

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

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## 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.

## Oxidation Model

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).

Cathcart Model:

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

Baker-Just Model:

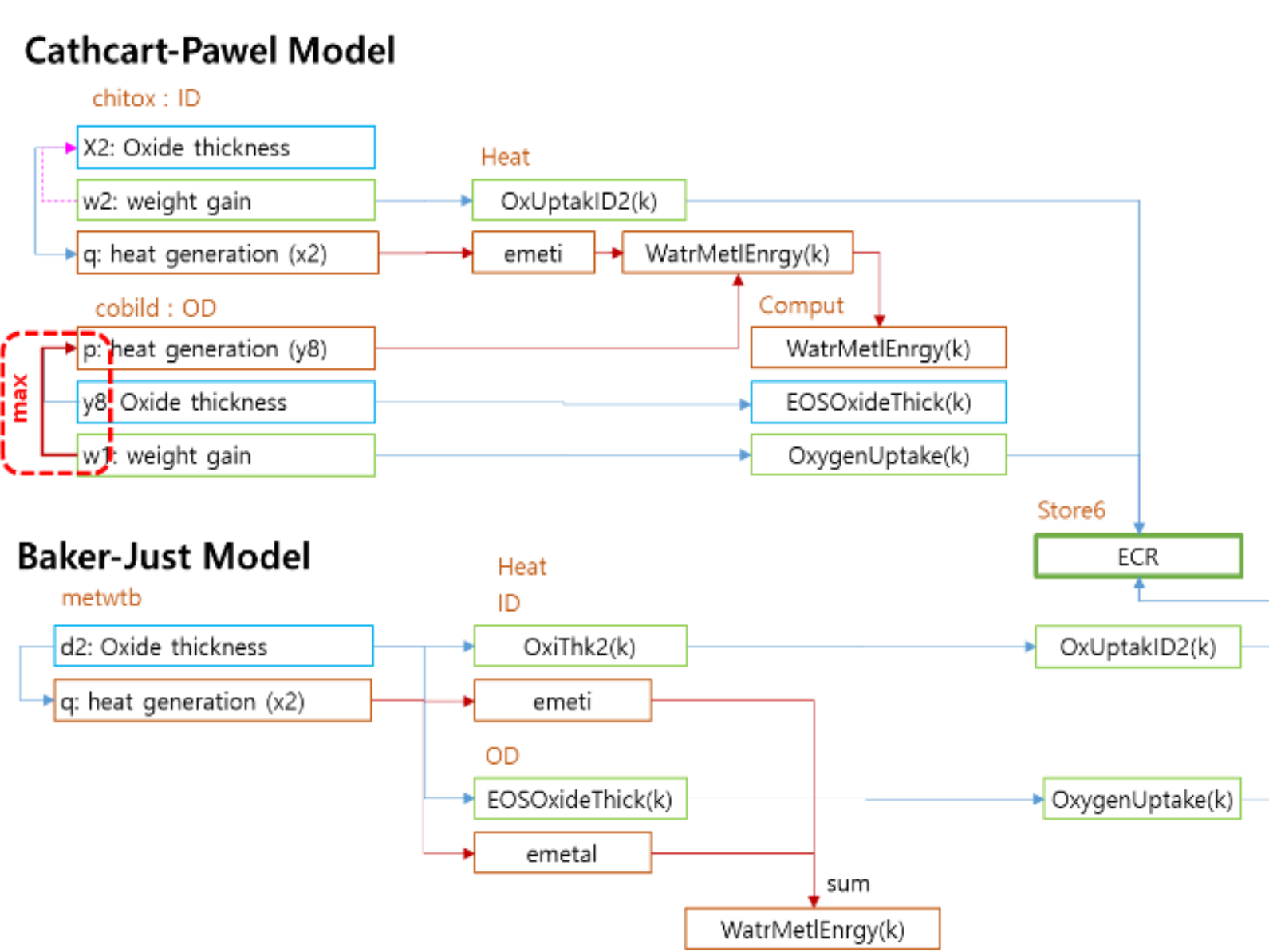
$$K_2^2 = K_1^2 + 1.883 \times 10^{-4} \exp\left(\frac{-45500}{R \cdot T}\right) \Delta t$$

