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Preliminary Modeling of Accident Tolerant Fuel Concepts under Accident Conditions

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Abstract. The catastrophic events that occurred at the Fukushima-Daiichi nuclear power plant in 2011 have led to widespread interest in research of alternative fuels and claddings that are proposed to be accident tolerant. Thus, the United States Department of Energy through its NEAMS (Nuclear Energy Advanced Modeling and Simulation) program has funded an Accident Tolerant Fuel (ATF) High Impact Problem (HIP). The ATF HIP is funded for a three-year period. The purpose of the HIP is to perform research into two potential accident tolerant concepts and provide an in-depth report to the Advanced Fuels Campaign (AFC) describing the behavior of the concepts, both of which are being considered for inclusion in a lead test assembly scheduled for placement into a commercial reactor in 2022. The initial focus of the HIP is on uranium silicide fuel and iron-chromium-aluminum (FeCrAl) alloy cladding. Utilizing the expertise of three national laboratory participants (INL, LANL, and ANL) a comprehensive mulitscale approach to modeling is being used including atomistic modeling, molecular dynamics, rate theory, phase-field, and fuel performance simulations.

In this paper, we present simulations of two proposed accident tolerant fuel systems: U_3Si_2 fuel with Zircaloy-4 cladding, and UO_2 fuel with FeCrAl cladding. The simulations investigate the fuel performance response of the proposed ATF systems under Loss of Coolant and Station Blackout conditions using the BISON code. Sensitivity analyses are completed using Sandia National Laboratories' DAKOTA software to determine which input parameters (e.g., fuel specific heat) have the greatest influence on the output metrics of interest (e.g., fuel centerline temperature). Early results indicate that each concept has significant advantages as well as areas of concern. Further work is required prior to formulating the proposition report for the Advanced Fuels Campaign.

Keywords: BISON, ATF, LOCA, SBO

INTRODUCTION

There has been an increased emphasis on research of accident tolerant fuels concept in recent years. Through the United States Department of Energy's NEAMS ATF HIP program, a multi national laboratory (INL, LANL, ANL) effort is underway to investigate the suitability of iron-chromium-aluminum (FeCrAl) claddings and U_3Si_2 fuel as alternative fuel rod materials. A comprehensive multiscale approach is planned that uses lower length scale methodologies such as density functional theory, molecular dynamics, rate theory and phase field to develop more mechanistically informed correlations for use in the macroscale fuel performance code BISON.

While the lower length scale models are under development, preliminary fuel performance simulations have been completed using empirical models based upon the limited existing experimental data for FeCrAl and U_3Si_2. In this paper we present initial simulations of two proposed ATF systems: U_3Si_2 fuel with Zircaloy-4 cladding, and UO_2 fuel with FeCrAl cladding. The simulations investigate the response of the systems under Loss of Coolant and Station Blackout conditions following a representative base irradiation. Two sets of results are presented for each case including comparisons between the ATF systems and the traditional UO_2/Zircaloy-4 system, as well as sensitivity analyses calculated by means of Sandia National Laboratory's DAKOTA software. In general, the preliminary results indicate that the ATF systems have improved performance during transient conditions than the current UO_2/Zircaloy-4. More rigorous investigations are required once the more mechanistically based models have been developed and implemented into the BISON code. Eventually, the results of this study will form part of the basis of the final report provided to the Department of Energy's Advanced Fuels Campaign.

MATERIAL MODELS

Given that the lower length scale models are under development, empirical correlations have been implemented into BISON. The materials of interest in this study are U_3Si_2 and the iron-chromium-aluminum (FeCrAl) alloy being developed at Oak Ridge National Laboratory (ORNL) known as C35M [1].

Uranium silicide is of particular interest because of its considerably higher thermal conductivity compared to UO_2, which will result in lower fuel temperatures and temperature gradients within the fuel. Lower thermal gradients are expected to result in less cracking of the fuel pellets. Less cracking and lower temperatures suggests that fission gas release will be less in U_3Si_2 than in UO_2. Moreover, U_3Si_2 has a higher uranium density than oxide fuel resulting in economic savings, as fuel enrichment is not necessary to achieve the same discharge burnup. Unfortunately the majority of existing experimental data for U_3Si_2 is for low temperature dispersion fuel used in research reactors. The applicability of the models developed using this data to U_3Si_2 in pellet form under Light Water Reactor (LWR) conditions is unclear.

