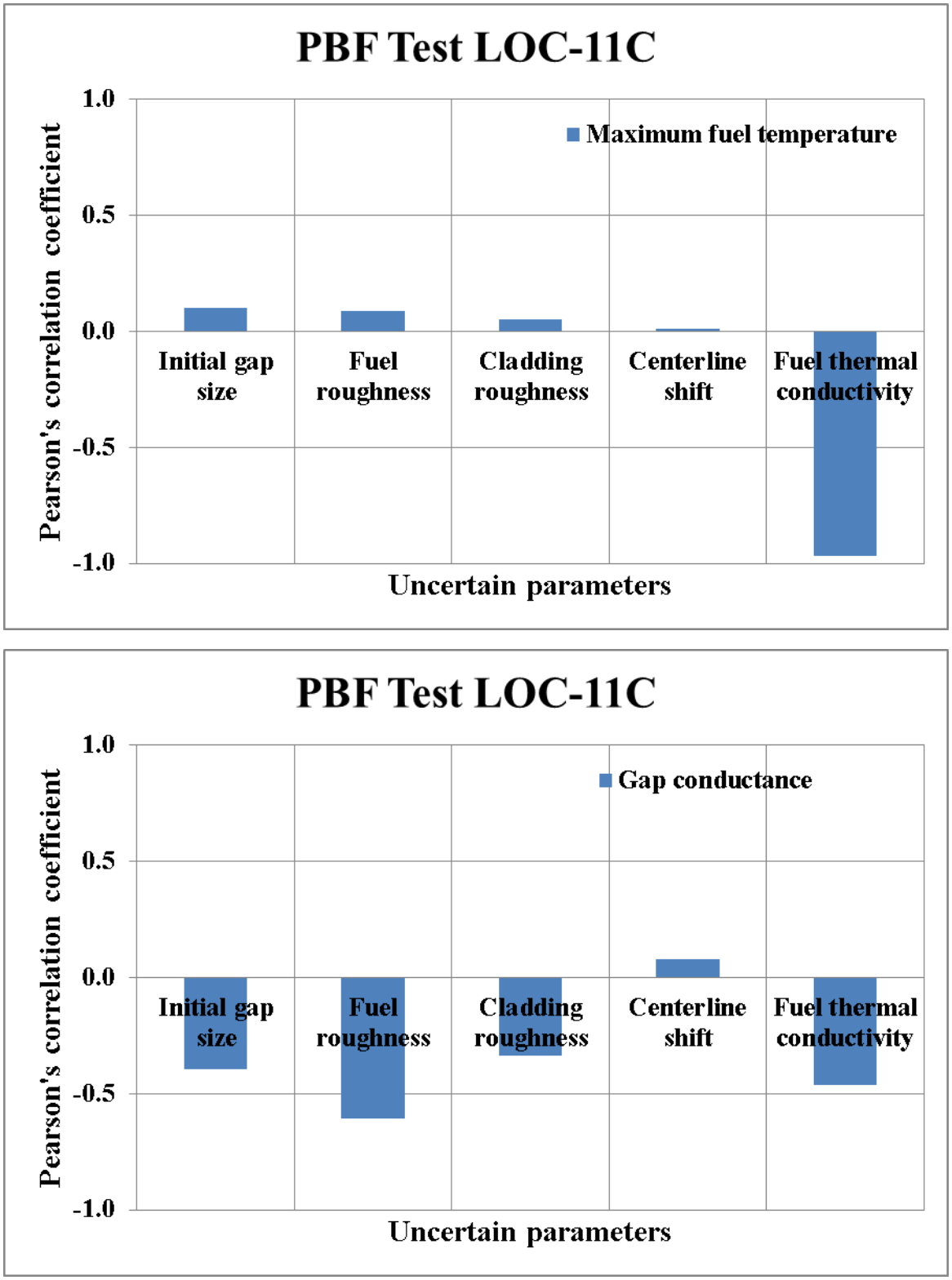



*Figure 41: Pearson's correlation coefficients, RELAP5, RS (Case 1-99-2)*

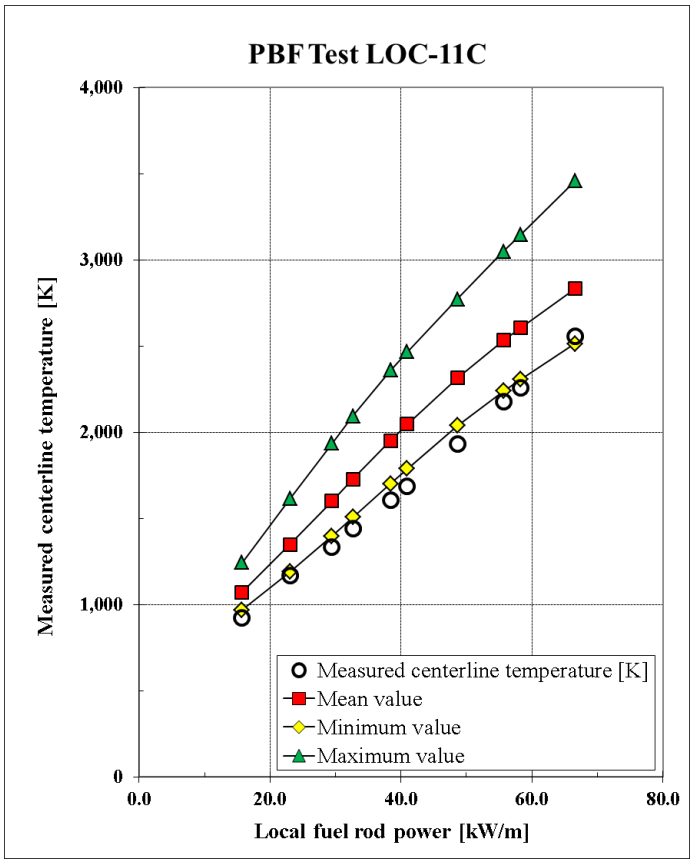



*Figure 42: Centerline temperatures, RELAP5, RS (Case 1-99-2)*

The results obtained for the Case 1-95 are shown in Figure 43, Figure 44, Figure 45, and Figure 46. Figure 43 and Figure 44 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range"). The last value (3275 K - Figure 43) is the upper tolerance limit.

Figure 45 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

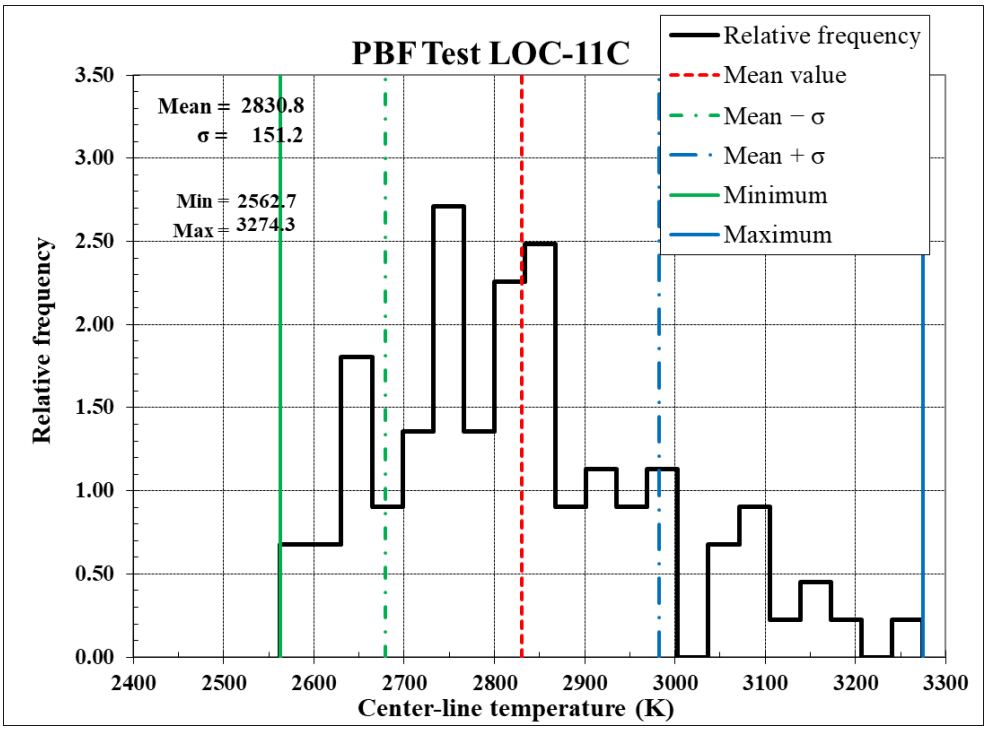



*Figure 43: Centerline temperature at t=10,000 s, RELAP5, RS (Case 1-95)*

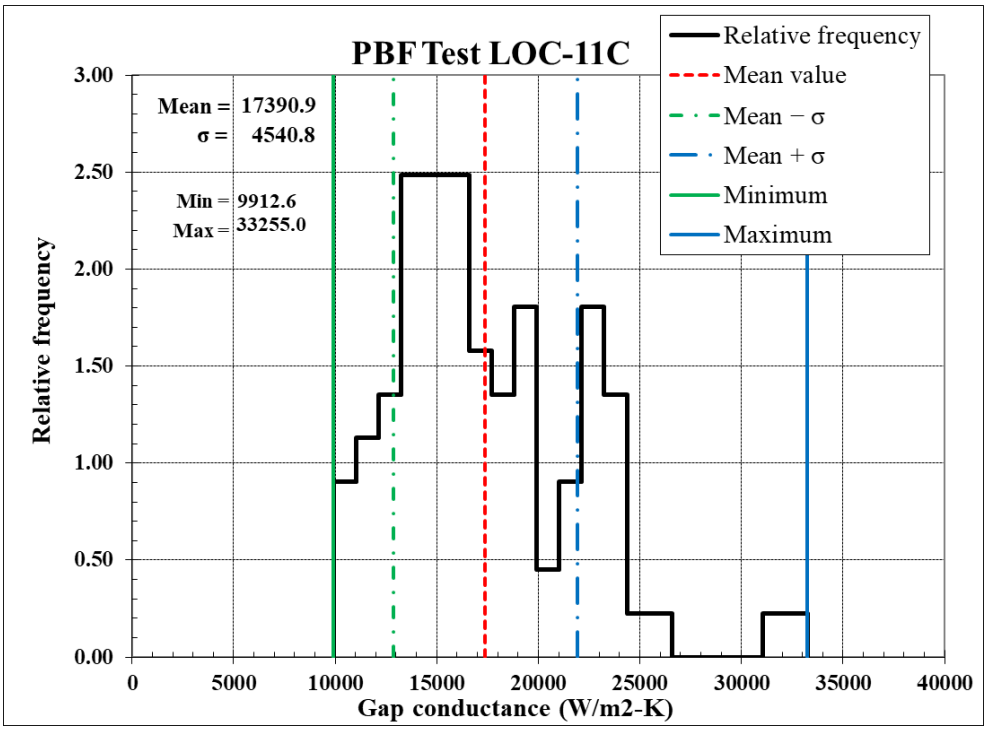



*Figure 44: Gap conductance at t=10,000 s, RELAP5, RS (Case 1-95)*

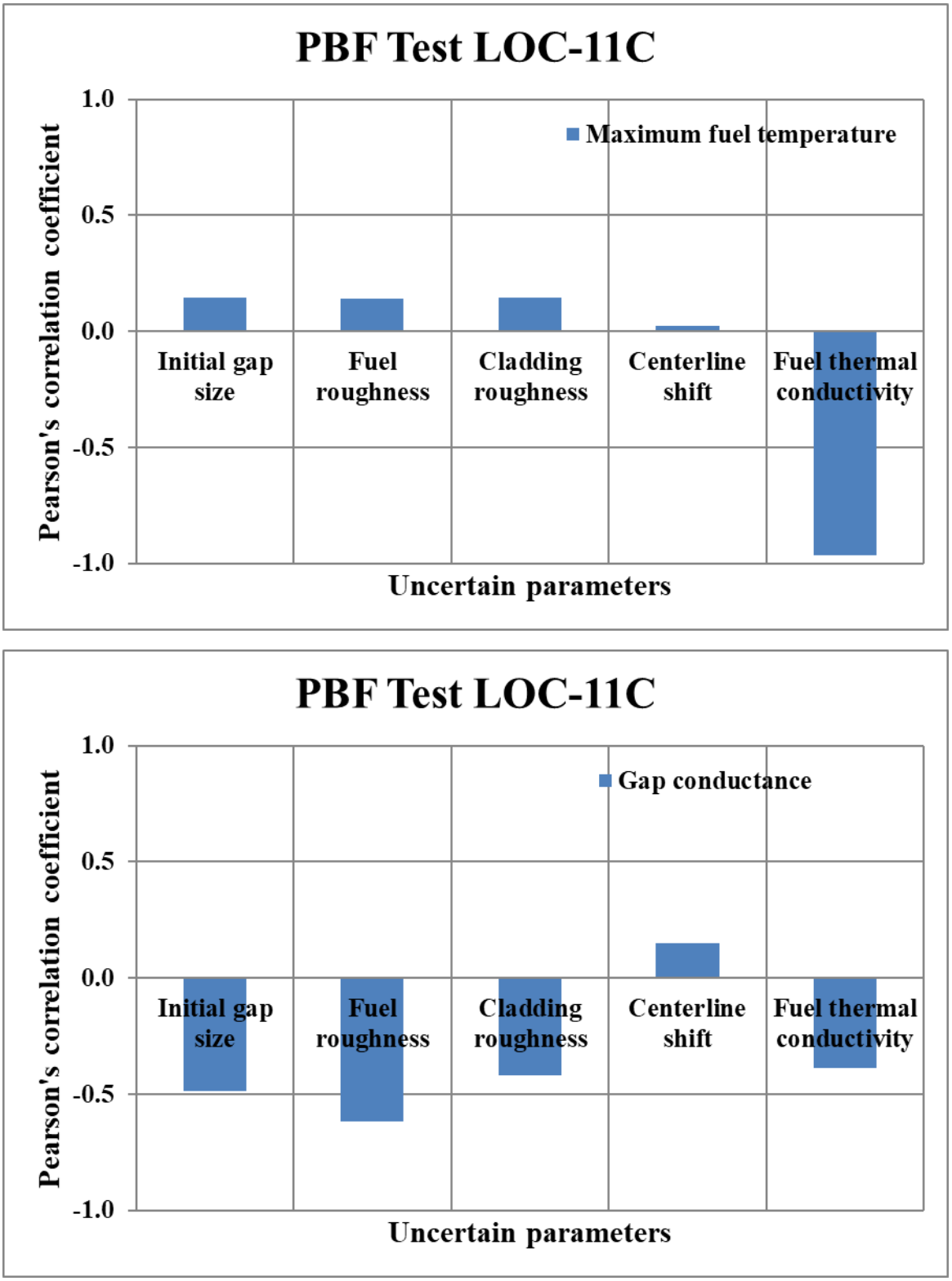



*Figure 45: Pearson's correlation coefficients, RELAP5, RS (Case 1-95)*

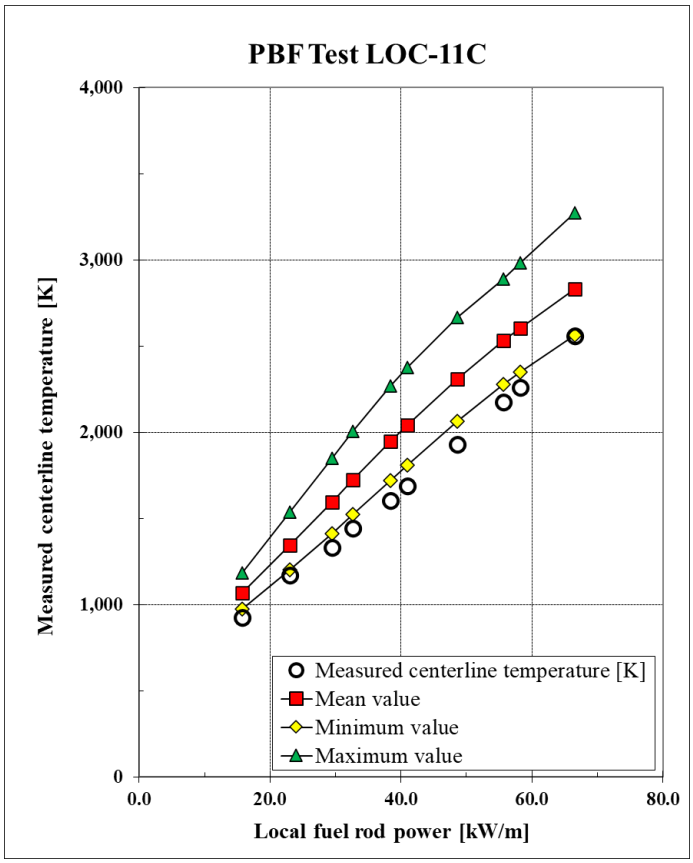



*Figure 46: Centerline temperatures, RELAP5, RS (Case 1-95)*

Table 10 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 10: Main parameters, REALP5, Cases 1*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2840 | 153 | 17.0 | 3.9 |
| Case 1-99-2 | 662 | 2832 | 144 | 16.5 | 4.0 |
| Case 1-95 | 95 | 2831 | 151 | 17.4 | 4.5 |

