

## Evaluation of Models in FRAPCON-4.0/FRAPTRAN-2.0 for Cladding Material Change

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### 1. Introduction

Currently, the Korean nuclear fuel vendor is preparing for an application for the commercial use of a new fuel with HANA cladding. Therefore, Korea Institute of Nuclear Safety (KINS) is initiating a research to improve the capability of the regulatory fuel performance codes, FRAPCON [1] and FRAPTRAN [2] incorporating the HANA cladding features. As a part of the implementation of this research, the identification of models from FRAPCON and FRAPTRAN to be modified for the cladding change is conducted in the present study. To determine the models needed to be modified under the cladding change, two independent approaches were applied in the present study. In the first approach, all models included in FRAPCON and FRAPTRAN were checked carefully to find any models directly related to properties affected by the cladding change. In the second approach, we tried to identify models need to be modified based on the in-depth review on the fuel system design criteria perspective. The results from these two approaches were consolidated and the necessary areas of modifications in FRAPCON and FRAPTRAN codes under the cladding change are finally identified in the conclusion.

### 2. Evaluation of FRAPCON/FRAPTRAN Cladding Models

In this section, cladding models and material properties in FRAPCON/ FRAPTRAN were checked. The four types of the cladding behavior model should be considered for changing the cladding material.

#### 2.1 Thermal model

The temperature gradient from pellet to coolant is calculated in FRAPCON as eq. (2.1) and affected by heat flux ( $q''$ ), geometry and cladding thermal conductivity( $k_c$ ).

$$\Delta T = \ln q''(z)r_0 \ln(r_0/r_i)/k_c \quad (2.1)$$

The cladding thermal conductivity is dependent on the cladding temperature. In FRAPTRAN, the temperature distribution of the cladding is obtained by applying the law for heat conduction as eq. (2.2).

$$\int \rho C_p \frac{\partial T}{\partial t} dV = \int k \bar{\nabla} T d\bar{s} + \int q dV \quad (2.2)$$

Eq. (2.2) includes the enthalpy change of an arbitrary infinitesimal volume, the heat transfer through the surface and heat generation within the volume with density, thermal conductivity, and specific heat of the material. Some thermal properties such as specific heat are calculated using interpolation in FRAPCON/FRAPTRAN. The thermal models of the cladding such as thermal conductivity, thermal expansion, specific heat and emissivity will be considered for HANA cladding.

#### 2.2 Mechanical model

FRAPCON/FRAPTRAN consider the thermal expansion, creep and plastic deformation of cladding for calculating deformation of cladding. During analysis of cladding deformation, radial displacement is considered between pellet and cladding. If radial displacement of pellet is smaller than the sum of the cladding displacement and gap size, the pellet isn't in contact with the cladding (open gap condition). For the opposite case, the pellet is in contact with the cladding (closed gap condition)

##### 2.2.1 Thermal and irradiation creep rate of cladding

In steady-state, thermal and irradiation creep rate of cladding in FRAPCON are as follows.

$$\dot{\epsilon}_{th} = A \frac{E}{T} \left( \sinh \frac{a_i \sigma_{eff}}{E} \right)^n \exp \left( \frac{-Q}{RT} \right) \quad (2.3)$$

$$\dot{\epsilon}_{irr} = C_0 \cdot \phi^{C_1} \cdot \sigma_{eff}^{C_2} \cdot f(T) \quad (2.4)$$

The constants and variables in eq.(2.3) and (2.4) are dependent on annealing, temperature and fast neutron flux. The thermal and irradiation creep rate models including variables will be considered for HANA cladding.

##### 2.2.2 Stress-strain behavior

The elastic deformation of the cladding in FRAPCON/FRAPTRAN is considered using Hook's law. The elastic modulus in eq.(2.5) is

dependent on the cladding temperature, oxidation, cold work and fast neutron flux.

$$\sigma = E \cdot \varepsilon \quad (2.5)$$

The plastic deformation of the cladding in FRAPCON/FRAPTRAN is calculated using Hollomon equation as follows.

$$\sigma = K \left[ \frac{\dot{\varepsilon}}{10^{-3}} \right]^m \varepsilon^n \quad (2.6)$$

Constants including strength coefficient(K) in eq. (2.6) are affected by the temperature, cold work and fast neutron flux. For evaluating the stress-strain behavior of HANA cladding in FRAPCON /FRAPTRAN, the two independent moduli (elastic modulus and shear modulus) and the variables including strength coefficient in eq.(2.6) will be checked.

