

COEFFICIENTS FOR I-131 SORPTION ON DIFFERENT SURFACES

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ABSTRACT

Sorption of fission product vapors on metallic surfaces and dust particles is an important safety aspect of HTR reactors. Safety analyses of these reactors are performed using computer codes, such as MELCOR, RADAX, SPECTRA. These codes have sorption models allowing to compute the sorption rates of different fission products on surfaces. The code users must supply the model coefficients applicable for the particular surface and isotope. This paper describes the work performed to find relevant experimental data and find the sorption coefficients that represent well the available data for iodine on different surfaces. The purpose of this work is to generate a set of coefficients that may be recommended for the computer code users. Calculations were performed using the computer code SPECTRA.

The following data was analyzed:

- Sorption of I-131 on graphite
- Sorption of I-131 on steel
- Sorption of I-131 on dust

The results are summarized as follows:

- The available data is provided in form of Langmuir isotherms.
- The Langmuir isotherms do not provide sufficient data to define all sorption coefficients. The Langmuir isotherm provides equilibrium data; the relaxation time (to get to equilibrium) needs to be guessed. In practice this means that one of the sorption coefficients must be guessed. In the present calculations the desorption coefficient was being guessed and then varied in sensitivity calculations. The calculations showed that surface concentration is not sensitive to the choice of the parameter.
- The sorption model in SPECTRA is capable to correctly reproduce the sorption behavior given by the Langmuir isotherms.

- Out of the calculated cases, the highest activity (surface concentration) is observed on the steel surface; the lowest on the graphite surfaces.
- The present work may serve as a useful guide of how to convert the Langmuir isotherm data into the input parameters required for computer code calculations.

1 INTRODUCTION

Sorption of fission product vapors on metallic surfaces and dust particles is an important safety aspect of HTR reactors. Safety analyses of these reactors are performed using computer codes, such as SPECTRA [1], RADAX [2], MELCOR [3]. These codes have sorption models allowing to compute the sorption rates of different fission products on surfaces. The code users must supply the model coefficients applicable for the particular surface and isotope. The sorption process has been theoretically investigated and described in literature [4], [5], [6], [7]. The principal difficulty in applying the sorption models in practice is lack of knowledge of coefficients applicable for each surface and each fission product vapor. The coefficients must be based on measured data, which are still quite scarce. The analysts must often guess values of certain model parameters because the available data is simply insufficient.

This paper describes the work performed to find relevant experimental data and find the sorption coefficients that represent well the available data for iodine on different surfaces. The purpose of this work is to generate a set of coefficients that may be recommended for the computer code users. The analytical work was performed using the computer code SPECTRA [1].

Sorption data for Iodine I-131 on different surfaces is available in the review of fission product plateout and liftoff in MHTGR systems, performed at Oak Ridge and

documented in reference [5]. The data available there include:

- Sorption of I-131 on graphite
- Sorption of I-131 on steel
- Sorption of I-131 on dust

The data is available in terms of Langmuir isotherms. Therefore the Langmuir isotherm is discussed first, in section 2. Next, conversion of the Langmuir isotherm data into the sorption model applied in SPECTRA and results of calculations are described in the sections 3, 3.2, and 3.3 for the graphite, steel, and dust. Results obtained for different surfaces are compared in section 4. Finally, summary and conclusions are given in section 5. The presented conversion may serve as a useful guide for the code users how to convert Langmuir isotherm data into the code-required input coefficients

2 LANGMUIR ISOTHERM

The sorption process is described in reference [5] by making use of the Langmuir isotherm. Written for an i -th isotope out of a total of N isotopes, it has the form:

$$C_{S,i} = \frac{LKP_i}{1 + K \sum_{i=1}^N P_i} \quad (1)$$

- $C_{S,i}$ surface concentration of the sorbed isotope i , [mol/m²]
 P_i partial pressure of the isotope i in equilibrium with $C_{S,i}$, [Pa]
 L concentration of the sorption sites, [kg/m²]
 K sorption equilibrium constant, [Pa⁻¹]

The term $\sum P_i$ is the element partial pressure summed for all isotopes. Therefore, whenever $\sum P_i$ is significant compared with unity, the sorbed concentration of the isotope i is coupled with sorbed concentrations of all other isotopes. In such case the transport behavior of, say, I-131, must be solved simultaneously with other isotopes. It has been shown in [5] that for iodine in the MHTGR primary system: $K \sum P_i \ll 1$, which results in simplification:

$$C_{S,i} = LKP_i \quad (2)$$

The above equation applies in the so-called Henrian regime. The surface coverage, $C_{S,i}$, is in this regime proportional to the partial pressure P_i , and independent of other isotopes, which provides a considerable computational simplification.