### 4.3.2 DS Standard Methodology

The SUE input data file for the DS-Standard methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, RELAP5
* ====================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      2    *    DS-STANDARD
*
*
105000   'GAP-PBF-LOC-11C.INP'              *  BASE INPUT FILE
115000   'GAP-PBF-LOC-11C.INP'              *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'c:\relap5-mod33jz\exe\relap5.exe' *  PROGRAM TO RUN
130000    1                                 *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   2          2
*
305001   httemp         100100101 *  Cell  1, centerline
305002   httemp         100100111 *  Cell 10, clad surface
305003   hgap             1001001 *  Gap conductance
*
*
* ======================================================================
*  END OF INPUT FILE
* ======================================================================
*
```

The RELAP5 input file (GAP-PBF-LOC-11C.INP) is the same as described in the previous section.

The results obtained for the DS-S methodology, referred to here as Case 2, are shown in Figure 47, Figure 48, Figure 49, and Figure 50. Figure 47 and Figure 48 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range").

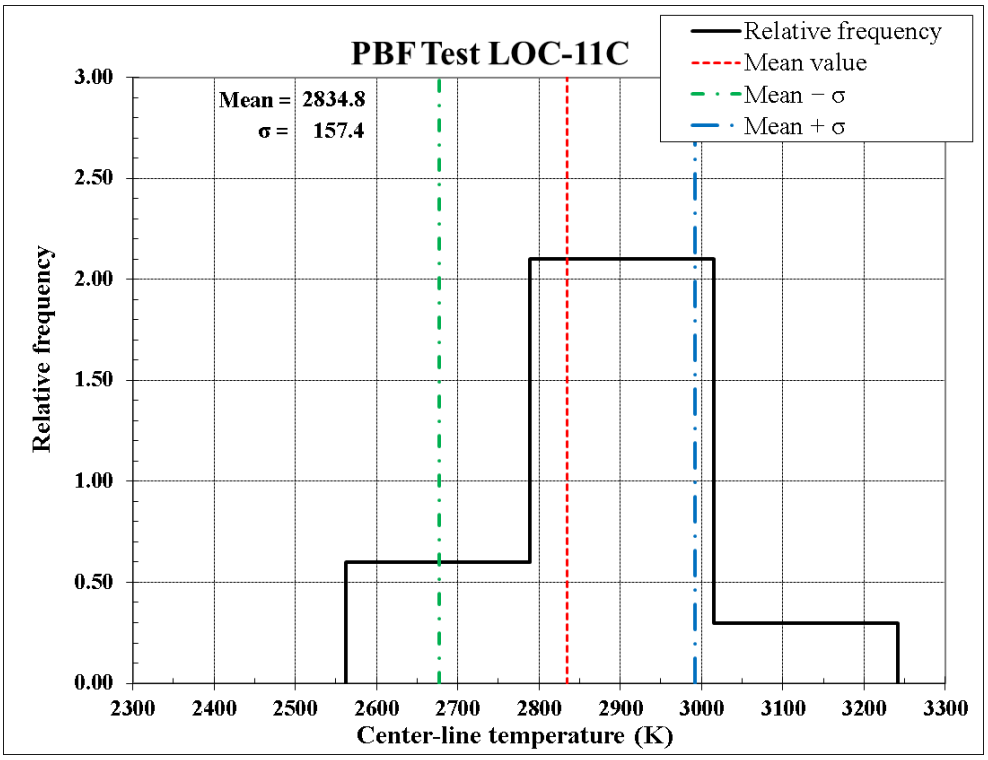



*Figure 47: Centerline temperature at t=10,000 s, RELAP5, DS-Standard (Case 2)*

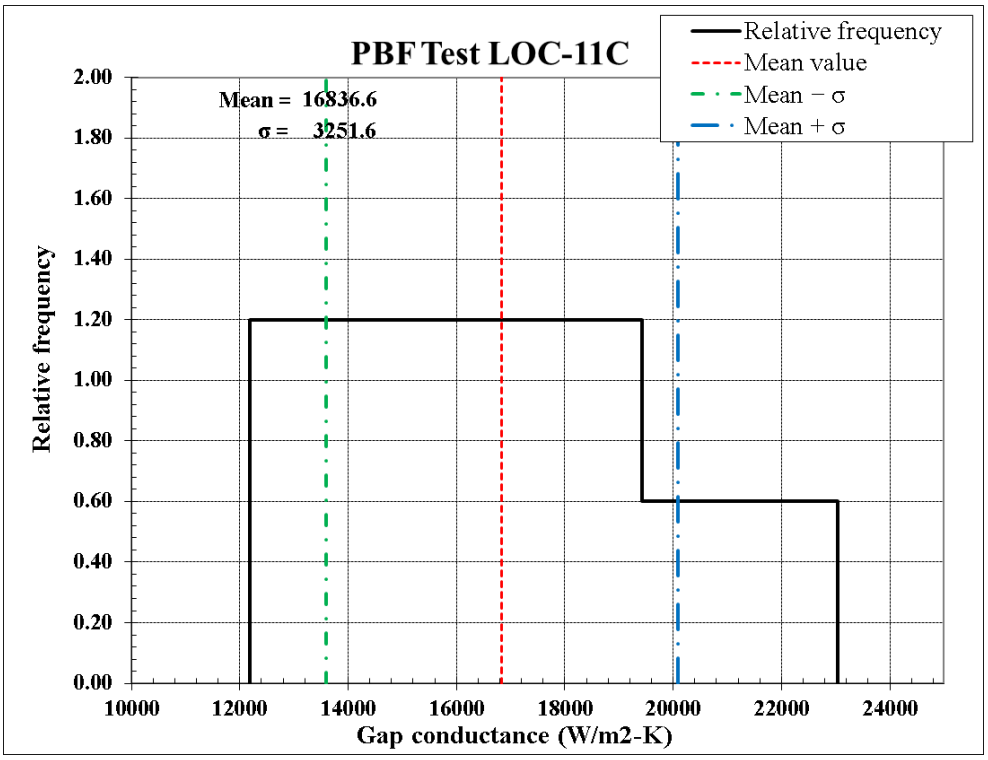



*Figure 48: Gap conductance at t=10,000 s, RELAP5, DS-Standard (Case 2)*

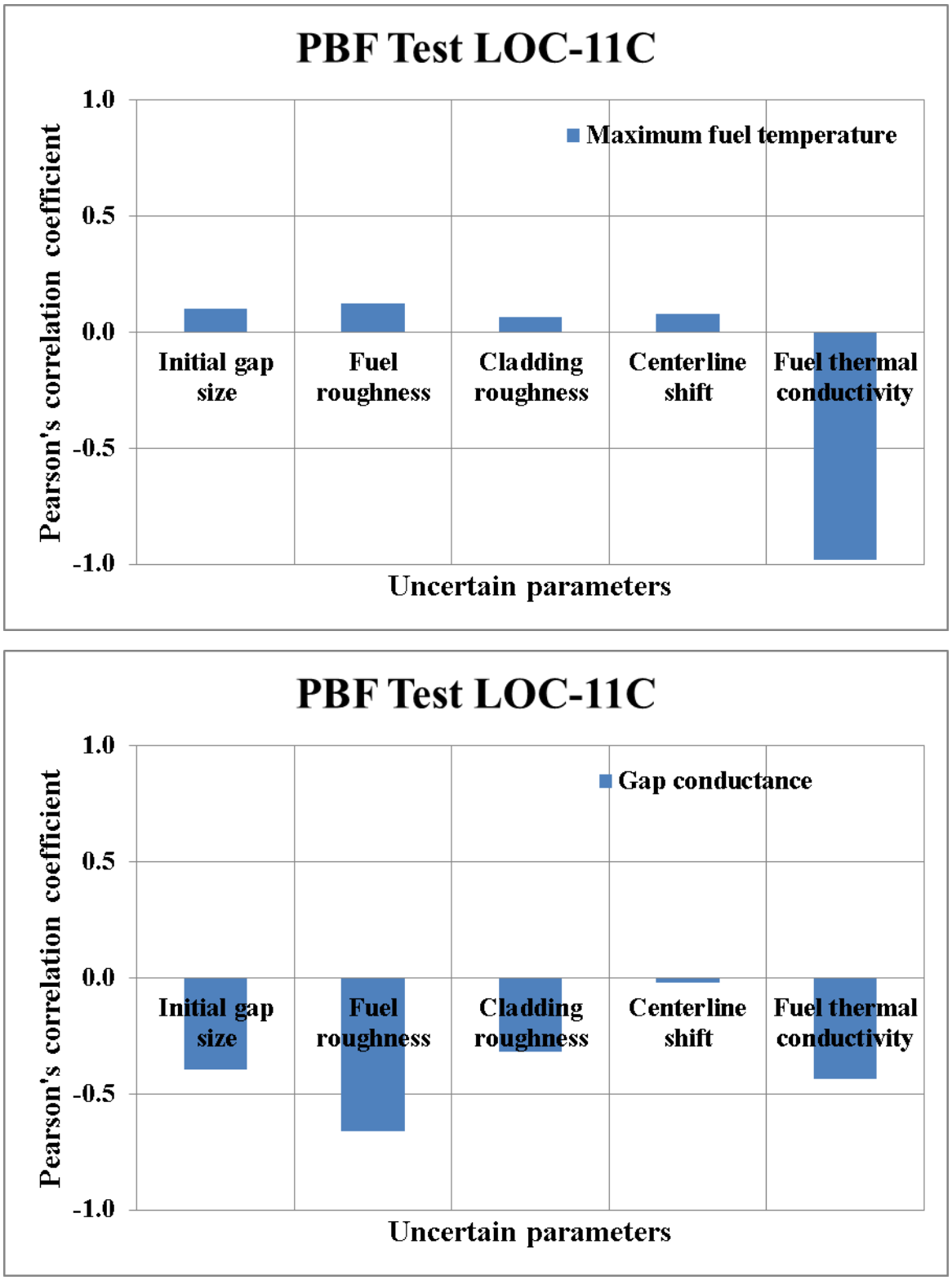



*Figure 49: Pearson's correlation coefficients, RELAP5, DS-Standard (Case 2)*

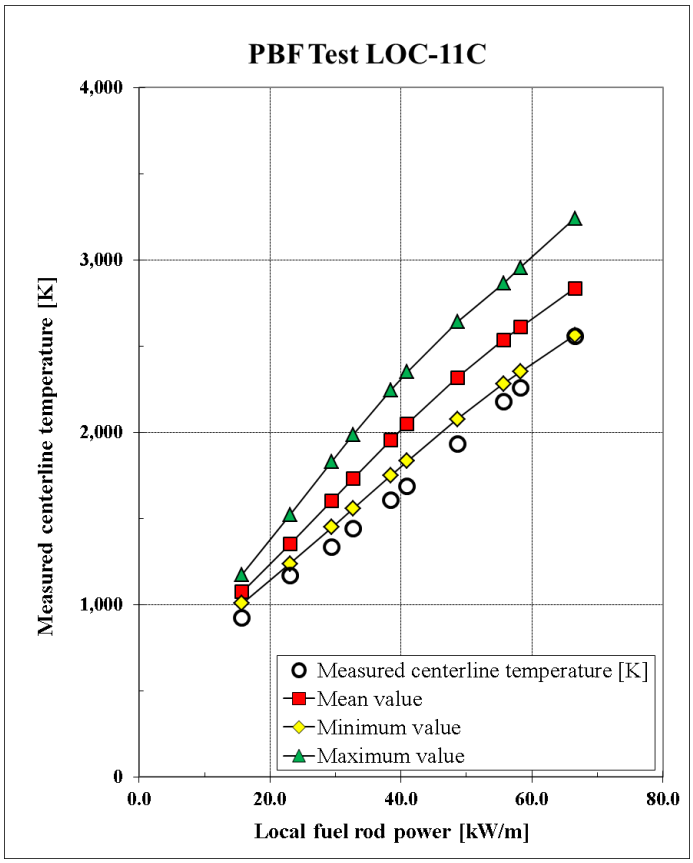



*Figure 50: Centerline temperatures, RELAP5, DS-Standard (Case 2)*

Figure 49 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

Table 11 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 11: Main parameters, REALP5, Cases 1 and 2*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2840 | 153 | 17.0 | 3.9 |
| Case 1-99-2 | 662 | 2832 | 144 | 16.5 | 4.0 |
| Case 1-95 | 95 | 2831 | 151 | 17.4 | 4.5 |
| Case 2 | 10 | 2835 | 157 | 16.8 | 3.3 |

### 4.3.3 DS Hadamard Methodology

The SUE input data file for the DS-Hadamard methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, RELAP5
* ====================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      3    *    3=DS-HADAMARD
*
*
105000   'GAP-PBF-LOC-11C.INP'              *  BASE INPUT FILE
115000   'GAP-PBF-LOC-11C.INP'              *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'c:\relap5-mod33jz\exe\relap5.exe' *  PROGRAM TO RUN
130000    1                                 *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   2          2
*
305001   httemp         100100101 *  Cell  1, centerline
305002   httemp         100100111 *  Cell 10, clad surface
305003   hgap             1001001 *  Gap conductance
*
*
* ======================================================================
*  END OF INPUT FILE
* ======================================================================
*
```

The RELAP5 input file (GAP-PBF-LOC-11C.INP) is the same as described in the previous section.

The results obtained for the DS-H methodology, referred to here as Case 3, are shown in Figure 51, Figure 52, Figure 53, and Figure 54. Figure 51 and Figure 52 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range").

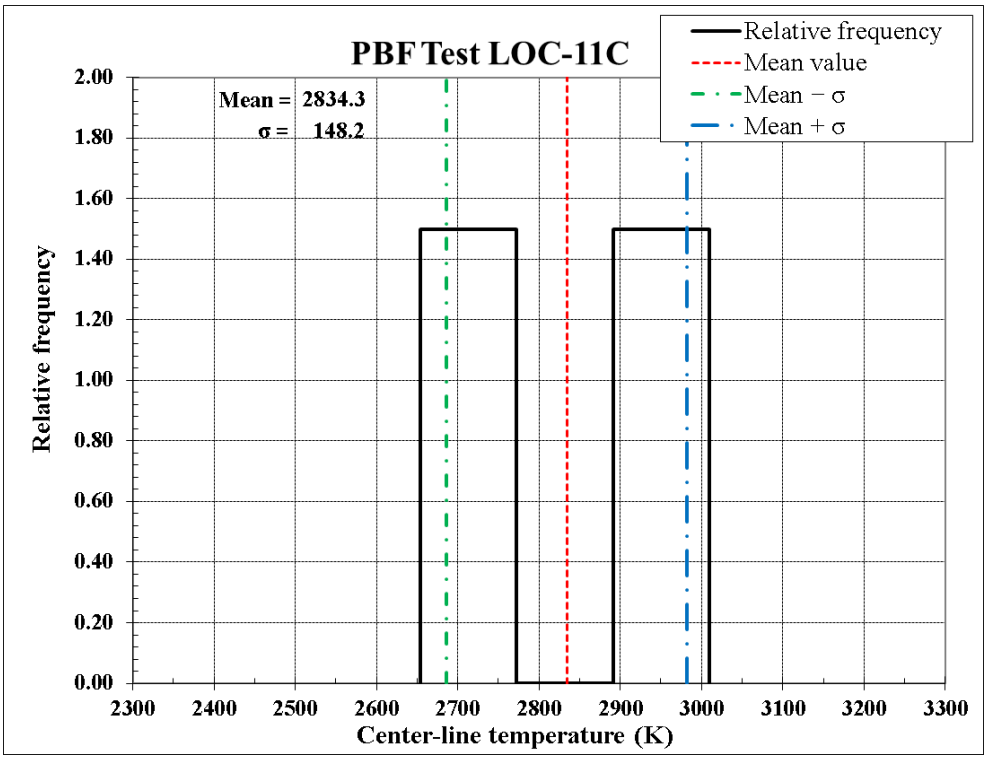



*Figure 51: Centerline temperature at t=10,000 s, RELAP5, DS-H (Case 3)*

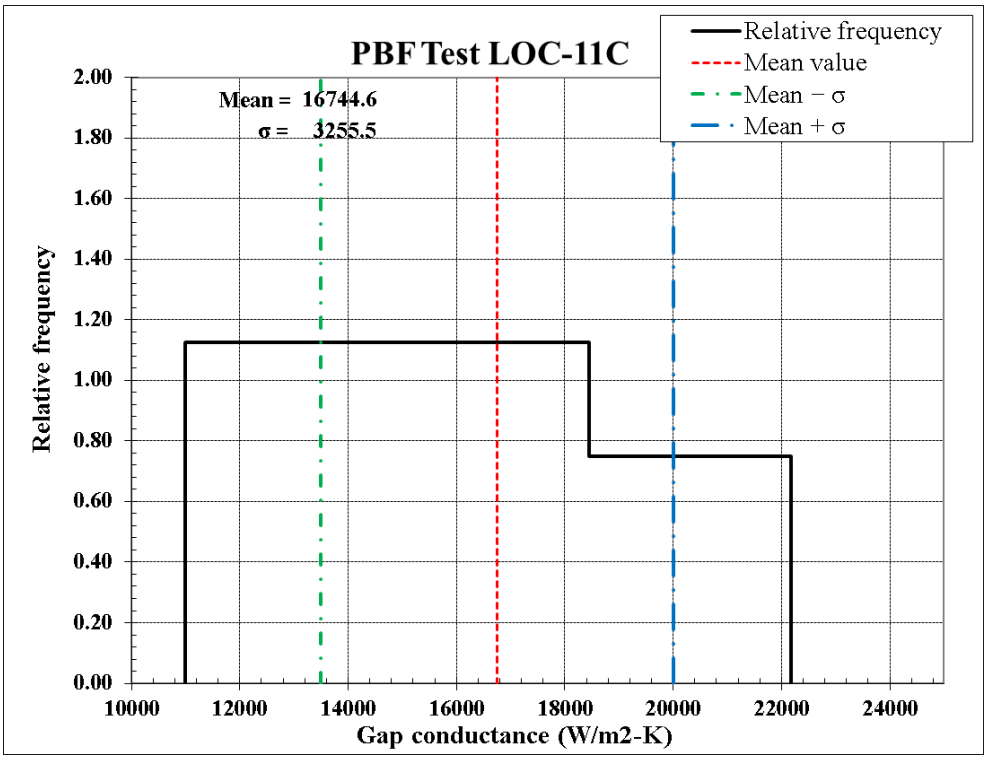



*Figure 52: Gap conductance at t=10,000 s, RELAP5, DS-H (Case 3)*

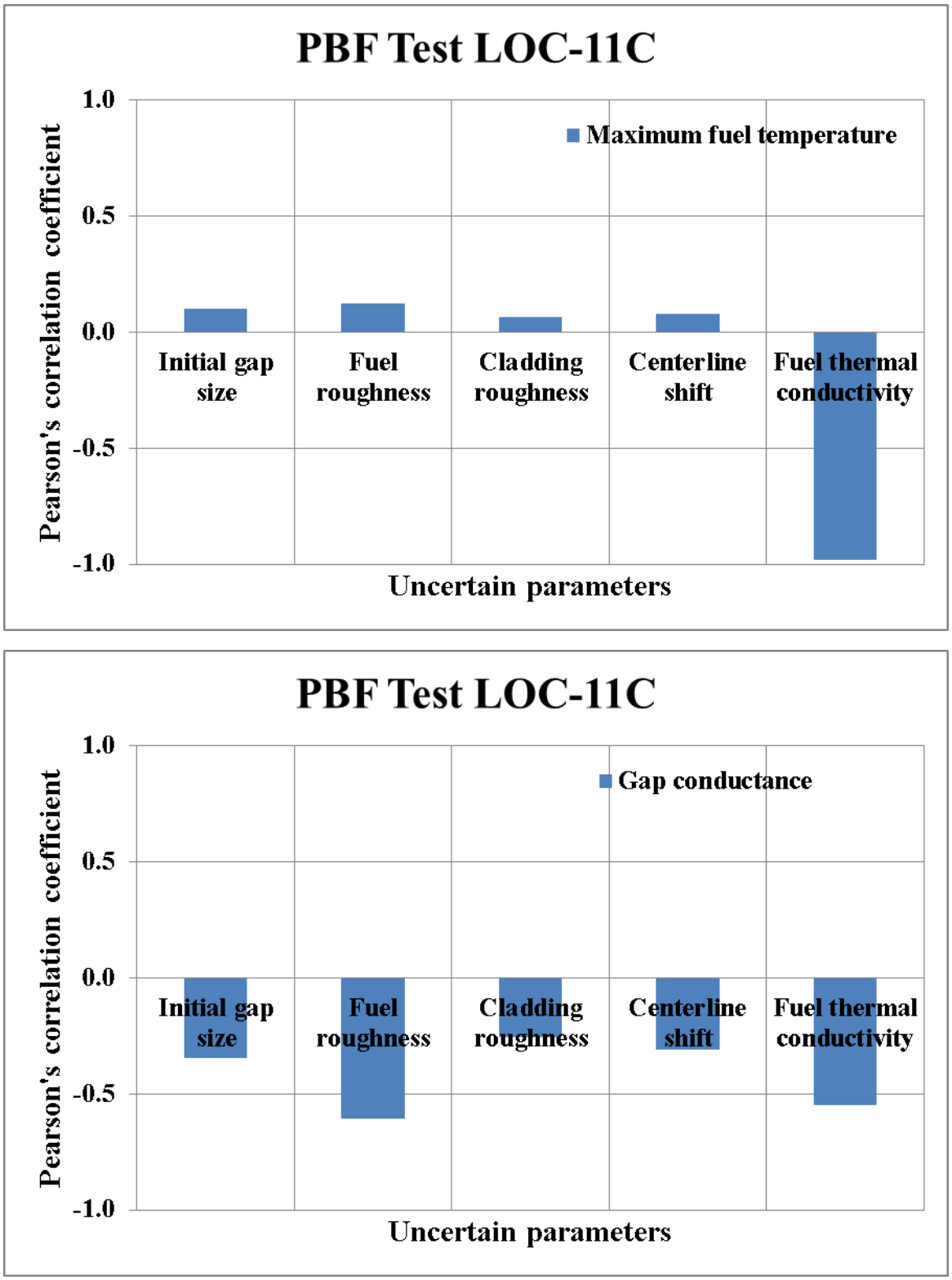



*Figure 53: Pearson's correlation coefficients, RELAP5, DS-H (Case 3)*

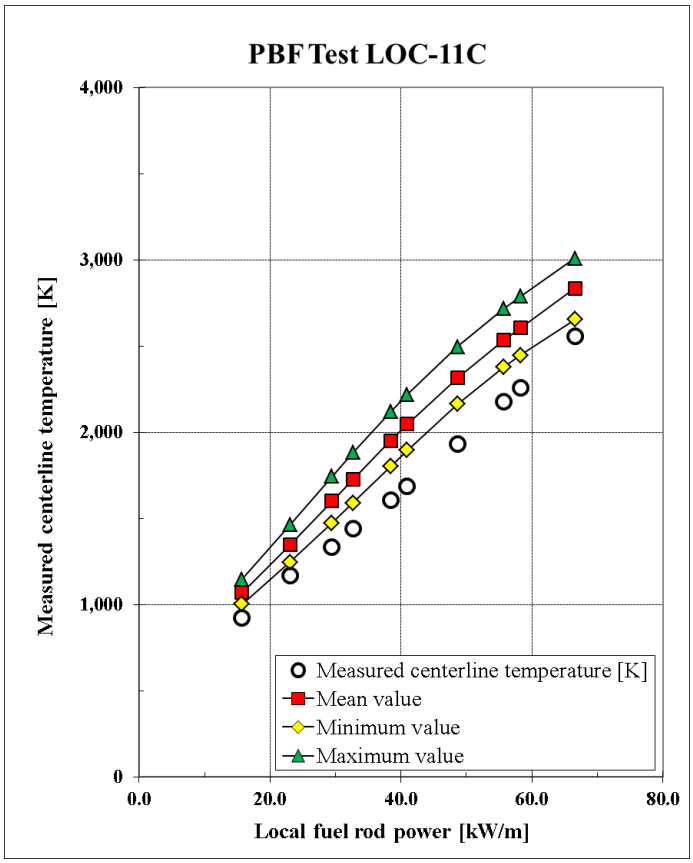



*Figure 54: Centerline temperatures, RELAP5, DS-H (Case 3)*

Figure 53 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

Table 12 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 12: Main parameters, REALP5, Cases 1, 2, and 3*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2840 | 153 | 17.0 | 3.9 |
| Case 1-99-2 | 662 | 2832 | 144 | 16.5 | 4.0 |
| Case 1-95 | 95 | 2831 | 151 | 17.4 | 4.5 |
| Case 2 | 10 | 2835 | 157 | 16.8 | 3.3 |
| Case 3 | 8 | 2834 | 148 | 16.7 | 3.3 |

