Comparative Study of Massih's and Findlay's Models for Fission Gas Diffusion

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1. Introduction

The diffusion coefficient is the key model parameter for fission gas release analysis, and hence the uncertainty of the diffusion coefficient model is the key model parameter uncertainty for fuel performance uncertainty analysis. The in-house fuel performance code being developed in KNF uses Findlay's model [1] as the default fission gas diffusion coefficient model for CANDU fuel. This paper indirectly derives the fission gas diffusion coefficient uncertainty of Findlay's model, based on the Massih fission gas diffusion coefficient uncertainty reported in FRAPCON-4 [2, 3]. Section 2 describes the methodology and the estimation analysis and Section 3 summarizes the results.

2. Methods and Results

This section describes the methodology applied for the indirect estimation of the in-house code fission gas diffusion coefficient uncertainty based on the Massih fission gas diffusion coefficient uncertainty.

Massih's model is the reference model for FRAPCON-4, and was validated against fission gas release measurements. The sensitivity analysis result on Massih's model for FRAPCON shows that most of the fission gas release measurement data were bounded by the code predictions using the fission gas diffusion coefficient bias factors between 0.5 (lower-bound bias factor) and 2.0 (upper-bound bias factor). This result can be utilized to indirectly set an upper uncertainty bound for the Findlay's fission gas diffusion coefficient without recourse to the validation fission gas release measurement data set.

2.1 Findlay's Diffusion Coefficient Model

Findlay has measured the in-reactor diffusional release of ^{85}Kr from specimens of known surface-to-volume ratio. Use of this type of measurement enables us to calculate release from a sphere whether the gas migrates atomically or as intergranular bubbles. Findlay obtained a diffusion coefficient, D, given by:

$$D = 7.8 \times 10^{-2} exp\,(\frac{-288\ kJ/mole}{R(T/10^3)})\ m^2 s^{-1} \quad (1)$$

where, D is the diffusion coefficient (m^2/s); T is the fuel temperature (K); and R is the gas constant (8.31 J/moleK).

2.2 Massih's Diffusion Coefficient Model

The original Massih model begins with a solution of the gas diffusion equation for constant production and properties in a spherical grain. Forsberg and Massih attempt to solve the equation for the case where there is re-solution of gas on the grain surface, which changes the outer boundary condition. Diffusion coefficient model which is used in modified Massih's fission gas release model in FRAPCON-4.0 is as follows:

$$D = 12 \times 2.14 \times 10^{-13} exp\,(\frac{-1.15 \times 22884}{1850}) \cdot B^{eff} \quad \text{for } T > 1850K$$

$$D = 12 \times Max[1.51 \times 10^{-17} exp\,\left(\frac{-9508}{T}\right), 2.14 \times 10^{-13} exp\,(\frac{-1.15 \times 22884}{T}) \cdot B^{eff}] \quad \text{for } T \leq 1850K$$

$$B^{eff} = \mathrm{Min}[20000, 100^{Max[0, Bu-21]/40}] \quad (2)$$

where, D is the diffusion coefficient (m^2/s); T is the fuel temperature (K); B^{eff} is the enhancement factor; and Bu is the fuel burnup (GWd/MTU).

2.3 Methodology of Uncertainty Estimation

Figure 1 shows the upper-bound and lower-bound diffusion coefficient curves for Massih's diffusion coefficient model along with the prediction by the prediction by the in-house code fission gas diffusion coefficient (Findlay's model).

The following steps are taken to find the upper-bound uncertainty bias factor for the in-house code fission gas diffusion coefficient (Findlay's model). (I) The in-house code is set as a reference code into which the Massih's model and its sensitivity analysis capability option are incorporated. (II) Three representing power histories experienced by a CANDU fuel element during the normal operation are analyzed. The nominal design bundle power envelope of 800kW, the reference high-power envelope of 860kW and the limiting power envelope of 935kW are analyzed. (III) Five diffusion coefficient analysis cases (see Table 1 below) for each of the three representing power histories are performed to find the upper uncertainty bound bias factor for the in-house code fission gas diffusion coefficient.

Of the three Findlay cases (1xF, 2xF and 3xF) for 800kW power history case, the Findlay case predicting the amount of fission gas release closest to that from the upper-bound Massih case (2xM) for the same power history case is selected to be a candidate for the upper-bound uncertainty bias factor for the in-house code fission gas diffusion coefficient (Findlay's model).