Construction of a Langmuir isotherm is quite simple, and is illustrated in Figure 1. For pressures above $1/K$ the surface concentration (surface load) is equal to L . For

pressures lower than $1/K$, the load increases linearly with pressure. Figure 1 shows a Langmuir isotherm for $L=10^{-5}$, $K=10^4$.

There are several key features of the Langmuir isotherm, worth remembering:

- Pressure at which line becomes flat is given by: $P_{\max} = 1/K$
- Maximum surface concentration: $C_{S,\max} = L$
- The ratio between the surface concentration and the vapor concentration (the slope) of the left part of the curve is given by: $C_S / P = KL$

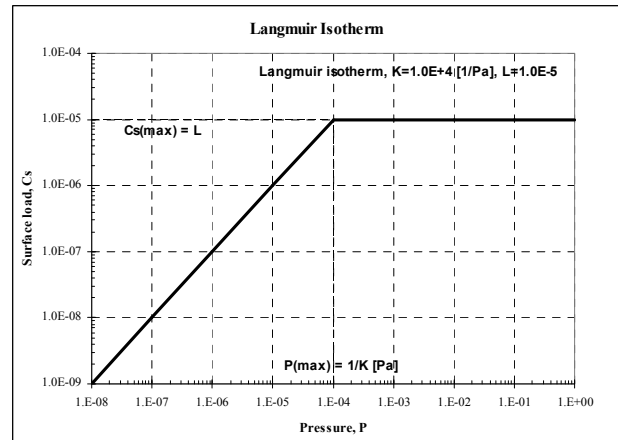


Figure 1 Langmuir isotherm

The Langmuir isotherm gives only an equilibrium value; there is no information about the time dependency of the sorption process. For example, suppose the vapor pressure is constant and equal to 10^{-5} . The Langmuir isotherm shown in Figure 1 ($L=10^{-5}$, $K=10^4$) predicts the equilibrium surface load of $C_S = 10^{-6}$. When a surface is subjected to a constant vapor pressure, the sorbed concentration will reach that equilibrium with a certain time constant, as illustrated in Figure 2.

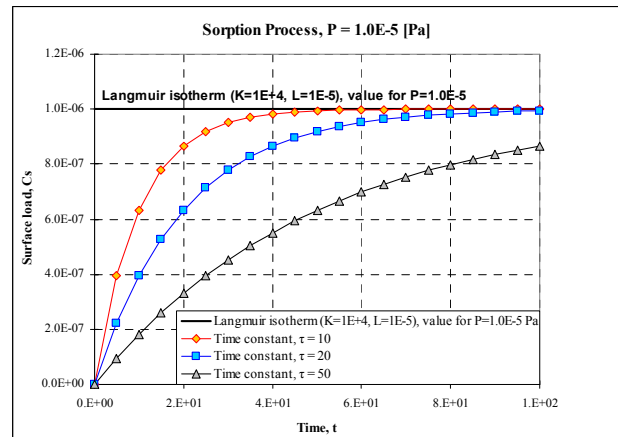


Figure 2 Time-dependent surface concentrations following a step change in vapor pressure

The information which line adequately represents reality is not available from the Langmuir isotherm and therefore the user has a certain degree of freedom in choosing the coefficients in the sorption model equation. This problem is further discussed in the next section.

3 SORPTION OF I-131 ON DIFFERENT SURFACES

3.1 Sorption of I-131 on Graphite

Several computer codes exist that are capable of analyzing sorption of fission products on surfaces. These are PATRAS, SPATRA [11], [12], RADAX [2], developed at Jülich, MELCOR [3], developed by Sandia, SPECTRA [1], developed at NRG. The codes have different models for calculating sorption phenomena. In SPECTRA two sorption models are available:

- Sorption Model 1 (SPECTRA model). A simpler model, similar to the one adopted in the MELCOR code.
- Sorption Model 2 (PATRAS/SPATRA model). A more detailed model adopted for the codes PATRAS, SPATRA.

Out of the two sorption models available in SPECTRA, the simpler Sorption Model 1 was used. The equation of the Sorption Model 1 is:

$$\frac{dM}{dt} = S = A(T) \cdot C_V - B(T) \cdot C_d \quad (3)$$

M surface load of isotope [kg/m³],
 C_V isotope concentration in the gas [kg/m³], with a maximum limit of C_{sat} , $C_V \leq C_{sat}$.
 C_d surface concentration [kg/m²]
 S sorption flux [kg/m²s]
 A, B temperature-dependent adsorption and desorption coefficients:

$$\begin{aligned} A(T) &= A_0 \cdot \exp\left(-\frac{A_A}{T}\right) \\ B(T) &= B_0 \cdot \exp\left(-\frac{A_B}{T}\right) \end{aligned} \quad (4)$$

Here A_0 , B_0 , A_A , A_B , are user-defined coefficients: The concentrations C_V , C_d are related to the Langmuir isotherm parameters as:

$$C_V = \left(\frac{1}{RT}\right) \cdot P \quad C_d = \left(\frac{M}{1000}\right) \cdot C_S$$

Here T is temperature and R is the gas constant, equal to R_u/M , where R_u is the universal gas constant, equal to 8314.5 [J/kmol K], and M is the molar weight. For I-131 $M_{I-131} = 131$ [kg/kmol] and $R = 63.4$ [J/kg K].