### 4.3.4 DS Simplex Methodology

The SUE input data file for the DS-Simplex methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, RELAP5
* ====================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      4    *    4=DS-SIMPLEX
*
*
105000   'GAP-PBF-LOC-11C.INP'              *  BASE INPUT FILE
115000   'GAP-PBF-LOC-11C.INP'              *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'c:\relap5-mod33jz\exe\relap5.exe' *  PROGRAM TO RUN
130000    1                                 *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF  IUPERR
200000     1       0       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   2          2
*
305001   httemp         100100101 *  Cell  1, centerline
305002   httemp         100100111 *  Cell 10, clad surface
305003   hgap             1001001 *  Gap conductance
*
*
* ======================================================================
*  END OF INPUT FILE
* ======================================================================
*
```

The RELAP5 input file (GAP-PBF-LOC-11C.INP) is the same as described in the previous section.

The results obtained for the DS-Simplex methodology, referred to here as Case 4, are shown in Figure 55, Figure 56, Figure 57, and Figure 58. Figure 55 and Figure 56 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range").

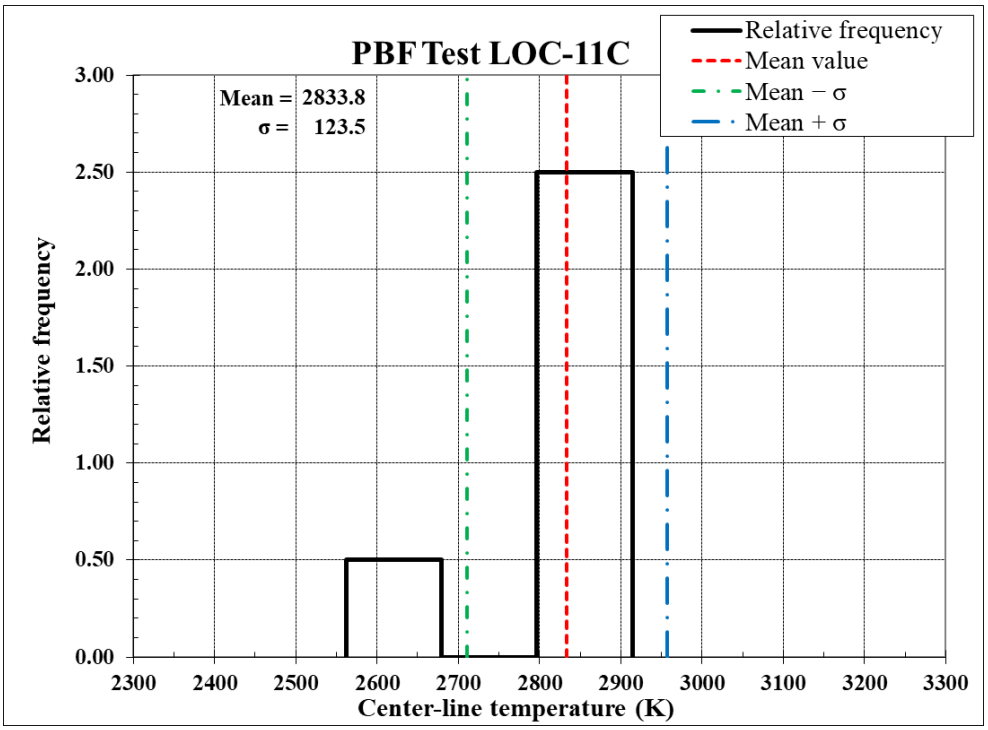



*Figure 55: Centerline temperature at t=10,000 s, RELAP5, DS-Simplex (Case 4)*

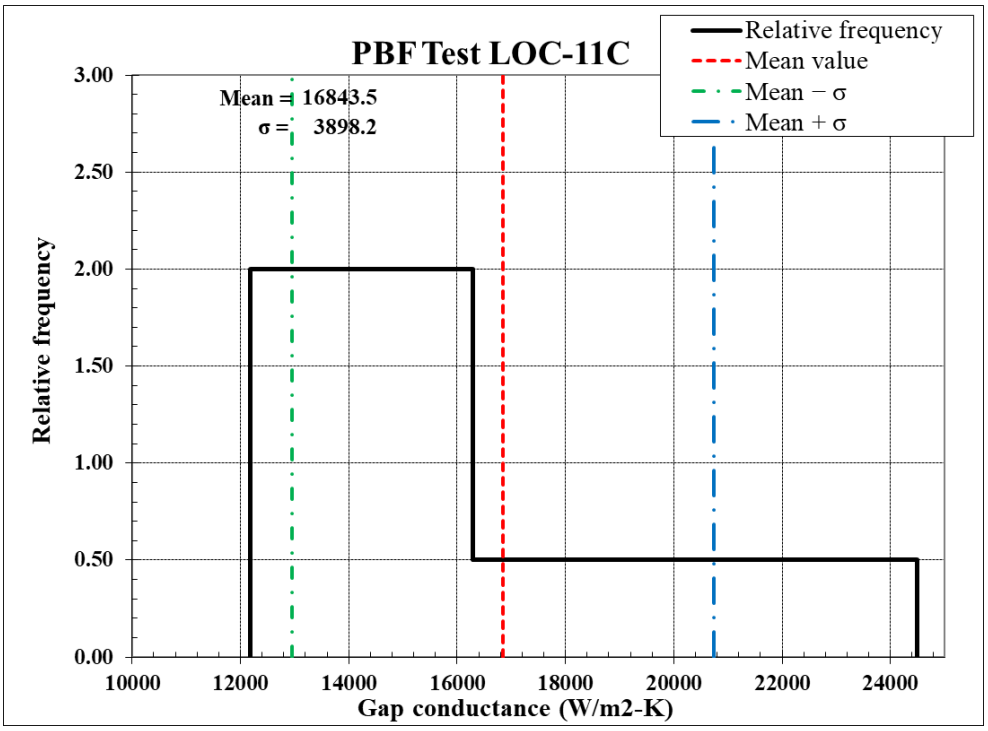



*Figure 56: Gap conductance at t=10,000 s, RELAP5, DS-Simplex (Case 4)*

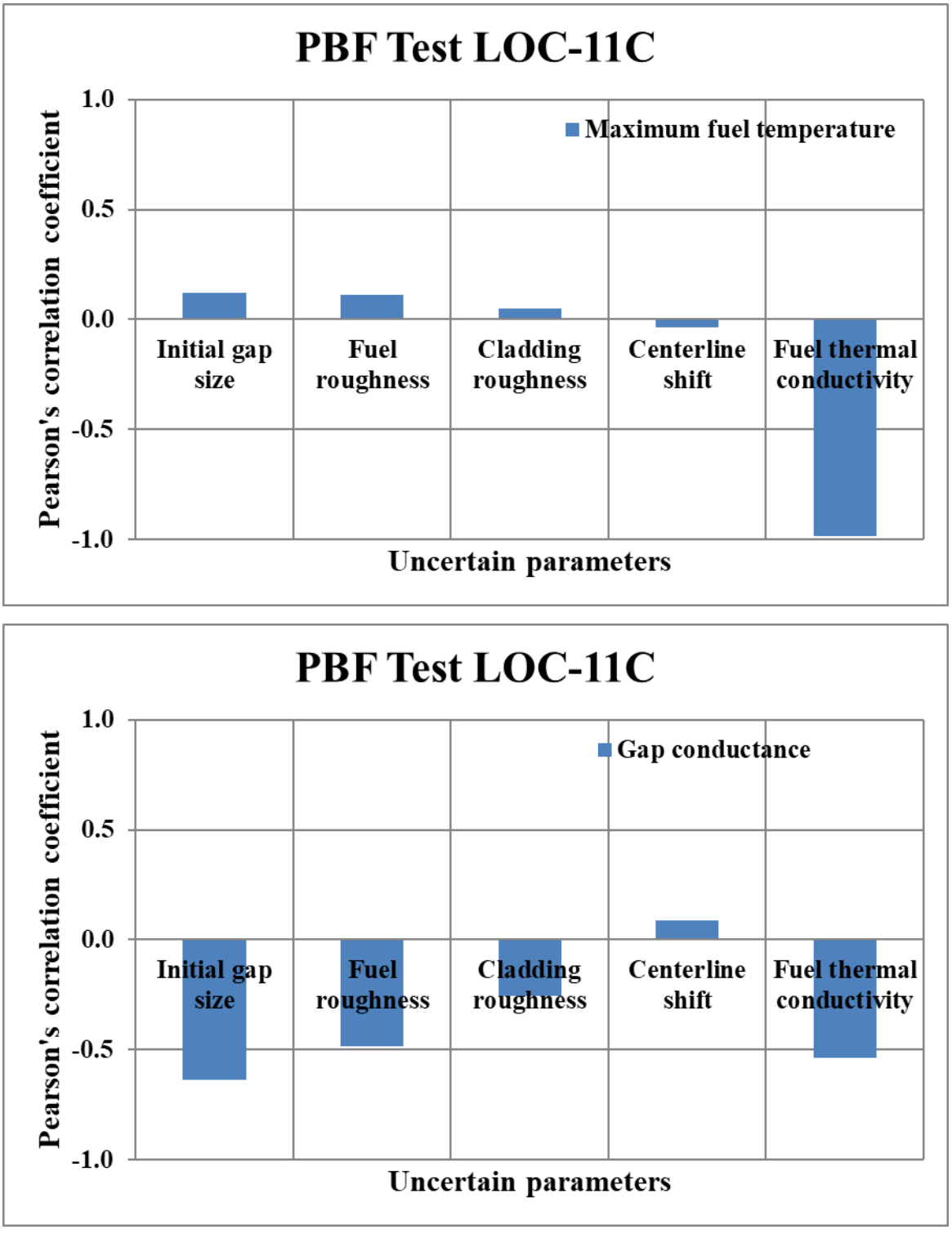



*Figure 57: Pearson's correlation coefficients, RELAP5, DS-Simplex (Case 4)*

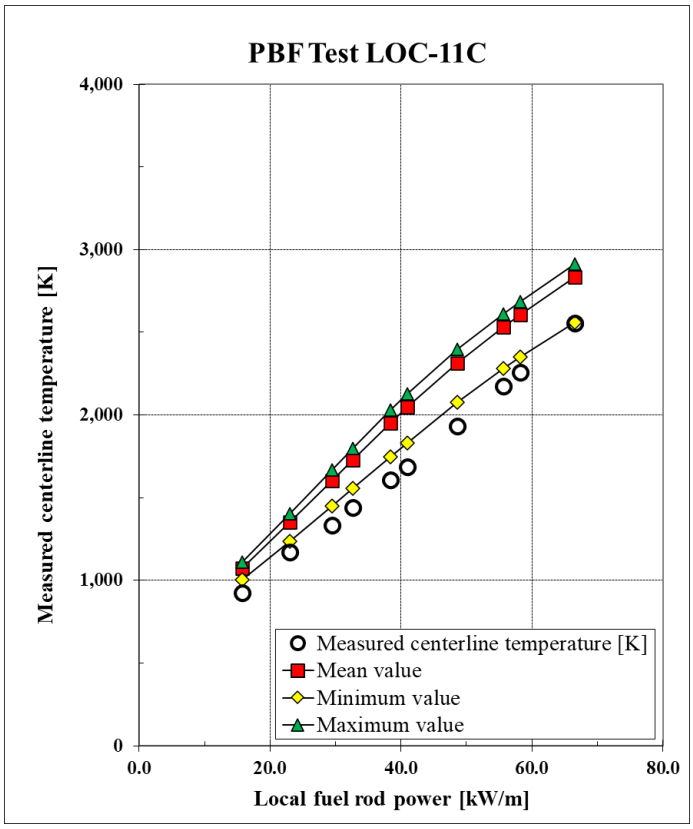



*Figure 58: Centerline temperatures, RELAP5, DS-Simplex (Case 4)*

Figure 57 shows the Pearson's correlation coefficients for the maximum fuel temperature and the gap conductance.

Table 13 presents a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 13: Main parameters, REALP5, Cases 1, 2, and 3*

| Case | Runs | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|---|
| | | Mean, $\mu$ | Std. dev. $\sigma$ | Mean, $\mu$ | Std. dev. $\sigma$ |
| Case 1-99-1 | 662 | 2840 | 153 | 17.0 | 3.9 |
| Case 1-99-2 | 662 | 2832 | 144 | 16.5 | 4.0 |
| Case 1-95 | 95 | 2831 | 151 | 17.4 | 4.5 |
| Case 2 | 10 | 2835 | 157 | 16.8 | 3.3 |
| Case 3 | 8 | 2834 | 148 | 16.7 | 3.3 |
| Case 4 | 6 | 2834 | 124 | 16.8 | 3.9 |

### 4.3.5 RS versus DS Methodologies

Comparison of the results obtained with the Deterministic Sampling (DS) and the Random Sampling (RS) methodologies is shown in Table 14 and Table 15. It is seen that both methodology types give very similar results. The DS methodologies allow to significantly reduce the number of runs. In the present case the DS methodologies required 6 - 10 runs, while the RS methodology requires hundreds of calculations.

*Table 14: Center-line temperatures, RS versus DS methodologies*

| **Methodology Type** | **Center-line T (K)** | |
|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| Random Sampling | 2831 - 2840 | 144 - 153 |
| Deterministic Sampling | 2834 - 2835 | 124 - 157 |

*Table 15: Gap conductance, RS versus DS methodologies*

| **Methodology Type** | **Center-line T (K)** | |
|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| Random Sampling | 16.5 - 17.4 | 3.9 - 4.5 |
| Deterministic Sampling | 16.7 - 16.8 | 3.3 - 3.9 |

## 4.4 PBF Test LOC-11C, RELAP5/SPECTRA Comparison

Before SPECTRA and RELAP5 results can be compared, one gap modeling aspect must be discussed. The gap conductance involves a term with surface roughness of fuel and cladding:

$$d_{\min} = C_d \cdot (r_f + r_c)$$

Here $r_f$, $r_c$, are the surface roughness of fuel and cladding respectively, and $C_d$ is constant. The value of $C_d$ recommended in literature ranges from 0.62 to 3.2. The default value of $C_d$ in SPECTRA is taken from the Ross and Stoute model and is equal to 1.5 [1]. RELAP5 uses a fixed value of 3.2 [2], not changeable by the user. The base calculations with SPECTRA (section 4.2) were performed using the default value $C_d$ =1.5 because this value gives better agreement with experiment for the PBF test LOC11C. However, for the sake of comparison with RELAP5, the value was changed to the same value as is used in RELAP5, $C_d$ =3.2. This was done in the UNPAR file:

```
*       Radiation        Gas conduction                          Solid conduction
*        Ef      Ec      Cd      Rf          Rc         Cj       C-s   Pa      Hc      n
341001   0.0     0.0     3.2   $002        $003         0.0      0.0   0       009    0.0*
```

All calculations were repeated. The new SPECTRA runs were given suffix "-Cd". These results are compared to the RELAP5 results from section 4.3 below, for the three methodologies:

- RS - section 4.4.1,
- DS-Standard - section 4.4.2,
- DS-Hadamard - section 4.4.2.

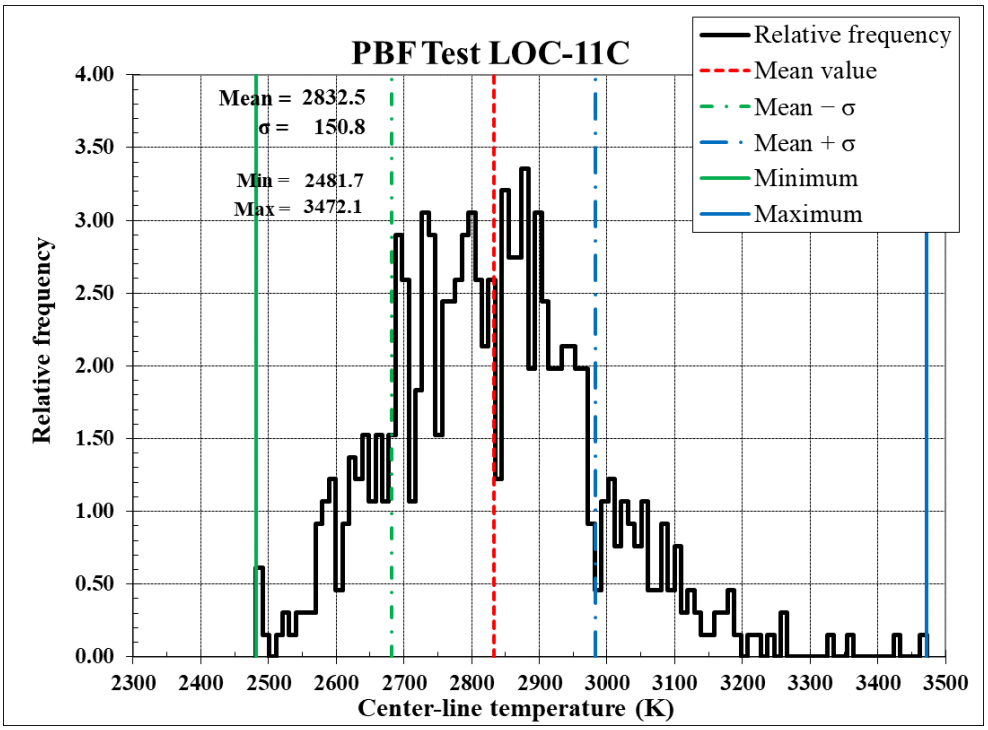
### 4.4.1 RS Methodology

Calculations were performed for 3 cases:

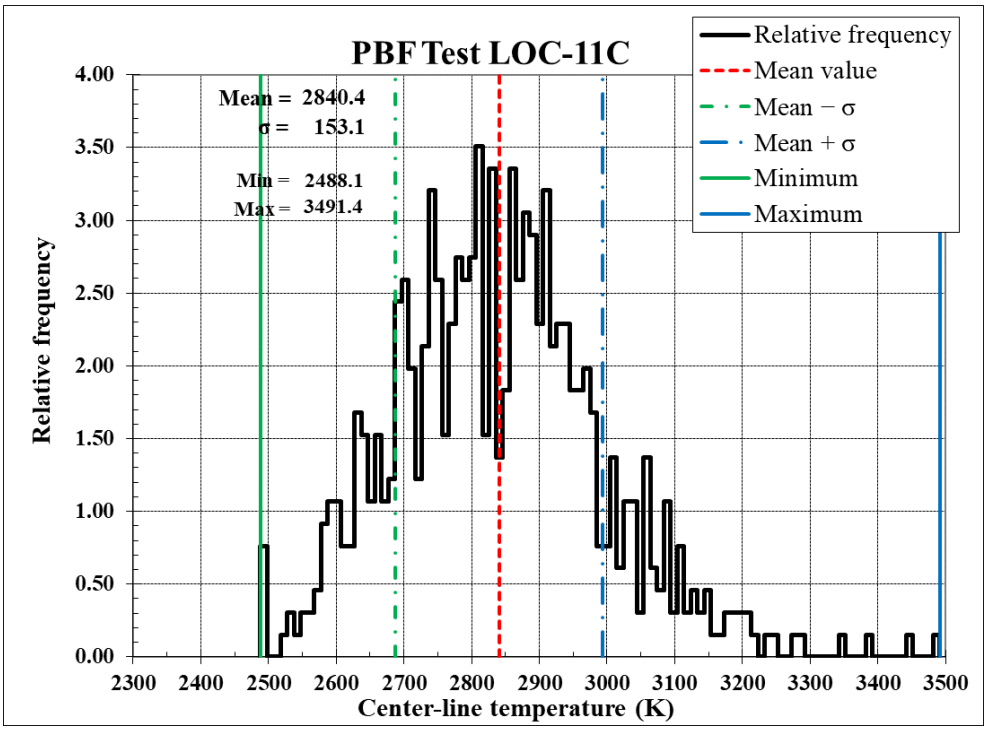
- Case 1-99-1: α=99%, β=99%, pseudo-random series 1.
- Case 1-99-2: α=99%, β=99%, pseudo-random series 2.
- Case 1-95: α=95%, β=95%.

The results are shown in Figure 59 through Figure 64.

- Case 1-99-1: Figure 59 and Figure 60.
- Case 1-99-2: Figure 61 and Figure 62.
- Case 1-95: Figure 63 and Figure 64.

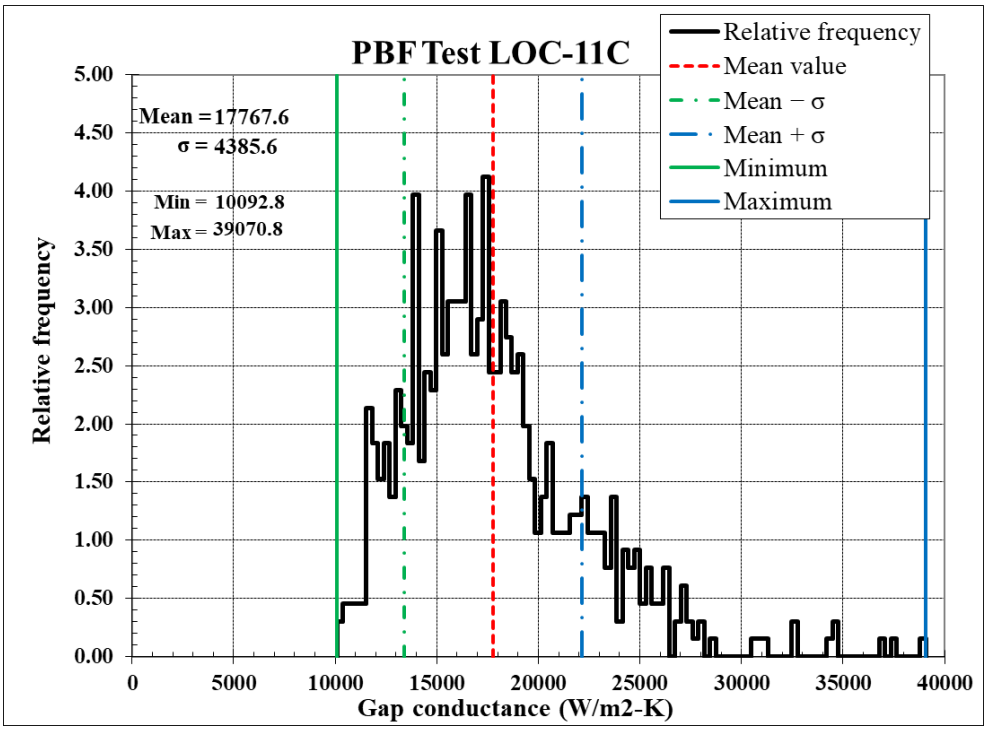



*(a) SPECTRA, Case 1-99-1-Cd*

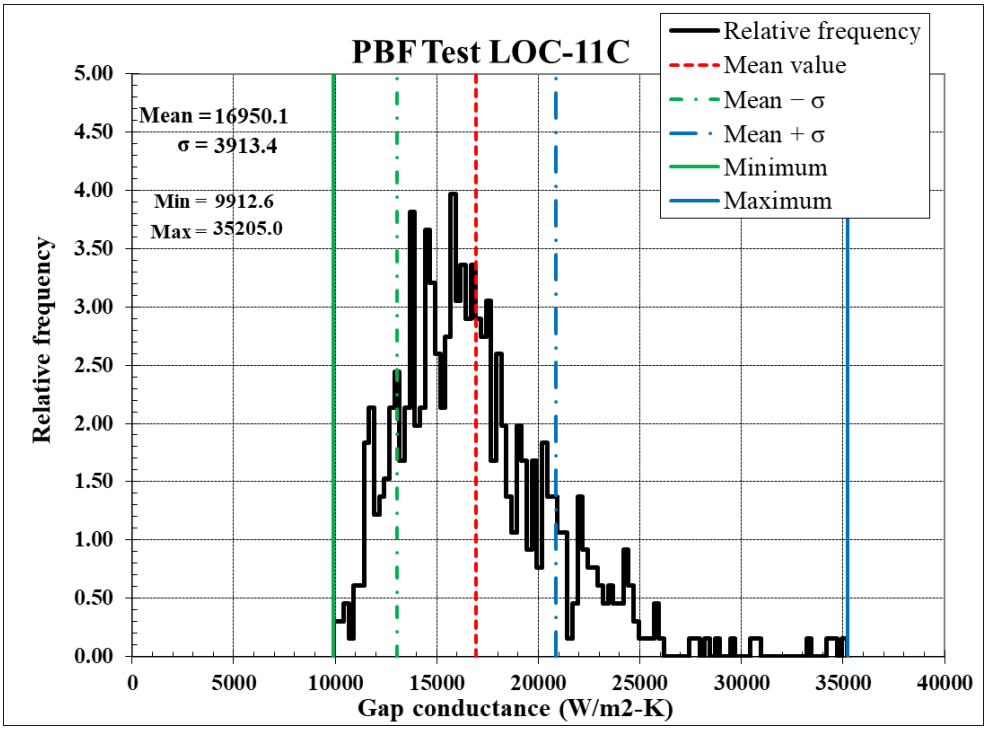



*(b): RELAP5, Case 1-99-1*

*Figure 59: Centerline temperature at t=10,000 s, RS*

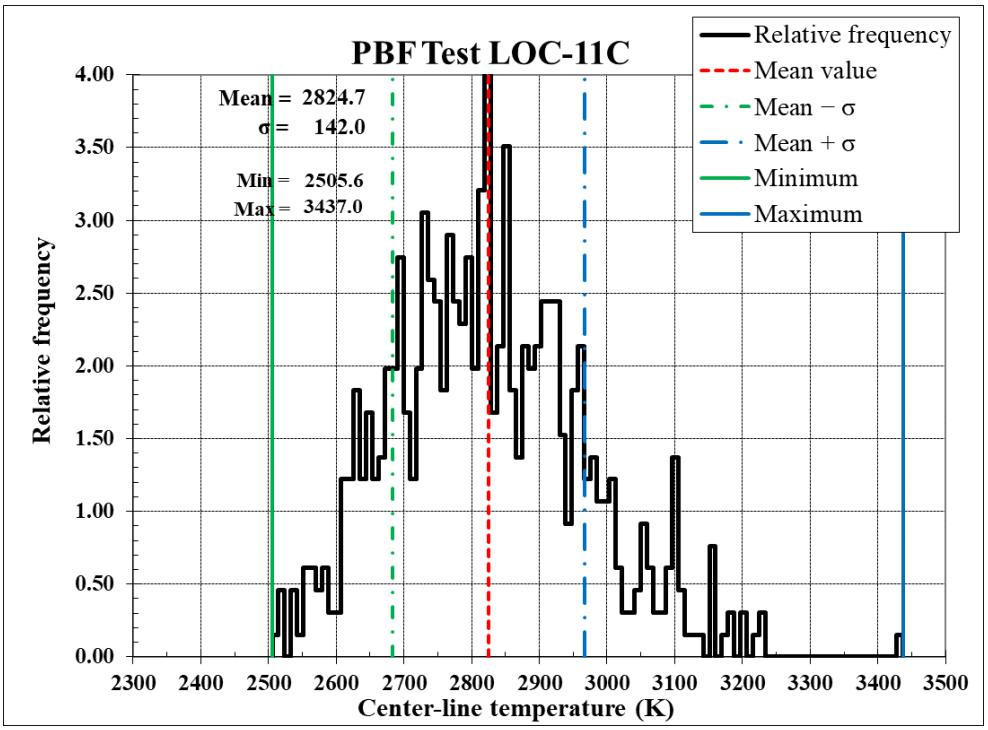



*(a) SPECTRA, Case 1-99-1-Cd*

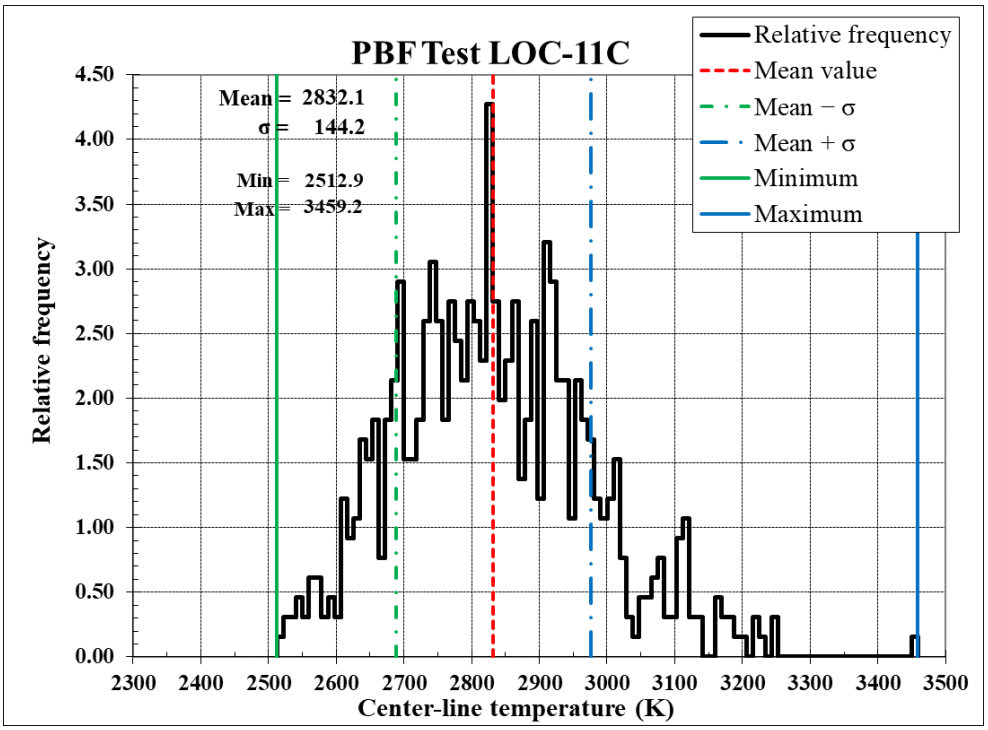



*(b): RELAP5, Case 1-99-1*

*Figure 60: Gap conductance at t=10,000 s, RS*

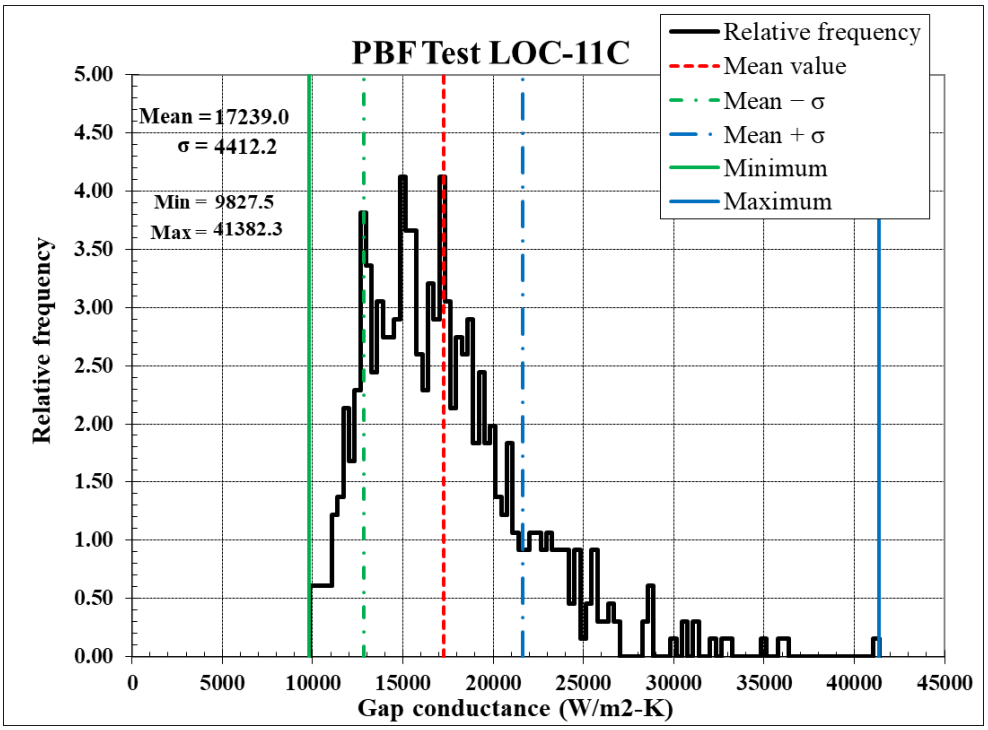



*(a) SPECTRA, Case 1-99-2-Cd*

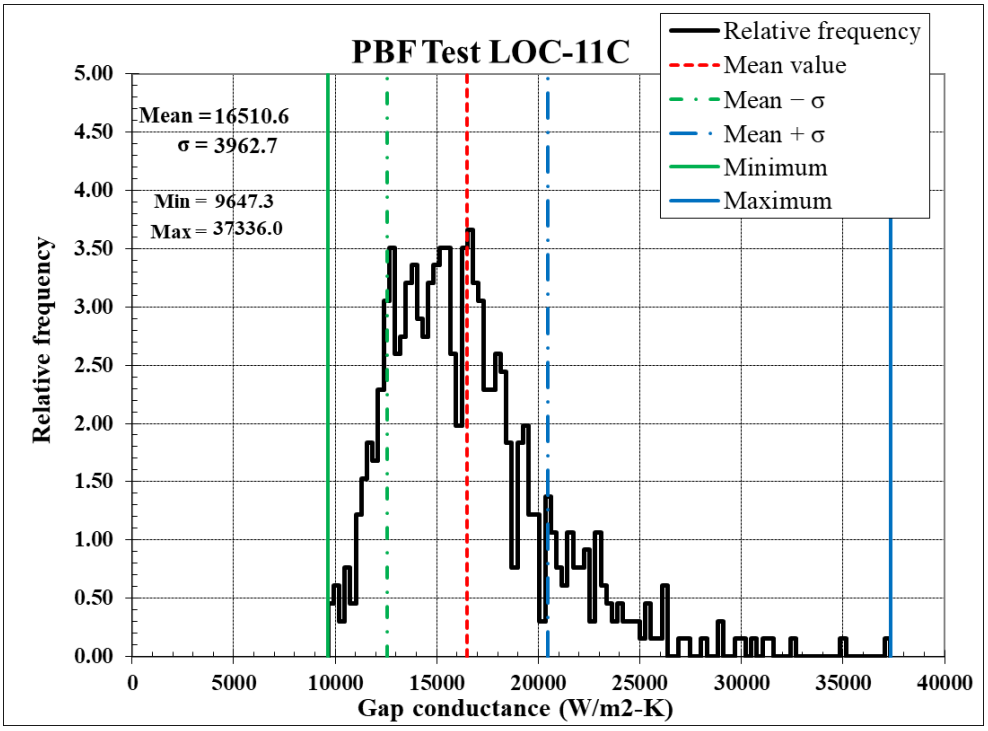



*(b): RELAP5, Case 1-99-2*

*Figure 61: Centerline temperature at t=10,000 s, RS*

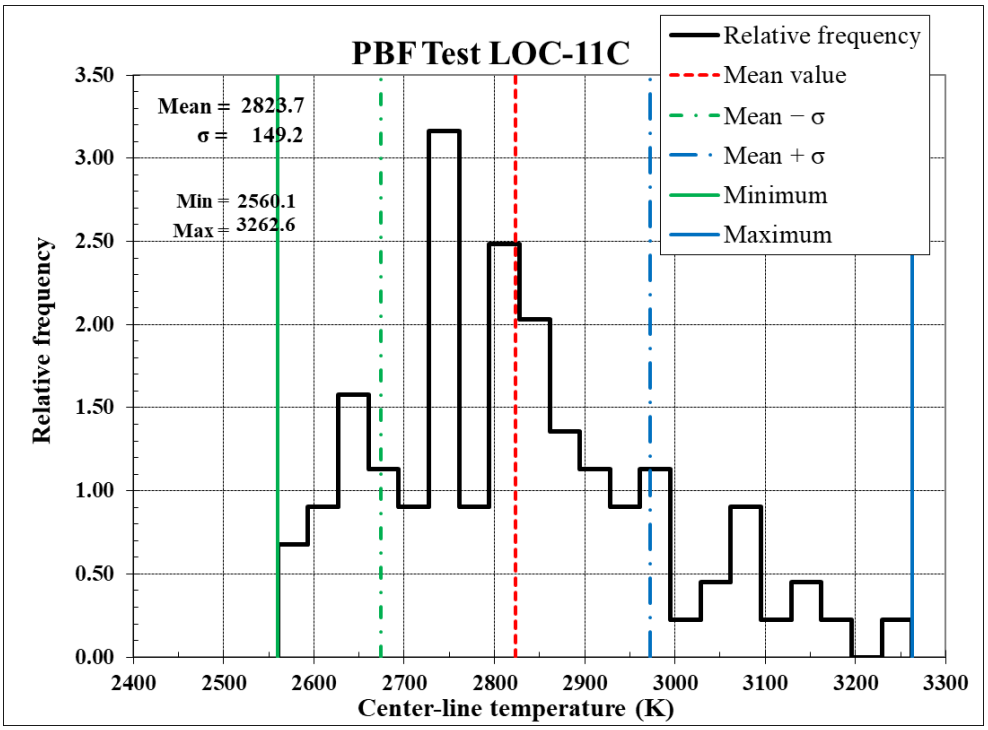



*(a) SPECTRA, Case 1-99-2-Cd*

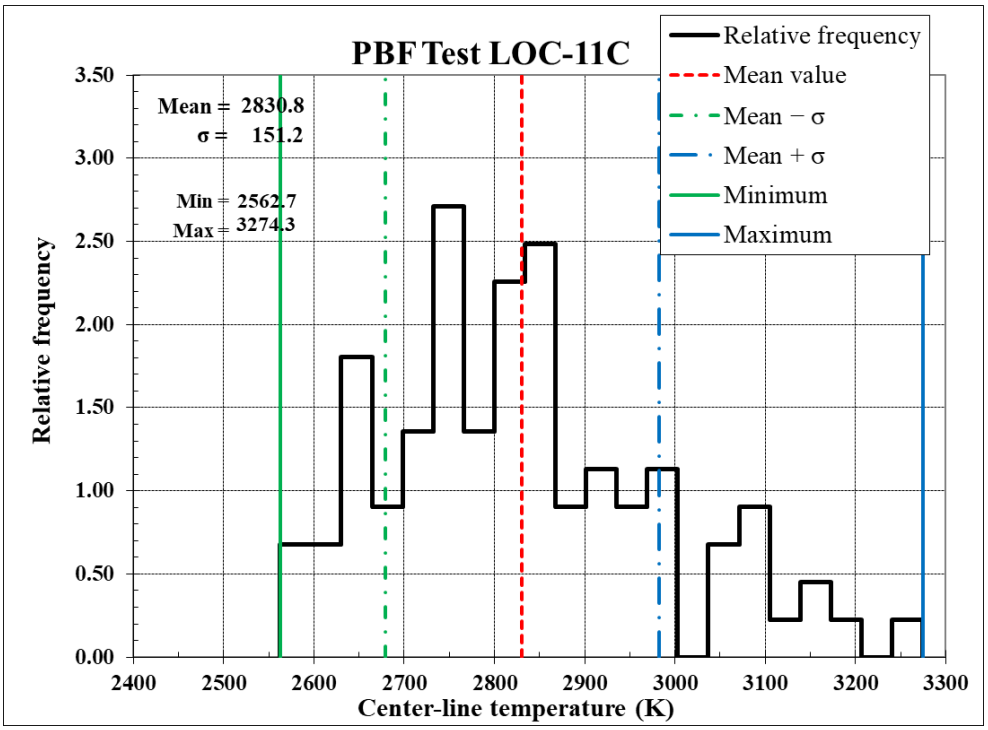



*(b): RELAP5, Case 1-99-2*

*Figure 62: Gap conductance at t=10,000 s, RS*

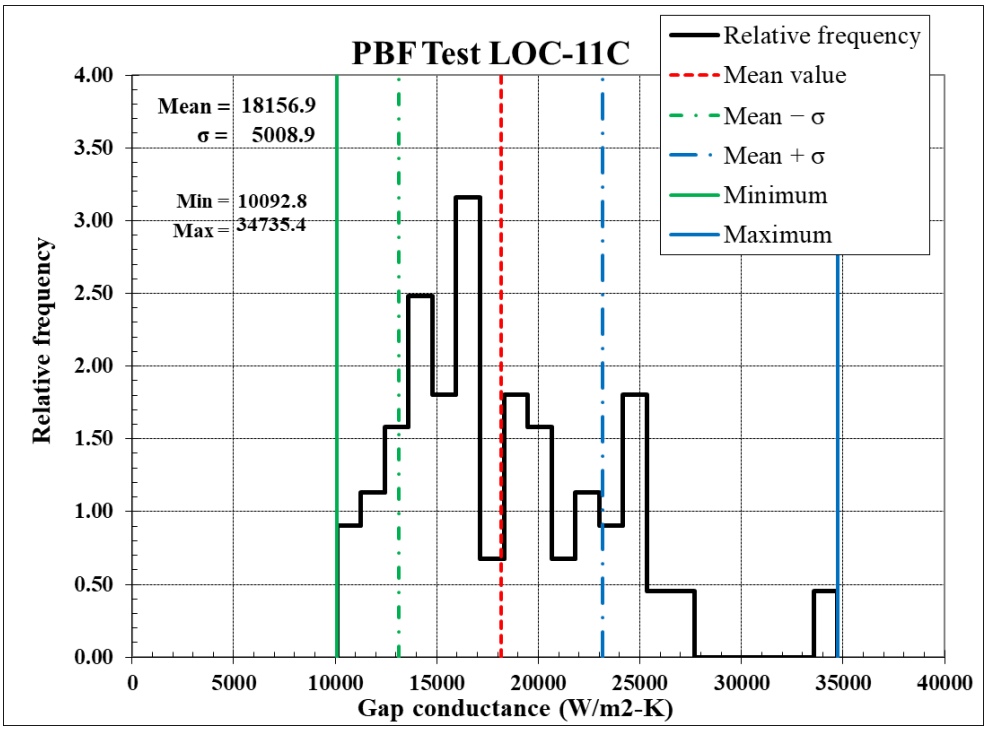



*(a) SPECTRA, Case 1-95-Cd*

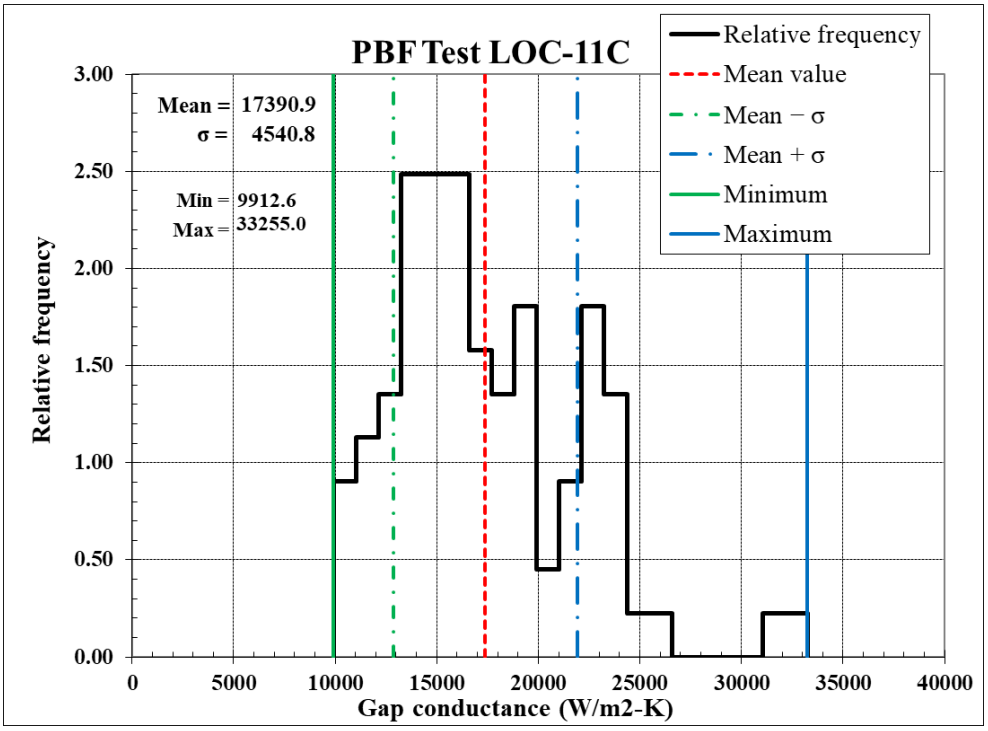



*(b): RELAP5, Case 1-95*

*Figure 63: Centerline temperature at t=10,000 s, RS (Case 1-95)*




*(a) SPECTRA, Case 1-95-Cd*




*(b): RELAP5, Case 1-95*

*Figure 64: Gap conductance at t=10,000 s, RS*

### 4.4.2 DS Standard, DS Hadamard, DS-Simplex Methodologies

The results for the DS-Standard methodology (Case 2) are shown in Figure 65 and Figure 66. The results for the DS-Hadamard methodology (Case 3) are shown in Figure 67 and Figure 68. he results for the DS-Simplex methodology (Case 4) are shown in Figure 69 and Figure 70.

### 4.4.3 Summary of Results

Table 16 and Table 17 present a summary of main parameters, including the mean value and the standard deviation of the fuel center-line temperature and the gap conductance at t=10,000 s, obtained from the figures shown above.

*Table 16: Main parameters, SPECTRA, Cases 1, 2, and 3 ("Cd")*

| Case | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| Case 1-99-1-Cd | 2833 | 151 | 17.8 | 4.4 |
| Case 1-99-2-Cd | 2825 | 142 | 17.2 | 4.4 |
| Case 1-95-Cd | 2824 | 149 | 18.2 | 5.0 |
| Case 2-Cd | 2828 | 155 | 17.4 | 3.5 |
| Case 3-Cd | 2827 | 145 | 17.5 | 3.6 |
| Case 4-Cd | 2825 | 122 | 17.8 | 4.6 |

*Table 17: Main parameters, REALP5, Cases 1, 2, and 3*

| Case | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| Case 1-99-1 | 2840 | 153 | 17.0 | 3.9 |
| Case 1-99-2 | 2832 | 144 | 16.5 | 4.0 |
| Case 1-95 | 2831 | 151 | 17.4 | 4.5 |
| Case 2 | 2835 | 157 | 16.8 | 3.3 |
| Case 3 | 2834 | 148 | 16.7 | 3.3 |
| Case 4 | 2834 | 124 | 16.8 | 3.9 |

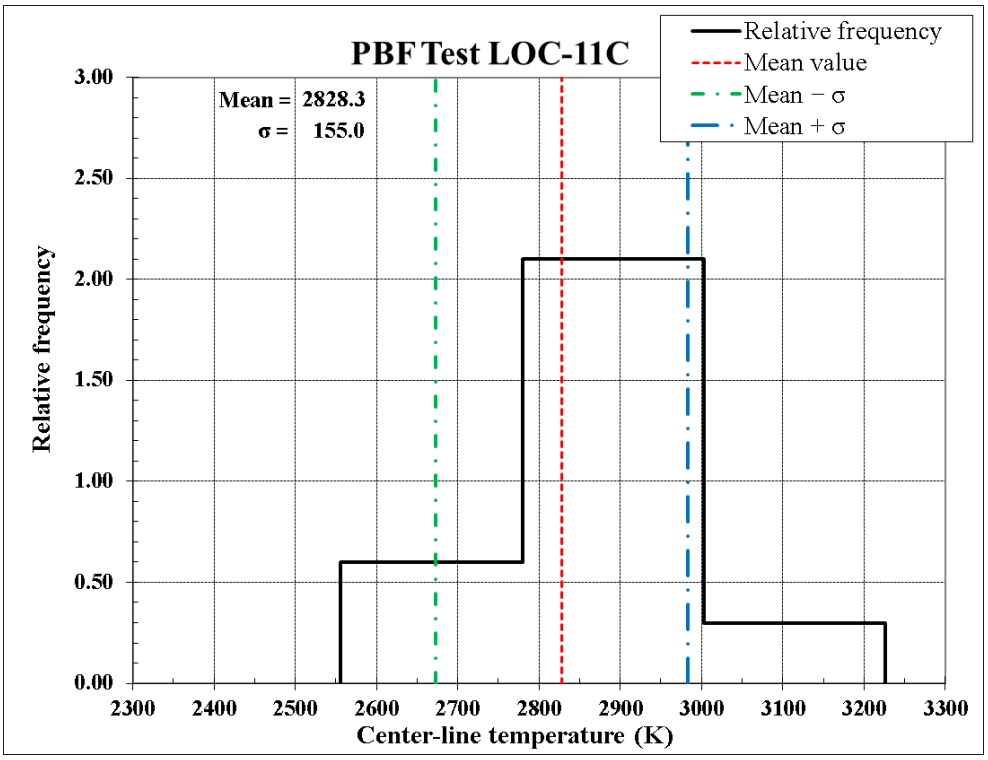
Comparison of the results obtained with the Deterministic Sampling (DS) and the Random Sampling (RS) methodologies is shown in Table 18 and Table 19. It is seen that both methodology types give very similar results. The DS methodologies allow to significantly reduce the number of runs. In the present case the DS methodologies required 6 - 10 runs, while the RS methodology requires hundreds of calculations.

*Table 18: Center-line temperatures, RS versus DS methodologies*