This candidate selection is repeated for 860kW and 935kW power history cases. The highest bias factors of the three candidates is conservatively set to be the final, upper-bound uncertainty bias factor for the in-house code fission gas diffusion coefficient. The inverse of the highest bias factor is assumed to be the lower-bound uncertainty bias factor for the fission gas diffusion coefficient for simplicity.

2.4 Results

The in-house code simulation for each of the analysis cases given in Table 1 was performed. The volume of fission gas release at two representative element burnups (average discharge burnup of 180 MWh/kgU and maximum discharge burnup 460 MWh/kgU) are given in Tables 2 and 3, respectively.

Tables 2 and 3 show that the upper-bound uncertainty bias factor candidate for each power history is 3.0 or 1.0. Therefore, the highest upper-bound uncertainty bias factor of all the analysis cases is 3.0. This highest bias factor of 3.0 is set to be the final, upper-bound uncertainty bias factor for the fission gas diffusion coefficient as per Step (III) of Section 2.3. The bias factor of 1/3, the inverse of the highest bias factor (3.0) is the lower-bound uncertainty bias factor for the in-house code fission gas diffusion coefficient (Findlay's model) as per Step (III) of Section 2.3.

Table 1: Analysis Cases

Power History	Diffusion Coefficient Case				
	1xM	2xM	1xF	2xF	3xF
800kW	√	√	√	√	√
860kW	√	√	√	√	√
935kW	√	√	√	√	√

Note: "1xM" and "2xM" mean 1 and 2 times of Massih diffusion coefficient from Equation (2) respectively. Similarly, "1xF", "2xF" and "3xF" mean 1, 2 and 3 times of Findlay diffusion coefficient from Equation (1) respectively.

Table 2: Fission Release Volume at Burnup of 180 MWh/kgU

Power History	Volume Fission Gas Release (mm^3) for Each Diffusion Coefficient Case					Uncertainty Bias
	1xM	2xM	1xF	2xF	3xF	
800kW	5060	**6207**	4879	5833	**6353**	**3.0**
860kW	6871	**8596**	**8578**	10246	11110	**1.0**
935kW	10466	**13105**	**17011**	19583	N/A	**1.0**

Table 3: Fission Release Volume at Burnup of 460 MWh/kgU

Power History	Volume Fission Gas Release (mm^3) for Each Diffusion Coefficient Case					Uncertainty Bias
	1xM	2xM	1xF	2xF	3xF	
800kW	6115	**7520**	5600	6681	**7276**	**3.0**
860kW	10085	**14445**	11037	13632	**14994**	**1.0**
935kW	17241	**23941**	**24069**	29435	N/A	**1.0**

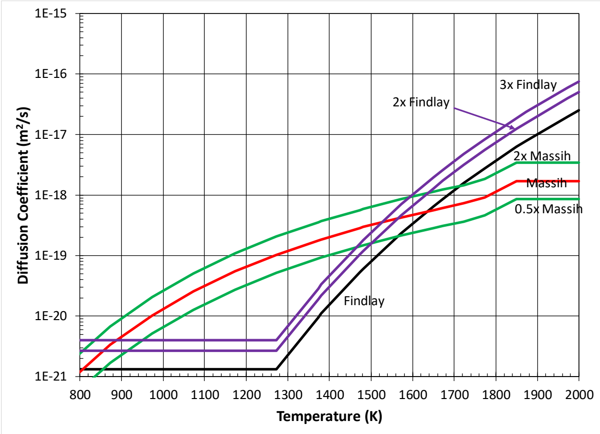

Figure 1: Diffusion Coefficient Curves for Massih's Model Along with Findlay's Model.

3. Conclusions

The in-house code fission gas diffusion coefficient uncertainty being developed in KNF was indirectly estimated based on the Massih fission gas diffusion coefficient uncertainty reported in FRAPCON-4 code.

The upper-bound uncertainty bias factor for the in-house code fission gas diffusion coefficient (Findlay's model) generating the amount of fission gas release closest to that from the upper-bound diffusion coefficient for Massih's model is found to be 3.0. The estimated upper-bound uncertainty bias factor covers the power histories and fuel burnup range experienced by a CANDU fuel element during the normal operation.

The lower-bound uncertainty bias factor is assumed to be the inverse of the upper-bound uncertainty bias factor of 3.0 and is 1/3.

REFERENCES

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