FeCrAl alloys are widely used in applications where low oxidation rates and high temperature performance is required (e.g., coatings on gas turbines blades). Compared to traditional zirconium based claddings, FeCrAl alloys have higher strength and oxidation resistance, but a lower melting point and higher neutron absorption cross-section. Therefore, thinner cladding walls, and slightly larger pellets with higher enrichment will be necessary to compensate for this neutronic penalty.

Based upon the existing data for U_3Si_2 and C35M empirical models have been developed and added to BISON. For areas where FeCrAl experimental data is non-existent (e.g., thermal conductivity of C35M) data from commercial alloys are used. For U_3Si_2, material models have been added for thermal conductivity and specific heat [2], gaseous and solid swelling [3], and fission gas release [4]. The fission gas release model used is the same as for UO_2 in the absence of data suggesting differences in fission gas release behavior. Since no thermal and irradiation creep data exists for U_3Si_2, the fuel is treated as an elastic material with a Young's modulus of 140 GPa, a Poisson's ratio of 0.17, and a thermal expansion coefficient of 15e-6 K^{-1} as per Metzger et al. [5]. For the laboratory optimized FeCrAl alloy C35M developed at ORNL, models have been added for the mechanical and thermal properties as a function of temperature, thermal and irradiation creep, volumetric swelling and oxidation. The mechanical properties (Young's modulus and Poisson's ratio) were obtained from Thompson et al. [6]. Thermal properties, namely specific heat and thermal conductivity, for the commercial alloy Kanthal APMT are used [7]. The high temperature thermal creep model for MA956 developed by Seiler et al. [8] is used in the absence of other data. Representative models have been added for isotropic swelling and irradiation creep of FeCrAl claddings based upon engineering judgment. The oxidation model adopts the parabolic rate constant suggested by Pint et al. [9], and the conversion from mass gain to oxide thickness proposed by Jönsson et al. [10] is used. In depth details and the equations behind the models used can be found in the BISON theory manual [11].

SIMULATION DESCRIPTIONS

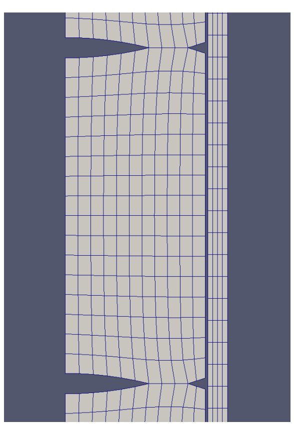
Fuel Performance

BISON is a multiphysics finite element based fuel performance code [12] built upon the MOOSE multiphysics computational framework [13]. In the preliminary analyses completed here a modified version of the BISON discrete ten pellet rodlet example problem was used as the finite element domain. A discrete pellet simulation is one that explicitly models the geometric features of fuel dishes and chamfers. To enable comparisons between the different systems, the initial rod diameter (cladding outer diameter) and fuel-to-cladding gap are the same in all cases. The cladding thickness is varied depending on whether the material is Zircaloy-4 or FeCrAl to simulate the thinner cladding required when FeCrAl is used to overcome the neutronic penalty. To compensate for the thinner cladding, the pellet diameter was increased for the UO_2/FeCrAl system. The specifications of the fuel rodlets are summarized in Table 1.

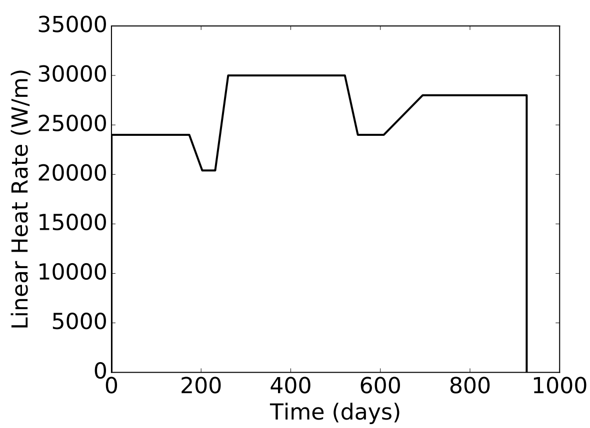
TABLE 1. Rodlet specifications for the three systems.