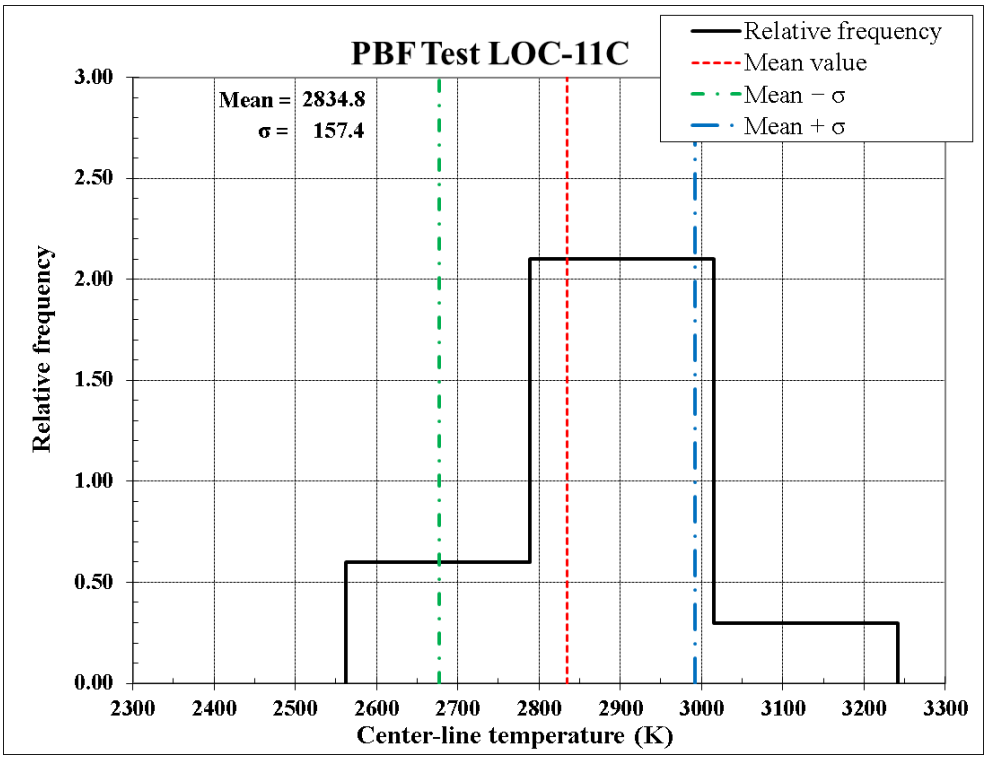
| **Methodology Type** | **Center-line T (K)** | |
|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| **SPECTRA** | | |
| Random Sampling | 2824 - 2833 | 142 - 151 |
| Deterministic Sampling | 2825 - 2828 | 122 - 155 |
| **RELAP5** | | |
| Random Sampling | 2831 - 2840 | 144 - 153 |
| Deterministic Sampling | 2834 - 2835 | 124 - 157 |

*Table 19: Gap conductance, RS versus DS methodologies*

| **Methodology Type** | **Center-line T (K)** | |
|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| **SPECTRA** | | |
| Random Sampling | 17.2 - 18.2 | 4.4 - 5.0 |
| Deterministic Sampling | 17.4 - 17.8 | 3.5 - 4.6 |
| **RELAP5** | | |
| Random Sampling | 16.5 - 17.4 | 3.9 - 4.6 |
| Deterministic Sampling | 16.7 - 16.8 | 3.3 - 3.9 |

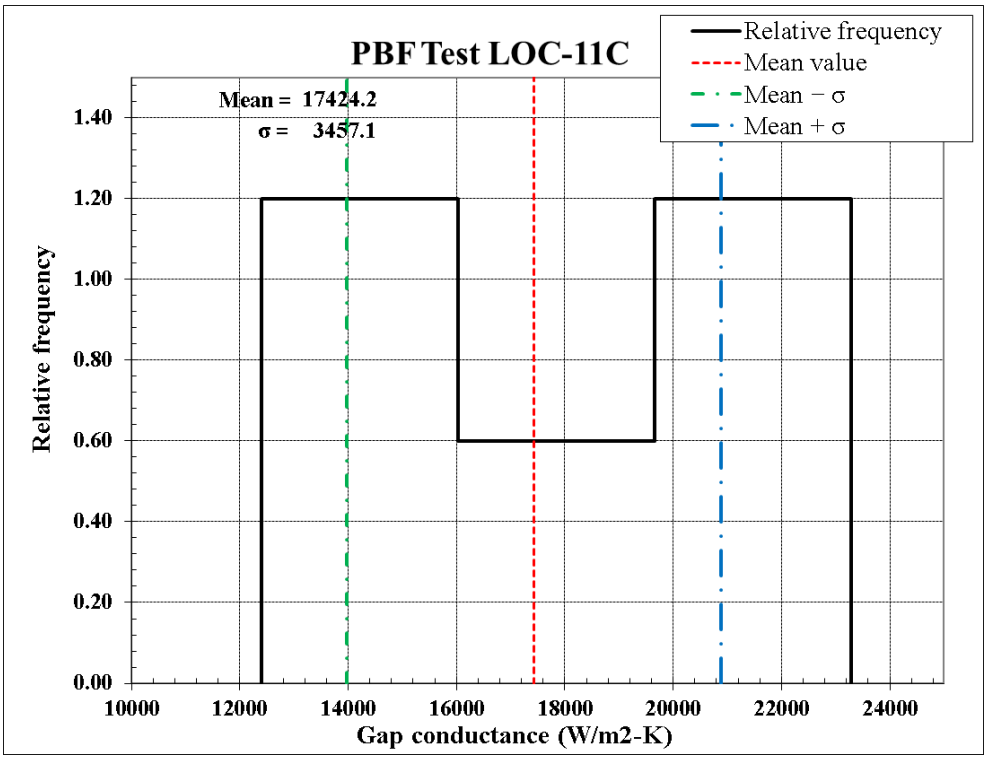



*(a) SPECTRA, Case 2-Cd*

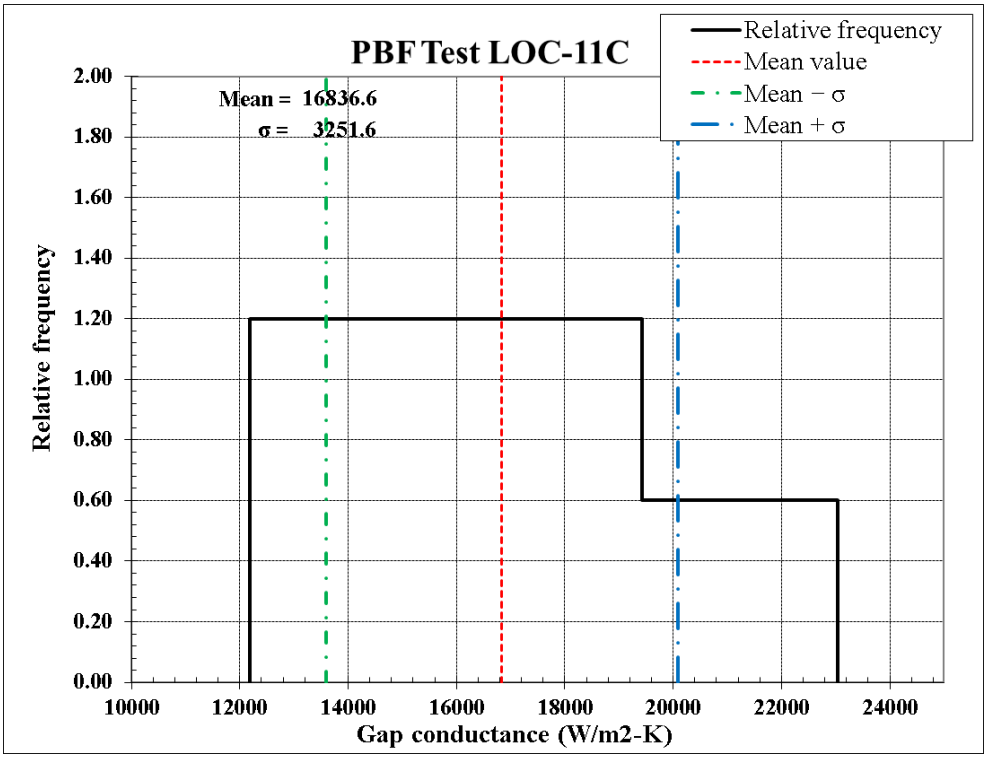



*(b): RELAP5, Case 2*

*Figure 65: Centerline temperature at t=10,000 s, RELAP5, DS-Standard (Case 2)*

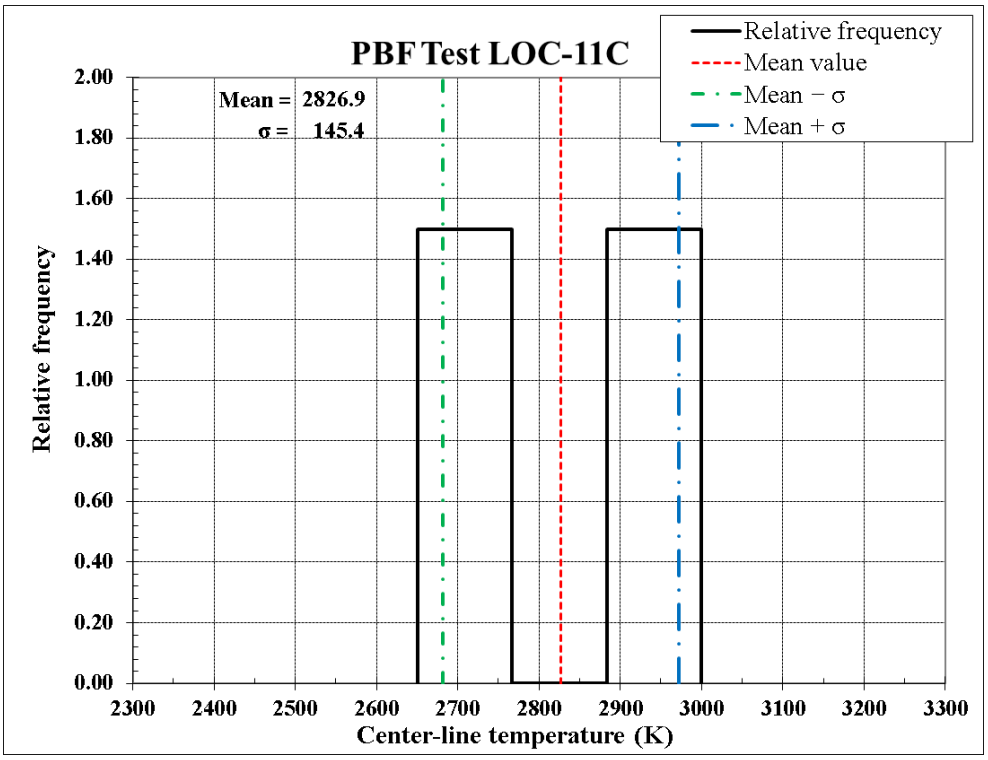



*(a) SPECTRA, Case 2-Cd*

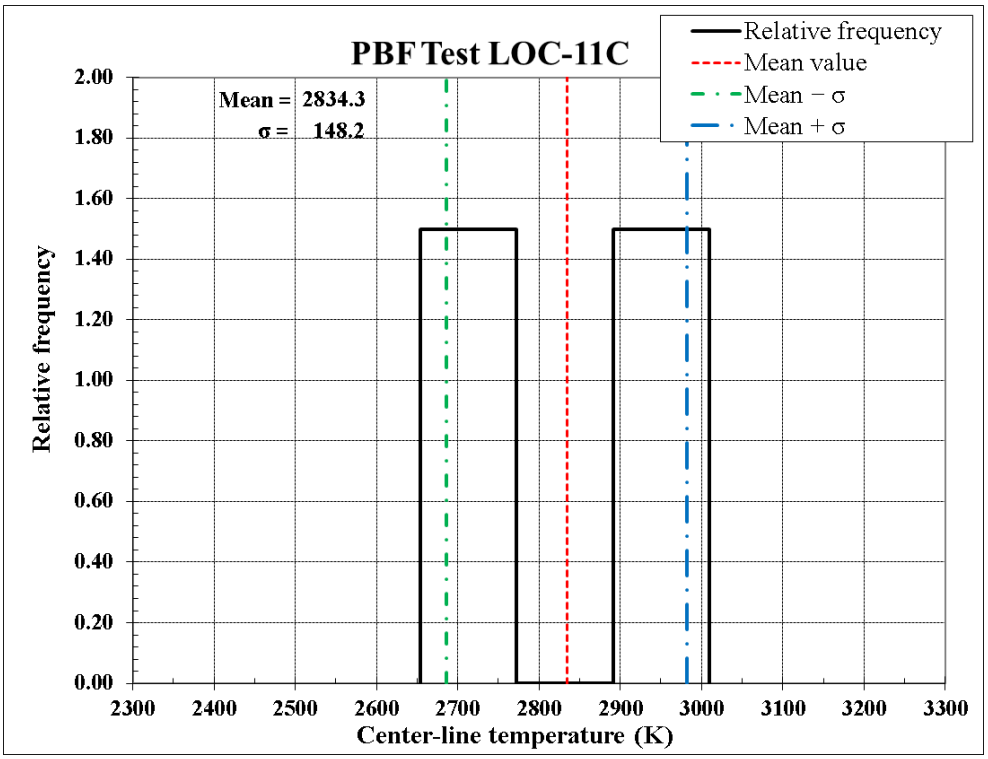



*(b): RELAP5, Case 2*

*Figure 66: Gap conductance at t=10,000 s, RELAP5, DS-Standard (Case 2)*

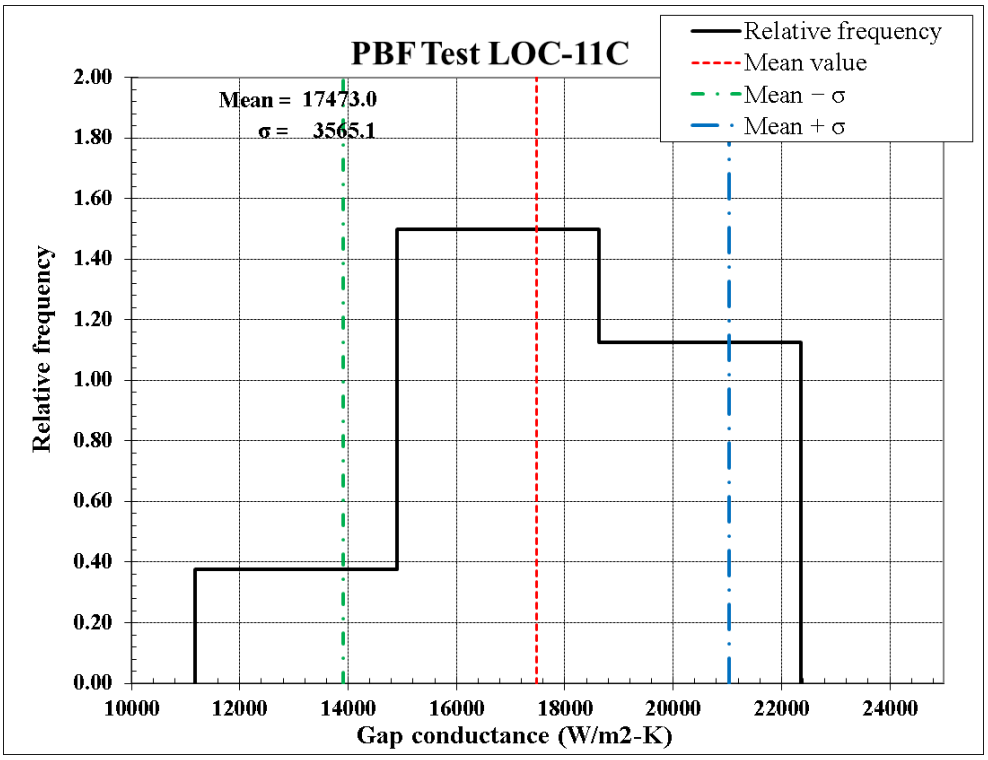



*(a) SPECTRA, Case 3-Cd*

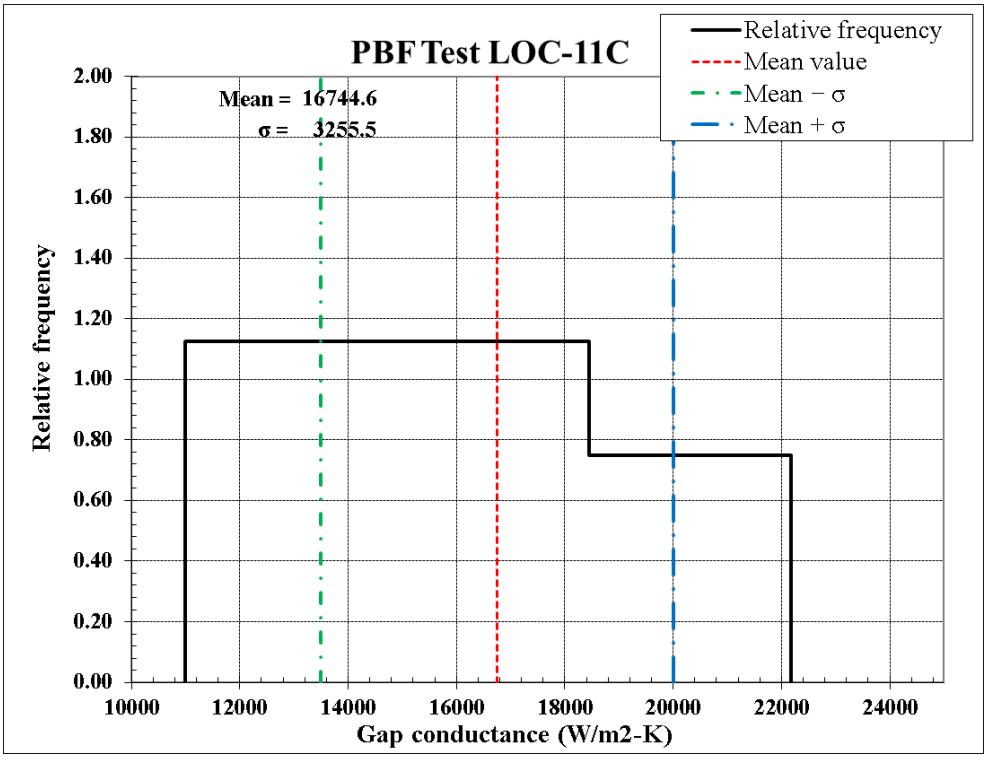



*(b): RELAP5, Case 3*

*Figure 67: Centerline temperature at t=10,000 s, RELAP5, DS-H (Case 3)*

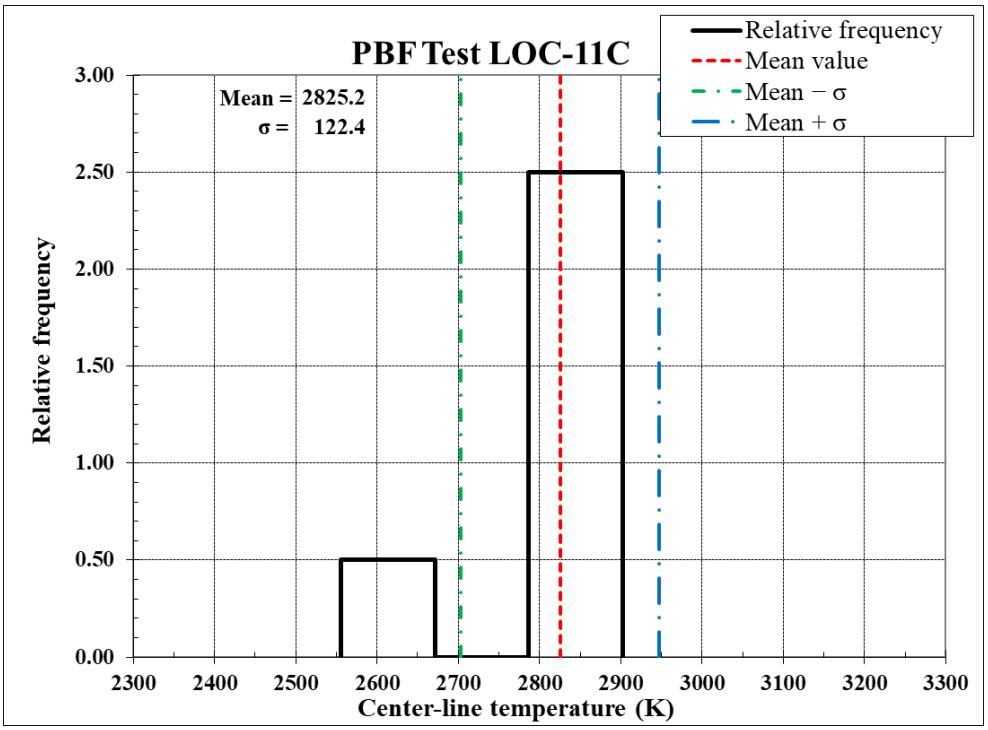



*(a) SPECTRA, Case 3-Cd*

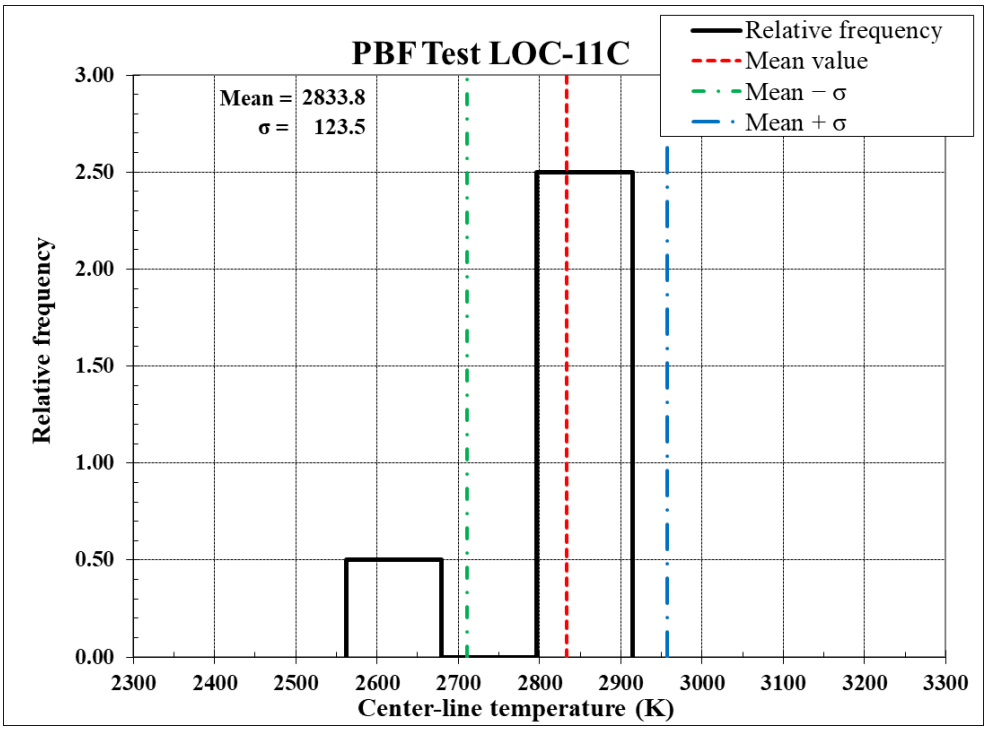



*(b): RELAP5, Case 3*

*Figure 68: Gap conductance at t=10,000 s, RELAP5, DS-H (Case 3)*

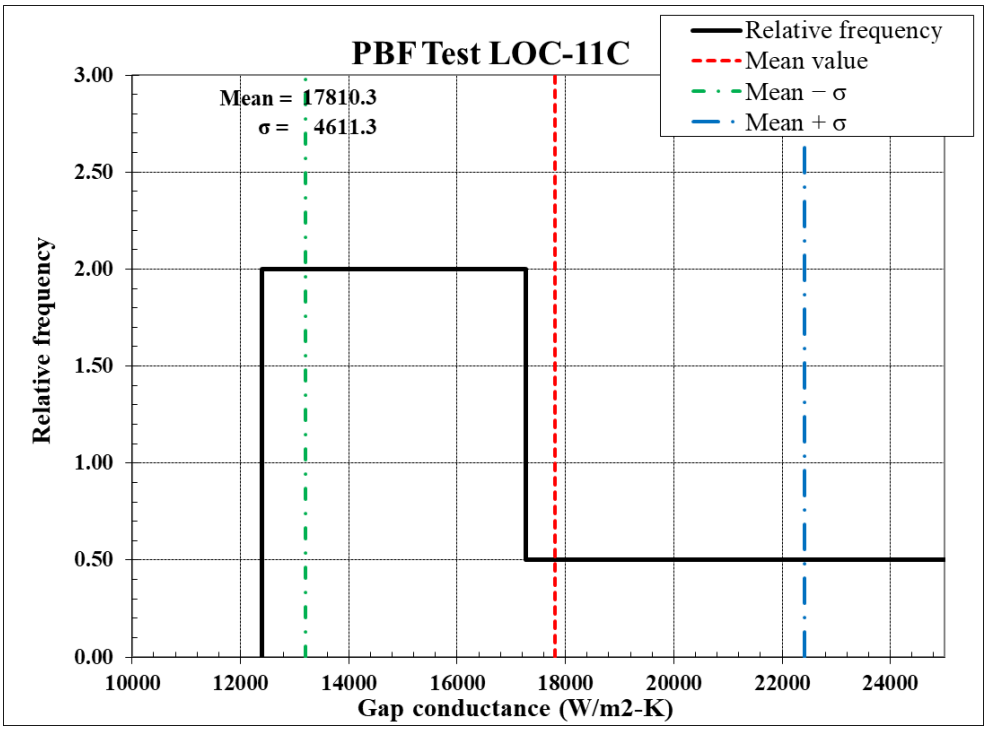



*(a) SPECTRA, Case 4-Cd*

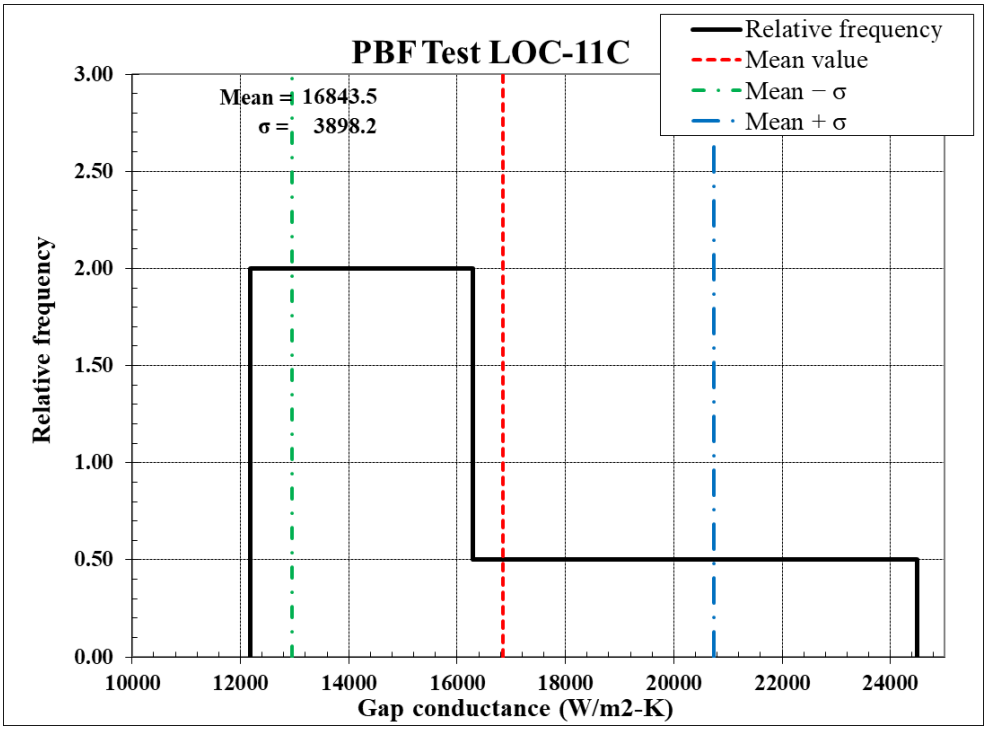



*(b): RELAP5, Case 4*

*Figure 69: Centerline temperature at t=10,000 s, RELAP5, DS-Simplex (Case 4)*




*(a) SPECTRA, Case 4-Cd*




*(b): RELAP5, Case 4*

*Figure 70: Gap conductance at t=10,000 s, RELAP5, DS-Simplex (Case 4)*

## 4.5 PBF Test LOC-11C, MELCOR Analysis

MELCOR [4] does not have a dynamic gap expansion model. Therefore, the case presented in this section is provided mainly as a showcase how to run MELCOR analyses. The gap is modeled as a node with gap material, which has certain (user-defined) thermal conductivity, *k* (W/m-K). The uncertain parameters are limited to only two:

- Gap conductance: the values entered are based on SPECTRA results shown in Table 9, mean value is assumed as μ = 27,000 (W/m$^2$-K), σ = 9,000 (W/m$^2$-K). The gap conductance is used to define the thermal conductivity of the gap material, *k* (W/m-K). Since the gap thickness is $10^{-4}$ m, the gap conductance is multiplied by the factor of $10^{-4}$ in order to obtain the thermal conductivity of the gap material.
- Thermal conductivity of $UO_2$: the same values as presented in section 4.2 and 4.3.

Only the DS-Hadamard methodology is used. The results are described in section 4.5.1.

### 4.5.1 DS Hadamard Methodology

The SUE input data file for the DS-Hadamard methodology is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, MELCOR
* ========================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      4    *    DS-HADAMARD
*
*
105000   'GAP-PBF-LOC-11C.GEN'                  *  BASE INPUT FILE
115000   'GAP-PBF-LOC-11C'                      *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'c:\MELCOR\EXE\MELGEN'                 *  PROGRAM TO RUN
130000    4                                     *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     2       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      1    27000.     9000.   0.0    0.0    *  GAP CONDUCTANCE
200002      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   3          2
*
305001   GAP-EDF.DAT  *  MELCOR EDF
305002   2
*
*
```

```
* ======================================================================
*  END OF INPUT FILE
* ======================================================================
*
```

