Implementation of the High Temperature Oxidation Model for the Zircaloy Cladding in the MERCURY

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1. Introduction

KAERI has been developing the FEM(Finite Element Method)-based nuclear fuel performance code, MERCURY to evaluate the behavior of nuclear fuel during accident conditions [1]. A widely used code system for evaluating the fuel performance in accident conditions is the NRC's FRAPTRAN [2]. The FRAPTRAN uses a so-called 1.5D analysis that divides the axial direction into several nodes and calculates radial changes at each node. Unlike this analysis system, codes that apply FEM to structural analysis are being developed as an analysis system to more reflect physical phenomena. In the USA, an FEM-based nuclear fuel performance code represented by BISON, has been developed and applied to integrated analysis system such as VERA and CASL [3].

In this paper, we describe the selection and implementation process of the high temperature oxidation model in the MERCURY code. In addition, the verification calculation result of the applied model is presented.

2. High-temperature Oxidation Model of Zircaloy Cladding

As a high-temperature oxidation model of the zircaloy cladding, the models of the Cathcart-Pawel(C-P) and the Bake-Just(B-J) are typically used. The B-J model is widely used for conservative calculations, and the C-P model is mainly used for best-estimate calculation. Since the FEM-based fuel performance code is for best-estimate analysis, the MERCURY is also based on the C-P model. The C-P model provides each model constant for four parameters of oxide(ϕ), alpha(α), Xi(ξ) layer growth and total oxygen consumed (τ) based on the Arhenius equation for temperaure as follows [4].

$$\delta_{\phi}^2 = 2 \cdot 0.01126 exp\left(-\frac{35890}{RT}\right), \left[\frac{cm^2}{s}\right] \quad (1)$$

$$\delta_{\alpha}^2 = 2 \cdot 0.7615 exp\left(-\frac{48140}{RT}\right), \left[\frac{cm^2}{s}\right] \quad (2)$$

$$\delta_{\xi}^2 = 2 \cdot 0.3412 exp\left(-\frac{41700}{RT}\right), \left[\frac{cm^2}{s}\right] \quad (3)$$

$$\delta_{\tau}^2 = 2 \cdot 0.1811 exp\left(-\frac{39940}{RT}\right), \left[\frac{(\frac{g}{cm^2})^2}{s}\right] \quad (4)$$

where, R is the gas constant, T is the cladding temperature.

The zirconium-based cladding tube generates the reaction heat during the high temperature oxidation process, and the heat of the metal-water reaction is determined by the amount of oxygen consumed. The relation for the metal-water reaction heat is defined in MATPRO [5] as follows.

$$\frac{0.74}{0.26}\frac{\Delta W}{\Delta t} 2\pi R_0 6.45 \times 10^6 \ \frac{J}{m} \quad (5)$$

where, ΔW is the weight gain during the time increment Δt and R_0 is initial radius of cladding.

The ECR(Equivalent Cladding Reacted) as a parameter expressing the mechanical integrity of the cladding tube in relation to the high temperature oxidation is expressed as follows [2].

$$\mathrm{ECR} = 100 \cdot \frac{(w_o + w_i)\frac{m_{Zr}}{m_{O_2}}\frac{1}{\rho_{Zr}}}{(r_o - r_i)\cdot(1+\varepsilon)} \quad (6)$$

where, w_o and w_i is weight gain of outer and inner surface, r_o and r_i is the initial radius of outer an inner surface, m is the molecular weight, ρ is density, and ε is strain. As described above, the reaction heat and the ECR are expressed as a function of the weight gain increased during the oxidation. Accordingly, in MERCURY, the weight gain for a time step will be calculated based on the total oxygen consumed correlation of C-P model, and the reaction heat and the ECR will be evaluated from this result.

3. Implementation of Oxidation Model

The difference from FRAPTRAN in the calculation scheme for the oxidation heat is compared in Fig. 1. FRAPTRAN first completes the temperature calculation in one time step, and then calculated the oxidation heat using the average temperature of beginning (BOS) and end of step (EOS). The obtained reaction heat is substituted into the heat generation of the next step. In contrast, MERCURY configures the oxidation heat and temperature at BOS into one matrix and determines the temperature at EOS. Therefore, MERCURY transfer the final temperature of the time step to the temperature of the next step. Since the temperature convergence is checked for each time step, and the time increment is readjusted by algorithm of MERCURY.