Equilibrium means that the source due to adsorption and removal due to desorption as well as radioactive decay are equal. In equilibrium, the source due to adsorption and removal due to both desorption and the radioactive decay are equal:

$$A(T) \cdot C_V = B(T) \cdot C_d + \lambda N \cdot \left(\frac{M}{N_A}\right) \quad (5)$$

λ decay constant [1/s]
 N number of molecules of the radioactive isotope per unit surface area [1/m²]
 N_A Avogadro number, equal 6.02×10^{26} [1/kmol]
 M molar weight, [kg/kmol]

The last term represents the radioactive decay converted into kg/m²s. Since $NM/N_A = C_d$, this equation is transformed to:

$$A(T) = [B(T) + \lambda] \cdot \frac{C_d}{C_V} \quad (6)$$

Finally:

$$A(T) = [B(T) + \lambda] \cdot KL \quad (7)$$

The decay constant, λ , for I-131 is equal to 10^{-6} s⁻¹, which corresponds to the half-life of about 8 days.

Case 1: desorption coefficient, $B(T) = 0.0$

As a first step the desorption is neglected, by setting $B(T) = 0.0$. In such case the adsorption is balanced mainly by the radioactive decay, and $A(T) = \lambda KL$.

For I-131 $\lambda = 1.0 \times 10^{-6}$ [s⁻¹]. Therefore: $A(T) = (1.0 \times 10^{-6}) (9.04 \times 10^{-8}) (5.13 \times 10^4) = 4.63 \times 10^{-9}$. Since the available data is known for one temperature only ($T = 400^\circ\text{C}$), the temperature dependence of A cannot be obtained. Therefore a constant value of A is used, with $A_0 = 4.6 \times 10^{-9}$, $A_A = 0.0$. Finally the value of C_{sat} is equal to $1/K$ in the appropriate units. Therefore $C_{sat} = 1/(5.13 \times 10^4) = 1.95 \times 10^{-5}$ [kg/m³]. The following value of 2.0×10^{-5} was used for the calculations:

Case 2: desorption coefficient, $B(T) = 1 \times 10^{-6}$

As a second choice the desorption coefficient of $B = 1 \times 10^{-6}$ is used (the value was based on analysis of Laminar Loop experiments [8], [9]). In such case: $A(T) = (1.0 \times 10^{-6} + 1.0 \times 10^{-6}) (9.04 \times 10^{-8}) (5.13 \times 10^4) = 9.27 \times 10^{-9}$. For the calculations the value was set to 9.3×10^{-9} . The value of C_{sat} is the same as above, 2.0×10^{-5} [kg/m³].

Case 3: desorption coefficient, $B(T) = 1 \times 10^{-5}$

Finally, a "large" value of B is assumed, 1.0×10^{-5} . The value of A is obtained as before: $A(T) = (1.0 \times 10^{-5} + 1.0 \times 10^{-6}) (9.04 \times 10^{-8}) (5.13 \times 10^4) = 5.10 \times 10^{-8}$. The following values were used for the second calculation:

Table 1 I-131 isotherms for Graphite

Parameter	Case 1	Case 2	Case 3
Adsorption, A ,	4.6×10^{-9}	9.3×10^{-9}	5.1×10^{-8}
Desorption, B ,	0.0	1×10^{-6}	1×10^{-5}
Saturation, C_{max} ,	2.0×10^{-5}	2.0×10^{-5}	2.0×10^{-5}

The sorption parameters are summarized in Table 1. Test runs were performed with a tabulated source of I-131. The source strength was increased in steps to cover the whole range of interest. The time behavior within a single step is illustrated in Figure 5 and Figure 6. Each step lasted 10^7 s. A large plot frequency was used (10^7 s) to make sure that the system is already at equilibrium when a plot point is made. Results are shown in Figure 3. It is seen in Figure 3 that the sorption model with the applied coefficients perfectly represents the Langmuir isotherm. The adequacy of the isotherm itself may be judged by comparing with experimental data shown in Figure 4. It is clear that the accuracy of the Langmuir isotherm is at best within an order of magnitude.

For each of the three cases results look practically the same so only the second case is shown in Figure 3. However, in each case the time behavior is different. This is illustrated in Figure 5, showing the surface concentrations plotted versus time for a single step of the vapor pressure increase. The difference between the three different versions of the sorption model is very small, considering that the adsorption constants were varied by three orders of magnitude. The reason is a feedback of the sorption mechanism on the vapor concentration, which is explained below.

