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Introduction

The purpose of this milestone report is to present the work completed in regards to material model development for U_3Si_2 fuel and highlight the results of applying these models to Reactivity Initiated Accidents (RIA), Loss of Coolant Accidents (LOCA), and Station Blackouts (SBO). With the limited experimental data available (essentially only the data used to create the models) true validation is not possible. In the absence of another alternative, code-to-code comparisons have been completed. Qualitative comparisons during postulated accident scenarios between U_3Si_2 and UO_2 fueled rods have also been completed demonstrating the superior performance of U_3Si_2.

Material Model Development

At the engineering scale, the material model development has primarily focused on the implementation of new gaseous swelling and thermal conductivity models developed using lower length scale rate theory and phase field modeling. In addition, a consistent set of material and behavioral models for U_3Si_2 have been decided upon for the code-code and qualitative rod comparisons shown in subsequent sections.

For U_3Si_2, material models have been added for thermal conductivity and specific heat [1], gaseous and solid swelling [2], and fission gas release [3]. 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 1.5×10^{-5} K^{-1} as per Metzger et al. [4]. Moreover, since limited cracking is expected to occur in U_3Si_2 no relocation model is used. While the radial power profile in U_3Si_2 is being determined by neutronics calculations, the traditional Lassman model for UO_2 is used.

Two new models in BISON are worth mentioning that are based upon lower length scale work completed by Yongfeng Zhang at Idaho National Laboratory and Yinbin Miao at Argonne National Laboratory. The first model is a thermal conductivity model developed using phase field calculations, known henceforth as the Zhang model. This model improves upon the current state of the art correlation of White et al. [1] by predicting the thermal conductivity of a variety of the secondary uranium silicide phases including U_3Si and U_3Si_5. The Zhang model reproduces the behavior for U_3Si_2 determined by White et al. The second model is a gaseous swelling model for U_3Si_2, subsequently known as the Miao model. The Miao gaseous swelling model is more sophisticated than the correlation developed from the data of Finlay et al. [2] and takes into account the effect of local power, local temperature, and temperature gradient within the fuel pellet. The Miao model has also been developed for both normal operating and transient conditions. The Zhang model has been fully incorporated into BISON whereas the Miao model is currently being implemented. Application of these two new models to accident scenarios is the subject of future work.

Verification

Prior to validating a new material model it must be verified to known analytical or universally accepted textbook solutions. Verification essentially ensures that the correlation or model of interest has been coded correctly and that BISON is performing the mathematical calculation as expected. Verification is completed in BISON in part by ensuring regression tests are included with every new model added to the code. A detailed description of the verification procedure can be found in Hales et al. [5]. Every model for U_3Si_2 that has been added to BISON has been accompanied with a regression test.

Simulation Model Development

As mentioned previously, limited experimental data exists for the behavior of U_3Si_2 under irradiation. In addition, the data that is available was used to develop the material models in use. This led to the lower length scale effort to develop more mechanistic (physics-based) models. While these models are under development important information can be garnered from simulations that compare the U_3Si_2 fuel to UO_2 for representative cases. In this FY, investigations of three accidents have been considered including RIA, LOCA, and SBO. The details of the simulations and select results are presented in the following subsections.

Application to a Reactivity Initiated Accident

The analysis of U_3Si_2 during a RIA was completed in collaboration with Brookhaven National Laboratory. The approach and results are detailed in a TopFuel 2016 paper that was accepted to be presented as a poster at the meeting. In brief, a RIA was simulated on fresh fuel from hot full power conditions (ALHR 33658 W/m) on a rod with AP-1000 dimensions. The power history and axial power profile were generated using the TRACE [6] and PARCS [7] codes respectively. Since, the BISON coolant channel model is not currently developed to handle the complex coolant conditions during a RIA, the cladding outer surface temperature was provided as an input to BISON from TRACE. The reactivity insertion corresponded to a $1 ramp. Figure 1 presents the normalized reactor power calculated by TRACE and the core-averaged axial power distribution calculated by PARCS. The normalized reactor power is converted to average linear heat rate (ALHR) in units of W/m for use in BISON. The simulations of the two rod systems (UO_2/Zircaloy-4 and U_3Si_2/Zircaloy-4) were terminated after 1 second of simulation time.