	UO_2/Zircaloy-4 System	**U_3Si_2/Zircaloy-4 System**	**UO_2/FeCrAl System**
Number of pellets	10	10	10
Pellet length (mm)	9.83	9.83	9.83
Pellet outer diameter (mm)	8.1915	8.1915	8.6345
Dish depth (mm)	0.3	0.3	0.3
Chamfer width (mm)	0.5	0.5	0.5
Chamfer height (mm)	0.16	0.16	0.16
Radial gap width (µm)	82.55	82.55	82.55
Clad thickness (mm)	0.5715	0.5715	0.35
Rodlet length (mm)	107.203	107.203	107.203
Rodlet diameter (mm)	9.4996	9.4996	9.4996
Initial fill pressure (MPa)	2.0	2.0	2.0
Initial fill gas	Helium	Helium	Helium
Initial grain size (µm)	20	20	20
Coolant inlet mass flux (kg/ m^2-s)	3800	3800	3800
Coolant inlet temperature (K)	583	583	583
Coolant pressure (MPa)	15.5	15.5	15.5

The mesh density used for the three systems was the same including 2448 QUAD8 finite elements producing 8242 nodes. Figure 1(a) shows a section of the rodlet to illustrate the mesh. The comparative simulations consisted of a nominal base irradiation followed by either a loss of coolant accident LOCA or station blackout (SBO). The base irradiation power history is illustrated in Figure 1(b). A flat axial profile was assumed for this short rodlet. The transients begin at 80050000 seconds (~926.5 days) in all cases. Each system (UO_2/FeCrAl, UO_2/Zircaloy-4, U_3Si_2/Zircaloy-4) is subject to a LOCA and SBO resulting in six different simulations. In the LOCA cases the transients last for 90 seconds and the station blackout lasts for a day (86400 s). To simulate the LOCA, the 1-D coolant channel model's inlet mass flux was dropped to 1 kg/m^2-s and the coolant pressure reduced to atmospheric over 10 seconds, thereby significantly reducing the cladding-to-coolant heat transfer coefficient. Meanwhile the power supplied to fuel is dropped to zero over two seconds where decay heat is turned on as a source term for the duration of the transient. For the SBO scenarios the transient is similar except the coolant pressure remains at 15.5 MPa while the coolant flow is decreased to 100 kg/m^2-s to simulate the low flow rate introduced by the direct current backup generators, and the power to the fuel is shut off.



(a)



(b)

FIGURE 1. (a) An illustration of the mesh density for the three systems and (b) the base irradiation power history.

Sensitivity Analyses

Due to the lack of experimental data and limited knowledge of the fuel performance response of the accident tolerant fuel concepts under postulated accident conditions such LOCAs and SBOs sensitivity analyses can be used to provide additional insight. There are numerous statistical methodologies available to determine the sensitivity of the output metrics of interest to uncertainties in select input parameters including Pearson and Spearman correlation coefficients, main effects studies, surrogate models, and variance based decomposition. In this work, BISON is coupled to the DAKOTA [14] sensitivity analysis software to perform main effects studies that illustrate the importance of uncertain input parameters on the fuel centerline temperature and total cladding hoop strain at the end of the transients for the UO_2/FeCrAl and U_3Si_2/Zircaloy-4 systems. The input parameters of interest in this study are presented in Table 2 for the UO_2/FeCrAl and Table 3 for the U_3Si_2/Zircaloy-4 including their maximum, minimum and mean values. Note that the creep correlations are scaled by orders of magnitude because it is expected that C35M will creep more than the current commercial FeCrAl alloys at higher temperatures. GB and IG stand for grain boundary and intergranular, respectively. These diffusion coefficients are varied in the U_3Si_2/Zircaloy-4 case due to the limited knowledge of fission gas behavior in silicide fuel.

TABLE 2. Parameters varied in the main effects analysis including their minimum, mean, and maximum values for the UO_2/FeCrAl system.

