Development of Two-Stage Two-Step Fission Gas Release Model

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1. Introduction

Since the LWR operation mode changed from annual to extended/high burn-up fuel cycles in the late 1980s, more attention has been paid to fission gas release phenomena There have been reports that fractional fission gas release is even accelerating with increasing burn-up. Therefore, for the development of high performance fuels, fission gas release is considered. In this study, two-stage two-step model is developed which incorporates two stage diffusion processes, grain lattice and grain boundary diffusion, coupled with the two step burn-up factor in the low and high burn-up regime.

2. Development of the Model

2.1. Two-Stage Model

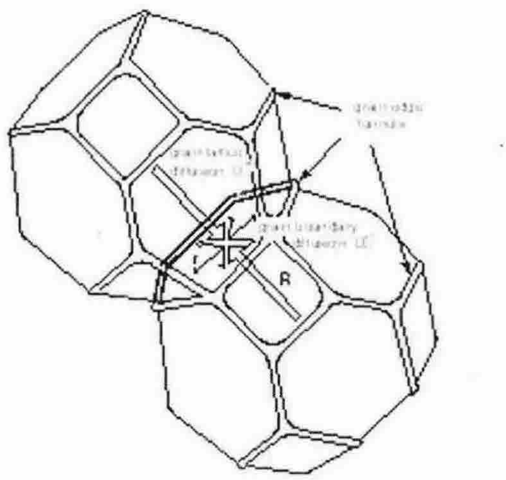

Figure 1. A schematic of two principal diffusion processes in the current two-stage two-step model with grain lattice diffusion D_v^{eff} and grain boundary diffusion D_{gb}^{eff}.

In the model, coupled with the bubble trap and the bubble resolution, fission gas transport is broken down into the two principal processes: the effective grain lattice diffusion, and the effective grain boundary diffusion. Figure 1 schematically shows the fundamental processes of the current two-stage model with the assumption that a grain has an ideal tetrakaidecahedron structure and fission gas bubbles at the grain edges are linked together to form grain edge tunnels that are finally connected to the open space inside the fuel rod.

Therefore, the governing equation for the effective grain lattice diffusion is then:

$$\frac{\partial C_v}{\partial t} = \beta + \frac{1}{R^2}\frac{\partial}{\partial R}\left(D_v^{eff} R^2 \frac{\partial C_v}{\partial R}\right) \qquad (1)$$

with the initial condition $C_v(R,0)=0$, and boundary conditions $C_v(0,t)=$ finite and $C_v(a,t)=\bar{C}_{gb}(t)$. In the equation, C_v is the volumetric fission gas concentration within the grain, β is the fission gas generation rate, and a is the equivalent radius of the grain. D_v^{eff} is defined as $D_v^{eff}=(b/b+g)D_{trap}^{in-pile}$ that was proposed by Speight for the application of Booth concept to the high burn-up cases.

Now, the fission gas atom concentration in the grain boundary is expressed as:

$$\delta\frac{\partial C_{gb}}{\partial t} = \delta\frac{1}{r}\frac{\partial}{\partial r}\left(D_{gb}^{eff} r \frac{\partial C_{gb}}{\partial r}\right) - 2D_v^{eff}\left(\frac{\partial C_v}{\partial R}\right)_{R=a} \qquad (2)$$

subject to the initial condition $C_{gb}(r,0)=0$, and the boundary conditions $C_{gb}(0,t)=$ finite and $C_{gb}(s,t)=0$. In Equation (2), C_{gb} is the fission gas concentration in the grain boundary, δ is the grain boundary thickness, and s is the equivalent radius of the grain surface.

Assuming the steady state, equation (2) is turned into the following boundary condition:

$$\alpha\left.\frac{\partial C_v}{\partial R}\right|_{R=a} - C_v(a,t) = 0 \qquad (3)$$

where, $\alpha = \frac{2}{\delta\beta_1^2}\frac{D_v^{eff}}{D_{gb}^{eff}}$

Then, according to the following definition, the fractional fission gas release is finally obtained:

$$F \cong \frac{4}{\sqrt{\pi}}\left(\frac{a}{\alpha+a}\right)^2\left(\frac{D_v^{eff}t}{a^2}\right)^{1/2} - \frac{3}{2}\left(\frac{a}{\alpha+a}\right)\left(\frac{D_v^{eff}t}{a^2}\right) \qquad (4)$$

As seen in the equation, multiples of the two-stage parameter, $a/(\alpha+a)$, appear in each term of the simple Booth solution, factorizing it with the new dimensionless property.

2.2. Two-Step Two-Stage Model

The successful depiction of two-stage model on the high burn-up behaviors leads to the development of current two-step two-stage model.