where,

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

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

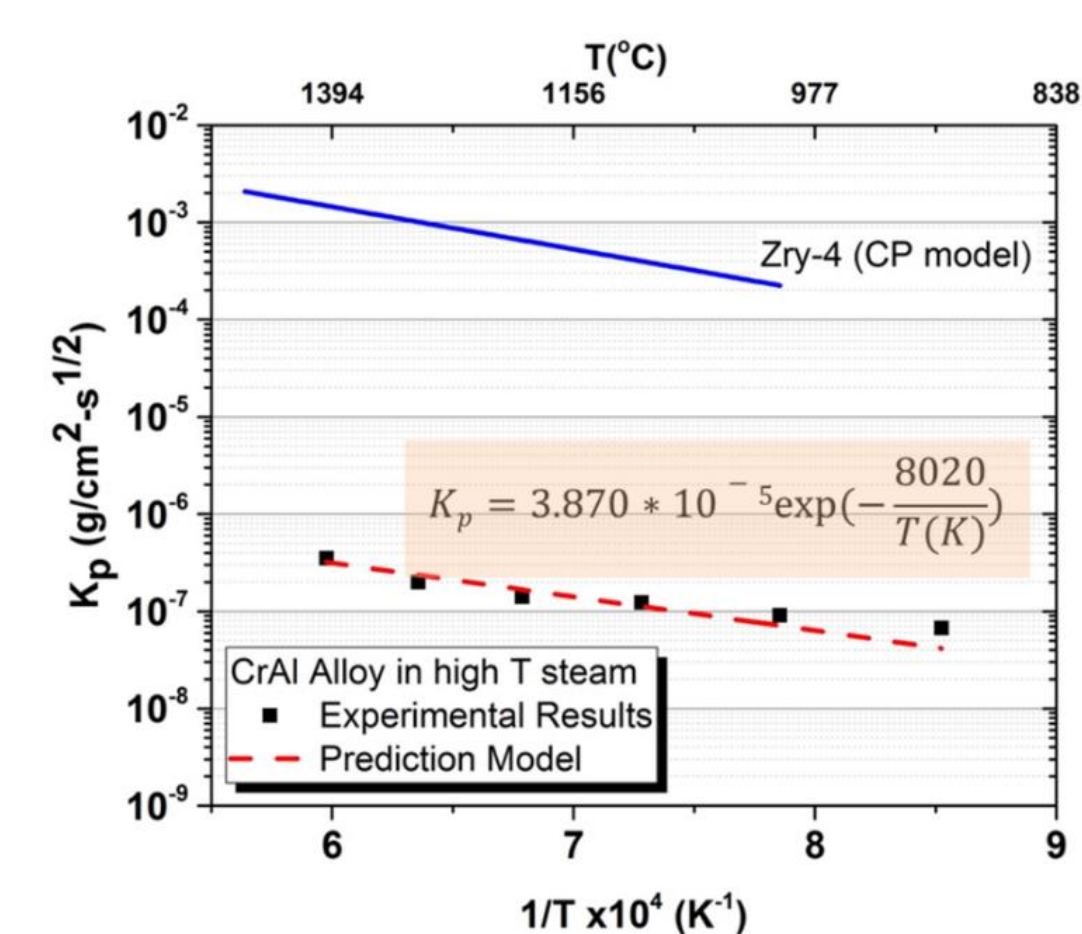
## Flow chart



The Calculation flow diagram of the high temperature oxidation model in FRAPTRAN-2.0

For the C-P model, the inner and outer cladding surface oxidation is calculated in a separated subroutine.

## Oxidation Model for Coating Material



KAERI has developed CrAl alloy as a coating material. The high temperature oxidation model has been suggested by Hong et al. (2016)

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

## Assumption for Oxidation Thickness and Heat

- It is necessary to convert the oxide film thickness based on the measured weight gain.
- Since the theory and experimental results for the oxidation reaction of CrAl alloy are not sufficient, it is assumed here that an oxide layer is formed only of  $Cr_2O_3$ , an oxide of Cr.
- From this assumption, the oxide film thickness is calculated as follows.