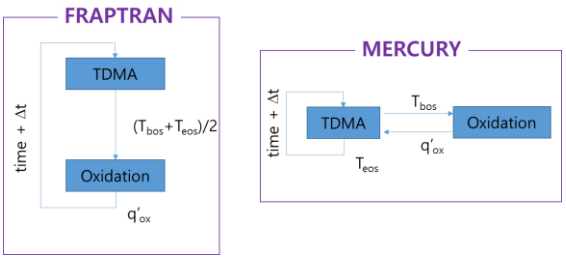

Fig. 1 The difference of the calculation scheme for oxidation heat between FRAPTRAN and MERCURY

3.1 Calculation of Oxidation Heat

The calculation flow chart for the heat of oxidation reaction is shown in Fig. 2. The oxidation reaction heat is considered when the temperature of the cladding exceeds 1073 K. When the temperature of the cladding exceeds 1073 K, the weight gain (wg2) is determined by the temperature and time increment for each node of current time step, and the determined weight gain includes the weight gain (wg1) of the previous step. The amount of oxidation increased at the current step becomes wg2 minus wg1.

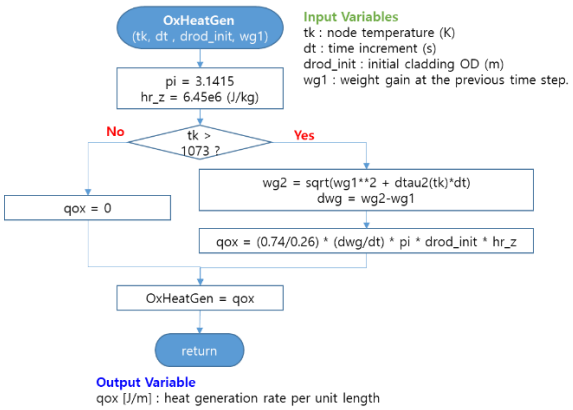

Fig. 2 Flow chart of oxidation heat calculation

3.2 Calculation of ECR

The ECR is a parameter for evaluating the mechanical integrity of cladding considering the oxidation, so the oxidation of inner and outer surfaces should be considered. To do this, it is necessary to designate a pair of nodes on the inner and outer surfaces of the grid mesh generated for FEM. ECR is calculated by the summation of the weight gain from a pair of inner and outer surfaces and initial radius of cladding. The flow chart for ECR is shown in Fig. 3.

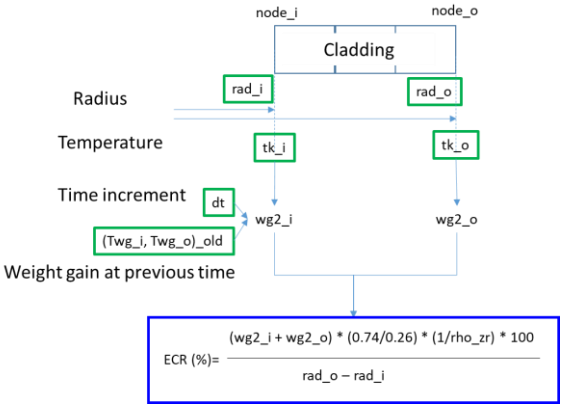

Fig. 3 Flow chart of ECR calculation

3.3 Verification of Oxidation Model

For the verification calculation, a simple geometry consisting of pellet and cladding was used. In order to remove the deformation of the cladding tube, the rod internal pressure was ignored, and the temperature of the outer surface was maintained constant at 800 ℃ and 1000 ℃. The weight gain results calculated using MERCURY are compared with the results of the correlation in Fig. 4. As shown in the figure, the two results are exactly the same. Through this, it was verified that the oxidation model was well implemented into the MERCURY code.

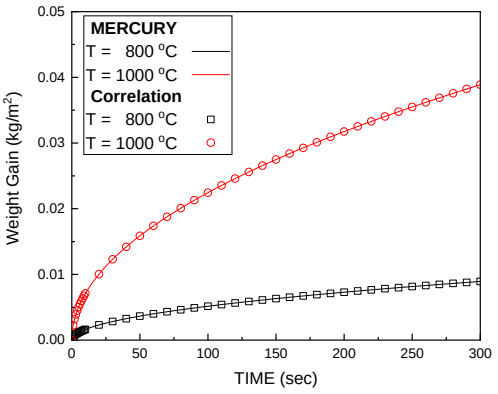

Fig. 4 Comparison of weight gain calculated by MERCURY and correlation

4. Conclusions

FEM-based MERCURY code is being developed for the evaluation of the fuel performance under accident conditions. The implementation and verification of the high-temperature oxidation model in the MERCURY code were performed.

The Cathcart-Pawel model, which is used as a high-temperature oxidation model of the cladding for the best-estimated analysis, is composed of functions. The high temperature oxidation reaction heat and ECR were calculated from the weight gain function.

Unlike FRAPTRAN, MERCURY uses the BOS temperature and oxidation reaction heat of the current calculation step to obtain the EOS temperature and then transfers it to the BOS of the next step.

It was confirmed that the weight gain over time by the high-temperature oxidation module of MERCURY was the same by comparing the results of the correlation.

The flow chart and modularization for calculating the ECR have been completed, but verification considering the nodal mapping between the inner and outer surfaces of the cladding is currently in progress.

Acknowledgement

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