The following MELCOR-specific issues need to be discussed:

- Calculations are performed in two steps. First MELGEN is executed that reads the input data file. Next the MELCOR is executed, which performs the time-dependent calculations. The MELGEN input is defined in SUE input. In the presented example the MELGEN input is GAP-PBF-LOC-11C.GEN. The MELGEN input should have the extension .GEN. The MELCOR input file must have the extension .COR. The SUE diagnostics file contains the run commands for the MELCOR runs only:

```
[...]

  CALCULATIONS OF:   4 RUNS

  COMMAND LINES EXECUTED:

 >start c:\MELCOR\EXE\MELCOR GAP-PBF-LOC-11C-001.COR
 >start c:\MELCOR\EXE\MELCOR GAP-PBF-LOC-11C-002.COR
 >start c:\MELCOR\EXE\MELCOR GAP-PBF-LOC-11C-003.COR
 >start c:\MELCOR\EXE\MELCOR GAP-PBF-LOC-11C-004.COR
 >start c:\MELCOR\EXE\MELCOR GAP-PBF-LOC-11C-000.COR

  ->  RUN STATISTICS
      ---------------------------------------------------------------------
      Analyzed runs           :     4
      Processor time (CPU) [s]:  0.328       ( 0.910E-04 [hrs] )
      Clock time     (RUN) [s]:   145.       ( 0.404E-01 [hrs] )
      ---------------------------------------------------------------------
```

- In order to allow simultaneous execution, the default file names, e.g., MEGOUT, MELOUT, etc. is changed by SUE. This is done automatically by supplementing the .GEN and *.COR files by the appropriate file definitions. In the current example, the input file name is GAP-PBF-LOC-11C. For the run number 001, it is: GAP-PBF-LOC-11C-001. The following records are automatically inserted in the *.GEN and *.COR files:

  - GAP-PBF-LOC-11C-001.GEN:

```
OUTPUTF  GAP-PBF-LOC-11C-001-G.OUT
DIAGF    GAP-PBF-LOC-11C-001-G.DIA
RESTARTF GAP-PBF-LOC-11C-001.RST
```

  - GAP-PBF-LOC-11C-001.COR:

```
OUTPUTF  GAP-PBF-LOC-11C-001.OUT
PLOTF    GAP-PBF-LOC-11C-001.PLT
DIAGF    GAP-PBF-LOC-11C-001.DIA
EXTDIAGF GAP-PBF-LOC-11C-001.EXD
MESSAGEF GAP-PBF-LOC-11C-001.MES
RESTARTF GAP-PBF-LOC-11C-001.RST
```

For the current methodology and two uncertain parameters, the number of runs is 4. The SUE output file is

```
[...]
 =IN=  TOTAL NO. OF RUNS AND DETERMINATION OF UNCERTAIN PARAMETERS

 =IN=  TOTAL NO. OF RUNS  : NRUNST = 4

 =IN=  DETERMINATION OF UNCERTAIN PARAMETERS
       DETERMINISTIC SAMPLING - HADAMARD MATRIX

FULL HADAMARD MATRIX

 \  J:
  \   1  2  3  4
 I \ -- -- -- --
  1   1  1  1  1
  2   1 -1  1 -1
  3   1  1 -1 -1
  4   1 -1 -1  1

REDUCED HADAMARD MATRIX

 \ RUN:
  \   1  2  3  4
PAR\ -- -- -- --
  1   1 -1  1 -1
  2   1  1 -1 -1

TRANSPOSED REDUCED HADAMARD MATRIX

 \ PAR:
  \   1  2
RUN\ -- --
  1   1  1
  2  -1  1
  3   1 -1
  4  -1 -1

================================================================================
 =IN=  END OF UNCERTAIN PARAMETERS DATA
================================================================================




================================================================================
 =IN=  PLOT PARAMETERS DATA
================================================================================

  RESULT FILE  :  MELCOR OUTPUT, EDF (IOUTPT = 3)

  OUTPUT FORMAT:  *.CSV, EXCEL FILES (IFORMT = 2)

  LIST OF PLOT PARAMETERS

  No.    NAME
  ---    ----------------
   1     GAP-EDF.DAT
   2     2

  MELCOR EDF FILE          : GAP-EDF.DAT
  NUMBER OF PLOT PARAMETERS:   2

================================================================================
 =IN=  END OF PLOT PARAMETERS DATA
================================================================================
```

```
================================================================================
 =SL=  VALUES OF UNCERTAIN PARAMETERS IN ALL RUNS
================================================================================

      VALUES OF PARAMETERS
 RUN            1            2
 --- ------------ ------------
 001  3.60000E+04  1.10000E+00
 002  1.80000E+04  1.10000E+00
 003  3.60000E+04  9.00000E-01
 004  1.80000E+04  9.00000E-01
 000  2.70000E+04  1.00000E+00

================================================================================
 =SL=  OUTPUT OF CALCULATED RESULTS
================================================================================

[...]

       MAXIMUM PEAK VALUE
       ==================
       TIME = 1.00000E+04

        RUN      VALUE
       -----  ------------
          1    2.57157E+03
          2    2.65077E+03
          3    2.91208E+03
          4    2.98009E+03

                  VALUE      RUN
              ------------  -----
       MEAN :  2.77863E+03
       SIGMA:  1.71477E+02
       MIN. :  2.57157E+03      1
       MAX. :  2.98009E+03      4

            PARAMETER RANGE         No. OF     RELATIVE
         MINIMUM       MAXIMUM       RUNS      FREQUENCY
       ------------  ------------  ------  ------------
        2.57157E+03   2.70774E+03       2    1.50000E+00
        2.70774E+03   2.84392E+03       0    0.00000E+00
        2.84392E+03   2.98009E+03       2    1.50000E+00
[...]
```

The results are shown in Figure 71 and Figure 72. Figure 71 and Figure 72 show relative frequencies, i.e. relative number of runs that give the value of the quantity of interest within a certain range (based on the *.OUT file - section 3.3.1, bottom: "relative frequency" versus "parameter range"). The results are summarized in Table 20. The gap conductance parameters are printed in italics, as these are input parameters to the analysis.

The method presented here was tested using MELCOR version 1.8.6 [4], however it is applicable also to the most recent MELCOR versions.

