Improvements to Modeling Capabilities of ATF Concepts in the BISON Fuel Performance Code

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INTRODUCTION

Research into accident tolerant materials for the fuel and cladding in Light Water Reactors has been at the forefront of the nuclear fuel research community since the events that occurred at the Fukushima Daiichi nuclear power plant in March 2011. Accident tolerant materials are defined as those that provide significantly increased response time in the event of an accident while providing similar or improved performance as the conventional UO2/zirconium-based cladding fuel rods during normal operation [1]. In particular, qualitative attributes for materials with improved accident tolerance include improved reaction (e.g., oxidation) kinetics with steam, resulting in lower hydrogen (or other combustible gases) generation rate, while maintaining acceptable thermo-mechanical properties, fuel-clad interactions, and fission-product behavior [1]. Through it’s Office of Nuclear Energy, the United States Department of Energy (U.S. DOE) has accelerated research in this area through the Fuel Cycle Research and Development (FCRD) Advanced Fuels Campaign (AFC). The goal of the AFC Accident Tolerant Fuel (ATF) program is to guide selection of promising concepts for insertion into a commercial reactor as part of a lead test rod or assembly in 2022.

Given the aggressive development schedule, it is impossible to perform a comprehensive set of experiments to provide material characterization data. Therefore, the AFC is utilizing computational analysis tools in an effort to understand the proposed accident tolerant materials. The two materials of interest in this work are iron-chromium-aluminum (FeCrAl) cladding and U3Si2. From a fuel performance standpoint, the correlations available to describe the behavior of these two materials is limited. Therefore, as additional experimental data becomes available and correlations are updated, the fuel performance models must be updated as well to assure that the material models reflect the latest experimental findings.

In this paper we demonstrate the importance of utilizing the latest state-of-the-art models for fuel performance simulations by comparing the change in the updated thermal conductivity model for U3Si2 fuel and oxidation model for FeCrAl cladding alloys using the BISON [2, 3] fuel performance code under normal operating conditions. The results indicate that the latest thermal conductivity model for U3Si2 results in fuel centerline temperatures that are on average approximately 3% higher than the previous model. For the oxidation behavior of FeCrAl alloys the new model predicts observable but small oxide thickness (~6 μm) compared to the previous model which predicted essentially zero oxide scale formation.

THERMAL CONDUCTIVITY OF U3Si2

Thermal conductivity of the fuel in a reactor is one of the most important material properties governing the evolution of centerline temperature and fuel behavior under irradiation. Currently, only correlations for fresh unirradiated U3Si2 fuel as a function of temperature exist. In the absence of correlations that take into account the degradation of thermal conductivity due to fission products, porosity, and other irradiation effects, these unirradiated conductivity correlations have been incorporated in BISON. The original thermal conductivity correlation for U3Si2 in BISON was based upon the data of White et al. [4] given by:

$$k = 0.0151 \times T + 6.004$$  \hspace{1cm} (1)

where $k$ is thermal conductivity (W/m-K) and $T$ is the temperature (K). The above correlation is valid from room temperature to 1773 K. A recent corrigendum by White et al. [5] to the paper that gives the above correlation has resulted in an updated thermal conductivity correlation for U3Si2 in BISON given by:

$$k = 0.0118 \times T + 4.996$$  \hspace{1cm} (2)

where the correlation is valid from room temperature to 1773 K. The key observation is that the thermal conductivity of the fuel with the new correlation is approximately 18-21% lower than the previous model. In the results and analysis section of this paper we compare important fuel performance parameters such as the fuel centerline temperature and fission gas release computed using the two thermal conductivity models during normal operating conditions to demonstrate the importance of using the most up-to-date models in fuel performance simulations.

OXIDATION KINETICS OF FECRAL

One of the primary advantages of FeCrAl alloys over conventional zirconium-based alloys is the improved oxidation kinetics. Oxidation experiments completed by Pint et al. [6] investigated the oxidation behavior of the commercial FeCrAl alloy Kanthal APMT™. The parabolic rate constant is exponentially dependent upon temperature:

$$k_p = k_o e^{-Q/RT}$$  \hspace{1cm} (3)

where $k_p$ is the parabolic rate constant (g²/cm⁴-s), $k_o$ is a constant equal to 7.84 g²/cm⁴-s, $R$ is the universal gas constant (8.3145 J/mol-K) and $Q$ is the activation energy with a value of 344000 J/mol. The mass gain due to the oxide formation is then calculated by

$$w_g = \sqrt{k_p t}$$  \hspace{1cm} (4)

where $w_g$ is the mass gain due to oxidation (mg/cm²). Then the oxide thickness is determined by multiplying the mass gain by the conversion factor of 5.35 μm/(cm²/mg) as proposed by Jönnsson et al [7]. It is important to note that the above...
oxidation kinetics model was developed for high temperature steam environments (1323 to 1748 K). However, in the absence of low temperature oxidation data at the time, the Pint et al. [6] model was also applied at normal operating conditions.