- With small sorption coefficients, a small amount of vapor is sorbed. Consequently the concentration of vapor in the gas becomes relatively large and this in the end causes faster sorption.
- With large sorption coefficients, a large amount of vapor is sorbed. Consequently the concentration of vapor in the gas becomes relatively small and this in the end causes smaller sorption.

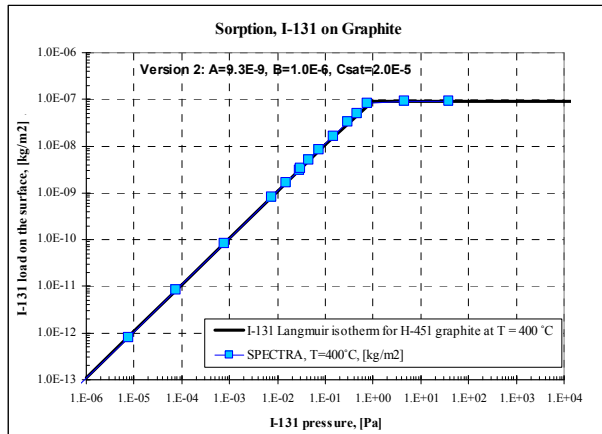


Figure 3 Sorption of I-131 on graphite, $A = 9.3 \times 10^{-9}$, $B = 1.0 \times 10^{-6}$, $C_{sat} = 2.0 \times 10^{-5}$

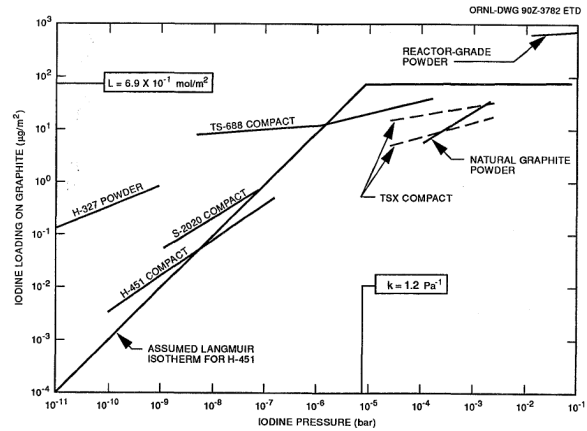


Figure 4 Sorption of I-131 on graphite, [5]

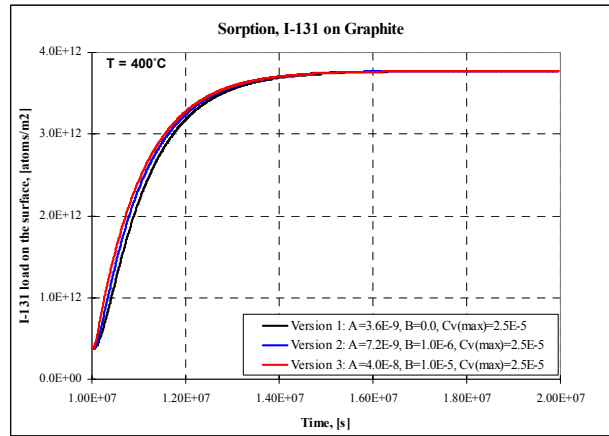


Figure 5 I-131 concentration on graphite, time-dependent graph

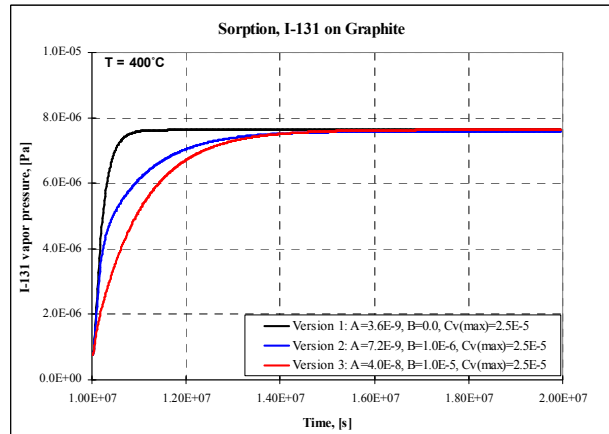


Figure 6 I-131 vapor pressure, time-dependent graph

The differences in the vapor pressures causes the sorbed mass to be very similar in each case. The vapor pressures are shown in Figure 6. It is therefore concluded that due to the self-stabilizing feedback described above, the sorption coefficients do not need to be known with very good accuracy. It is only important that the ratio between

the adsorption on one hand and the desorption plus the decay on the other hand, is correctly captured. This ratio can easily be derived from the Langmuir isotherm, as has been shown in above.

