Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 10-11, 2007

Adaptive Two-zone Method for a Fission Gas Release under an Imperfect Sink

Jin-Sik Cheon, Yang-Hyun Koo, Byung-Ho Lee, Je-Yong Oh, Dong-Seong Sohn
Korea Atomic Energy Research Institute

1. Introduction

A fission gas release has been evaluated under various operating conditions, which is frequently focused on to describe the gas behavior at a grain boundary. The boundary is treated to behave thermodynamically as a perfect sink. Also an irradiation induced resolution flux from the boundary has been introduced to model the incubation period after a Speight's argument [1].

We have proposed an adaptive two-zone method which is capable of providing an accuracy comparable to that of the FEM with very fine meshes at an early release stage as well as at a higher release under a perfect sink boundary condition [2]. This improvement is accomplished by implementing two strategies. Firstly the interface of the two regions is moved in proportion to the released fraction. Secondly the number of DOFs is reduced to guarantee the profile of a gas concentration to decrease monotonically from the center to the surface.

In this paper, the adaptive two-zone method is further extended to deal with the FGR problem with an imperfect sink due to an irradiation-induced resolution flux.

2. Adaptive two-zone method under imperfect sink

The diffusion equation in spherical coordinates,

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

is solved with the boundary conditions, $c_g = c_s$ at $r = a$ and $\partial c_g / \partial r = 0$ at $r = 0$, where a is the grain radius, D the effective diffusion coefficient of a gas atom, and β the gas atom generation rate. c_s and β are defined depending on how the irradiation-induced resolution flux near a grain boundary is taken into consideration.

Diffusive flux within the matrix to the boundary is assumed to be balanced by the resolution flux from the boundary. An imperfect boundary condition [3] is arranged

$$c_s = \frac{\lambda b N}{2D} \qquad (2)$$

where b is the rate of a resolution of the intergranular atoms, N the gas atoms per unit area of a grain face, and λ the thickness of a resolution layer.

As the gas is accumulated on a grain face via a resolution, N is saturated at N_{sat}. The saturation concentration is fixed at a certain value for all the temperatures. During the calculations, N is evaluated from the balance:

$$\int \beta dt = \bar{c}_g + 3N/2a + R \qquad (3)$$

where $\bar{c}_g$ is the average gas concentration in the grain, and R is the number of released gas atoms per unit volume of a fuel. After a saturation, all the gas arriving at a grain boundary is released. Gas released fraction to the free volume is determined by

$$f = 1 - \frac{\bar{c}_g + 3N_{sat}/2a}{\int \beta dt}. \qquad (4)$$

Three nodal points are required; $\rho_1 = 0.4$, $\rho_3 = 0.9$, and ρ_2. The interface ρ_2 is updated by the linear equation. The concentrations at ρ_1, ρ_2, and ρ_3 are represented by c_1, c_2, and c_3, respectively. In this problem the gas concentration at the grain face, c_0 is necessary since it varies with time. The concentration profile in each region is described by the quadratic trial functions, C_1 and C_2 which are a function of ρ_2.

In a comparison with our previous work [2], we impose a multi-point constraint (MPC) to the variational equation before a gas saturation on a grain face. The constraint is

$$c_0 = \Lambda\left(G - R - \bar{c}_g \right), \qquad (5)$$

where $\bar{c}_g = k_1 c_1 + k_2 c_2 + k_3 c_3 + k_0 c_0$ and $\Lambda = \lambda b a / 3D$.

The Lagrange multiplier method adds the constraint to the original variational equation, yielding

$$\delta \int_0^a 4\pi \left[\frac{D_{eff}}{2}\left(\frac{c_g}{r} \right)^2 + \frac{c_g^2}{2\delta t} - \left(\frac{c_g^0}{\delta t} + \beta \right) c_g \right] r^2 dr + \delta\lambda_c 4\pi a^3 \left[c_0 - \Lambda\left(G - R - \bar{c}_g \right) \right] = 0, \qquad (6)$$

where λ_c is the Lagrange multiplier, and $G = \int \beta dt$.

Inserting the trial functions into Eq. (6) and minimizing the integral with respect to c_1, c_2, c_3, c_0, and λ_c leads to a set of equations

$$\mathbf{K}\mathbf{c}_\mathbf{g} = \mathbf{b}. \qquad (7)$$

By virtue of a small difference of ρ_2 relative to ρ_{20}, ρ_2 at a previous time increment [2], **b** is simply approximated by

$$b_i \approx (\hat{b}_{i,0} + \hat{b}_{i,1}(\rho_{20} - \rho_2))/b_i$$

where b_i and $\hat{b}_{i,j}$ are the denominator and the coefficient of the numerator, respectively.