Basically α is D_v^{eff}/D_{gb}^{eff} with the unit of centimeter since δ is on the order of 10^{-8} cm, β_1 is $2.405/s$ where s is the equivalent radius of a grain surface which is on the order of 10^{-4} cm, and thus $2/\delta\beta_1^2$ is close to unity. Thus, the ratio of diffusivities α is rewritten in the following way:

$$\alpha \cong \frac{D_v^{eff}}{D_{gb}^{eff}} = \frac{D_{v0}e^{-Q_v/RT}}{D_{gb0}e^{-Q_{gb}/RT}} = \alpha_0 e^{-(Q_v - Q_{gb})/RT}$$

$$= \alpha_0 e^{-Q_v\left(1-\frac{Q_{gb}}{Q_v}\right)/RT}$$

Then, burn-up factor f_{Bu} is introduced in the following way:

$$\alpha = \alpha_0 e^{-f_{Bu}Q_v/RT} \qquad (5)$$

where, $f_{Bu} = 1 - Q_{gb}/Q_v$

Finally, the fractional release of fission gas atoms is obtained as:

$$F = \frac{4}{\sqrt{\pi}}\left(\frac{1}{1+\alpha' e^{-f_{Bu}Q_v/RT}}\right)^2 \left\{\left(\frac{D_0}{a^2}\right)\exp\left(\frac{-Q_v}{RT}\right)t\right\}^{\frac{1}{2}} \qquad (6)$$

where, $\alpha' = \alpha_0/a$

The burn-up factor f_{Bu} is treated step-wisely in this two-step two-stage model, depending on the fuel burn-up. Until the burn-up reaches the threshold burn-up it remains zero since Q_{gb} stays close to Q_v, never exceeding, in the low burn-up regime. On the other hand, it begins to increase linearly up to the unity in high burn-up regime because Q_{gb} linearly decrease down to zero at ultimate high burn-up.

3. Model Validation and Discussion

For the derivation of constituent parameters and the validation of the model FRAPCON-3 code and its in-pile measurement data sets are used.

First, ten data sets that are all distributed by the FRAPCON-3 code authority are chosen for the derivation of best fitting parameters of the model. In this best fitting analysis the threshold burn-up is assumed to be 25,000 MWd/MTU. Finally derived best-fit parameters are as follows:

$\alpha' = 1.06$

$f_{Bu} = Max(0, Bu - 25000)/72000$

$(D_0/a^2) = 0.018$ /sec

$Q = 44906$ cal/mol

Then, current model predictions are examined using those best-fit parameters and compared with those by other popular models, especially contained in FRAPCON-3 code. As shown in Figure 2, over whole burn-up range up to 70,000 MWd/MTU its prediction is in much better agreement with the experimental measurements than that by any model in the FRAPCON-3 code such as ANS 5.4, modified ANS5.4, and Forsberg - Massih model except one measurements data set. It is easily understood when the burn-up factors of the models are compared and reviewed.

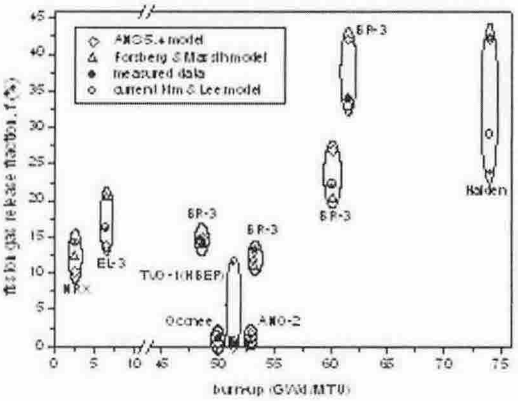

Figure 2. Current two-step two-stage model prediction results and their comparison using the same in-pile data sets used for FRAPCON model validation.

4. Conclusions

Based on the recent theoretical model, two-step two-stage model is developed with the incorporation of step-wisely divided burn-up factor in the low and high burn-up regime. In the model the two-step factor is introduced to the two-stage parameter of the two-stage model in order to simulate the decreasing activation energy for the fission gas atoms diffusion through the grain boundary with fuel burn-up increase.

FRAPCON-3 code and its in-pile measurement data sets are used for the derivation of constituent parameters in the model and its validation. Results reveals that over whole burn-up range up to 70,000 MWd/MTU its prediction is in much better agreement with the experimental measurements than that by any model in the FRAPCON-3 code such as ANS 5.4, modified ANS5.4, and Forsberg - Massih model. This excellent agreement may confirm that two-step burn-up factor and two-stage parameter introduced to this model are based on sound mechanistic foundation.

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