### 2.3 Corrosion model

#### 2.3.1 Waterside corrosion

In steady-state, the cladding is oxidized by occurring metal-water reaction. The oxide thickness is converted to weight gain( $\Delta w$ ) in FRAPCON as follows.

$$\Delta w_{i+1} = \Delta w_i + f(R, T, \lambda, \gamma, Q, q'', k, \Delta w_i) \quad (2.7)$$

The calculation of the corrosion for cladding in FRAPCON is used to Garzarolli's correlation and have different form according to the cladding type. At first, the confirmation of whether Garzarolli's correlation is applicable to HANA cladding. If the correlation can be used to evaluate HANA, the material properties Q and k in eq.(2.7) have to reflect the experimental data of HANA.

#### 2.3.2 Hydrogen pickup

The fraction of the hydrogen by the metal-water reaction that is absorbed locally by the cladding is called the hydrogen pickup fraction [1]. FRAPCON considers a constant hydrogen pickup fraction for pressurized water reactor conditions. The constant for hydrogen pickup is dependent on the cladding type. The hydrogen pickup fraction is also needed as one of the material properties that should be considered for evaluating the behavior of HANA cladding in pressurized water reactor conditions.

#### 2.3.3 High-temperature corrosion

In the high temperature environment like Loss of Coolant Accident (LOCA), the cladding corrosion in

FRAPTRAN is calculated using Baker-Just and Cathcart-Pawel model as eq.(2.8)

$$K_2 = \sqrt{K_1^2 + 2Ae^{(-B/RT)}\Delta t} \quad (2.8)$$

The oxide thickness(K) is calculated using Baker-Just when the average cladding temperature is greater than 1000 K. If it's more than 1073 K, Cathcart-Pawel is used. It would be necessary to consider whether to apply the model first and then, find the variables in eq.(2.8) for HANA cladding.

### 2.4 Failure model

#### 2.4.1 Pellet-cladding mechanical interaction (PCMI)

In reactivity initiated accident (RIA), PCMI may be occurred by a combination of differential thermal expansion between the pellet and cladding and fission product induced swelling of the pellet. FRAPTRAN calculates a uniform plastic elongation that is a function of temperature and hydrogen concentration. Equations using the calculation of the uniform plastic elongation will be consider whether to apply the model for HANA. Simultaneously, the calculation of the hoop stress corresponding to the uniform plastic elongation is also considered and it's related to the stress-strain behavior in section 2.2.2.

#### 2.4.2 Ballooning

In the postulated accident, there is a possibility that the cladding is ballooning because of thermal expansion and swelling of the pellet and increase of internal pressure for fission products. FRAPTRAN calculates the effective plastic strain with the plastic instability strain. If the effective plastic strain is greater than the cladding instability strain, FRAPTRAN starts to the calculation of cladding ballooning using BALON2 model and that should be considered for applying HANA cladding. Also, the calculation of the hoop stress corresponding to the strain limit will be considered and it's related to the stress-strain behavior in section 2.2.2.

## 3. Evaluation of FRAPCON/FRAPTRAN Models Based on Fuel System Design Bases

### 3.1 Fuel System Design Bases

The fuel system design bases was required to provide fuel system safety. The basis consists of fuel system damage, fuel rod failure, and fuel coolability [3]. Recently, PNNL (Pacific Northwest National Laboratory) reclassified the fuel system design basis depending on assembly performance and fuel rod

performance [4]. Assembly performance is related to the structure of assembly whereas fuel rod performance considers single rod. Because the simulation of FRAPCON/FRAPTRAN is specialized on the single rod, the analysis of fuel design bases was considered to the fuel rod performance in this study.

### 3.2 Evaluation of FRAPCON/FRAPTRAN Models Related to Fuel System Design Bases

The change of the material of cladding means the change of the material properties. According to material property correlation of Luscher et al. [5], the correlations used in FRAPCON/FRAPTRAN related to cladding material were nine: cladding specific heat, cladding thermal conductivity, cladding oxide thermal conductivity, cladding surface emissivity, cladding thermal expansion, cladding elastic modulus and shear modulus, cladding axial growth, creep rate, and cladding Meyer hardness. Therefore, this section confirms whether each fuel system design was evaluated in the FRAPCON/FRAPTRAN and derives models which are related to cladding material change (using nine cladding correlation or unique parameters of cladding material) in evaluated by the fuel analysis code.

Among these design bases, the models related to the cladding change are described in normal & AOO and accident conditions in sections 3.2.1 and 3.2.2 respectively. FRAPCON and FRAPTRAN could not evaluate the fatigue, inner hydriding, cladding collapse, overheating of cladding, bursting, and violent expulsion of fuel.

