

A Variational Approach for the Solution of the Diffusion Equation with a Moving Interface and Optimal Trial Functions

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1. Introduction

A distinctive feature in a fuel performance code relative to others is the consideration of the gas release due to fissions during an operation [1]. A lot of models have been developed to understand the fission gas release where the flux of gas atoms to the grain boundaries is described by a diffusion equation with different boundary conditions. The solutions of the equation are sought analytically as well as numerically [2-4]. Among the numerical treatments, the variational principle applied to the equation is regarded as a suitable method in the sense of its accuracy and efficiency. A finite element method is this kind of approach. The accuracy of the FEM depends principally on how well the trial functions accurately represent the profile of the gas concentration.

We have tried to increase the accuracy of the variational approach not only by introducing the moving interface strategy between the two concentric regions for the model of the spherical grain, but also by adaptively choosing the optimal trial functions.

2. Adaptive variational method

The diffusion equation in spherical coordinates,

$$\frac{\partial c_g}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(D_g r^2 \frac{\partial c_g}{\partial r} \right) + \beta \quad (1)$$

is solved with the boundary conditions, $c_g = 0$ at $r = r_g$ and $\partial c_g / \partial r = 0$ at $r = 0$, where r_g is the grain radius, D_g the gas atom diffusion coefficient, and β the rate of gas atom generation.

2.1 Investigation of previous works

An attempt to apply the variational principle to the problem of the fission gas release was made by Matthews and Wood [3]. The spherical grain is divided into two concentric regions of almost an equal volume. Three nodal points are required; the midpoint radius of region I ($\rho_1 = 0.4$), the interface between the regions ($\rho_2 = 0.8$), and the midpoint radius of region II ($\rho_3 = 0.9$), where $\rho = r/r_g$. The concentrations at these points are represented by c_1 , c_2 , and c_3 , respectively. Quadratic functions are employed to represent the concentration profile. The two-zone approximation was reported to be unlikely to give

satisfactory results at a low release less than 2% [3].

We have further examined the accuracy of the calculation by increasing the number of the concentric regions. This was accomplished by using a commercial finite element code, ABAQUS. The released fraction at the low times seemed to be inaccurately calculated even if the number of the finite elements was increased by as many as 10. In such a case, the concentration near the grain boundary was evaluated to be higher than those at the inner points of the grain. In addition, another critical problem arose especially in the two-region approximation, where the radial coordinate corresponding to the apex of the trial function for the outer region, ρ_{2v} is larger than ρ_2 at the early moments.

2.2 Adaptive method for the enhanced accuracy

The exact solution of Eq. (1) is given for a zero initial condition and constant gas generation rate in the reference [5]. The normalized distribution of the gas concentration is nearly flat in most of the grain. It also exhibits an abrupt drop near the surface at an early time, whose radial coordinate moves inward in proportion to the released fraction. The maximal concentration is always located at the center of the grain. The distribution of the gas concentration is described well by the quadratic function later on. Finally those problems mentioned in 2.1 do not appear in the exact solution. These observations mean that the interface of the regions needs to move inward, and that the trial functions should guarantee the monotonous decrease of the concentration with an increasing radial coordinate.

As for the moving interface, we calculated the locus of the radial point as a function of the released fraction where the concentration is equal to a constant less than unity times its maximum using the exact solution above. This locus is ρ_2 . The application of the same relationship is assumed to be applicable to the case of a varying gas generation rate. 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 0.7.

Trial functions are modified with the 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 . In this case the degree of freedom is reduced

from three to two. Furthermore c_1 is set to be equal to c_2 for the latter case, thus the degree of freedom is one. The trial functions are selected adaptively during the calculation according to the previous criteria.

Several iterations are required to satisfy the convergence criteria of the released fraction at every time step.

3. Verification of the adaptive method

The present method was compared with the original one by Matthews and Wood [3] for the cases of a constant and varying gas generation. The reference solutions were obtained using the ABAQUS code with 50 elements. We have used the diffusion coefficient of the gas atoms in the reference [6]. The grain radius is assumed to be 5 μm .

