Adaptive Two-zone Method Applied to the Fission Gas Release under an Irradiation-induced Re-solution Condition

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1. Introduction

Numerous models have been developed to predict the fission gas release where the flux of gas atoms to the grain boundaries is described by a diffusion equation. Among the numerical solution methods, the variational principle has been regarded as a suitable method in the sense of its accuracy and efficiency.

The assumption of a perfect sink for a grain boundary results in a steep gradient near the outer layer of the grain at an early stage of a FGR. A suitable re-meshing technique in combination with proper trial functions is needed to treat such a steep gradient by relocating the finite element nodes [1]. The adaptivity, however, should be implemented with the number of meshes as small as possible due to the high number of the FGR calculations during a fuel performance analysis.

The two-zone method by Matthews and Wood [2], is most appropriate since it requires two elements with three degrees of freedom to model the spherical grain. On the other hand, it is known to have a lower accuracy for a low release. In our previous work [3], we proposed an adaptive two-zone approach to provide an accuracy comparable to that of the FEM with very fine meshes at an early stage as well as at a higher release.

In this paper, the adaptive two-zone method is applied to the FGR problem under an irradiation-induced re-solution boundary condition.

2. Adaptive two-zone method

The diffusion equation in spherical coordinates,

$$\frac{\partial c_g}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_{eff} r^2 \frac{\partial c_g}{\partial r} \right) + \beta_{eff}\,, \qquad (1)$$

is solved with the boundary conditions, $c_g = 0$ at $r = a$ and $\partial c_g / \partial r = 0$ at $r = 0$, where a is the grain radius, D_{eff} the effective diffusion coefficient of a gas atom, and β_{eff} the rate of an effective gas generation. The effect of an irradiation-induced re-solution on the gas generation rate near a grain boundary is described by

$$\beta_{eff} = \begin{cases} \beta & \text{for } 0 \le r < a - 2\lambda, \\ \beta + \dfrac{bN}{4\lambda} & \text{for } a - 2\lambda \le r < a, \end{cases} \qquad (2)$$

where β is the number of gas atoms produced per fission event, λ the re-solution depth, b the resolution parameter, and N the number of gas atoms per unit area of a grain boundary.

A variation treatment on Eq. (1) leads to

$$\delta \int_0^a 4\pi \left[\frac{D_{eff}}{2}\left(\frac{dc_g}{dr}\right)^2 + \frac{c_g^2}{2\delta t} - \left(\frac{c_g^0}{\delta t} + \beta_{eff} \right) c_g \right] r^2 dr = 0 \qquad (3)$$

The concentrations at these points are represented by c_1, c_2, and c_3. For this purpose, we have prepared the quadratic trial functions, C_1 and C_2 as a function of ρ_2 with $\rho_1 = 0.4$ for the two regions, respectively. ρ_3 is the mid point of ρ_2 and 1. The upper limit of ρ_2 is set to be 0.8.

Trial functions are modified with additional criteria; $\partial C_2 / \partial \rho = 0$ at $\rho = \rho_2$ if ρ_{2v} is larger than ρ_2 or if c_1 is less than c_2. Here the condition $\partial C_2 / \partial \rho = 0$ leads to,

$$\rho_{2v} = \frac{c_2(3+\rho_2) - 4c_3(1+\rho_2)}{4(c_2 - 2c_3)}\,. \qquad (4)$$

Furthermore c_1 is set to be equal to c_2 if c_1 is less than c_2. The trial functions are selected adaptively during the calculation according to the previous criteria.

Inserting the trial functions into Eq. (3) and minimizing the integral with respect to c_1, c_2, and c_3, leads to a set of equations,

$$\mathbf{K}\mathbf{c_g} = \mathbf{b}\,, \qquad (5)$$

where $\mathbf{K}$ represents the global stiffness matrix, $\mathbf{c_g}$ the concentration vector, and $\mathbf{b}$ the load vector. When DOF = 1 for the perfect boundary condition, Eq. (6) and Eq. (7) provide the simplest relation for $\mathbf{K}$ and $\mathbf{b}$, respectively.

