Development and Verification of the Standalone Code for High-Temperature Oxidation Analysis of an Accident Tolerant Fuel

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1. Introduction

There are active researches being conducted globally on Accident Tolerant Fuel (ATF) to enhance nuclear safety by drastically reducing the oxidation heat and hydrogen generation of nuclear fuel during accidents. To achieve this, research and licensing preparations are underway to form a coating layer using corrosion-resistant metals such as Cr or CrAl on the outer surface of the existing cladding, which is previously composed of a single layer.

This paper is about a study on the performance improvement of accident condition nuclear fuel evaluation code (MERCURY) [1] based on the finite element method (FEM) for analyzing multi-layered corrosion-resistant metal-coated claddings. MERCURY is a code that evaluates the performance of a multidimensional entire fuel rod, which takes a significant amount of time for mechanical and thermal analysis. Therefore, to develop and verify the high-temperature oxidation analysis code of the coated claddings, it is first implemented as a standalone code for ease of use. As the property data for the coating claddings is very limited, the module is developed based on published data and coded to make it easy to apply when the property model is secured in the future. To verify that the implemented code is running well, the values calculated from the high-temperature oxidation analysis module are compared with the arithmetic calculation values of the experimental model over time at a given temperature.

2. High-temperature oxidation analysis code

To develop a coating cladding oxidation analysis code based on Fortran90, the oxidation module calling statements of MERCURY are separated and the main program ATF_OX_MERCURY.f90 is constructed. These assign arguments used in the oxidation module. The main program receives information on temperature exposure time, and whether the current element being calculated is on the inner or outer surface of the coated cladding to call the subprogram Oxidation.f90. The oxidation module uses the information received from the main program to calculate the oxide thickness, weight gain, oxidation reaction heat, and the resulting ECR, and sends the results back to the main program. The other subprograms, Kinds.f90 and Module.f90, are modules that declare the variables used in the oxidation module and are used without modification to the existing MERCURY to prevent errors during the integration process with MERCURY in the future. The Kind module defines the precision of integers and real numbers used in the code. The Module declares the variables used various modules.

3. Oxidation module implementation

3.1 Weight gain and oxide thickness calculation

The currently available high-temperature oxidation weight gain experimental results for coated cladding have been reported in reference [2].

$$K_p = 3.87 \times 10^{-5} \exp(-8020/T) \quad (1)$$

Where,
K_p : weight gain [$(g/cm^2)/s^{1/2}$]
T : temperature [K]

The function “dtau2_coat” is coded to reflect this, which determines the weight gain constant based on the given temperature. The input of this function is the temperature, and the output is the weight gain constant [$(kg/m^2)^2/s$] calculated as the square of the equation above.

The equation above is for weight gain, so the conversion equation for oxide thickness is calculated using the Equation (2). However, this equation only considers the composition of Cr_2O_3 for the oxide layer, and modifications may be necessary depending on the actual material used in future.

$$\delta_{eff} = W/(\rho \times w_f) \quad (2)$$

Where,
δ_{eff} : effective oxide thickness [m]
W : total oxygen uptake (kg/m^2)
ρ : density of Cr_2O_3 (= 5220 kg/m^3)
w_f : weight fraction of oxygen in Cr_2O_3 (= 0.3158)

The “dox2_coat” function is coded according to the above equation to calculate the oxide thickness. The

input to this function is temperature, and the output is the oxide thickness [m^2/s] of coating cladding. Since there is no data available for cases where coating is applied, a virtual value is output for the alpha layer thickness.

3.2 Oxidation reaction heat calculation

The heat generated during the oxidation process of the cladding tube should be taken into account when calculating the total heat of the fuel rod. The oxidation of the coating layer generates heat that is determined by the oxidation reaction heat of the coating material, which is typically a chromium oxide(Cr_2O_3) for most corrosion-resistant metallic materials. In other words, assuming only Cr_2O_3 as the oxide for the coating material, the reaction heat per unit mass of chromium ($Q_{Cr_2O_3} = 3.87 \times 10^6$ J/kg) is used. However, modifications may be required in the future depending on the oxide used in the coating layer.

The reaction heat is defined as the "hr_coat" parameter in the code. Currently, only the outer coating of accident-tolerant nuclear fuel cladding is considered, so if an element is on the outer surface of the coating, the weight gain is calculated using the previously defined "dtau2_coat" function. In this case, the oxidation reaction heat per unit length due to the added weight gain is calculated using the following equation.

$$q = (0.684/0.316) \times (dW_g/dt) \times \pi d_0 \times Q_{Cr_2O_3} \quad (3)$$

Where,

dW_g : weight gain increment [(kg/m^2) /s]

dt : time increment [s]

d_0 : initial cladding outer diameter [m]

$Q_{Cr_2O_3}$: oxidation reaction heat generation per unit mass [J/kg]

The inputs for the oxidation reaction heat calculation include the current cladding tube temperature, time increment, initial outer diameter of the cladding tube, weight gain from the previous time step, and an identifier for the inner and outer surface of the cladding. The output is the oxidation reaction heat per unit length [W/m] and the weight gain [kg/m^2] for the current time step.