	Minimum	Mean	Maximum
Thermal creep scaling factor	1.0	50.5	100.0
Irradiation creep scaling factor	1.0	5.5	10.0
Volumetric swelling scaling factor	0.8	1.0	1.2
Young's modulus scaling factor	0.8	1.0	1.2
Fuel enrichment (%)	5	6.5	8

TABLE 3. Parameters varied in the main effects analysis including their minimum, mean, and maximum values for the U_3Si_2/Zircaloy-4 system.

	Minimum	Mean	Maximum
GB diffusion coefficient scaling factor	1.0	5000.0	10000.0
IG diffusion coefficient scaling factor	1.0	5000.0	10000.0
Thermal conductivity scaling factor	0.8	1.0	1.2
Gas swelling scaling factor	0.8	1.0	1.2
Specific heat capacity scaling factor	0.95	1.0	1.05

RESULTS AND ANALYSIS

Loss of Coolant Accidents

The results of the LOCA simulations are presented in Figures 2, 3, and 4. Figure 2 highlights the comparison between the three systems for the baseline cases. In these cases the uncertain material models are taken as their default value. The plots show the evolution of the fuel centerline temperature and cladding hoop strain during the LOCA (i.e., t = 0 is the end of the base irradiation). The rapid decrease in the fuel centerline temperature at the beginning of the LOCA is due to the removal of power to the fuel. Once the mass flux has decreased to its very small minimum value at 10 s the temperature begins to rise due to the decay heat and severely degraded heat transfer coefficient. It is observed that the two ATF systems result in lower centerline temperature at the end of the 90 s transient. The strain evolution in Figure 2b clearly illustrates the significant hoop strain experienced by Zircaloy during the LOCA. The sharp transition in the UO_2 case at 10 s corresponds to the significant reduction in heat transfer on the surface of the cladding. Both the UO_2/Zircaloy-4 and U_3Si_2/Zircaloy-4 cases begin following an exponential increase in strain due to the significant deformation experienced by Zircaloy during the LOCA. The UO_2/FeCrAl observes superior performance in terms of cladding deformation, as the strain remains very low.

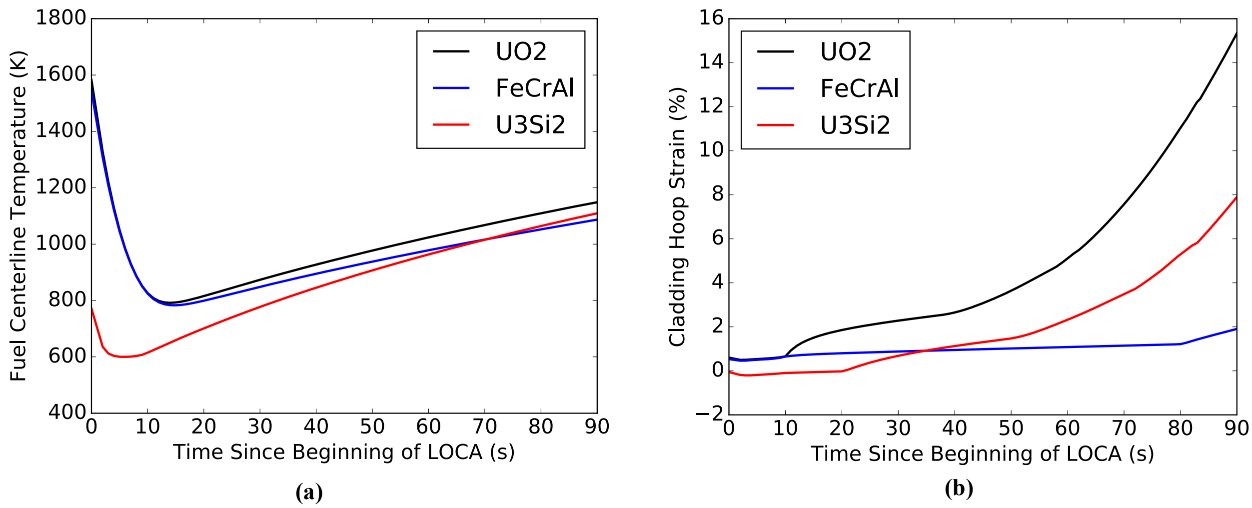
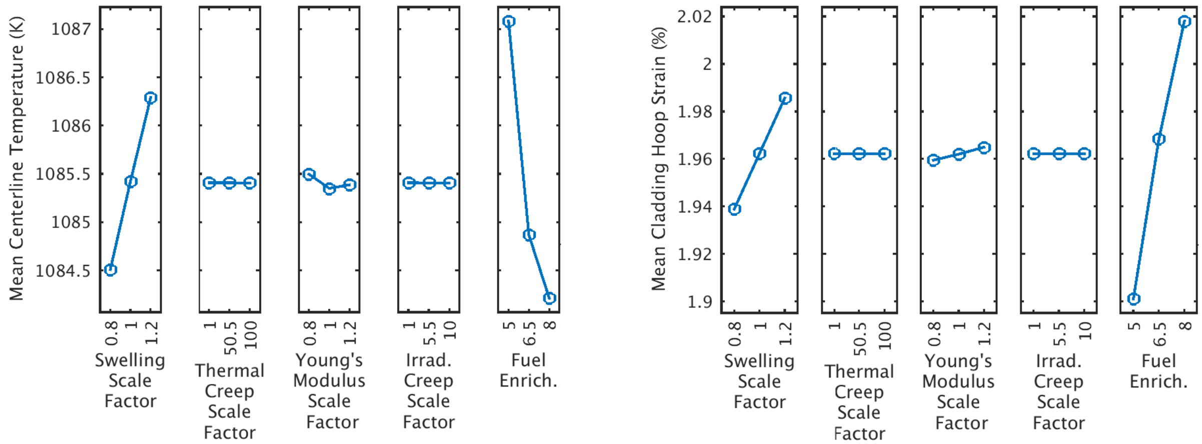