The saturation concentration of I-131 on the graphite surface is 10^{-7} kg/s, which corresponds to the number concentration of: $N_{I-131} = 4.2 \times 10^{17}$ [atoms/m²].

3.2 Sorption of I-131 on Steel

In case of steel, the Langmuir isotherms are given in [5] for four temperatures: $T = 400^\circ\text{C}$, 600°C , 700°C , and 800°C . The data is shown in Figure 9 (reproduced from [5]). The values of K and L has been read from this graph and are given in Table 2.

Table 2 I-131 isotherms for steel.

Parameter	$T = 400^\circ\text{C}$ $T = 673 \text{ K}$	$T = 600^\circ\text{C}$ $T = 873 \text{ K}$	$T = 700^\circ\text{C}$ $T = 973 \text{ K}$	$T = 800^\circ\text{C}$ $T = 1073 \text{ K}$
K , [Pa ⁻¹]	1×10^{-4}	1×10^{-3}	2×10^{-2}	5×10^{-1}
L , [$\mu\text{g}/\text{cm}^2$]	4	2	1	0.5

As shown in the previous sections, the conversion of Langmuir isotherms to SPECTRA input requires assuming one of the sorption parameters. For simplicity it is assumed that $B = 0.0$. In such case:

$$A(T) = \lambda KL \quad C_{sat}(T) = 1/K$$

The values of $A(T)$ and $C_{sat}(T)$ are given in Table 3 together with the values of K and L converted into appropriate units.

Table 3 I-131 isotherms for steel, input parameters

Parameter	$T = 400^\circ\text{C}$ $T = 673 \text{ K}$	$T = 600^\circ\text{C}$ $T = 873 \text{ K}$	$T = 700^\circ\text{C}$ $T = 973 \text{ K}$	$T = 800^\circ\text{C}$ $T = 1073 \text{ K}$
K , [m ³ /kg]	4.27×10^{-8}	5.54×10^{-7}	1.24×10^{-7}	3.41×10^{-6}
L , [kg/m ²]	4.00×10^{-5}	2.00×10^{-5}	1.00×10^{-5}	5.00×10^{-6}
$A = \lambda KL$, [m/s]	1.71×10^{-2}	1.11×10^{-3}	1.24×10^{-3}	1.70×10^{-3}
$C_{sat} = 1/K$, [kg/m ³]	2.34×10^{-9}	1.80×10^{-8}	8.10×10^{-8}	2.94×10^{-7}

There are two possible ways of preparing data for SPECTRA:

- Correlations for $A(T)$, $B(T)$, and $C_{sat}(T)$
- Tabulated $A(T)$, $B(T)$, and $C_{sat}(T)$

Use of both methods is made for the present data. The use of tabulated data option is obviously an easier and more accurate choice. Nevertheless it is sometimes convenient to use the equations, for example for comparison with other codes that are using such equations. Therefore both methods are discussed subsequently below.

Correlations for $A(T)$, $B(T)$, and $C_{sat}(T)$

With this option the A , B , and C_{sat} are calculated from the following correlations:

$$A(T) = A_0 \cdot \exp\left(-\frac{A_A}{T}\right)$$

$$B(T) = B_0 \cdot \exp\left(-\frac{A_B}{T}\right)$$

$$C_{sat}(T) = C_0 \cdot \exp\left(-\frac{A_C}{T}\right)$$

The model coefficients: A_0 , A_A , B_0 , A_B , C_0 , A_C , must be defined by the user. In the present case $B(T)$ is assumed to be zero, therefore only $A(T)$ and $C_{sat}(T)$ need to be determined. The values of $A(T)$ and $C_{sat}(T)$ are plotted in Figure 7 and Figure 8.

