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An extension of the two-zone method for evaluating a fission gas release under an irradiation-induced resolution flux

Jin-Sik Cheon *, Yang-Hyun Koo, Byung-Ho Lee, Jae-Yong Oh, Dong-Seong Sohn

Korea Atomic Energy Research Institute, P.O. Box 105, Yuseong, Daejeon 305-600, Republic of Korea

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Abstract

This paper describes an extension of the adaptive two-zone method whose accuracy is substantially enhanced when compared to the original formulation by Matthews and Wood. A diffusive problem under the presence of an irradiation-induced resolution flux is evaluated by applying a variational principle to the diffusion equation. Prior to a gas saturation in the grain boundaries, a constraint associated with a gas balance is added to the variational equation. The spherical grain is divided into two regions whose interface is relocated as the ratio of the number of gas atoms within a grain to that generated. The distribution of the gas concentration is calculated over the grain. During the calculations, the number of degrees of freedoms is reduced to provide a profile which decreases monotonically along the radius. Numerical verifications show that the present approach is viable in computing a gas release accurately and efficiently in fuel performance codes.

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1. Introduction

Fission gas release in a nuclear fuel is modeled by describing a gas transport from a pellet to a free volume. During these complex processes, gas behavior on the grain boundaries plays a key role in determining the diffusive flux from the interior of the pellet [1]. Grain boundary is thermodynamically regarded to behave as a perfect sink to which all the atoms arriving at it are absorbed.

Applying the assumption of a perfect sink to the diffusion problem does not lead to a satisfactory explanation for an incubation observed during a fission gas release. After Speight's argument [2], an irradiation-induced resolution flux has been widely introduced to account for the delay of a gas release. The resolution flux is proportional to the number of gas atoms in the bubbles on a grain boundary. As the gas atoms on a grain boundary reach a certain critical value, the gas atoms are assumed to vent.

A few solutions exist for the gas atoms accumulated on a grain boundary before a saturation [2–4]. In addition, a gas release after a saturation can be evaluated [4,5]. Even with these semi-analytical solutions, it is necessary to obtain their responses through several iterations when time-varying histories are considered. On the other hand there are several numerical solution methods for which the gas concentrations are calculated at nodal points in advance: finite difference method [6], finite element method (FEM) [7,8], and finite volume method [9]. These numerical attempts are more attractive in the sense that they are rather easily extended to versatile situations such as the modification of a boundary condition, time-varying problems, etc. Meanwhile some loss of their accuracy has to be accepted if the number of nodes is not enough and their distribution is not appropriate so that a steep gradient near a grain boundary is not described well and the resolution flux is not computed accurately.

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* Corresponding author. Tel.: +82 42 868 2648; fax: +82 42 864 1089.
E-mail address: jscheon@kaeri.re.kr (J.-S. Cheon).

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Recently the authors proposed an adaptive two-zone method [10] for which the coordinate of a nodal point changes as a function of the released fraction. This method not only overcomes an inaccuracy at a lower release range, but also it has an efficiency comparable to the Fosberg–Maissh algorithm [11].

In this paper, the adaptive two-zone method is further developed to deal with a fission gas release under an imperfect sink. A system of equations are derived by applying a variational principle to the diffusion equation under a non-homogeneous boundary condition. The gas accumulated at the grain boundaries and its release to the free volume are computed from the profile of the gas concentration. It is also of importance to compare these results with those from previous analytic solutions and the FEM.

2. Fission gas release under irradiation-induced resolution condition

The diffusion equation in spherical coordinates,

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

is solved with the boundary conditions, $c_g = c_\lambda$ 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. The values c_λ and β are defined depending on how the irradiation-induced resolution flux near a grain boundary is taken into account.

Following Speight's argument [2], although there is controversial discussion on its validity [12], the diffusive flux within the matrix to the boundary is assumed to be balanced by the resolution flux from the boundary, i.e.

$$\frac{Dc_\lambda}{\lambda} = \frac{bN}{2}, \tag{2}$$

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

When the perfect sink boundary condition is preserved, all the atoms due to a resolution provide an additional flux at a depth of λ, or an additional source term which is distributed uniformly throughout a layer [6]. In combination with the perfect sink boundary condition, the solutions are obtained by adding the resolution flux to the source term. On the other hand, the diffusion equation under the resolution flux is also solved by adopting an imperfect boundary condition [4,5,9]. Rearranging Eq. (2) yields the boundary condition

$$c_\lambda = \frac{\lambda bN}{2D}. \tag{3}$$

As the gas is accumulated on a grain face via a resolution, N is saturated at a value of N_{sat}. The saturation concentration is fixed for all the temperatures [13].

During the computations, N is evaluated from a balance among the gas atoms generated, those remaining within a grain, those in a grain boundary, and those released:

$$\int \beta\,\mathrm{d}t = \bar{c}_g + 3N/2a + R, \tag{4}$$

where $\bar{c}_g$ is the average gas concentration in the grain, and R is the number of gas atoms released 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

$$f = 1 - \frac{\bar{c}_g + 3N_{\mathrm{sat}}/2a}{\int \beta\,\mathrm{d}t}. \tag{5}$$

2.1. Steady-state condition

Speight [2] suggested an approximate method for the rate of an accumulation of gas atoms at a grain face. It is given by

$$\frac{\mathrm{d}N}{\mathrm{d}t} = 4\beta\left(\frac{Dt}{\pi}\right)^{1/2}\left(1 - \frac{Nb\lambda}{2D\beta t}\right). \tag{6}$$

The solution [6] for Eq. (6) is written in the form of

$$N = A'(u^2 - 2u + 2 - 2\exp(-u)), \tag{7}$$

where $A' = \beta\pi D^2/8(b\lambda)^3$ and $u = 4b\lambda(t/D\pi)^{1/2}$.

Gas release after the saturation of a grain boundary was obtained by Turnbull [5], based on the assumption of a uniform gas concentration within a grain. It was evaluated that the fractional release shows an overestimation after an incubation when a variation of the gas concentration across the grain is pronounced under certain conditions such as a high temperature, and a low resolution rate [6]. Thus the following numerical methods are desirable to seek a reference solution.

2.2. Time-varying condition

Nuclear fuels are normally irradiated under varying power conditions. Even when a pin power remains constant, the fuel temperature varies with time due to a change in the gap conductance, a reduction of the thermal conductivity of a pellet, etc. Therefore a suitable algorithm is required to obtain a gas accumulation on a grain boundary and a fission gas release after a saturation under varying temperature conditions.

A few iterations are inevitable to develop a transient solution for all the algorithms which have been developed up to now. Based on the Booth [14] solutions, a composite release equation proposed by Turnbull [15] provides the fractional release by solving an effective time iteratively. Also an integro-differential equation for the gas accumulated on a grain face and the gas release were rigorously derived by Forsberg and Massih [4]. However, it still needs to be treated numerically for time-varying conditions.