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The Review of Models and Correlations in FRAPCON-4.0 and FRAPTRAN-2.0 for Fuel Pellet Material Change

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1. Introduction

ATF (Accident Tolerant Fuel) is being developed for (1) offering better performance in the normal and AOOs (Anticipated Operational Occurrences) conditions and (2) providing additional coping time to operators during the postulated accident. To meet these requirements, the materials of the fuel rods, especially cladding and pellet would be changed. Also, with the development of the ATF, the prediction capability of fuel analysis codes should be improved for an in-depth regulatory review of the ATF design. Currently, FRAPCON-4.0 [1] and FRAPTRAN-2.0 [2] are used as fuel performance analysis codes for regulatory audit calculation.

In the previous research, a list of the models and correlations of the codes affected by the cladding material change was identified. And the list was evaluated in detail for the application of HANA-6 cladding [4]. In conjunction with the previous research, in the present study, the models and correlations are analyzed again but we focus on fuel pellet change this time. From the thorough review of the fuel system design bases from Safety Review Guidelines for Light Water Reactors [5], a list of the models and correlations affected by the pellet material change was derived for the FRAPCON-4.0 and FRAPTRAN-2.0 codes.

2. Identification of FRAPCON/FRAPTRAN Correlations and Models affected by Fuel Pellet Material Changes using Fuel System Design Bases

The material of the fuel pellet is related to several behaviors of the fuel rod, such as fission gas generation, fission gas release, pellet centerline temperature, and mechanical interaction between pellet-cladding. PNNL-19417 Rev.2 [6] identified the eight material property correlations related to the fuel pellet, described in the following table.

Table 1. Pre-identified Pellet material property correlations in FRAPCON-4.0/FRAPTRAN-2.0[6]

No.	Material Property Correlations	Note
①	Fuel Melting Temperature	Thermal property
②	Fuel Specific Heat Capacity	Thermal property
③	Fuel Enthalpy	Thermal property
④	Fuel Thermal Conductivity	Thermal property
⑤	Fuel Emissivity	Thermal property
⑥	Fuel Thermal Expansion	Thermal property
⑦	Fuel Densification	Mechanical property
⑧	Fuel Swelling	Mechanical property

In this study, the design bases of the fuel system described in Safety Review Guidelines chapter 4.2 were reviewed in detail. Each design base was analyzed to find the relationship with fuel pellet material change. As a result, three models (mechanical, thermal, and rod internal pressure) and five additional material correlations beyond Table 1 were identified to be subject to change due to the fuel pellet modification. Three typical design bases are described: stress and strain, rod internal gas pressure, and overheating of the fuel pellet.

2.1. Stress and strain design base – mechanical model

The stress and strain design base is related to the mechanical model of the fuel. This design base limits the stress-strain of cladding to avoid failure of the fuel rod. At the beginning of life, the pellet and cladding of as-fabricated fuel are separated. The helium gas fills the gap to prevent the cladding collapse. During the gap opening, the stress of the cladding is independent of the deformation of the fuel pellet.

As the fuel burns, the pellet swells by the fission gas. Then, the swelled pellet and the crept cladding contact each other. After the gap closure, the pellet deformation strains the cladding.

In FRAPCON-4.0 and FRAPTRAN-2.0, the cladding strain could not affect the deformation of the pellet because the codes assume the ‘rigid pellet’.

The codes simulate the radius of the pellet in a closed-gap as follows:

$$\mathbf{R_H} = \sum_{i=1}^{N} \Delta \mathbf{r_i}\left[1 + \alpha_{T_i}\left(T_i - T_{ref}\right) + \varepsilon_i^s + \varepsilon_i^d\right] \tag{2.1}$$

Formula 2.1 uses the coefficient of thermal expansion α_{T_i} (⑥), the densification strain ε_i^d (⑦), and the swelling strain ε_i^s (⑧) to calculate the pellet radius.

In summary, the material coefficients (⑥,⑦,⑧) in the FRAPCON-4.0 needs to be updated to reflect the mechanical property of the material due to the fuel pellet change.

2.2. Rod internal gas pressure design base – fission gas model

The rod internal gas pressure design base is related to the fission gas model. This design base limits the rod’s internal gas pressure under the system pressure. As described in section 2.1, the cladding and pellet would contact during the fuel burn. If this closed gap re-opens due to a rapid increase of rod internal pressure, decreased heat transfer could make pellet temperature suddenly rise and break the cladding. Also, if the rod's internal pressure exceeds the lift-off pressure of the cladding, DNB could widely spread to surrounding rods. Therefore, the internal pressure of the fuel should be limited.