Recent autoclave experiments under PWR, BWR-HWC (hydrogen water chemistry), and BWR-NWC (normal water chemistry) conditions were completed by Terrani et al. [8]. Here, only the PWR and BWR-NWC cases are of interest. The experiments were conducted at normal operating temperatures 330°C and 290°C for PWR and BWR, respectively. Parabolic oxide growth kinetics govern the mass gain as a result of the formation and growth of the chromium rich chromite (FeCr2O4) layer:

\[ w = k \sqrt{t} \]  

where \( k \) is the parabolic oxidation rate constant (mg/cm²-h¹/²) and \( t \) is the time (hr). The thickness of the chromite layer is then given by:

\[ \delta = \frac{w}{\rho_{ox}} \]  

where \( \rho_{ox} \) is assumed to be the density of oxygen in chromite (1440 kg/m³) [8].

The parabolic rate constants used from [8] in the BISON model are 3.96 × 10⁻³ and 4.51 × 10⁻⁴ mg/cm²-h¹/² for PWR and BWR-NWC coolant conditions, respectively. These correspond to the FeCrAl alloy with composition of Fe-13Cr-4Al which most closely represents the C35M FeCrAl alloy, which is the leading candidate for inclusion in a LWR lead test rod or assembly. In the results and analysis section of this paper we compare oxide thickness predicted by the two different oxidation models presented here during normal operating conditions to demonstrate the importance of using the most up-to-date models in fuel performance simulations.

RESULTS AND ANALYSIS

In the analyses completed, a modified version of the BISON 10-pellet axisymmetric example problem is used as the finite element domain. The geometric details of the models for both UO₂/FeCrAl and U₃Si₂/Zircaloy-4 rodlets have been presented elsewhere [9]. In brief the outer diameter and cold gap thickness of the rodlets were kept the same. To account for a neutronic penalty associated with the larger thermal absorption cross-section in FeCrAl alloys, the cladding thickness was reduced and fuel diameter increased in the UO₂/FeCrAl case. The rodlets were subjected to a normal operating power history consisting of a ramp to 25 kW/m over 3 hours and holding constant for 3.2 years while important fuel performance parameters were extracted for analysis. In the simulations of the U₃Si₂/Zircaloy-4 rodlet fuel centerline temperature was extracted to assess the effect of the updated thermal conductivity model explained earlier. For the UO₂/FeCrAl rodlet simulations the oxide thickness was extracted to compare the predictions between the old and new oxidation models described previously.

The comparison results for the U₃Si₂/Zircaloy-4 rodlets is shown in Figure 1. As expected the White et al. 2015 correlation predicts lower fuel centerline temperatures for all times during the irradiation. The significant change in slope of the curves is the point at which fuel to cladding mechanical contact begins. While expected, this comparison illustrates the importance of using state-of-the-art correlations for fuel performance analyses, particularly when experimental data is limited for the materials of interest.

Oxide thickness predictions for the UO₂/FeCrAl rodlet using the two oxidation models is shown in Figure 2. In order to compare the oxide thickness predictions the ordinate is plotted on a logarithmic scale. It is observed that the old (Pint et al. 2015) model predicted essentially zero oxide thickness formation. This can be attributed to the application of the high temperature oxidation model to low operating temperatures. Since the activation is large in the parabolic rate constant formula given by Equation 3, the calculated parabolic rate constant at low temperatures is extremely small resulting in negligible oxide formation. The new (Terrani et al. 2016) model predicts a noticeable oxide thickness of approximately 6 μm. However, this thickness is still negligible when compared with the oxide thickness observed using conventional zirconium-based alloys.

CONCLUSIONS

In this paper we demonstrated the importance of using the state-of-art correlations for fuel performance modeling when predicting the behavior of the potential accident tolerant materials such as FeCrAl cladding and U₃Si₂ fuel by comparing old and new/updated models. After updating the thermal conductivity model for U₃Si₂, the centerline temperatures were observed to be on average approximately 3% higher. In the case of oxidation kinetics of FeCrAl during normal operation, the predicted oxide thickness was found to be about 6 μm using the new model whereas the old model predicted nearly zero oxide growth. As additional data becomes available for other behavior models, such as creep, the correlations available within BISON should be updated accordingly.
Fig. 2. Oxide thickness comparisons for the UO$_2$/FeCrAl rodlet using the old (Pint et al. 2015) and new (Terrani et al. 2016) oxidation kinetics models.

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REFERENCES