Similarly a set of equations after a gas saturation are derived by using the boundary condition, $c_0 = c_{sat}$. We can make the gas concentration to decrease monotonically by reducing the number of DOFs of the system. The number of DOFs could be decreased by imposing a homogeneous constraint to the system of equations.

We employ the same procedures as those reported [2] for a convergence criterion as well as an automatic time integration. Prior to the grain-face saturation, the number of gas atoms on a grain face is chosen to determine a convergence. After a saturation, it is checked by means of the released fraction. At every time step, several iterations are required to satisfy a convergence criterion. Time increment of the next time step is predicted by comparing the fractional release between the consecutive time steps.

In a reference problem with an irradiation-induced resolution flux, the computational time of the adaptive two-zone method is comparable to that of the case with a perfect sink boundary condition.

3. Application of the adaptive method to imperfect sink case

The reference solutions were obtained by using a FEM code with 50 quadratic elements. A grain radius of 5 μm and A thickness of the resolution layer of 0.01 μm are used in the calculations. It is assumed that the number of gas atoms on a grain face is saturated at 2×10^{19} atoms/m^2. We have used the diffusion coefficient of the gas atoms in the reference [4].

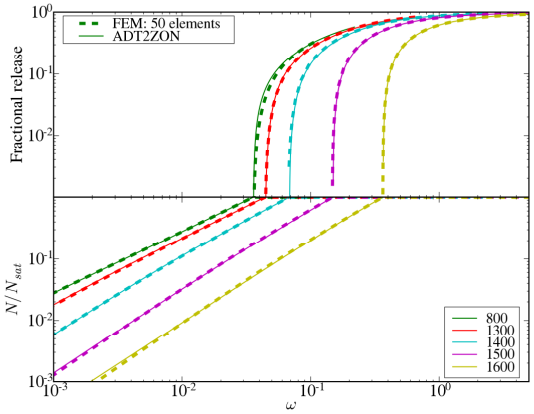

Figure 1. Calculated fractional gas release as a function of normalized time for $b = 3\times10^{-5}$ s^{-1}.

Fig. 1 shows the calculated results for the gas atoms at a grain boundary, and the fractional gas release as a function of the normalized time (Dt/a^2) for $b = 3\times10^{-5}$ s^{-1}. It appears that discrepancies are nearly absent between the reference FEM results and those from the present method.

Fig. 2 shows an application of the present method to a time-varying condition. The gas release begins after an operation for about 2×10^6 sec. The calculated fractional gas release is in good agreement with that from the reference FE solution.

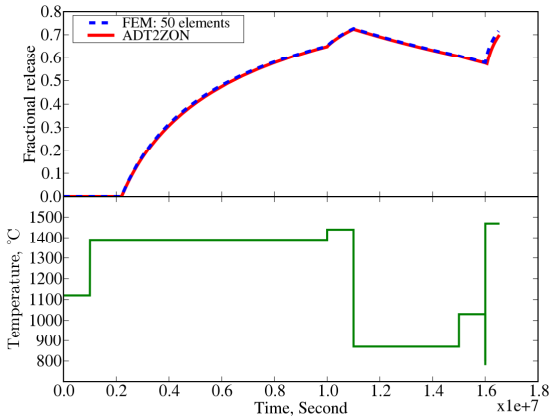

Figure 2. Calculated fractional gas release under a variable power condition for $b = 3\times10^{-6}$ s^{-1}.

4. Conclusion

An adaptive variational method was extended in order to apply it to a fission gas release problem under an imperfect sink at a grain boundary. The proposed MPC technique was suitable for treating the non-homogeneous boundary condition. It was demonstrated that the FGR under constant and varying gas generations can be calculated with an accuracy comparable to that of the FEM with fine meshes.

REFERENCES

[1] M. Speight, Nucl. Sci. Eng., 37 (1969) 180.
[2] J.-S. Cheon, Y.-H. Koo, B.-H. Lee, J.-Y. Oh, D.-S. Sohn, J. Nucl. Mater., 359 (2006) 139.
[3] K. Forsberg, A. R. Massih, J. Nucl. Mater., 135 (1985) 140.
[4] D. M. Dowling, R. J. White, M. O. Tucker, J. Nucl. Mater., 110 (1982) 37.