

## Application of High Temperature Oxidation Model for Coated Cladding in FRAPTRAN-2.0

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### 1. Introduction

After the Fukushima accident, improving the safety of nuclear power plants has been raised as an important issue. In particular, the development of the accident tolerant fuel, such as reducing the generation of hydrogen in the Zirconium alloy cladding during the accident condition has been studied worldwide. As a technology that can be applied in the short term, the coating technology on the cladding surface is being developed. The coated cladding have to apply each oxidation model to the inner and outer surface of the cladding. It is necessary to modify the nuclear fuel performance code FRAPTRAN, which is currently used in the accident conditions. This paper describes the results of applying the oxidation model of the coating material developed by KAERI into FRAPTRAN-2.0 code [1].

### 2. Oxidation Model of FRAPTRAN-2.0

The FRAPTRAN (Fuel Rod Analysis Program Transient) is the fuel performance code to calculate the transient performance of light-water-reactor fuel rods during reactor transients and hypothetical accidents, which has been developing by U.S. NRC. The FRAPTRAN-2.0 has 2 sub-options to specify the modeling of the metal-water reaction, one is the Cathcart correlation(C-P model), and the other is the Baker-Just model(B-J model). From the user manual, the Cathcart option is recommended for a best-estimate calculation, and the B-J model is the option to use in licensing calculation. The B-J model is the reaction correlation of zirconium metal, however Cathcart model suggests the thicknesses and the total oxygen consumed. Each of the two models is expressed in terms of the the oxide thickness as follows [1].

Cathcart model:

$$K_2^2 = K_1^2 + 2 \cdot 1.126 \times 10^{-6} \exp\left(\frac{-35890}{R-T}\right) \Delta t \quad (1)$$

B-J model:

$$K_2^2 = K_1^2 + 1.883 \times 10^{-4} \exp\left(\frac{-45500}{R-T}\right) \Delta t \quad (2)$$

where,

$K_1$ : oxide thickness at beginning of time step (m)

$K_2$ : oxide thickness at end of time step (m).

The calculation flow diagram of the oxidation model in the code is shown in Fig. 1. The oxidation model is used to calculate the amount of heat additionally generated by the oxidation reaction and to calculate the

ECR(Equivalent Clad Reacted) based on the oxide thickness. In the C-P model, the inner and outer cladding oxidation is calculated in a separated subroutine, but in the B-J model, it is calculated in one subroutine.

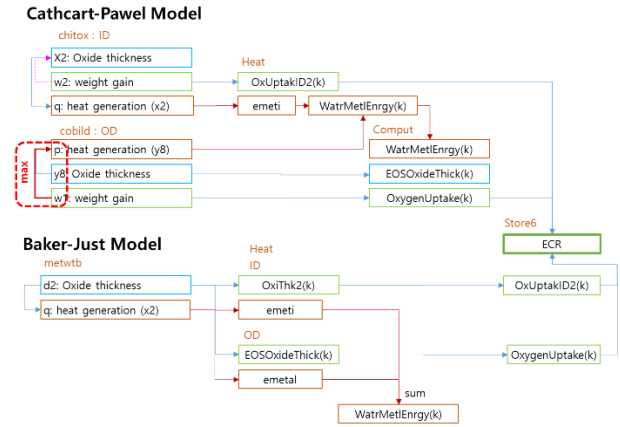


Fig. 1 The calculation flow diagram of the oxidation model in FRAPTRAN-2.0

### 3. Oxidation Model for Coated Cladding

#### 3.1 Oxidation model for coating material

KAERI has developed CrAl alloy as a coating material that can improve the oxidation resistance of coated cladding. The high temperature oxidation model of the developed coating material has been suggested as follows [2].

$$K_p = 3.870 \times 10^{-5} \exp\left(\frac{-8020}{T(K)}\right) \quad (3)$$

The oxidation model of the coated cladding calculates the amount of oxidation of CrAl alloy used as a coating material. Therefore, Equation (4) can applied to convert the oxide film thickness based on the measured weight gain. Since the theory and experimental results for the oxidation reaction of CrAl are not sufficient, however, it is assumed here that an oxide layer is formed only of  $\text{Cr}_2\text{O}_3$ , an oxide of Cr. From this assumption, the oxide film thickness is calculated as follows.

$$\delta_{eff} = \frac{W}{\rho \cdot w_f} \Big|_{\text{Cr}_2\text{O}_3} \quad (4)$$

$\delta_{eff}$ : effective oxide thickness (m)

W: total oxygen uptake ( $\text{kg/m}^2$ )

$\rho$ : density of  $\text{Cr}_2\text{O}_3$  ( $= 5220 \text{ kg/m}^3$ )

$w_f$ : weight fraction of oxygen in  $\text{Cr}_2\text{O}_3$  ( $= 0.3158$ )

In addition, the heat of oxidation reaction was estimated as shown in Table 1 below.

