Verification of Mechanistic Modeling on the Distribution of Fission Products in the Fuel Pellet via Method of Manufactured Solutions at Steady-State

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1. Introduction

The source term analysis during a severe accident is one of the most important issues in the accident management plan since the source term is initial and boundary conditions for the evaluation of the environmental impact from the severe accident [1]. For the source term analysis, a fission product release from the reactor core (or fuel) is considered as the first step.

In the conventional computer codes for a severe accident analysis such as MELCOR [2], MAAP [3], CORSOR model has been widely used [4]. The CORSOR model is a simplified model based on the assumption that the release characteristic of fission products can be categorized into several groups, according to the similarity in terms of chemical behaviors. And the release characteristics can be modelled as a set of Bateman equations on the aforementioned groups. Even though the CORSOR model has advantages in terms of fast-running and easy implementation in the code, the model is not based on the detailed description on the fission product behaviors so that it is difficult to apply the model if the accident scenario and the type of reactor fuel are different from the ones that are considered to obtain the coefficients in the model. It is, therefore, necessary to develop a model based on the fission product behaviors, so called mechanistic model, so that we can apply the model in general manner.

As a beginning step of the developing mechanistic modeling, we would like to implement a model on the fission product distributions in the fuel pellet at steady-state. And we also perform verification of the aforementioned implementation via method of manufactured solution (MMS) [5].

2. Modeling on Fission Product Distribution in the Fuel and Verification via MMS at Steady-State

2.1 Modeling on fission product distributions in the pellet

The main mechanisms of the fission product behaviors in the pellet are diffusion and convection via porous media [6]. The distribution of the fission product concentration in the pellet can be calculated via the following Eq :

$$\alpha \frac{\partial C(i)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left\{\beta_f \cdot D(i)\cdot r\cdot \frac{\partial C(i)}{\partial r} - r\cdot u\cdot C(i)\right\} + s_p(i), \qquad (1)$$

where

$C(i)$: concentration of fission product i

D(i) : diffusion coefficient of the fission product i at free volume,

$s_p(i)$: generation rate of fission product i into porous media in the fuel pellet,

α : total porosity in the fuel pellet,

β_f : interconnected porosity in the fuel pellet,

u : superficial velocity of gas in the pellet.

For the steady-state, the Eq. (1) is simplified as the follow :

$$\frac{1}{r}\frac{\partial}{\partial r}\left\{\beta_f \cdot D(i)\cdot r\cdot \frac{\partial C(i)}{\partial r} - r\cdot u\cdot C(i)\right\} + s_p(i) = 0. \qquad (2)$$

In this paper, we use one-dimensional finite difference method (FDM) to discretize the Eq. (2). For the convection term in Eq. (2), upwind explicit scheme is considered for simplicity. Then the following equation is obtained for the n-th cell in the fuel pellet :

$$\begin{aligned}
&-\left[\frac{\left\{\beta_f \cdot D(i)\cdot r_{n-1/2}\right\}}{\Delta r_n^2} + \frac{r_n \cdot u_n}{\Delta r_n}\right] C(i)_{n-1} \\
&+\left[\frac{\left\{\beta_f \cdot D(i)\cdot r_{n-1/2}\right\}}{\Delta r_n^2} + \frac{\left\{\beta_f \cdot D(i)\cdot r_{n+1/2}\right\}}{\Delta r_n^2} + \frac{r_n \cdot u_n}{\Delta r_n}\right] C(i)_n \qquad (3) \\
&-\left[\frac{\left\{\beta_f \cdot D(i)\cdot r_{n+1/2}\right\}}{\Delta r_n^2}\right] C(i)_{n+1} = r_n \cdot s_p(i),
\end{aligned}$$

where

r_n : distance of the n-th cell from the center of the pellet,

$r_{n-1/2}$: distance of the left boundary of n-th cell from the center of the pellet,

$r_{n+1/2}$: distance of the right boundary of n-th cell from the center of the pellet,

Δr : size of the cell in the calculation.

With the boundary condition of the pellet, i.e., no fission product outside of the pellet at steady-state, the Eq. (3) is implemented in an in-house code.

2.2 Method of manufactured solution for the verification of fission product distribution at steady-state

For the verification of the in-house code at steady-state, it is necessary to compare an analytic solution of Eq. (2) with the numerical results obtained from the code. However, due to complexity of Eq. (2), it is difficult to obtain the analytic solution. Therefore, in this paper, a method of manufactured solution (MMS) is used to verify the code.

In the MMS, a manufactured solution is inserted to the Eq. (2) so that the right-hand-side (RHS) is modified via arithmetic operations. Then with slight modification of the RHS, we can obtain numerical solutions and compare them with the manufactured solution to verify the in-house code.

In this paper, we assume that the manufactured solution has the following form :

$$MS(r) = A_1 \cdot \cos(B_1 \cdot r) + P_1 \cdot r^2 + Q_1 \cdot r + R_1, \quad (4)$$

where A_1, B_1, P_1, Q_1, R_1 are constants determined considering the boundary conditions.