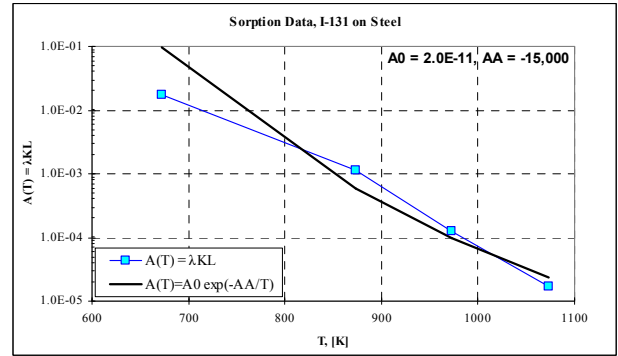


Figure 7 Values of $A(T)$ and data fit equation

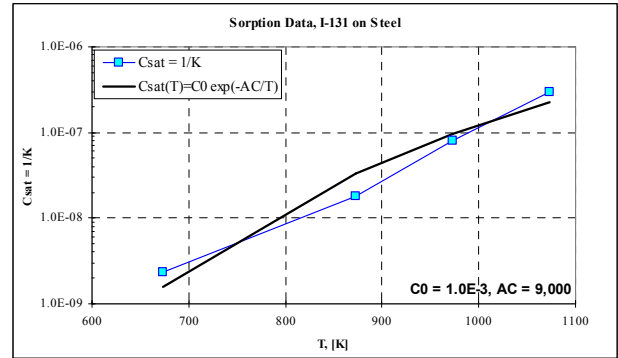


Figure 8 Values of $C_{sat}(T)$ and data fit

The coefficients were established using a simple trial and error method and comparing the plotted lines representing the fit equations with the tabulated data. The obtained values are: $A_0 = 2.0 \times 10^{-11}$, $A_A = -1.5 \times 10^4$, $B_0 = 0.0$, $C_0 = 1.0 \times 10^{-3}$, $A_C = 9.0 \times 10^3$. The fit lines for $A(T)$ and $C_{sat}(T)$ are shown in Figure 7 and Figure 8. The final formulae for the sorption model applied on steel surfaces are:

$$A(T) = 2.0 \times 10^{-11} \exp\left(\frac{15,000}{T}\right)$$

$$C_{sat}(T) = 1.0 \times 10^{-3} \exp\left(-\frac{9,000}{T}\right)$$

Results are provided in Figure 10. The source data is provided in Figure 9, copied from reference [5]. The fit equations give somewhat different values of $A(T)$ and $C_{sat}(T)$ than the source. Because of these differences, the calculated isotherms in Figure 10 are somewhat different from the isotherms in the source data Figure 9. However, the experimental data scatter is still larger therefore the use of the fit equations is justified.

Tabulated $A(T)$, $B(T)$, and $C_{sat}(T)$

With this option the data given in Table 3 is directly used in SPECTRA. Results are provided in Figure 11. The isotherms are now much closer to those provided in the source data. In fact they can be as close as the values of K and L can be read from the Figure 9. The decrease of sorption sites ("saturation concentration") from about $4 \mu\text{g}/\text{cm}^2$ ($4 \times 10^{-5} \text{ kg}/\text{m}^2$) at 400°C (strictly speaking reference [5] gives 3.6 but it is here rounded up) down to $0.5 \mu\text{g}/\text{cm}^2$ ($5 \times 10^{-6} \text{ kg}/\text{m}^2$) at 800°C is obtained exactly by the use of the tables.

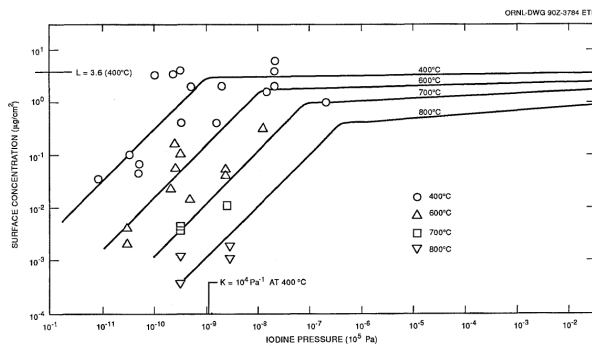


Figure 9 Sorption of I-131 on steel, [5]

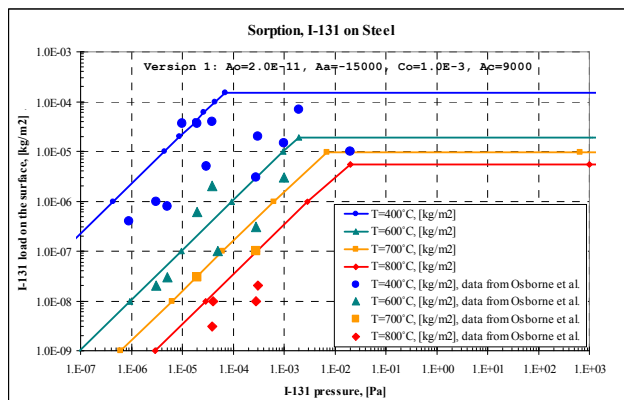


Figure 10 Sorption of I-131 on steel, $A_0 = 2 \times 10^{-11}$, $A_A = -15000$, $C_0 = 10^{-3}$, $A_C = -9000$

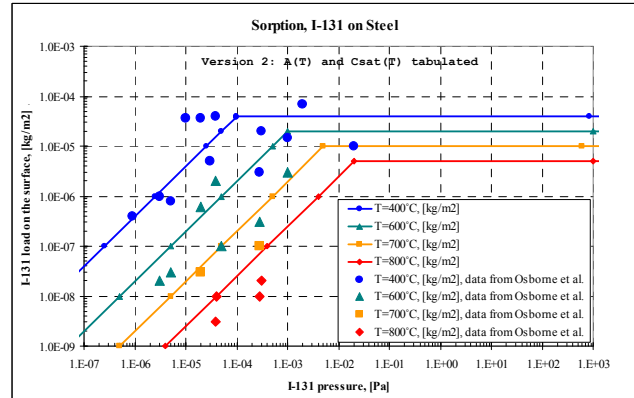


Figure 11 Sorption of I-131 on steel, tabulated $A(T)$ and $C_{sat}(T)$

The saturation concentration of I-131 on the graphite surface is $10^{-4} - 10^{-5} \text{ kg}/\text{m}^2$, depending on temperatures. The corresponding number concentration is: $N_{I-131} = 5.57 \times 10^{20} \text{ [atoms}/\text{m}^2]$ at 400°C and $N_{I-131} = 5.47 \times 10^{19} \text{ [atoms}/\text{m}^2]$ at 800°C .