The fission gases (Krypton, Xenon) are released from the grain boundary of the pellet. Helium and Nitrogen also increase the rod's internal pressure. FRAPCON uses several models to simulate the fission gas release, and among them, the modified Forsberg-Massih model was reviewed in this study. The modified Forsberg-Massih model is based on the diffusion equation considering the gas generation, diffusion, concentration, and saturation on the grain boundary. The model is described as follows:

$$\frac{dC}{dt} = D(t)\Delta_r C(r,t) + \beta(t) \tag{2.2}$$

$$\text{Boundary condition: } \begin{cases} C(r,0) = 0 \\ C(a,t) = \frac{b(t)\lambda N(t)}{2D} \end{cases}$$

The material properties of the pellet used in formula 2.2 are discovered as follows:

- Diffusion constant [m^2/s] (⑨) is used to calculate the fission gas and Nitrogen diffusion.
- Resolution rate (⑩) and hypothetical grain radius (⑪) are used to calculate the gas concentration and resolution into the grain.
- Surface tension (⑫) is used to calculate the saturation concentration in grain [atoms/m^2].

In addition, the released fission gas is accommodated in the free volume of the fuel rod and raises the internal pressure. The inner volume of the cladding includes the pellet chamfer, the pellet dishes, the pore of the pellet, and the plenum of the rod. The material coefficients of the pellet which used to compute the total rod internal space are as follows:

- The densification (⑦) and swelling (⑧) of the pellet change the free volume.
- The fission gas could fill the pore of the pellet. The porosity of the pellet (⑬) needs to be considered.

In summary, the material coefficients (⑦,⑧) and material properties (⑨,⑩,⑪,⑫,⑬) needed to be properly reflected in the FRAPCON-4.0 to correctly simulate the internal pressure of the rod with changed pellet material.

2.3. Overheating of fuel pellet design base –thermal model

The overheating of the fuel pellet design base is related to the thermal model of the fuel. This design base defines the fuel failure criteria due to overheating, especially fuel centerline melting. FRAPCON-4.0 and FRAPTRAN-2.0 calculate the temperature distribution in the fuel rod from the coolant to cladding, gap and plenum gas, and pellet surface to center in turn. The material properties of the pellet used for the thermal analysis are as follows:

FRAPCON-4.0:
- Pellet thermal conductivity (④) and emissivity (⑤) are used to calculate the heat transfer through the gap.
- Pellet thermal conductivity (④) is used to calculate heat transfer inside the pellet in a steady state.

FRAPTRAN-2.0:
- Pellet thermal conductivity (④) and emissivity (⑤) are used to calculate the heat transfer through the gap.
- Pellet heat capacity (②) and thermal conductivity (④) are used to calculate heat transfer inside the pellet in a transient state.

The calculated pellet centerline temperature is compared with the melting temperature (①). Also, the pellet enthalpy correlation (③) needed to be updated for thermal analysis.

In summary, the material coefficients (①,②,③,④,⑤) needed to be properly modified in the FRAPCON-4.0 and FRAPTRAN-2.0 to correctly simulate the thermal distribution of the fuel pellet with material change.

3. Conclusions

From the review of the limited number of design bases of the fuel system, five additional material property correlations from the three models were derived. The summarized correlations in conjunction with the result from PNNL-19417 Rev.2 [6] were as follows:

Table 2. Pellet material property correlations in FRAPCON-4.0/FRAPTRAN-2.0

No.	Material Property Correlations	Relevant Models	Note
①	Fuel Melting Temperature	Thermal model	Thermal property
②	Fuel Specific Heat Capacity	Thermal model	Thermal property
③	Fuel Enthalpy	Thermal model	Thermal property
④	Fuel Thermal Conductivity	Thermal model	Thermal property
⑤	Fuel Emissivity	Thermal model	Thermal property
⑥	Fuel Thermal Expansion	Mechanical model	Thermal property
⑦	Fuel Densification	Mechanical, fission gas models	Mechanical property
⑧	Fuel Swelling	Mechanical, fission gas models	Mechanical property
⑨	Fission Gas Diffusion constant	Fission gas model	Mechanical property
⑩	Fission Gas Resolution rate	Fission gas model	Mechanical property
⑪	Fuel Grain Radius	Fission gas model	Mechanical property
⑫	Fuel Surface Tension	Fission gas model	Mechanical property
⑬	Fuel Porosity	Fission gas model	Mechanical property

The models and correlations of fuel performance analysis codes (FRAPCON-4.0 and FRAPTRAN-2.0) which need some modifications were identified for the changed fuel pellet by reviewing the fuel system design bases. Before this study, eight material correlations were already derived that related to the fuel pellet [6]. However, through the current study, additional five material correlations and three model areas were identified to be modified for the fuel pellet change. It was clearly shown that three models (mechanical, rod internal gas pressure, and thermal model) were mostly linked with the material change of the pellet.

Table 2 from the present study can be used to improve the fuel performance analysis codes for in-depth regulation on the pellet-changed fuel, like the fuel employing LAS (La2O3-Al2O3-SiO2). The sensitivity analysis regarding the correlations in Table 2 will be conducted in the further research to be followed.

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