3. Numerical Results

In the numerical analysis, we consider the radius of fuel pellet as 0.4095 cm, which is a typical value for the LWR fuel pellet. The coefficients in the manufactured solutions are listed on Table 1. For the numerical analysis, we consider various cases in terms of number of cells in the fuel pellet the computation conditions for the in-house codes are shown in Table 2. The numerical solution with 819 cells is compared with the manufactured solution in Fig. 1.

Table 1. Coefficients in the manufactured solution

Coefficients	Value
A_1	1.200
B_1	3.927
P_1	-2.872
Q_1	0.150
R_1	0.465

Table 2. Computation conditions for the in-house code

Parameters	Value
Number of cells	10
	50
	100
	500
	819
Matrix equation solver	Gaussian elimination for tridiagonal matrix

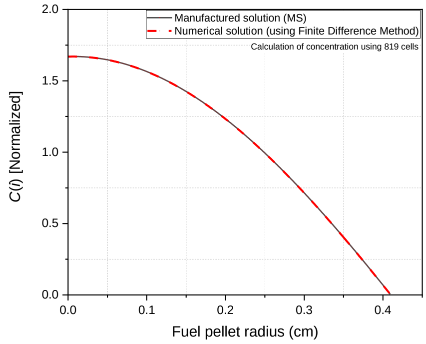

Fig. 1. Comparison of numerical solutions with the manufactured solution

As shown in Fig. 1, the numerical solutions show excellent agreement with the manufactured solution, i.e., the average difference between the two solution is less than 0.2%. The results of the sensitivity on the number of cells are shown in Fig. 2 and the change of relative errors with the various number of cells are shown in Fig. 3. As shown in Figs. 2 and 3, the relative errors decrease as the number of cells increases. Note that the difference between the result with 10 cells and the manufactured solution is caused by the boundary condition which impose the concentration of the fission product in the imaginary cell next to the outer boundary of the fuel pellet as zero.

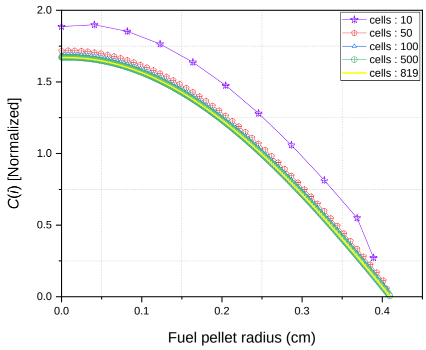

Fig. 2. Comparison on the various number of cells in the calculation

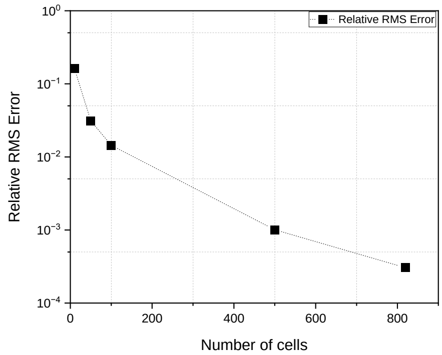

Fig. 3. Relative Root Mean Square (RMS) errors vs Number of cells

4. Conclusions

In this paper, for the detailed analysis on the fission product release from the reactor core, we implemented mechanistic model on the distribution of fission products in the fuel pellet at steady-state into an in-house code as a beginning step for mechanistic modeling of fission product behaviors. We verified the code with the method of manufactured solution.

From the numerical analyses, the in-house code shows good agreement with the manufactured solution. if the number of cells in the fuel pellet is sufficient to describe the boundary condition of the outside of the fuel.

As future work, a proper boundary condition for the outside of the fuel pellet will be formulated in order to make the numerical solutions with small number of cells in the pellet consistent with the ones with large number of cells, which is necessary for the severe accident analysis since a huge number of calculations on the mechanistic modeling is required in the analysis of fission product release. The formulation on the transient analysis is also required to analyze the fission product release during a severe accident as well as verification with manufactured solutions and validation with experimental data.

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REFERENCES

[1] B. R. Sehgal et al., *Nuclear Safety in Light Water Reactors – Severe Accident Phenomenology*, Elsevier, Oxford, U.K. 2012.
[2] R. O. Gaunnt, et al., *MELCOR Computer Code Manuals Vol. 1: Primer and Users' Guide, Version 2.2.9541*, SAND2017-0455, Sandia National Laboratories, NM, 2017.
[3] T. Kindred, *Modular Accident Analysis Program 5 (MAAP5) Applications Guidance*, 3002010658, EPRI, Palo Alto, CA, 2017.
[4] M. R. Kuhlman et al., *CORSOR User's Manual*, NUREG/CR-4173, Battelles' Columbus Laboratories, Coloumbus, OH, 1985.
[5] C. J. Roy, Review of code and solution verification procedures for computation simulation, *J. Comp. Phys*. 205 pp. 131-156, 2005
[6] N. E. Bixler et al., *VICTORIA 2.0: A Mechanistic Model for Radionuclide Behavior in a Nuclear Reactor Coolant System Under Severe Accident Conditions*, NUREG/CR-6131, Sandia National Laboratory, NM, 1998.