3.3 Sorption of I-131 on Dust

For sorption of I-131 on dust reference the [5] (section 5.2.3) following data of Osborne [10], provides the following isotherm:

$$\begin{aligned} \circ & K = 10^3 & [\text{Pa}^{-1}] \\ \circ & L = 4 \times 10^{-6} & [\text{mol}/\text{m}^2] \end{aligned}$$

The data is valid for 400°C . This is concluded from the context, although it is not clearly stated in the text. The procedure to use Langmuir isotherm to produce SPECTRA input has been discussed in the previous two sections, therefore it is given here without any further explanations.

Step 1 - conversion of units:

$$\begin{aligned} K &= 10^3 \text{ Pa}^{-1} \times (RT) = (63.5 \times 673) \rightarrow 4.27 \times 10^7 \text{ m}^3/\text{kg} \\ L &= 4 \times 10^{-6} \text{ mol}/\text{m}^2 \times (M_{I-131}/1000) = 0.131 \rightarrow 5.24 \times 10^{-7} \text{ kg}/\text{m}^2 \end{aligned}$$

Step 2 - assume the desorption coefficient: (1) small, (2) equal, and (3) large, compared to the decay constant, $\lambda = 10^{-6} \text{ 1/s}$.

- Case 1: $B = 0.0$
- Case 2: $B = 1.0 \times 10^{-6}$
- Case 2: $B = 1.0 \times 10^{-5}$

Step 3 - calculate A and C_{sat}

$$\begin{aligned} C_{sat} &= 1/K = 1/1.05 \times 10^4 = 2.34 \times 10^{-8} \text{ kg}/\text{m}^3 \\ A &= (B + \lambda)KL, \text{ where } KL = 4.27 \times 10^7 \times 5.24 \times 10^{-7} = 22.4 \text{ m} \\ \text{Case 1: } A &= (0 + 10^{-6}) \times 22.4 = 2.24 \times 10^{-5} \text{ m/s} \\ \text{Case 2: } A &= (1 \times 10^{-6} + 10^{-6}) \times 22.4 = 4.48 \times 10^{-5} \text{ m/s} \\ \text{Case 3: } A &= (1 \times 10^{-5} + 10^{-6}) \times 22.4 = 2.46 \times 10^{-4} \text{ m/s} \end{aligned}$$

Results are shown in Figure 12. The fastest sorption is of course obtained with larger coefficients, however as

shown in section 3, the surface concentrations are quite insensitive to the choice of the sorption parameters. The saturation concentration of I-131 on the dust surface is 5×10^{-7} kg/s, which corresponds to the number concentration of: $N_{I-131} = 2.3 \times 10^{18}$ [atoms/m²]

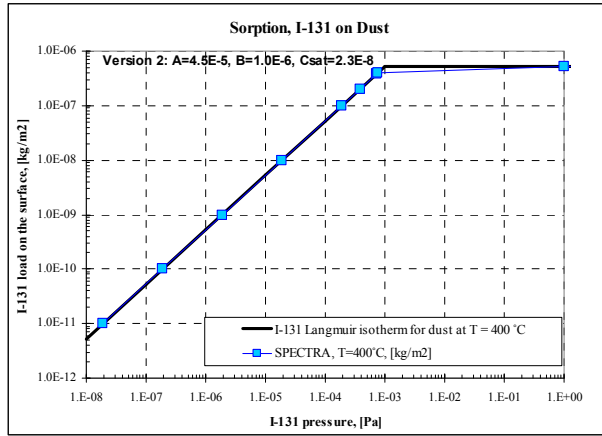


Figure 12 Sorption of I-131 on dust,
 $A = 4.5 \times 10^{-5}$, $B = 1.0 \times 10^{-6}$, $C_{sat} = 2.3 \times 10^{-8}$

4 COMPARISON OF SORPTION ON DIFFERENT SURFACES

Figure 13 shows comparison of Langmuir isotherms for dust, graphite, and steel. The highest activity (I-131 concentration) is observed on the steel surface; the lowest on the graphite surfaces.