#### 3.2.1 Normal and AOO Condition

##### A. Stress and strain design bases

- a) Evaluation in the code : O
- b) Relation to cladding material : O

Cladding stress and strain were limited to protect rod integrity and hermeticity of cladding. FRAPCON and FRAPTRAN use the FRACAS-I model to analyze fuel mechanical response. The FRACAS-I model uses elastic and shear modulus of cladding to calculate stress and strain when the open gap or closed gap conditions.

##### B. Oxidation, hydriding, and the CRUD design bases

- a) Evaluation in the code : O
- b) Relation to cladding material : O

Cladding oxidation and hydriding were limited to remain ductility and strength of cladding.

FRAPCON and FRAPTRAN use the corrosion model and hydrogen pickup model to evaluate oxide weight gain and hydrogen containment. The corrosion model uses cladding oxide thermal conductivity and cladding material parameter, activation energy. Likewise, hydrogen pickup model uses hydrogen pickup fraction from coolant to cladding, a unique material parameter.

##### C. Rod internal pressure design bases

- a) Evaluation in the code : O
- b) Relation to cladding material : X

Rod internal pressure was limited to prevent gap re-open, that is, re-separation of pellet and cladding after their contact. Gap re-open would increase pellet temperature rapidly. In addition, if rod internal pressure is higher than coolant pressure, a wide DNBR spread could be induced. FRAPCON uses a rod internal pressure model considering fission gas/Nitrogen/Helium generation and release, but they are not related to cladding material.

##### D. Overheating of fuel pellet design bases

- a) Evaluation in the code : O
- b) Relation to cladding material : O

Pellet temperature was limited to protect the fuel rod from pellet centerline melting. FRAPCON and FRAPTRAN use the thermal model to calculate the temperature from coolant-cladding-gap to pellet and plenum gas. In the FRAPCON model, oxide and cladding thermal conductivity, and emissivity were used and in the FRAPTRAN model, oxide and cladding thermal conductivity, Meyer hardness were used.

##### E. Pellet-Cladding interaction design bases

- a) Evaluation in the code : O
- b) Relation to cladding material : O

Cladding strain and pellet centerline melting were limited to inhibit the failure by interaction or mechanical interaction between the pellet and cladding. FRAPCON and FRAPTRAN use the FRACAS-I model like sections 3.2.1 A and thermal model like section 3.2.1 D.

#### 3.2.2 Accident Condition

##### A. Excessive fuel enthalpy design bases

- a) Evaluation in the code : O
- b) Relation to cladding material : O

The rapid enthalpy increase during a short time due to the RIA accident could bring fuel rod failure by PCMI. DNBR was a criterion to determine the failure of cladding. FRAPTRAN does not calculate

DNBR, but rather the code could simulate the cladding failure by PCMI in low-temperature. If the plastic hoop stress exceeds the limit of uniform plastic elongation in a specific node of the fuel rod, this rod is considered to be failed. 3.2.1 A, mechanical model was used in calculation of stress, and 3.2.1 B, cladding hydrogen concentration was used to decide uniform elongation.

- B. Mechanical fracturing design bases
- a) Evaluation in the code : O
  - b) Relation to cladding material : O

To determine the fuel rod failure caused by the external mechanical force, FRAPTRAN uses the FRACAS-I model in 3.2.1 A to calculate the stress and strain.

- C. Cladding embrittlement design bases
- a) Evaluation in the code : O
  - b) Relation to cladding material : X

Cladding embrittlement was limited to remain the fuel coolability when the ECCS was activated by the LOCA. The maximum temperature of cladding (1204 °C) and cladding maximum ECR (17%) were limited. FRAPTRAN uses Cathcart-Pawel and Baker-Just models to calculate the oxide thickness. These models do not use the cladding material properties. However, it is required to be considered if this model could be acceptable when the cladding material is changed.

- D. Generalized cladding melting design bases
- a) Evaluation in the code : O
  - b) Relation to cladding material : X

If the cladding melts broadly, the structure of the reactor core would not remain. The generalized cladding melting was limited to maintaining structure. But the limitation of cladding embrittlement is stricter than the melting limit. FRAPTRAN uses section 3.2.2 C to satisfy the melting design bases.