FIGURE 2. Comparison of the (a) centerline temperature and (b) cladding hoop strain during for the three fuel systems during a LOCA transient.

Figure 3 illustrates the main effects plots for the UO_2/FeCrAl system during the LOCA transient. In a main effects study the output metric of interest (e.g., centerline temperature) is shown on the ordinate axis, whereas the various input parameters are plotted along the abscissa. Each subplot in a particular diagram represents the main effects of that input parameter. To provide guidance on how to interpret the results of a main effects study initially focus on the swelling scale factor subplot in Figure 3a. The point for a swelling scale factor of 0.8 represents the mean centerline temperature for all of the simulations that had the swelling scale factor set to 0.8. A monotonic upward slope when an input variable is varied indicates a positive correlation with the output metric. Subsequently, a monotonic downward slope represents a negative correlation between the input parameter and output metric. Lines that are close to horizontal imply no correlation between input and output. Note that all of the data points represent the mean values at the last timestep of the transient.

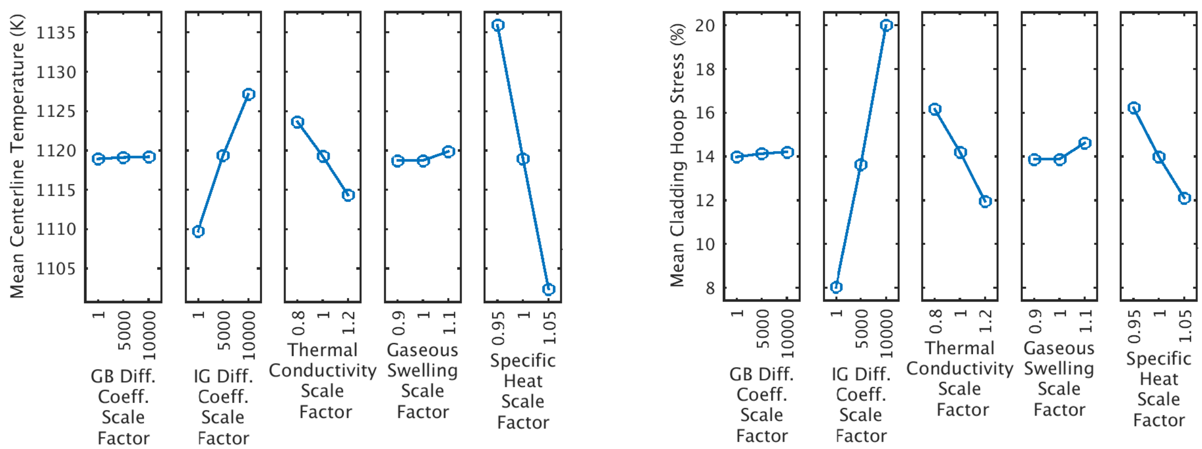
For the UO_2/FeCrAl system the main effects study highlights the importance of the swelling scaling factor and the fuel enrichment. The centerline temperature and cladding hoop strain are both positively correlated with the swelling strain. Contrarily, the fuel enrichment is negatively correlated with centerline temperature but positively correlated with the hoop strain. Higher enrichment leads to a larger burnup within the fuel, particularly in the rim region at the periphery of the pellet. The swelling correlation in BISON is burnup dependent, thus, increased enrichment results in larger fuel swelling. Larger fuel swelling results in contact between the fuel and cladding earlier in the LOCA transient resulting in a decreased centerline temperature. Subsequently, the