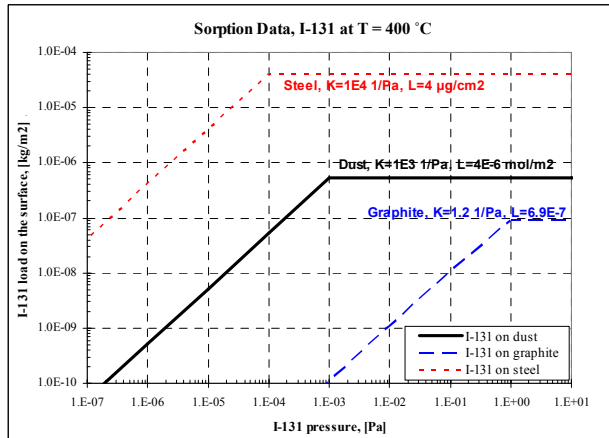


Figure 13 Sorption on structures and dust

5 SUMMARY AND CONCLUSIONS

The following data was analyzed:

- Sorption of I-131 on graphite
- Sorption of I-131 on steel

- Sorption of I-131 on dust

Calculations were performed using the SPECTRA Sorption Model 1:

$$S = A(T) \cdot C_v - B(T) \cdot C_d$$

with the following alternative sets of coefficients:

Sorption of I-131 on graphite:

$$\begin{aligned} A &= 4.6 \times 10^{-9}, & B &= 0.0, & C_{sat} &= 2.0 \times 10^{-5} \\ A &= 9.3 \times 10^{-9}, & B &= 1.0 \times 10^{-6}, & C_{sat} &= 2.0 \times 10^{-5} \\ A &= 5.1 \times 10^{-8}, & B &= 1.0 \times 10^{-5}, & C_{sat} &= 2.0 \times 10^{-5} \end{aligned}$$

Sorption of I-131 on steel, $B = 0.0$

$$A = 2 \times 10^{-11} \times \exp(15,000/T), C_{sat} = 10^{-3} \times \exp(-9,000/T)$$

A tabulated versus T , C_{sat} tabulated versus T

Sorption of I-131 on dust:

$$\begin{aligned} A &= 2.24 \times 10^{-5}, & B &= 0.0, & C_{sat} &= 2.34 \times 10^{-8} \\ A &= 4.48 \times 10^{-5}, & B &= 1.0 \times 10^{-6}, & C_{sat} &= 2.34 \times 10^{-8} \\ A &= 2.46 \times 10^{-4}, & B &= 1.0 \times 10^{-5}, & C_{sat} &= 2.34 \times 10^{-8} \end{aligned}$$

The results are summarized as follows:

- The available data is provided in form of Langmuir isotherms.
- The Langmuir isotherms do not provide sufficient data to define all coefficients of the sorption model. The Langmuir isotherm provide equilibrium data; the relaxation time (to get to equilibrium) needs to be guessed. In practice this means that one of the coefficients of the sorption model must be guessed. In the present calculations the desorption coefficient, $B(T)$, was being guessed and then varied in sensitivity calculations. The calculations showed that surface concentration is not sensitive to the choice of the parameter.
- Out of the calculated cases, the highest activity (surface concentration) is observed on the steel surface; the lowest on the graphite surfaces.
- The present work may serve as a useful guide of how to convert the Langmuir isotherm data into the input parameters required for computer code calculations.
- The Sorption Model in SPECTRA is capable to correctly reproduce the sorption behavior given by the Langmuir isotherms.

NOMENCLATURE

$A(T), B(T)$	temperature-dependent adsorption and desorption coefficients
C_d	isotope concentration on the surface [kg/m ²]
C_s	isotope concentration on the surface [mol/m ²]

C_V	isotope concentration in the gas volume [kg/m ³]	[9]	Dr. Wiedmann, "Data Set for Cs Plateout on Incoloy 800", PNP-5137-BF-GHRA 001241, October 24, 1984.
K	sorption equilibrium constant, [Pa ⁻¹]		
L	concentration of the sorption sites, [kg/m ²]	[10]	M.F. Osborne, et al., "Iodine Sorption on Low Chromium Alloy Steel", ORNL/TM-7755, 1982.
M_{I-131}	molar weight of = 131 [kg/kmol]		
P	partial pressure of fission product vapor, [Pa]	[11]	T. S. Kress, F. H. Neill, "A Model for Fission Product Transport and Deposition under Isothermal Conditions", ORNL-TM-1274, 1965.
R	gas constant, for iodine vapor equal to $R_u/M_{I-131} = 63.4$ [J/kg K]		
R_u	universal gas constant, equal to 8314.5 [J/kmol K]	[12]	N. Iniotakis, „Rechenprogramm PATRAS, Programmbeschreibung“, KFA IRB-IB-7/84, Research Center Jülich, 1984.
S	sorption flux, [kg/m ² s]		
T	temperature, [K]		

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