Transactions of the Korean Nuclear Society Autumn Meeting
Changwon, Korea, December 17~18, 2020

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

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## Introduction

- A widely used code system for evaluating the fuel performance in accident conditions is the NRC's FRAPTRAN. 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.
- 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
- 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.

## Oxidation Model

- Since the FEM-based fuel performance code is for best-estimate analysis, the MERCURY is based on the C-P model which is mainly used for best-estimation calculation.
- 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 temperature (Cathcart et al., 1977).

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

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

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

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

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

## Reaction Heat & ECR

- 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(NUREG/CR-6150, 1997) as follows.

$$P = \frac{0.74}{0.26}\frac{\Delta W}{\Delta t} 2\pi R_0 6.45 \times 10^6 \frac{J}{m}$$

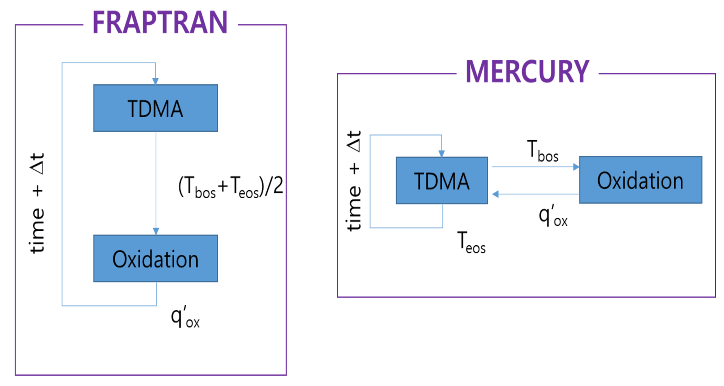
where, ΔW is the weight gain during the time increment Δt and $R_0$ is initial radius of cladding.

- 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.

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

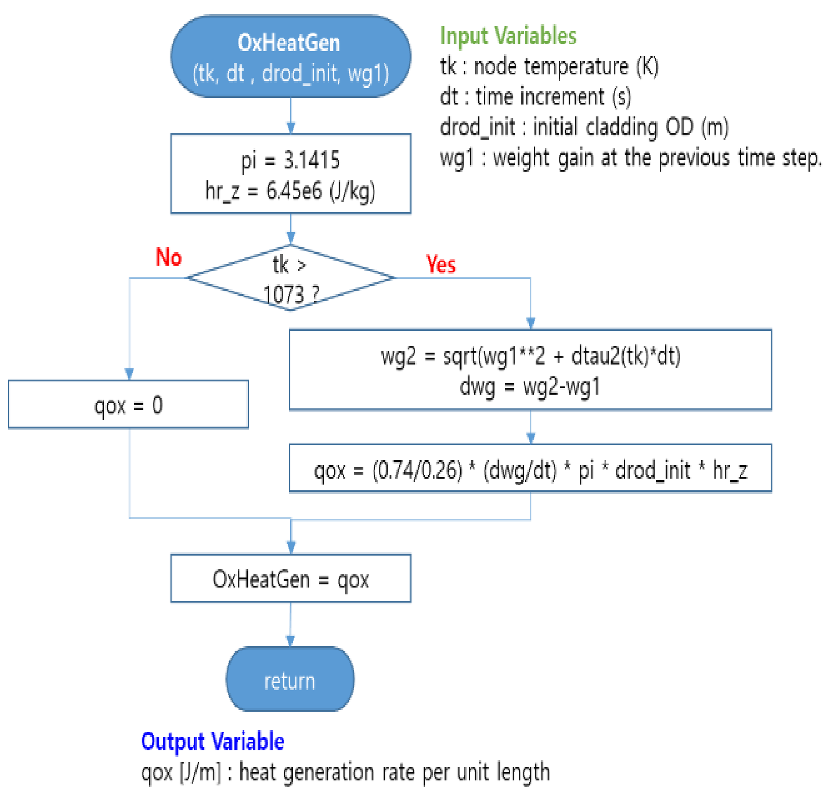
## Calculation Scheme

- 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.