Table 1 Reaction heat of Cr<sub>2</sub>O<sub>3</sub>

Cr <sub>2</sub> O <sub>3</sub> Reaction Heat						
Reaction	4Cr	+	3O <sub>2</sub>	→	2Cr <sub>2</sub> O <sub>3</sub>	+Q
$\Delta h_f^o$ (kJ/mol)	0		0		2*(-1128)	-2256

$Q = 2256 \text{ (kJ/mol)} / (4 \times 51.9961) \text{ (g/mol)}$   
 $= 10.85 \times 10^6 \text{ J/kg of Cr}$

- Standard Enthalpy of formation at 25 °C [3]:  
Cr<sub>2</sub>O<sub>3</sub> = -1128 (kJ/mol)
- Atomic weight :  
Cr = 51.9961 g/mol

### 3.2 Implementation of ATFMW

The oxidation model of coated cladding described above is coded with the subroutine 'atfmw', and the flow chart for implementing into FRAPTRAN is shown in Fig. 2. It is a combination of the calculation flow of the C-P and B-J models built into FRAPTRAN. For the oxidation of the inner surface, the subroutine 'chitox' applied with the C-P model is used, and for the coated outer surface, the developed subroutine 'atfmw' is used.

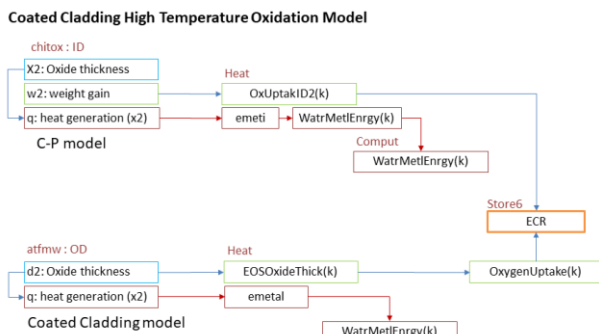


Fig. 2 Flow chart of the high temperature oxidation model for the coated cladding.

### 3.3 Verification of the oxidation model for a coated cladding

In order to oxidation model for coated cladding, a hypothetical input as shown in Fig. 3 was applied to the cladding surface. The high temperature of 1073 K or higher was loaded to the surface of the cladding, where oxidation reactions could occur. In Fig. 4, the thickness of the oxide film on the inner and outer surfaces of the cladding was compared, and in Fig. 5, the total ECR of the cladding was compared. In the outer surface oxidation, it was evaluated that the oxide film thickness was formed as much as 3000 times less due to the improved oxidation resistance of the coating layer. In the current calculation scenario, the cladding burst occurs in 34.5 seconds, after which oxidation of the inner surface proceeds. Therefore, since the existing C-P model was used to the internal oxidation of the zircaloy cladding,

similar oxide thickness were shown when the ATF model was used. When the ATF model was used, there is almost no oxidation on the outer surface, and only the internal oxidation after burst occurs. Therefore, compared to the case of applying the C-P model on both surfaces, the total ECR of ATF model shows almost half the value as expected. As a result, it was verified that the oxidation model of the currently applied coated cladding works properly.

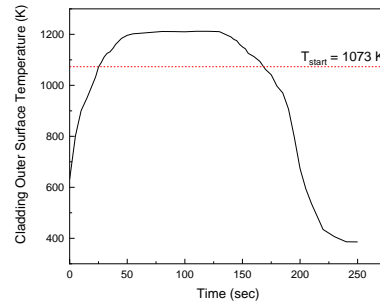


Fig. 3 The temperature history for verification of ATF oxidation model

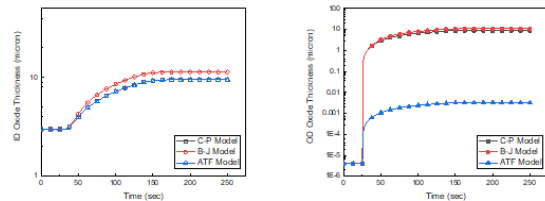


Fig. 4 The oxide thickness of inner and outer cladding of ATF oxidation model

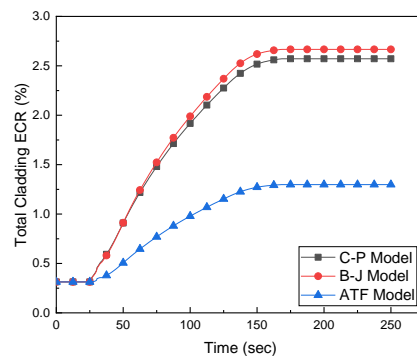


Fig. 5 The total cladding ECR of ATF oxidation model

## 4. Conclusions

In order to evaluate the oxidation characteristics of the coated cladding that can be applied as an accident tolerant fuel cladding, and the oxidation model of the coating material, CrAl was developed and implemented to the fuel performance code, FRAPTRAN-2.0.

In the coated cladding, each oxidation model is applied to the inner and outer surfaces, respectively. The

oxidation model should evaluate the change in thickness of the cladding tube and the reaction heat of oxidation. In order to the oxidation reaction heat of CrAl, a coating material developed by KAERI, it was assumed that the oxide layer was converted to Cr<sub>2</sub>O<sub>3</sub>.

The developed oxidation module was evaluated using a scenario of the hypothetical high temperature condition was loaded to the outer surface of the cladding. The behavior of the oxide thickness and ECR on the inner and outer surface were verified with FRAPTRAN-2.0. The fuel performance code system that can evaluate the high-temperature oxidation behavior in accident conditions for the coated cladding tube as an accident tolerant fuel has been developed.

#### **Acknowledgement**

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