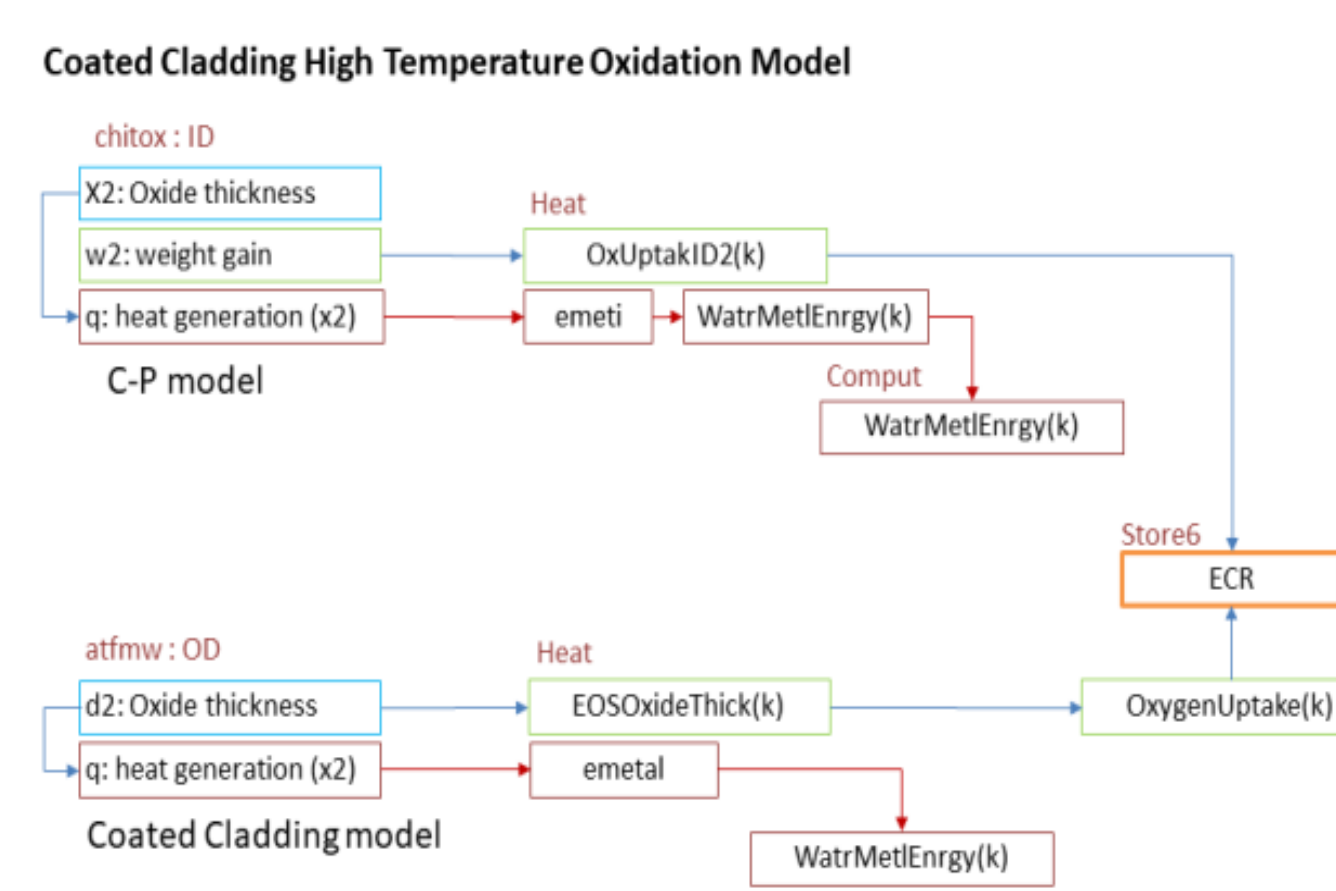
$$\delta_{eff} = \frac{w}{\rho \cdot w_f} \Big|_{Cr_2O_3}$$

The heat generation of oxidation reaction was estimated by assumption of  $Cr_2O_3$  reaction.

