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Numerical Approach of Grain Shape Effect on the Diffusional Fission Gas Release

Oh-Hyun Kwon*, Hye-In Shin, Young-Ho Heo, Jae-Ik Kim, Kyeong-Lak Jeon
KEPCO Nuclear Fuel Co. Ltd., 1047, Daedeokdaero, Yuseong-gu, Daejeon 305-353, Korea
**Corresponding author: ohkwon@knfc.co.kr*

1. Introduction

In the realm of nuclear fuel performance, much precise prediction of fission gas release is desirable because fission gas release significantly affects thermal and mechanical responses of fuel rod.

The equiaxed grain growth phenomenon is well known for the UO_2 fuel under the normal operation of commercial reactors. In this equiaxed grain growth zone, the fuel grain is usually simulated by a spherical geometric model. It is also well known that the columnar grain can be readily identified in the irradiated fuel at high powers [1]. For instance, the columnar grain growth occurred in CANDU fuel as shown in Fig. 1 [2]. And columnar grain growth was indicated in BWR [3]. Early study revealed that the columnar grain growth can occur by pore migration resulting from a sublimation mechanism at temperatures higher than 1700°C with gradients higher than 200°C/mm [4]. From a photographic analysis, the columnar grain can be depicted by a cylinder of which axis lies in perpendicular to the axial axis of cylindrical pellet. The influence of columnar grain growth on grain boundary sweeping has been already modeled by some investigators and incorporated into some computer models [5].

However, as far as the authors know, no models have been reported in open literatures to take into account of the diffusion of gas atoms in the columnar grain by taking the grain shape as a cylindrical one. In the computer models for fission gas release analysis, spherical geometric model is applied for columnar grain as well as equiaxed grain. This may be the reason that grain boundary sweeping is considered as the primary parameter in contributing to fission gas release rather than gas atom migration at high powers. However, it is still needed to develop more accurate computer models to understand the influence of different geometric models of fuel grain on gas atom migration. This study aims to evaluate the influence of different geometric models of fuel grain on gas atom migration under high temperature conditions.

2. Numerical Methods

Fission gas migrates from grain inside to grain boundary by various mechanisms such as single gas atom migration, bubble migration and resolution, and grain boundary sweeping. The bubble migration is not considered in this study because the small intra-granular bubbles are generally accepted to be immobile at the condition without great temperature gradients due to their octahedral shape and solid fission products contained in them [6-8]. Grain boundary sweeping is also not considered in this study to focus the subject on the evaluation of different grain shapes on fission gas diffusion, as mentioned before.

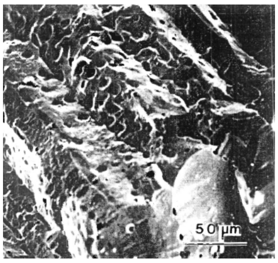

Fig. 1. Microstructure in UO_2 Pellets Irradiated in Canadian Reactors

2.1 Diffusion equation

The general form of diffusion equation is as follows.

$$\frac{\partial C}{\partial t} = D_{eff} \cdot \nabla^2 C + \beta \qquad (1)$$

Where,

C = fission gas concentration
t = time
β = gas generation rate per volume
D_{eff} = effective diffusion coefficient of single gas atom
∇^2 = Laplacian operator
for the spherical coordinate,

$$\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}$$

for the cylindrical coordinate,

$$\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}$$

The concentration gradient at the center is zero and the perfect sink bounding conditions at the grain surface are used. The fractional release of fission gas is calculated.

2.2 Spatial nodalization

Fig 2 shows the two different geometric models of fuel grain. Non-uniform grids were generated in geometric progression to give finer meshes toward grain surface. This discretization method was found to be much efficient in solving the diffusion equation where the concentration was rapidly changed near the boundary. In order to solve the diffusion equation (1), finite difference method with Crank-Nicolson numerical scheme is adopted. The gas atom diffusion coefficient was used given in the literature [9].

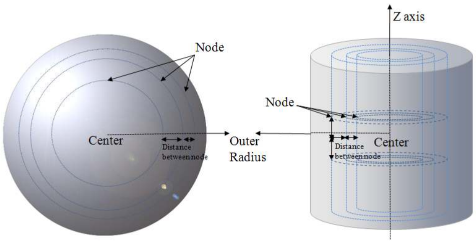

Fig. 2. The configuration and nodalization of the spherical geometric model (left) and cylindrical geometric model (right)

3. Results and Discussion

Fig. 3 shows the calculated fractional releases from the spherical and cylindrical grains at 1800°C under the constant gas generation rate condition. For the comparison, the grain volumes of the two different grains were assumed to be same each other. The fission gas release from the cylindrical grain was much more than that from the spherical grain, and the amount of fission gas release of the cylindrical grain greatly increased as the ratio of length to diameter, L/D increased and also the grain surface to volume ratios is increased. This occurred due to the decrease in the distance of gas atom migration to the boundaries. Under the constant volume condition, the diameter of the cylindrical grain was shorter than that of the spherical grain, as presented in Table 1. The decrease in the diameter of the cylindrical grain contributed to the much release.

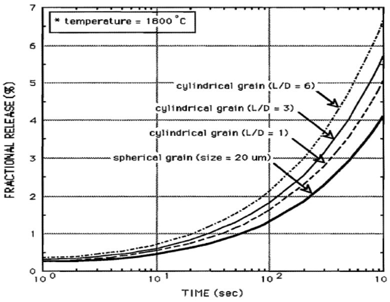

Fig. 3. The calculated fractional release from the spherical and cylindrical grains at the constant volume condition

Table 1: The change in the size of cylindrical grain

L/D	Constant volume*		Constant surface*	
	Length (μm)	Diameter (μm)	Length (μm)	Diameter (μm)
1	17.5	17.5	16.3	16.3
3	36.3	12.1	32.1	10.7
6	57.7	9.6	47.1	7.9

* In the constant volume condition, the volume of the cylindrical grain was equal to that of the spherical grain (20 μm). In the constant surface condition, the surface area of the cylindrical grain was equal to that of the spherical grain (20 μm)

Fig. 4 shows the calculated fractional releases from the two different grains. The operating conditions were considered to be same with those of Fig. 3. The diameter and the length of the cylindrical grain under the constant surface area condition were more reduced than those of the cylindrical grain under the constant volume condition, as presented in Table 1. Comparing the fractional releases under the constant volume and surface area conditions, the fractional release under the constant surface area condition much increased due to the decrease in the distance of gas atom migration to the boundaries in both axes.

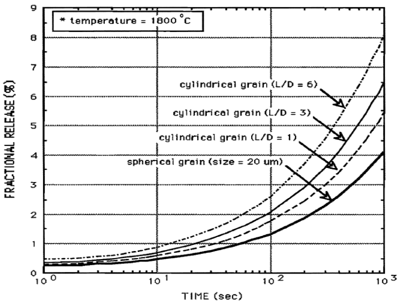

Fig. 4. The calculated fractional release from the spherical and cylindrical grains at the constant surface condition

4. Conclusions

Generally, fission gas release to a grain boundary depends on the surface to volume ratio of a grain. However, in this paper, a cylindrical grain shape was considered in order to numerically quantify the gas atom release in the columnar grain of UO_2 fuel. The fractional release calculated by the cylindrical geometric model was compared with that by the spherical geometric model under the constant volume or constant surface area conditions. It was shown that the fractional release with the cylindrical geometric model is much more than that with the spherical geometric model, due to the decrease in the diffusion distance. As a further study, the parameters affecting fission gas release such as sweeping, diffusion, resolution, and etc. are considered for more accurate quantification.

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