harder the contact occurring between the fuel and cladding the larger the strain. Interestingly, the large scaling factors on the thermal and irradiation creep appear to have no influence, indicating that the creep strain is still significantly low. It is prudent to note that the range of centerline temperature and cladding hoop strain is small.

The results of the main effects study for the U_3Si_2/Zircaloy-4 system during the LOCA are shown in Figure 4. In this case the range of the output metrics is much larger than the UO_2/FeCrAl system indicating that uncertainty in U_3Si_2 behavioral models have a more significant impact on the centerline temperature and hoop strain. As expected the significant uncertainty assumed on the intergranular diffusion coefficient results in large variations in the centerline temperature and cladding hoop stress. The larger diffusion coefficients give rise to increased stress due to greater fission gas release to the plenum increasing the internal pressure and inducing larger stress on the cladding. In addition, increasing the thermal conductivity results in lower temperatures and strains. Surprisingly, uncertainty in the specific heat capacity has a significant correlation with the centerline temperature for such a long duration transient. Usually, the specific heat only has an affect during very short duration transients (e.g., reactivity insertion accidents). The plots indicate that the grain boundary diffusion coefficient and gaseous swelling have minimal effects. It is anticipated that at very high burnups (>60 MWd/kgU) gaseous swelling would be the most dominant behavior due to the rapid increase in gaseous swelling at high burnups. In this study the burnup after the base irradiation was approximately 5.01 % FIMA (47.67 MWd/kgU) which is just above the threshold for gaseous swelling of 5% FIMA in the current BISON model.



(a) (b)

FIGURE 3. Main effects plots for the UO_2/FeCrAl system during for the LOCA transient.

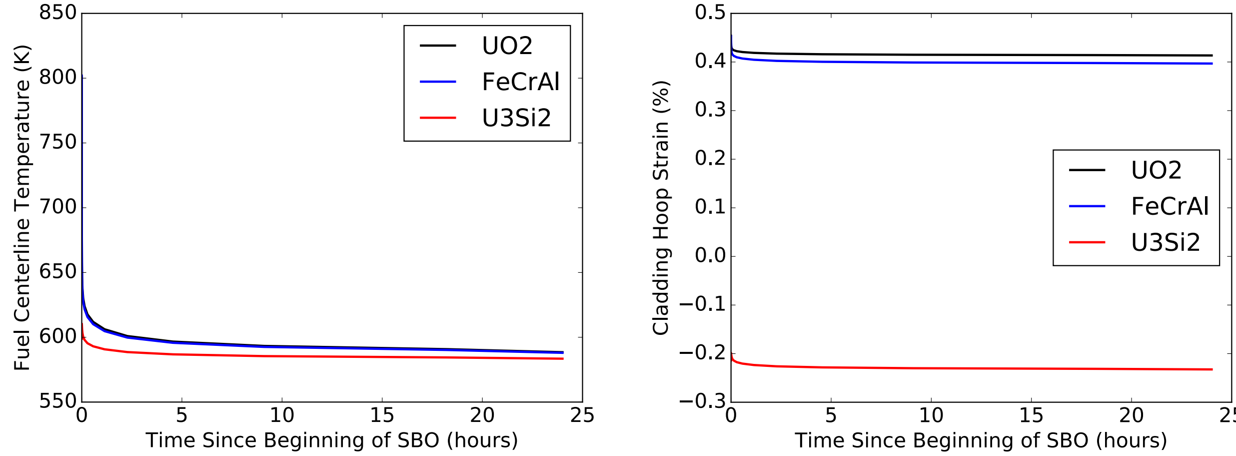


(a) (b)