*Table 20: Main parameters, MELCOR, Case 3*

| Case | Center-line T (K) | | Gap conductance(kW/m$^2$-K) | |
|---|---|---|---|---|
| | **Mean, $\mu$** | **Std. dev. $\sigma$** | **Mean, $\mu$** | **Std. dev. $\sigma$** |
| Case 3 | 2779 | 171 | *27.0* | *9.0* |

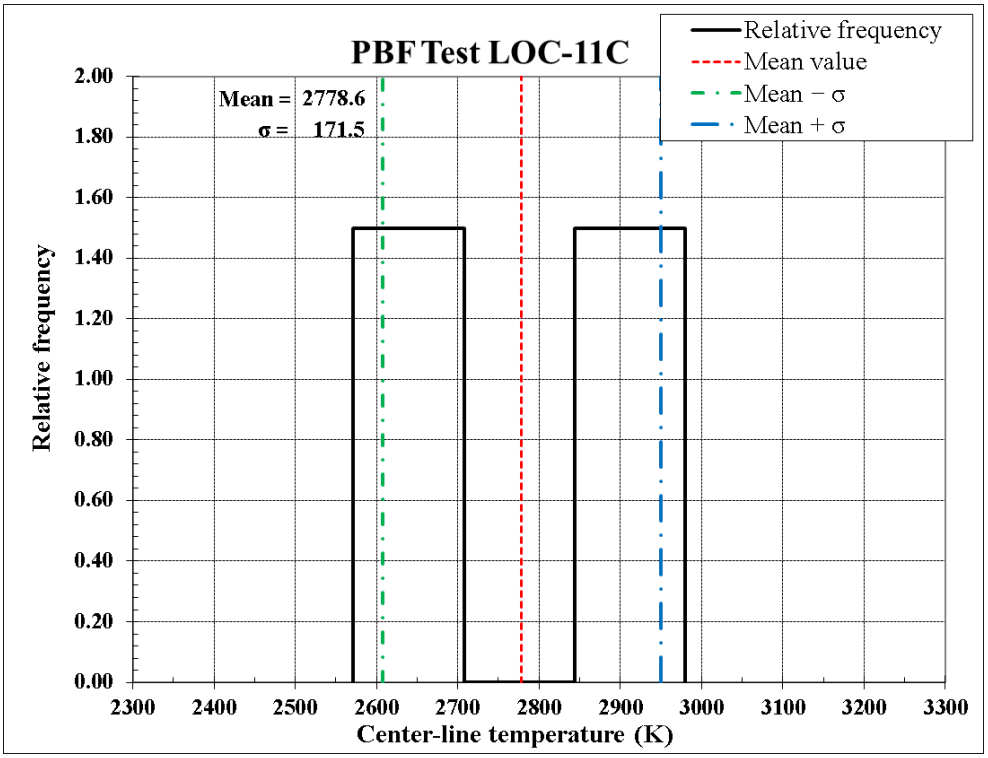



*Figure 71: Centerline temperature at t=10,000 s, MELCOR, DS-H (Case 3)*

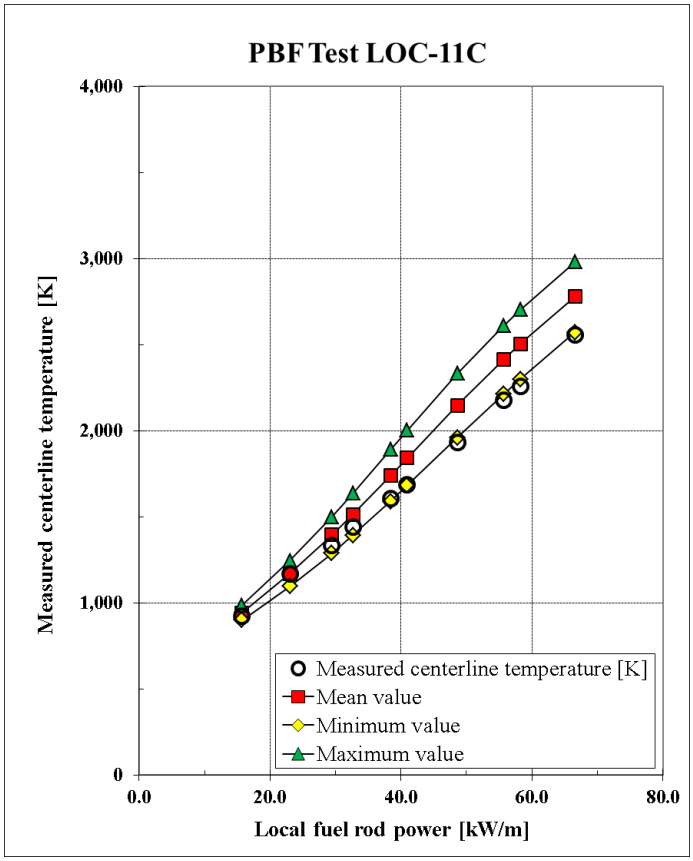



*Figure 72: Centerline temperatures, MELCOR, DS-H (Case 3)*

## 4.6 PBF Test LOC-11C, Analysis with "Other Code"

SUE may also be used with other codes, provided that the quantities of interest may be written to a simple text file or CSV file (see section 3.1.14). A test case was set up to demonstrate this capability. The test case is performs analysis using the DS-Hadamard methodology. SPECTRA code is used. The quantities of interest are written to a file "QOI" using the External Data File (EDF Package) in SPECTRA. The SUE input data file is presented below.

```
*
= SUE INPUT FOR: GAP-PBF-LOC-11C, SPECTRA AS "OTHER CODE"
* ========================================================
*
*
*  1.)   MAIN DATA
*
*        IMTSEL - Selection of methodology
100000      3    *    3=DS-HADAMARD
*
*
105000   'GAP-PBF-LOC-11C.SPE'                    *  BASE INPUT FILE
115000   'GAP-PBF-LOC-11C.SPE'                    *  FILE CONTAINING UNCERTAIN PARAMETERS
125000   'C:/SPECTRA/Z-EXE/SPECTRA.EXE'           *  PROGRAM TO RUN
130000    10                                      *  MAX. NUMBER OF SIMULTANEOUS RUNS
*
*
*  2.)   UNCERTAIN INPUT PARAMETERS
*
*        INPOPT  NINTDF
200000     1       0
*
*        IDISTR = DISTRIBUTION TYPE, 1=NORMAL, 2=UNIFORM
*
*        IDISTR    MEAN     SIGMA   MIN    MAX
200001      2    0.100E-3   0.0     0.88   1.12   *  INITIAL GAP SIZE
200002      1    3.300E-6   0.3     0.0    0.0    *  FUEL SURFACE ROUGHNESS
200003      1    1.780E-6   0.3     0.0    0.0    *  CLAD SURFACE ROUGHNESS
200004      1    0.90       0.1     0.0    1.1111 *  CENTERLINE SHIFT
200005      1    1.0        0.1     0.0    0.0    *  FUEL THERMAL CONDUCTIVITY
*
*
*  3.)   OUTPUT PARAMETERS
*        IOUTPT     IRORMT
300000   5          0
*
305000   QOI
*
305001   QOI1
305002   QOI2
305003   QOI3
30
*
*
* ========================================================================
*  END OF INPUT FILE
* ========================================================================
*
```

The results are identical to those presented in section 4.2.3, and therefore are not presented here.

# 5 Summary and Conclusions

## 5.1 Summary

This report describes the development and application of a user-friendly and robust uncertainty and sensitivity calculation tool, developed primarily for system thermal-hydraulic codes. It is however quite general and applicable for any code, e.g., CFD.

The tool has been developed and assessed for the application of the statistical methodology, which propagates uncertainties in input and physical model variables to output results. As a demonstration, the thermal behavior of the LWR fuel rod has been investigated and compared to the measured data. Within the present study a relatively small number of input variables were considered. A key aspect being the identification of reliable uncertainty information on the different parameters and models involved.

## 5.2 Conclusions

The main conclusions from the test case calculations performed are as follows.

- The Deterministic Sampling (DS) methodologies give very similar results as the Random Sampling (RS) methodology. The DS methodologies allow to significantly reduce the number of runs when the number of uncertain parameters is small. In the present case the DS methodologies required 6 - 10 runs, while the RS methodology requires hundreds of calculations.
- Verification of SUE was performed using SPECTRA, RELAP5, and MELCOR. Calculations are described in this report. Further verification was performed by comparing SUE / RELAP5 results with RAVEN / RELAP5 results [23] for an analysis of Reactivity Initiated Accident using Wilks and hot spot methodology. It was shown that the RAVEN / RELAP5 analyses can be redone by SUE / RELAP5 and exactly the same results are obtained (unless random sampling is used).

## 5.3 Recommendations for Future Work

The following additions/improvements are planned to be implemented in the future.

- Currently none identified.

# References

[1] M.M. Stempniewicz, "SPECTRA Sophisticated Plant Evaluation Code for Thermal-Hydraulic Response Assessment, Volume 1 – Program Description, Volume 2 – User's Guide, Volume 3 – Verification and Validation, Volume 4 – Code Structure, Development, Hardware and Software Requirements"
https://marekstempniewicz/files/Spectra-Vol1.pdf
https://marekstempniewicz/files/Spectra-Vol2.pdf
https://marekstempniewicz/files/Spectra-Vol3.pdf
https://marekstempniewicz/files/Spectra-Vol4.pdf

[2] "RELAP5/MOD3.3 Code Manual, Volume I: Code Structure, System Models and Solution Methods", NUREG/CR-5535/Rev P4-Vol I, October 2010.

[3] "RELAP5/MOD3.3 Code Manual, Volume IV: Models and Correlations", NUREG/CR-5535/Rev P4-Vol IV, October 2010.

[4] 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.

[5] Jong-Rong Wang, Chiung-Wen Tsai, Hao-Tzu Lin, Chunkuan Shih, "Performing Uncertainty Analysis of IIST Facility SBLOCA by TRACE and DAKOTA", NUREG/IA-0428, September 2013.

[6] Horst Glaeser, "GRS Method for Uncertainty and Sensitivity Evaluation of Code Results and Applications", Hindawi Publishing Corporation, Science and Technology of Nuclear Installations, Volume 2008, Article ID 798901, 7 pages, doi:10.1155/2008/798901

[7] N.W. Porter, "Wilks' formula applied to computational tools: A practical discussion and verification", Annals of Nuclear Energy 133 (2019) 129–137.

[8] "PREMIUM: A Benchmark on the Quantification of the Uncertainty of the Physical Models in System Thermal-hydraulic Codes - Methodologies and Data Review", Nuclear Safety, NEA/CSNI/R(2016)9, April 2016.

[9] A. Cutrono Rakhimov, D.C. Visser, E.M.J. Komen, "Uncertainty Quantification method for CFD applied to the turbulent mixing of two water layers – II: Deterministic Sampling for input uncertainty", Nuclear Engineering and Design 348 (2019).

[10] C. Fedon, E.Y. Garcia Cervantes, L. Salamon, B. Erasmus, "Application of deterministic sampling methods for uncertainty quantification in manufacturing tolerances in neutron physics", Nuclear Engineering and Design 373 (2021).

[11] E.Y. Garcia Cervantes, B. Erasmus, S. van der Marck, C. Fedon, "Quantification of uncertainties due to manufacturing tolerances using deterministic sampling methods", Nuclear Engineering and Design 382 (2021).

[12] Hadamard matrix, https://en.wikipedia.org/wiki/Hadamard_matrix

[13] D. Blanchet, K. Mikityuk, P. Coddington and R. Chawla, "An Uncertainty Assessment Methodology for Materials Behaviour in Advanced Fast Reactors", https://www.psi.ch/sites/default/files/import/fast/PublicationsEN/FB-DOC-07-012.pdf

[14] D. Rochman, "Nuclear Data Uncertainties for Typical LWR Fuel Assemblies and a Simple Reactor Core", https://oa.upm.es/49831/1/INVE_MEM_2017_270635.pdf

[15] S. S.Wilks, "Determination of sample sizes for setting tolerance limits," Annals of Mathematical Statistics, vol. 12, no. 1, pp. 91–96, 1941.

[16] S. S. Wilks, "Statistical prediction with special reference to the problem of tolerance limits," Annals of Mathematical Statistics, vol. 13, no. 4, pp. 400–409, 1942.

[17] J. R. Larson, et al. PBF-LOCA Test Series Test LOC-11 Test Results Report. NUREG/CR-0618, TREE-1329. Idaho National Engineering Laboratory. April 1979. https://inis.iaea.org/search/searchsinglerecord.aspx?recordsFor=SingleRecord&RN=11499829

[18] https://www.wallstreetmojo.com/uniform-distribution/

[19] https://en.wikipedia.org/wiki/Pearson_correlation_coefficient

[20] https://en.wikipedia.org/wiki/Spearman%27s_rank_correlation_coefficient

[21] https://www.scribbr.com/statistics/pearson-correlation-coefficient/

[22] N.E. Todreas, M.S. Kazimi, "Nuclear Systems II - Elements of Thermal-Hydraulic Design", ISBN 1-56032-079-6, 2001.

[23] M.M. Stempniewicz, "UQ Analysis of HFR Using Wilks and EHSF Methodologies - SUE / RELAP5 Analysis of Reactivity Initiated Accident", 26246/23.259712, May 2023.

[24] J.P. Hessling, "Deterministic Sampling for Propagating Model Covariance", SIAM/ASA J. Uncertainty Quantification, Vol. 1, pp. 297–318, 2013.

[25] S. Julier and J. Uhlmann, Unscented filtering and nonlinear estimation, Proc. IEEE, 92 (2004), pp. 401–422

[26] https://en.wikipedia.org/wiki/Gram-Schmidt_process

[27] J.D. Bartos, "Simplex testing", email dated 5:24 PM, June 6, 2024.

# List of tables

# List of figures

# Appendix A Sampling

## A.1 Theoretical Background

Sampling is performed by dividing the distribution function into a number intervals of equal length, followed by the random selection of a value representative for each interval. The number of intervals is a user-defined parameter, with a minimum of 3 and a maximum of 10001. The width of a single interval is equal to:

$$\Delta x = \frac{x_{\max} - x_{\min}}{NINTDF - 1}$$

The interval boundaries are defined as follows. For the first and the last interval the interval thickness is 0.5 Δ*x*. For other intervals, it is equal to Δ*x*. The boundary points are:

- For the first and the last point:

$$x_b(1) = x_{\min} \qquad x_b(N) = x_{\max}$$

- For other points:

$$x_b(i) = x_{\min} + \Delta x \cdot (i - 0.5)$$

The representative value for each interval is given by:

$$x(i) = x_{\min\, x} + \Delta x \cdot (i - 1)$$

This method is selected for its general applicability. In the case of uniform distribution, sampling could be performed by simply $x_{min}$ + RND()*($x_{max}$–$x_{min}$), where RND() is the computer-generated random number in the range 0.0 < RND() < 1.0. Thus, a continuous range of samples would be obtained. However, this could not be done for the normal distribution (or other distribution given by a function such that the inverse of the cumulative distribution, $F(x) = \int f(x)$, cannot be found analytically). With the applied method, there is a discrete number of values that may be sampled, equal to NINTDF. With increasing number of NINTDF the result will approach a continuous range. For consistency, the method is applied for both normal and uniform distributions.

The effect of NINTDF is illustrated below for the uniform distribution and normal distribution. The distribution functions *f*(*x*) and the cumulative distribution functions, *F*(*x*), are given by:

- Uniform:

$$f(x) = \frac{1}{x_{\max} - x_{\min}}$$

$$F(x) = \frac{x - x_{min}}{x_{max} - x_{min}}$$

- Normal:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left[ -\frac{1}{2} \cdot \left( \frac{x-\mu}{\sigma} \right)^2 \right]$$

$$F(x) = \frac{1}{2} \cdot \left[ 1 + erf\left( \frac{x-\mu}{\sqrt{2}\sigma} \right) \right]$$

The following values are assumed for the considered example:

- Mean value: $\mu = 0.5$
- Standard deviation $\sigma = 0.15$
- Minimum value: $x_{min} = 0.0$
- Maximum value: $x_{max} = 1.0$

First, the case of uniform distribution is shown. Figure A-1 shows the values obtained for NINTDF = 3. In this case we have three intervals:

| Interval range | Value | Probability |
|---|---|---|
| 0.00 - 0.25 | 0.00 | 0.25 |
| 0.25 - 0.75 | 0.50 | 0.50 |
| 0.75 - 1.00 | 1.00 | 0.25 |

Consequently, with these parameter SUE will sample:

- the value of x = 0.00 with probability of 0.25
- the value of x = 0.50 with probability of 0.50
- the value of x = 1.00 with probability of 0.25

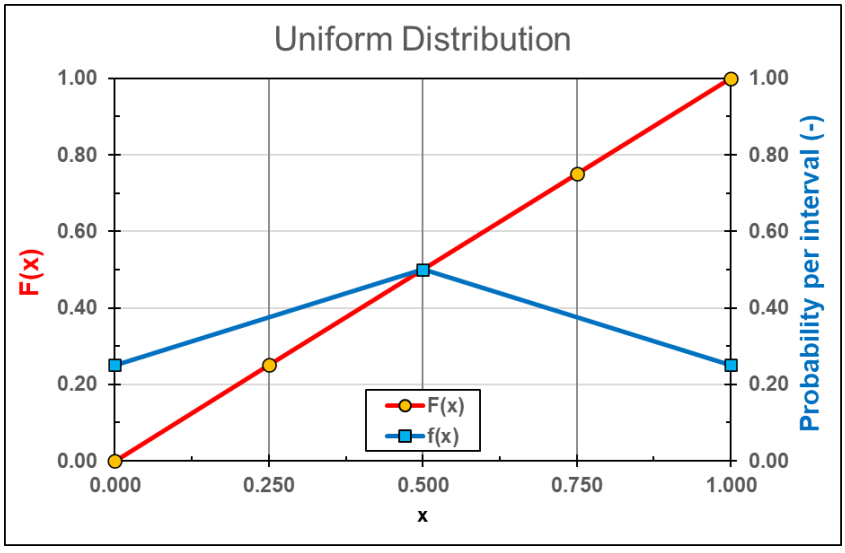


*Figure A-1: Sampling, uniform distribution, NINTDF=3*

Figure A-2 shows the values obtained for NINTDF = 11. In this case we have ten intervals:

| Interval range | Value | Probability |
|---|---|---|
| 0.00 - 0.05 | 0.00 | 0.05 |
| 0.05 - 0.15 | 0.10 | 0.10 |
| 0.15 - 0.25 | 0.20 | 0.10 |
| 0.25 - 0.35 | 0.30 | 0.10 |
| 0.35 - 0.45 | 0.40 | 0.10 |
| 0.45 - 0.55 | 0.50 | 0.10 |
| 0.55 - 0.65 | 0.60 | 0.10 |
| 0.65 - 0.75 | 0.70 | 0.10 |
| 0.75 - 0.85 | 0.80 | 0.10 |
| 0.85 - 0.95 | 0.90 | 0.10 |
| 0.95 - 1.00 | 1.00 | 0.05 |

Consequently, with these parameter SUE will sample:

- the value of x = 0.00 with probability of 0.05
- the value of x = 0.10 with probability of 0.10
- the value of x = 0.20 with probability of 0.10
- [...]
- the value of x = 0.80 with probability of 0.10
- the value of x = 0.90 with probability of 0.10
- the value of x = 1.00 with probability of 0.05

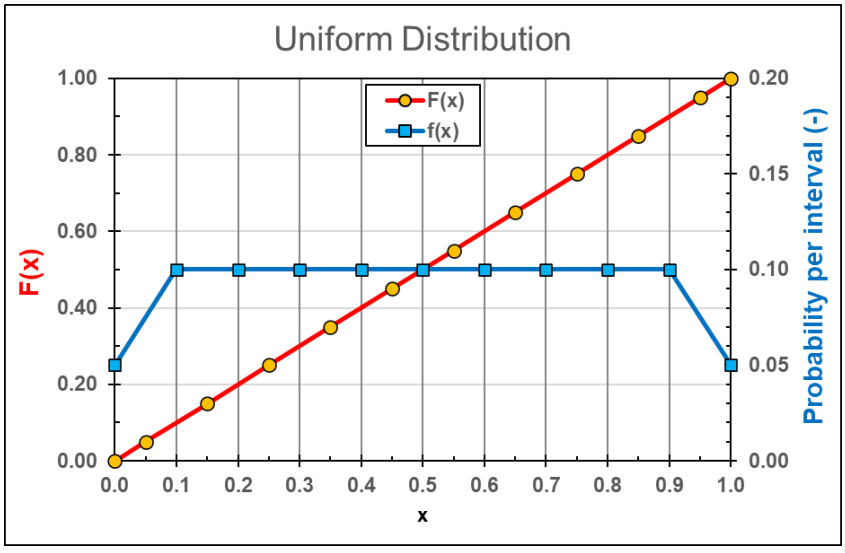



*Figure A-2: Sampling, uniform distribution, NINTDF=11*

Figure A-3 shows the values obtained for NINTDF = 101. In this case we have hundred intervals:

| Interval range | Value | Probability |
|---|---|---|
| 0.000 - 0.005 | 0.00 | 0.005 |
| 0.005 - 0.015 | 0.01 | 0.010 |
| 0.015 - 0.025 | 0.02 | 0.010 |
| 0.025 - 0.035 | 0.03 | 0.010 |
| [...] | | |
| 0.965 - 0.975 | 0.97 | 0.010 |
| 0.975 - 0.985 | 0.98 | 0.010 |
| 0.985 - 0.995 | 0.99 | 0.010 |
| 0.995 - 1.000 | 1.00 | 0.005 |

Consequently, with these parameter SUE will sample:

- the value of x = 0.00 with probability of 0.005
- the value of x = 0.01 with probability of 0.010
- the value of x = 0.02 with probability of 0.010
- the value of x = 0.03 with probability of 0.010
- [...]
- the value of x = 0.97 with probability of 0.010
- the value of x = 0.98 with probability of 0.010
- the value of x = 0.99 with probability of 0.010
- the value of x = 1.00 with probability of 0.005

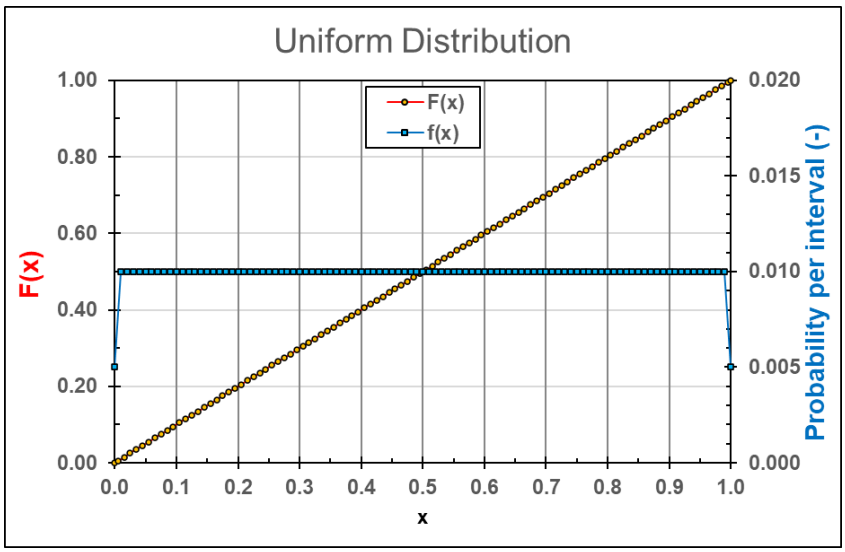



*Figure A-3: Sampling, uniform distribution, NINTDF=101*

Next, the case of uniform distribution is shown. Figure A-4 shows the values obtained for NINTDF = 3. In this case we have three intervals:

| Interval range | Value | Probability |
|---|---|---|
| 0.00 - 0.25 | 0.00 | 0.04779 |
| 0.25 - 0.75 | 0.50 | 0.90442 |
| 0.75 - 1.00 | 1.00 | 0.04779 |

Consequently, with these parameter SUE will sample:

- the value of x = 0.00 with probability of 0.04779
- the value of x = 0.50 with probability of 0.90442
- the value of x = 1.00 with probability of 0.04779

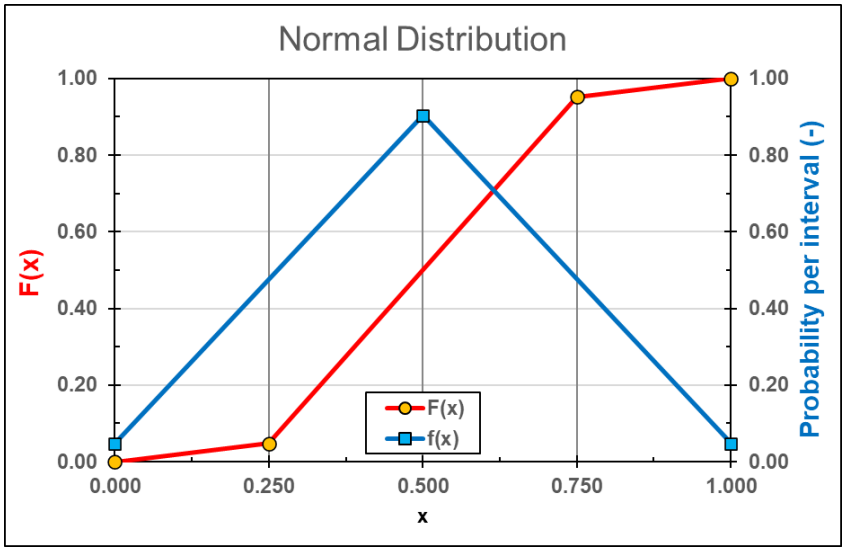



*Figure A-4: Sampling, normal distribution, NINTDF=3*

Figure A-5 shows the values obtained for NINTDF = 11. In this case we have ten intervals:

| Interval range | Value | Probability |
|---|---|---|
| 0.00 - 0.05 | 0.00 | 0.00135 |
| 0.05 - 0.15 | 0.10 | 0.00847 |
| [...] | | |
| 0.45 - 0.55 | 0.50 | 0.26112 |
| [...] | | |
| 0.85 - 0.95 | 0.90 | 0.00847 |
| 0.95 - 1.00 | 1.00 | 0.00135 |

Consequently, with these parameter SUE will sample:

- the value of x = 0.00 with probability of 0.00135
- the value of x = 0.10 with probability of 0.00847
- [...]
- the value of x = 0.50 with probability of 0.26112
- [...]
- the value of x = 0.90 with probability of 0.00847
- the value of x = 1.00 with probability of 0.00135

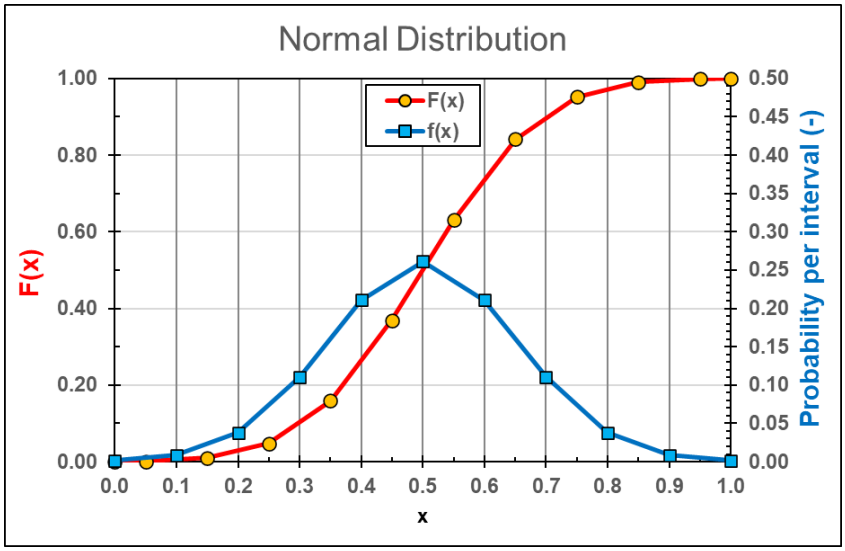



*Figure A-5: Sampling, normal distribution, NINTDF=11*

Figure A-6 shows the values obtained for NINTDF = 101. In this case we have hundred intervals:

| Interval range | Value | Probability |
|---|---|---|
| 0.000 - 0.05 | 0.00 | 0.00048 |
| 0.005 - 0.15 | 0.01 | 0.00013 |
| [...] | | |
| 0.495 - 0.505 | 0.50 | 0.02659 |
| [...] | | |
| 0.985 - 0.995 | 0.99 | 0.00013 |
| 0.995 - 1.000 | 1.00 | 0.00048 |

Consequently, with these parameter SUE will sample:

- the value of x = 0.00 with probability of 0.00048
- the value of x = 0.01 with probability of 0.00013
- [...]
- the value of x = 0.50 with probability of 0.02659
- [...]
- the value of x = 0.99 with probability of 0.00013
- the value of x = 1.00 with probability of 0.00048

In conclusion, use of a large number intervals leads to a better representation of an ideal random sampling, at the expense of slightly larger computational time. However, typically the execution time is primarily governed by the execution of codes that are run, so in practice the number of intervals does not affect the execution time.

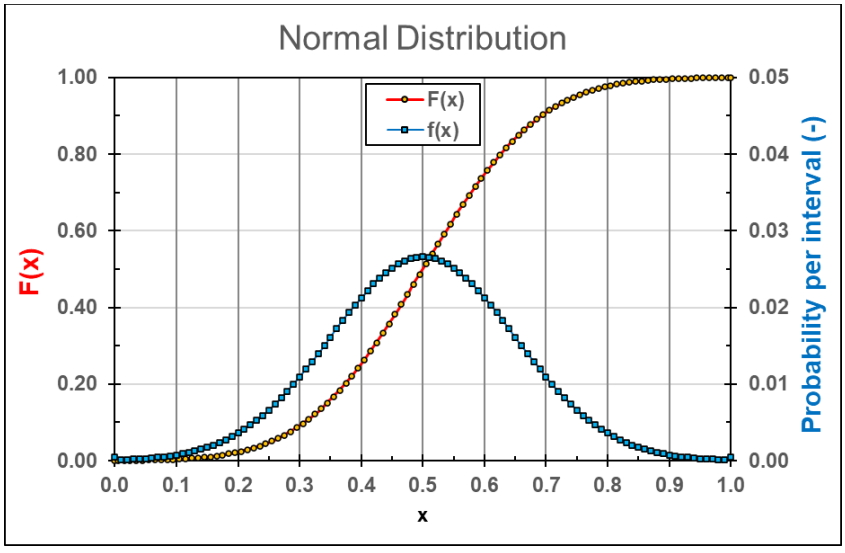



*Figure A-6: Sampling, normal distribution, NINTDF=101*

## A.2 Practical Results - Influence of NINTDF

In order to check the influence of the number of intervals on sampling results, sensitivity calculations were performed using NINTDF from ~$10^2$ to ~$10^9$. The sensitivity calculations were performed for the RELAP5, RS Case 1-95 (section 4.3.1). The results are shown in Figure A-7 and A-8. The results are summarized as follows:

- Visible (but small) differences are seen for NINTDF of ~$10^2$ ÷ ~$10^4$.
- For NINTDF of ~$10^5$ ÷ ~$10^9$. there are no visible differences on the graphs.
- A significant CPU time is required for sampling for NINTDF of >$10^8$.

Based on the above results, the value of NINTDF of ~$10^6$ was selected as the default value (section 3.1.8). Values significantly larger than $10^8$ are not recommended.

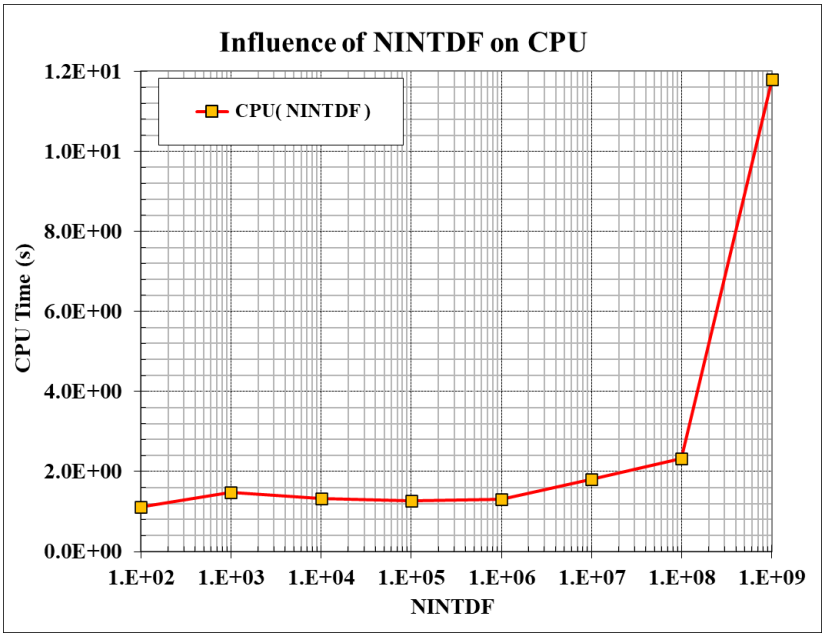
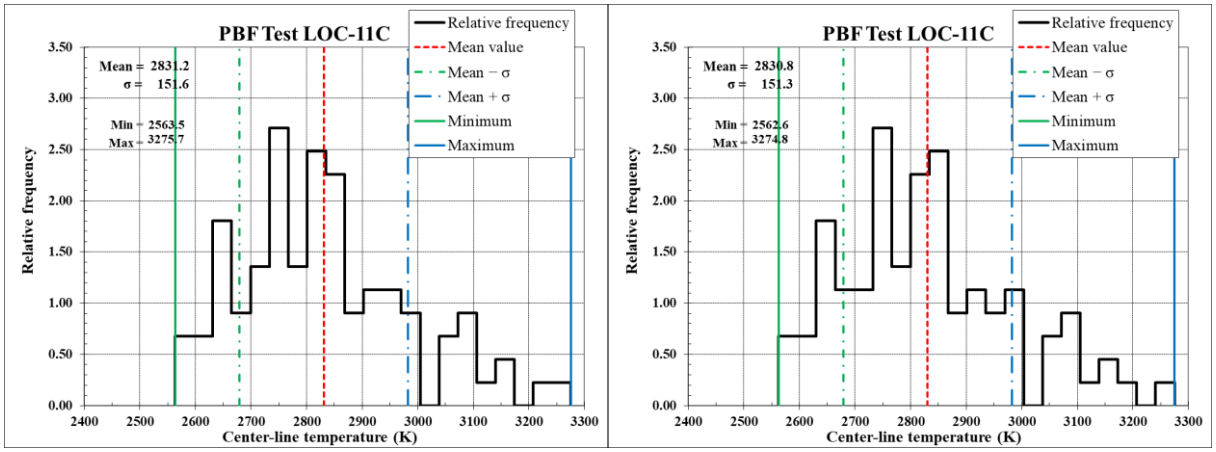
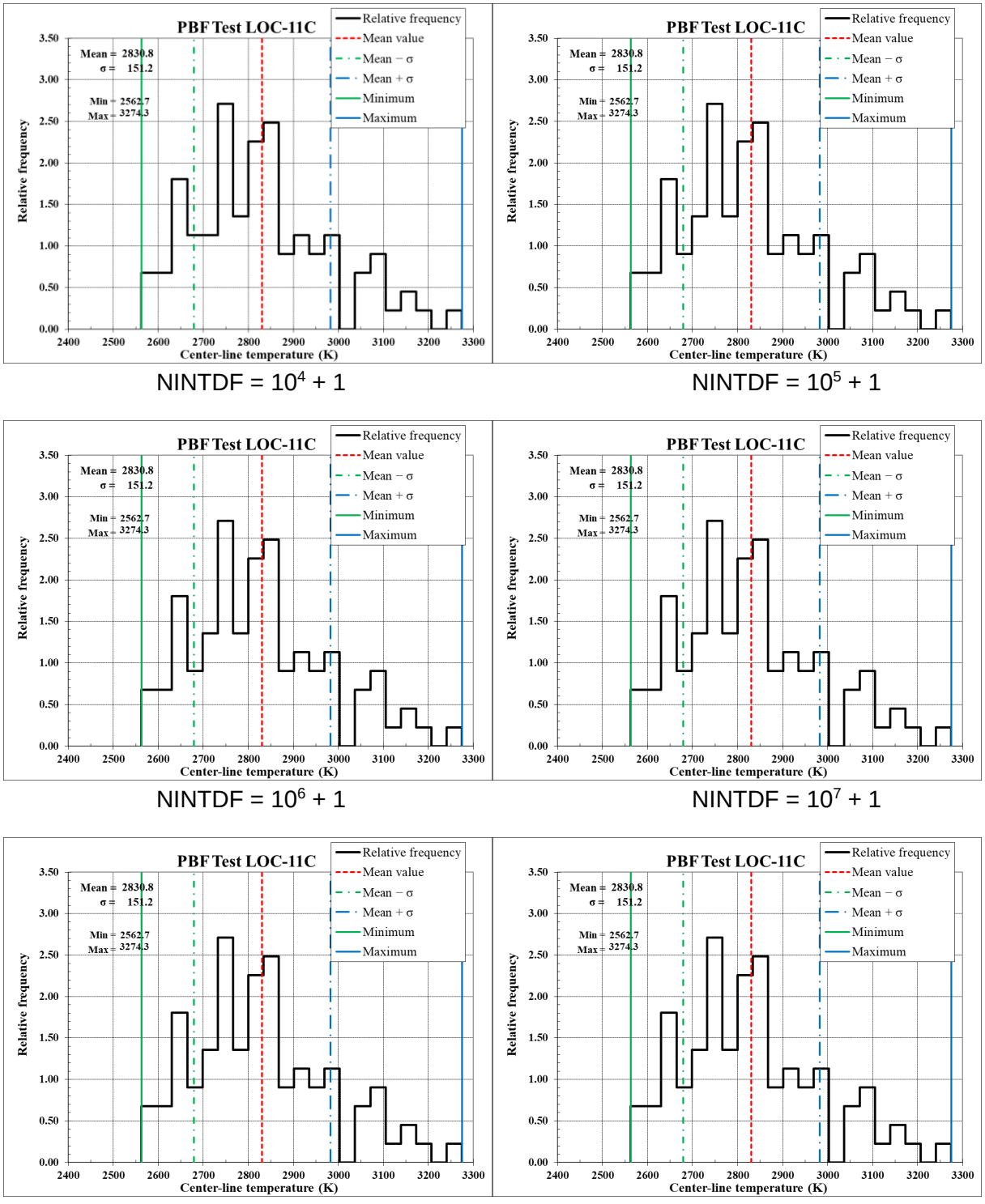



*Figure A-7: Influence of NINTDF on CPU*




NINTDF = $10^2$ + 1 NINTDF = $10^3$ + 1




NINTDF = $10^4$ + 1 NINTDF = $10^5$ + 1

NINTDF = $10^6$ + 1 NINTDF = $10^7$ + 1

NINTDF = $10^8$ + 1 NINTDF = $10^9$ + 1

*Figure A-8: Maximum fuel temperature, RELAP5, RS Case 1-95 (section 4.3.1)*

# Appendix B Project Archive

All documentation as well as the source code, the executable, and the input / output files from the example tests are located in the directory:

**\SUE**

- Source code:

```
\INPUT0\      general input procedures
\INPOUT\      input/output procedures specific to SUE
\SOLVER\      the main body of the SUE solver
\SUE\         the main program, version identifiers, availability limits
```

- Executable:

```
\Z-EXE\       the executable code
```

- Documentation

```
\Z-MANUALS\
      \Doc-Report   SUE description
      \Doc-Source   Literature references
```

- Test Problems

```
\Z-INPUTS\
SPECTRA runs:
      \GAP-SPE-1-95       IMTSEL=1, RS, sec. 4.2.1
      \GAP-SPE-1-99-1     IMTSEL=1, RS, sec. 4.2.1
      \GAP-SPE-1-99-2     IMTSEL=1, RS, sec. 4.2.1
      \GAP-SPE-2          IMTSEL=2, DS-Standard, sec. 4.2.2
      \GAP-SPE-3          IMTSEL=3, DS-Hadamard, sec. 4.2.3
      \GAP-SPE-4          IMTSEL=4, DS-Simplex, sec. 4.2.4
      \GAP-SPE-5-1        IMTSEL=5, EHSF, IHSDEF=1, sec. 4.2.6
      \GAP-SPE-5-1        IMTSEL=5, EHSF, IHSDEF=2, sec. 4.2.6
      \GAP-SPE-6          IMTSEL=6, User-defined matrix, sec. 4.2.7
      \GAP-SPE-1-95-Cd    Influence of Cd, sec. 4.4
      \GAP-SPE-1-99-1-Cd
      \GAP-SPE-1-99-2-Cd
      \GAP-SPE-2-Cd
      \GAP-SPE-3-Cd
      \GAP-SPE-4-Cd
      \GAP-SPE-3-ABS      absolute versus relative input, effect of INPOPT
      \GAP-SPE-3-DEP      conductivity input as dependent parameters
RELAP5 runs:
      \GAP-REL-1-95       IMTSEL=1, RS, sec. 4.3.1
      \GAP-REL-1-99-1     IMTSEL=1, RS, sec. 4.3.1
      \GAP-REL-1-99-2     IMTSEL=1, RS, sec. 4.3.1
      \GAP-REL-2          IMTSEL=2, DS-Standard, sec. 4.3.2
      \GAP-REL-3          IMTSEL=3, DS-Hadamard, sec. 4.3.3
      \GAP-REL-4          IMTSEL=3, DS-Simplex, sec. 4.3.4
MELCOR runs:
      \GAP-MEL-3          IMTSEL=3, DS-H, sec. 4.5
Other code runs:
      \GAP-XXX-3          IMTSEL=3, DS-H, sec. 4.6
```

# Appendix C Distribution list

| **External recipient** | ***Digital*** | ***Hardcopy*** | ***Date*** |
|---|---|---|---|
| | ☐ | ☐ | |
| | ☐ | ☐ | |
| | ☐ | ☐ | |
| **Internal recipient** | ***Digital*** | ***Hardcopy*** | ***Date*** |
| M.M. Stempniewicz | ☒ | ☐ | 2024-11-30 |
| E.A.R. de Geus | ☒ | ☐ | 2024-11-30 |
| M.L.F. Slootman | ☒ | ☐ | 2024-11-30 |
| P.A. Breijder | ☒ | ☐ | 2024-11-30 |
| D.C. Visser | ☒ | ☐ | 2024-11-30 |
| C. Fedon | ☒ | ☐ | 2024-11-30 |
| F. Roelofs | ☒ | ☐ | 2024-11-30 |
| E.M.J. Komen | ☒ | ☐ | 2024-11-30 |
| I. de Kock | ☒ | ☐ | 2024-11-30 |