- E. Fuel rod ballooning design bases
- a) Evaluation in the code : O
  - b) Relation to cladding material : O

In the accident condition, DNBR could be spread to nearby rods due to the fuel rod ballooning. ECCS evaluation considers the flow blockage regarding the ballooning. FRAPTRAN uses the BALON2 model to set limiting stress or calculate limiting strain; provided that the hoop stress or hoop strain over the limitation, the rod failed. BALON2 model uses cladding temperature, emissivity, and cold work to calculate the strain limit.

- F. Structural deformation design bases
- a) Evaluation in the code : O
  - b) Relation to cladding material : O

To determine the maintaining of core coolability and to evaluate the structural response of fuel assembly when external force was applied, FRAPTRAN uses the low-temperature PCMI model in 3.2.2 A for RIA and the ballooning model, BALON2 which measure the burst stress, in 3.2.2 E for LOCA.

#### 4. Conclusions

FRAPCON/FRAPTRAN models analysis was performed with two separated parts; chapter 2 specifically focused on cladding models in the FRAPCON/FRAPTRAN, and chapter 3 broadly checked the entire model upon the fuel design bases.

Because the models were independently evaluated in two separated directions, some models were derived in both chapters like the waterside corrosion model whereas other models were picked in the only single chapter like the rod internal gas pressure model. Each model was included on the list if the model was evaluated as cladding-related at least in one of the chapters. The list of models influenced by cladding change was consolidated in Table 1 and Table 2 as below.

Table 1. The model list related to cladding change : FRAPCON models

Fuel Rod Thermal Response	Fuel Rod Surface Temperature
	Cladding Temperature gradient
	Fuel-Cladding Gap Temperature Gradient
	Plenum Gas Temperature
Fuel Rod Mechanical Response : The FRACAS-I Model	Stress-strain(open gap)
	Stress-strain(closed gap)
	Creep
Waterside Corrosion and Hydrogen Pickup	Waterside Corrosion
	Hydrogen Pickup Fraction

Table 2. The model list related to cladding change : FRAPTRAN models

Fuel and Cladding Temperature	Gap Conductance
	Heat Conduction and Temperature Solution

Fuel Rod Mechanical Response : The FRACAS-I Model	Stress-strain(open gap)
	Stress-strain(closed gap)
	Creep
High-Temperature Oxidation	High-Temperature Oxidation
Cladding Failure Models	Low-Temperature PCMI Cladding Failure
	Cladding Ballooning

The list of models could be applicable in further studies to evaluate fuel rods with cladding change.

### Nomenclature

A : Thermal strain rate variable [K/MPa/hr],  
Cathcart-Pawel and Baker-Just model constant [m<sup>2</sup>/s]  
B : Cathcart-Pawel and Baker-Just model constant [J/mole]  
a<sub>i</sub> : Thermal strain rate variable [MPa<sup>-1</sup>]  
C<sub>p</sub> : Specific heat [J/kg·K]  
C<sub>0</sub>, C<sub>1</sub>, C<sub>2</sub> : Irradiation strain rate variable [MPa<sup>-1</sup>]  
E : Elastic modulus [Pa]  
K : Strength coefficient, Oxide thickness [m]  
k : Thermal conductivity [W/ m·K·s]  
k<sub>c</sub> : Cladding thermal conductivity [W/m·K]  
m : Strain rate sensitivity constant  
n : Strain hardening exponent  
Q : Thermal strain rate parameter [KJ/mole],  
Weight gain parameter [cal/mole]  
R : Universal gas constant [KJ/mole·K]  
T : Temperature [K]  
t : Time [s]  
q : Volumetric heat generation [W/m<sup>3</sup>]  
q" : Heat flux [W/cm<sup>2</sup>]  
r<sub>i</sub> : Cladding inside radius [m]  
r<sub>o</sub> : Cladding outside radius [m]  
V : Volume [m<sup>3</sup>]  
w : Weight gain [g/cm<sup>2</sup>]  
ρ : Density [kg/m<sup>3</sup>]  
ε<sub>th</sub> : Thermal strain rate [m/m/hr]  
ε<sub>irr</sub> : Irradiation strain rate [m/m/hr]  
φ : Fast neutron flux [n/m<sup>2</sup>·s]  
σ<sub>eff</sub> : Effective stress [Pa]  
σ : Stress [Pa]  
ε : Strain  
λ : Oxide thermal conductivity [W/cm·K]  
γ : Weight gain parameter [cm<sup>3</sup>/g]

### Acknowledgements

This work was supported by the Nuclear Safety Research Program through the Korean Foundation

of Nuclear Safety (KOFONS), granted financial resource from the Nuclear Safety and Security Commission (NSSC), Republic of Korea (Grant No. 2106002).

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