## Oxidation Heat Model of MERCURY

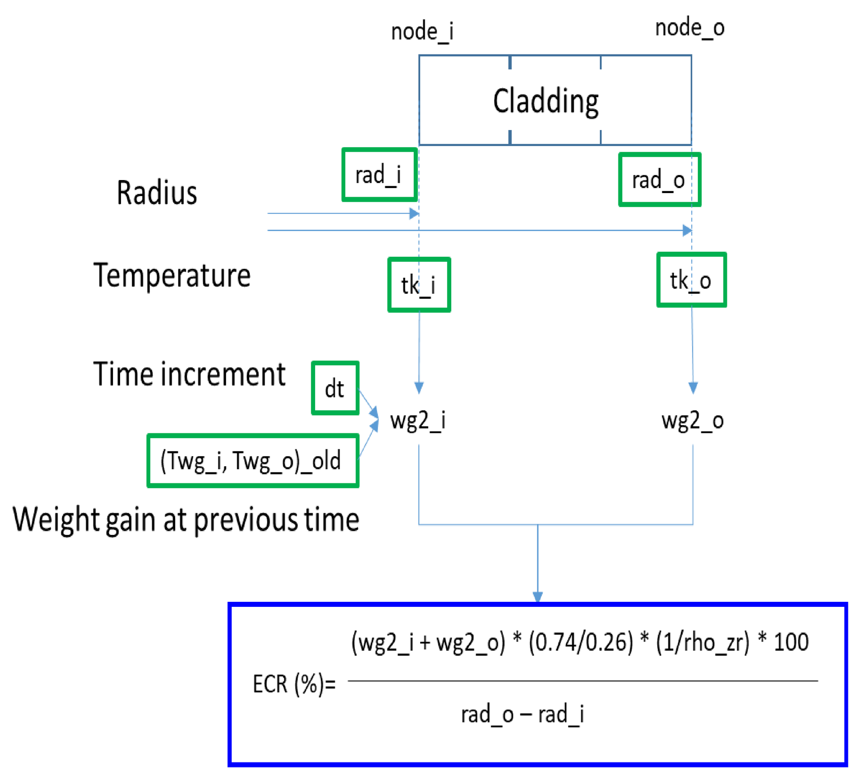
Flow chart for calculation of the heat of oxidation reaction




- 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 increment includes the weight gain (wg1) of the previous step.
- The amount of oxidation increased at the current step becomes difference between 'wg2(new)' and 'wg1(old)'.

## Calculation of ECR

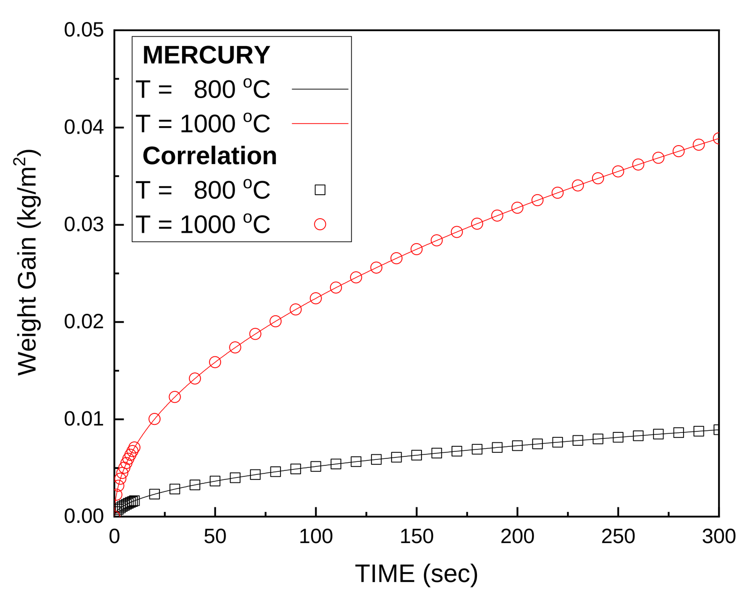
Flow chart for calculation of the ECR from oxygen weight gain




- 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.
- For ECR calculation, 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.

## Verification

Comparison of weight gain calculation by MERCURY and correlation.




- 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. the two results are exactly the same. Through this, it was verified that the oxidation model was well implemented into the MERCURY code.

## 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**

This work has been carried out under the Nuclear R&D Program supported by the Ministry of Science and ICT. (NRF-2017M2A8A4015024)

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