Table 1 Reaction heat of  $Cr_2O_3$

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
$\Delta h_p^\circ$ (kJ/mol)	0	0	2*(-1128)	-2256
Q = 2256 (kJ/mol) / (4*51.9961) (g/mol) = 10.85 x 106 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				

## Implementation of 'ATFMW'

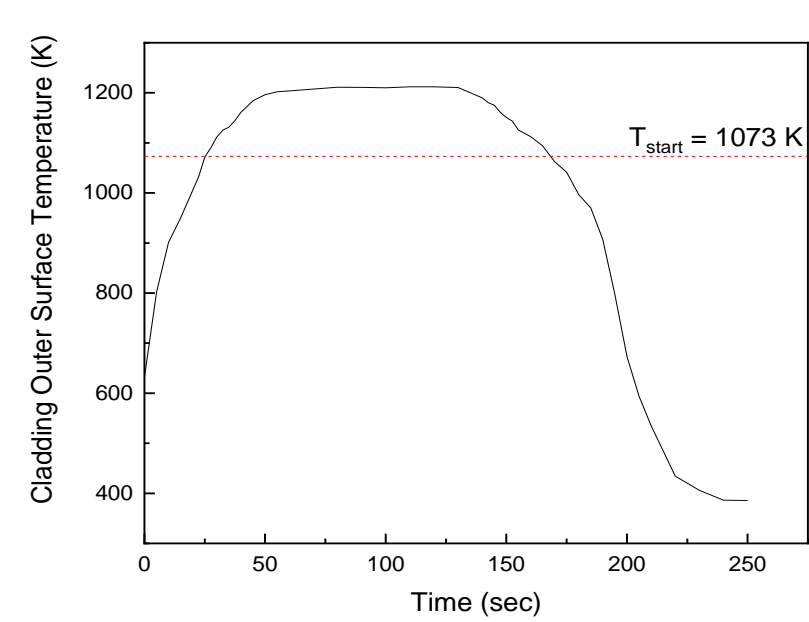


The oxidation model of coated cladding described above is coded with the subroutine 'atfmw', and the flow chart for implementing into FRAPTRAN

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.

## Verification

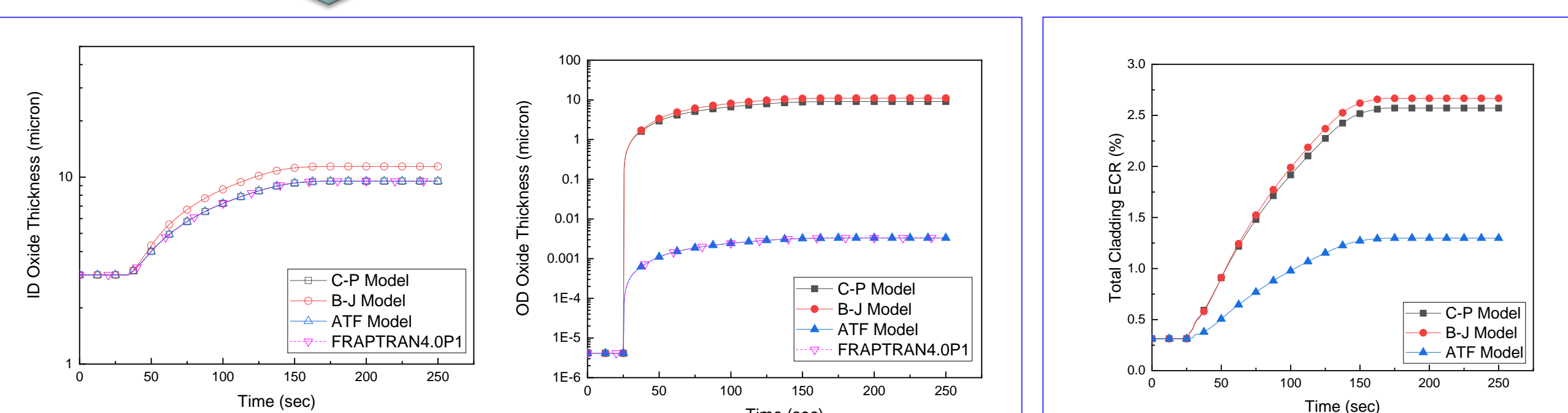
### Hypothetical cladding temperature input



After the cladding burst at 34.5s, the existing C-P model was used to the internal oxidation of the zircaloy cladding.

When the ATF model was used, there is almost no oxidation on the outer surface due to high oxidation resistance.

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.



Oxide thickness of inner and outer cladding of ATF oxidation model

Total ECR of ATF oxidation model

## 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  $Cr_2O_3$ .
- 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.

### Acknowledgement

This work has been carried out under the Nuclear R&D Program supported by the Ministry of Science and ICT. (NRF-2017M2A8A5015064)