FIGURE 4. Main effects plots for the U_3Si_2/Zircaloy-4 system during for the LOCA transient.

Station Blackouts

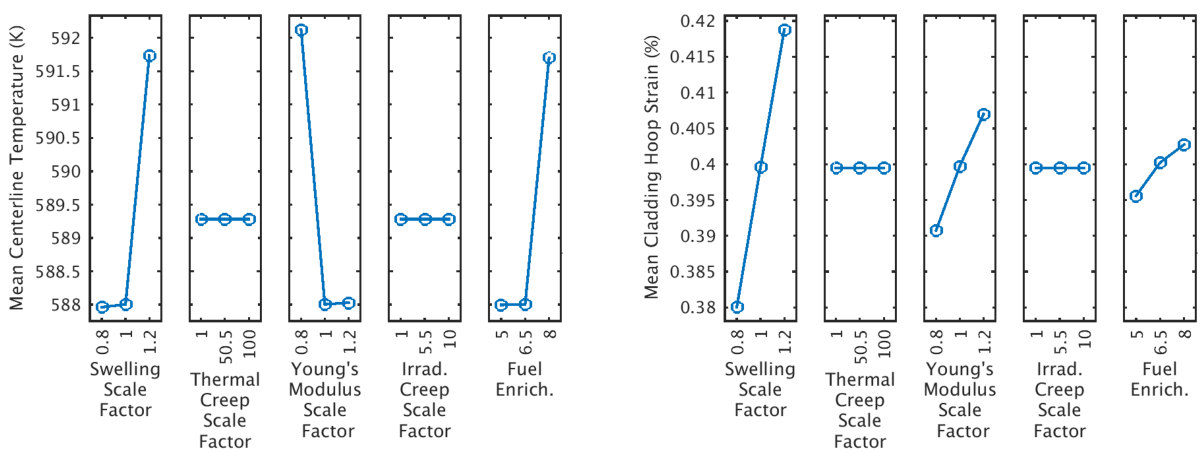
The results of the SBO simulations are presented in Figures 5, 6 and 7. Figure 5 presents the comparison between the three systems for the baseline cases. The plots show the evolution of the fuel centerline temperature cladding hoop strain during the station blackout transient. For the SBO plots the beginning of the transient (t=0) in the plot is taken as the time when the mass flux equals 100 kg/m^2-s. This value represents the minimal flow provided by the DC backup generators. It is observed that the centerline temperature approaches the coolant inlet temperature rapidly. This can be attributed to the size of the rodlet considered. The coolant channel model takes the bottom of the rodlet as the inlet and because the rodlet is only 107.2 mm long it can still be cooled quickly with minimal coolant flow. Subsequently, because the fuel and cladding temperatures remain low, the stress induced in the cladding is minimal. Thus, simulations of full-length fuel rods are required to provide conclusive qualitative comparisons of the three systems during a station blackout event. It should be noted that the reduced flow does decrease the rate of cooling from full power.



(a) **(b)**

FIGURE 5. Comparison of the (a) centerline temperature and (b) cladding hoop strain for the three fuel systems during a postulated SBO transient.