3.3 ECR calculation

The calculation of cladding ECR is designed to be performed at the end of each time step, so no special measures are required. The inputs for the ECR calculation include the time increment, inner and outer surface temperatures of the cladding, axial position of the deformed inner and outer radii of the cladding, and weight gain of the inner and outer surfaces. The output is the ECR (Equivalent Cladding Reacted [%]).

$$ECR = \frac{W_{g.i}\left(\frac{m_{Zr}}{m_{O_2}} \times \frac{1}{\rho_{Zr}}\right) + W_{g.o}\left(\frac{m_{Cr_2}}{m_{O_2}} \times \frac{1}{\rho_{Cr_2}}\right)}{(r_{outer} - r_{inner})} \times 100$$

Where,

$W_{g.i}$, $W_{g.o}$: total weight gain of inner and outer surfaces [kg/m^2]

m , ρ : moles and density [-, kg/m^3]

$r_{outer} - r_{inner}$: deformed cladding thickness [m]

4. Verification of high-temperature oxidation code

The completeness of the ATF_OX_MERCURY code can be verified by comparing the calculated values from the experimental correlation equation to the results obtained from the code. The arithmetic calculation of the experimental correlation equation is performed separately using Python language, and the results are compared with those from ATF_OX_MERCURY. The calculation conditions are involved between 1178.15 K and 1777.15 K comparing the accumulated oxidation characteristics values over a fixed period of time while maintaining a constant cladding temperature. The cladding temperature is selected based on the temperature used in the development of the C-P model [3].

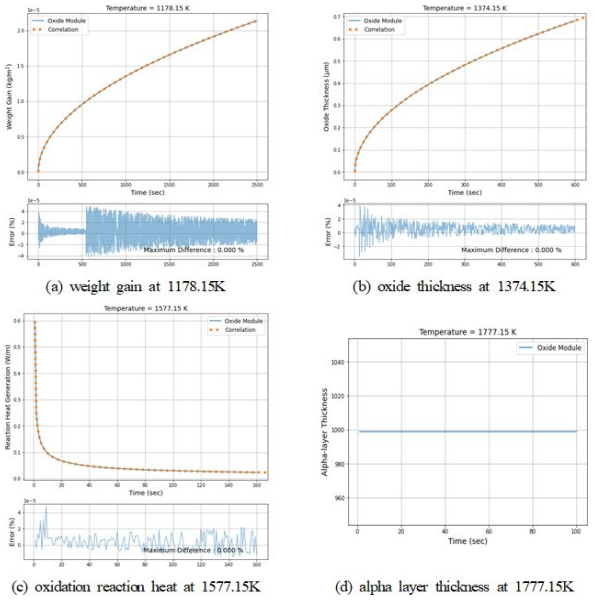
In this paper, only the comparison between the code results and experimental values of weight gain at 1178.15 K (Figure 1(a)), oxide thickness at 1374.15 K (Figure 1(b)), oxidation reaction heat at 1577.15 K (Figure 1(c)), and alpha layer thickness at 1777.15 K (Figure 1(d)) are indicated due to the limited space available.

As shown in Figure 1, it has been confirmed that the weight gain, oxide thickness, and oxidation reaction heat calculated at each temperature condition match well when they are below 1×10^{-5}. However, since there is no data available on the alpha layer thickness of the coated cladding, all values over time are output as a virtual value of '999'.

5. Conclusions

Through this research, the following conclusions and future plan are drawn.

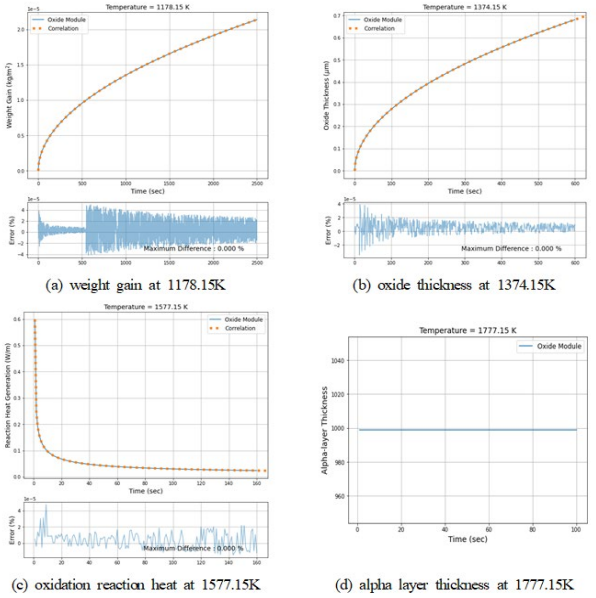
- A standalone code has been developed for analyzing high-temperature oxidation of ATF cladding. It consists of 1 main program and 3 sub-programs. By comparing the accumulated oxidation characteristics such as weight gain, oxide layer thickness, oxidation reaction heat, and alpha layer thickness while maintaining a constant temperature of the cladding between 1178.15~1777.15 K for a certain period of time, the



(a) weight gain at 1178.15K (b) oxide thickness at 1374.15K

(c) oxidation reaction heat at 1577.15K (d) alpha layer thickness at 1777.15K

Fig. 1. Verification results of high-temperature oxidation analysis code



(a) weight gain at 1178.15K (b) oxide thickness at 1374.15K

(c) oxidation reaction heat at 1577.15K (d) alpha layer thickness at 1777.15K

Fig. 1. Verification results of high-temperature oxidation analysis code

completeness of the developed code has been verified.

- In the future, the confirmed high-temperature oxidation code will be directly transferred to MERCURY as a single module, and the integrated verification calculation will be completed by demonstrating that the oxidation characteristics obtained through the input statements of MERCURY match the arithmetic calculation values of the experimental model.

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