Fractional gas release was calculated for a series of temperature and gas generation conditions. Fig. 1 shows an example of the response of the gas released fraction as a function of the time. Except for the very low times, the present method gave results within a deviation of 0.5 % with respect to the reference solution. The two-zone method without an adaptivity, however, underestimated the released fraction by $\sim 3.5\%$. The released fraction at time = 2000 sec was calculated to be 0.0068, 0.0072, and 0.018 from the ABAQUS, the adaptive two-zone method, and the original two-zone method with a quadrature adjustment for the average gas concentration, respectively.

Fig. 2 shows the calculated fractional gas release as a function of the time when the temperature is changed as shown. The present method gave a response comparable to the reference solution even though it was overestimated slightly during a temperature decrease. The original two-zone method was unsuccessful for the current case.

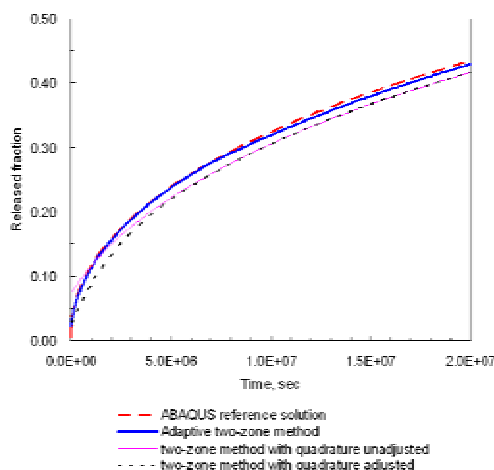


Figure 1. Calculated fractional gas release as a function of time at 1200 °C.

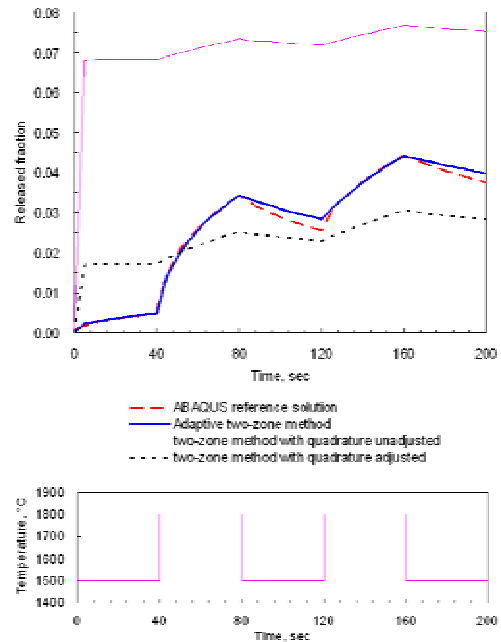


Figure 2. Calculated fractional gas release as a function of time for varying gas generation.

4. Conclusion

An adaptive variational method was developed to solve the diffusion equation for a gas release effectively and accurately. This approach is more precise than the conventional two-zone method by Matthews and Wood, especially for a lower gas release. It also provided a reasonable means for the condition of a varying gas generation. Further studies are needed to optimize the present method, and to apply it to the diffusion problems with different boundary conditions.

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REFERENCES

- [1] Y.H. Koo, B. H. Lee, D. S. Sohn, *Annals of Nuclear Energy*, 26 (1999) 47.
- [2] A.H. Booth, Report CRDC-721, 1957.
- [3] J.R. Matthews, M.H. Wood, *Nuclear Engineering and Design*, 56 (1980) 439.
- [4] K. Lassmann, H. Benk, *Journal of Nuclear Materials*, 280 (2000) 127
- [5] H.S. Carslaw and J.C. Jaeger. *Conduction of Heat in Solids*, Oxford University, London (1959), p243.
- [6] D.M. Dowling, R.J. White, M.O. Tucker, *Journal of Nuclear Materials*, 110 (1982) 37.