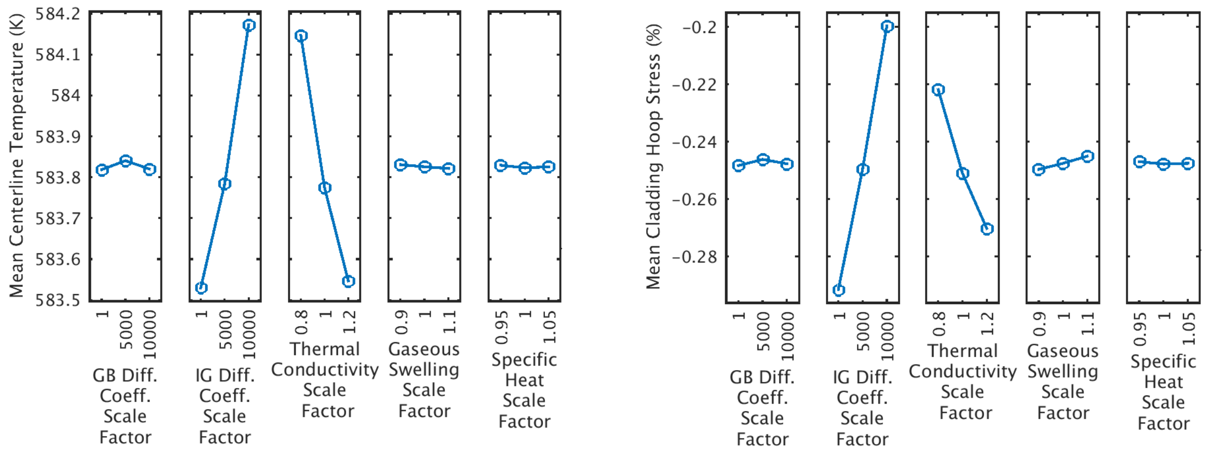
The UO_2/FeCrAl system's main effects study for the SBO scenario is shown in Figure 6. Since the temperatures in the baseline cases approach the coolant inlet temperature expectations of much variation during the SBO scenario were low. However, it was found that the cladding hoop strain had strong positive correlations between the Young's modulus and swelling factor. Comparing this to the LOCA case it can be concluded that at the end of the SBO there is no contact between the fuel and cladding because the Young's modulus correlates with the strain. Whereas, in the LOCA case shown previously, the Young's modulus has no effect indicating contact had been established at the end of the transient.



(a) **(b)**

FIGURE 6. Main effects plots for the UO_2/FeCrAl system during for the SBO transient.

The U_3Si_2/Zircaloy-4 system experienced minute variation in the centerline temperature and cladding hoop strain with respect to the uncertainties in the inputs for the SBO case as shown in Figure 7. Strong correlations are still observed for the integranular diffusion coefficient and thermal conductivities. An important observation is that for the SBO transient which lasted 24 hours compared to the LOCA that lasted 90 seconds, that the specific heat has no correlation with the output parameters. This is expected for the long duration transients.



(a) **(b)**

FIGURE 7. Main effects plots for the U_3Si_2/Zircaloy-4 system during for the SBO transient.

CONCLUSION

In this paper, we investigated the fuel performance response of two accident tolerant fuel concepts, compared to the UO_2/Zircaloy-4 system used in todays LWRs. under postulated LOCA and SBO conditions. It was observed that U_3Si_2/Zircaloy4 and UO_2/FeCrAl have superior performance during a 90 s LOCA than traditional UO_2/Zircaloy4 fuel rods. For the postulated SBO analyzed in this work, it was found that the centerline temperature and cladding strains remained well below any values of concern. This is attributed to the shortness of the rod studied and how the coolant channel model treats the inlet as the bottom of the rod. Thus, the short rodlet could be cooled very quickly. An analysis of a full-length fuel rod is required to obtain improved qualitative comparisons between the three systems under SBO conditions.

Sensitivity analyses were completed using the DAKOTA softwared coupled to BISON to obtain main effects plots. It was found that for UO_2/FeCrAl uncertainty in the creep correlations had no effect on the calculated centerline temperature or cladding hoop stress. Overall, it was observed that uncertainty in the material models for FeCrAl had negligible influence on the outputs considered. Contrarily, in the LOCA in particularly, the uncertainty in the U_3Si_2 material and behavioral models had significant influences on the calculated centerline temperature and cladding hoop strain.

Additional simulations and advanced sensitivity analysis techniques are required to gain improved understanding of the behavior of the proposed ATF concepts under accidents conditions prior to formulating the proposition report for the Advanced Fuels Campaign

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