$$\mathbf{K} = \frac{-56 D_{eff}\, dt \left(6 + 3\rho_2 + {\rho_2}^2\right) + 4a^2\left(-8 - 3\rho_2 + {\rho_2}^2 + 4{\rho_2}^3 + 6{\rho_2}^4\right)}{420\, dt\, a^2 \left(-1+\rho_2\right)} \qquad (6)$$

$$\mathbf{b} = \sum_{i=0}^{3} b_i (\rho_{20} - \rho_2)^i\,, \qquad (7)$$

where ρ_{20} is the coordinate of the interface ρ_2 at a previous time step, and b_i s are given by

$$b_0 = \frac{\left(4+3\rho_2+2\rho_2{}^2+\rho_2{}^3\right)}{30}\beta + \frac{\left(8+11\rho_2+10\rho_2{}^2+6\rho_2{}^3\right)}{105}\frac{c_{20}}{\delta t},$$

$$b_1 = \frac{\left(11+20\rho_2+18\rho_2{}^2\right)}{210}\frac{c_{20}}{\delta t}$$

$$b_2 = \frac{\left(-3-\rho_2+11\rho_2{}^2\right)}{105\left(-1+\rho_2\right)}\frac{c_{20}}{\delta t}$$

$$b_3 = \frac{\left(1-16\rho_2+8\rho_2{}^2\right)}{210\left(-1+\rho_2\right)^2}\frac{c_{20}}{\delta t} \quad (8)$$

where fourth and fifth-order terms are neglected.

The average gas concentration is given by

$$\overline{c}_g = \frac{c_2}{10}\left(4+3\rho_2+2\rho_2{}^2+\rho_2{}^3\right), \quad (9)$$

In the case of the re-solution boundary, only **b** is slightly modified in Eq. (5).

3. Application of the adaptive method to the irradiation-induced re-solution case

The reference solutions were obtained using the ABAQUS [4] code with 50 elements. The grain radius is assumed to be 5 μm.

The reference solutions were compared with the one from the present method through a modification of **b** to deal with the re-solution case. In Fig. 1, the calculated fractional gas releases are shown as a function of the time for $b = 10^{-5}$ s^{-1} and $\lambda = 10^{-8}$ m. The difference between the two results is nearly absent except for around the time for a grain face saturation.

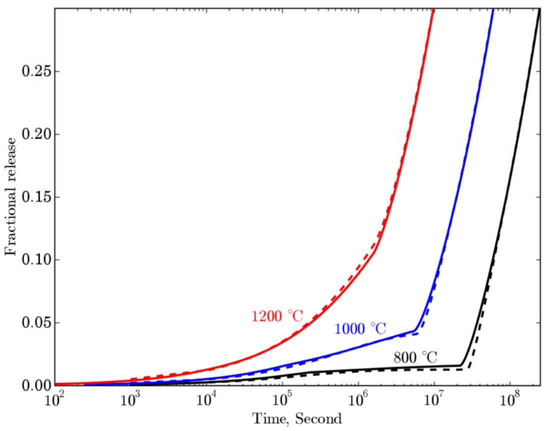

Figure 1. Calculated fractional gas release as a function of time for $b = 10^{-5}$ s^{-1} and $\lambda = 10^{-8}$ m.
(Solid line; ABAQUS, Dotted line; Present method).

We have also calculated the fractional gas release at a constant temperature under various resolution parameters. The adaptive two-zone method correctly predicts the dependency of the fractional release for the normalized time. It is confirmed that the case under $b = 0$ is reduced to that of the perfect sink boundary condition.

The application of the present method to the time-varying condition is found in Fig. 2. The transient begins after a steady condition holding at 900 °C for 10^7 sec. The calculated fractional gas release for $b = 10^{-5}$ s^{-1} and $\lambda = 10^{-8}$ m is in a good agreement with those from the reference solutions.

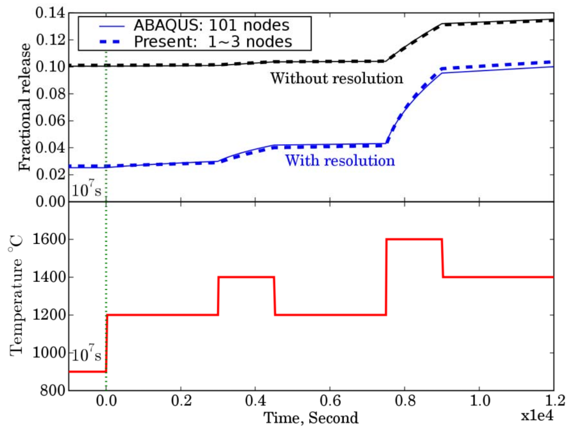

Figure 2. Calculated fractional gas release under a variable power condition for $b = 10^{-5}$ s^{-1} and $\lambda = 10^{-8}$ m .

4. Conclusion

An adaptive variational method was further extended in order to apply to the fission gas release problem under an irradiation-induced re-solution boundary condition. It was demonstrated that the FGR under constant and varying gas generation can be calculated with an accuracy comparable to that of the FEM with very fine meshes.

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