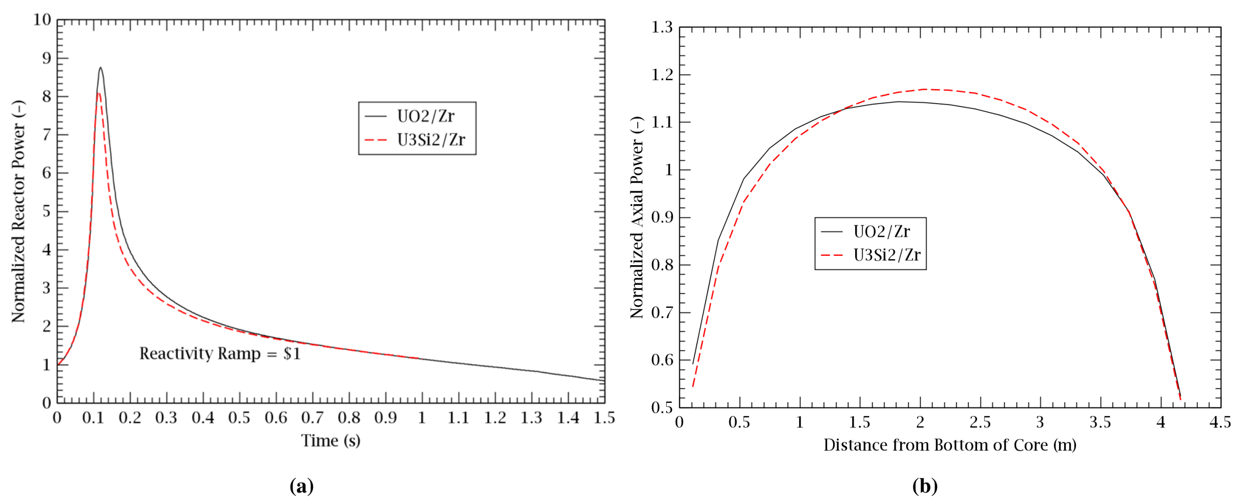
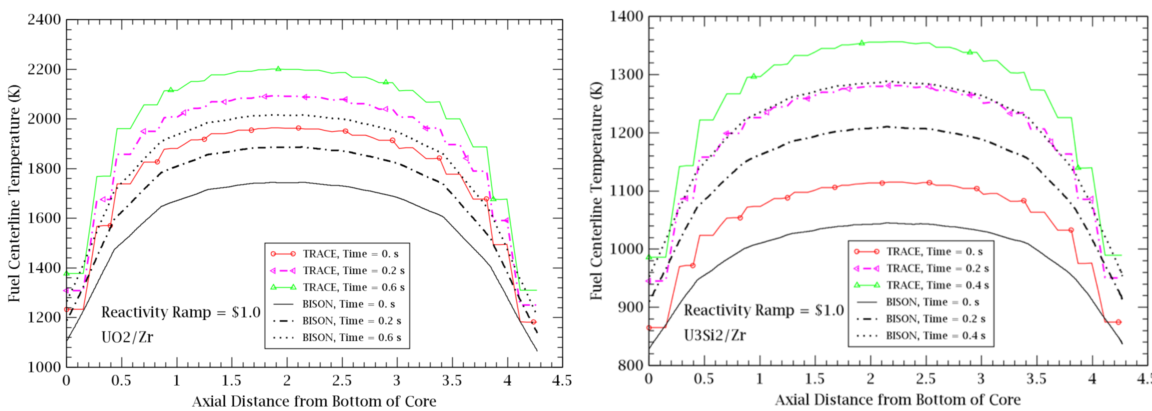


Figure 1: Illustration of the (a) normalized power history calculated by TRACE and (b) axial power profile calculated by PARCS applied to the UO_2/Zircaloy-4 and U_3Si_2/Zircaloy-4 rods for the RIA scenario.

A code-to-code comparison was completed between BISON and TRACE for the fuel centerline temperature for both rods. Figure 2 presents the axial temperature variation at simulation times of 0.0 (start of RIA), 0.2 and 0.6 s. The difference between the BISON and TRACE simulations are due to the gap conductance and thermal expansion models used by the codes. The important observation to make when comparing Figure 2a and 2b is that the centerline temperature is consistently lower for the U_3Si_2/Zircaloy-4 rod. This preliminary conclusion is a positive argument for using U_3Si_2 as an accident tolerant fuel. However, the melting temperature of U_3Si_2 is lower than that for UO_2, reducing the net benefit.



(a) **(b)**

Figure 2: Axial temperature profile during the RIA for (a) the UO_2/Zircaloy-4 and (b) the U_3Si_2/Zircaloy-4 rods at times of 0.0, 0.2 and 0.6 s.

Application to a Loss of Coolant Accident

The investigation of U_3Si_2 during a LOCA scenario was completed by utilizing a modified version of the BISON 10 pellet example problem. Both a UO_2 and a U_3Si_2 fueled rodlet were subjected to the base irradiation power history shown in Figure 3 followed by a LOCA transient representative of a large break LOCA. A flat axial profile was assumed for this short rodlet. The transient begins at the conclusion of the base irradiation (≈926.5 days). To simulate the LOCA, the 1-D coolant channel model's inlet mass flux was dropped to 1 kg m^{-2} $s^{-1}$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. The transient was terminated after 90 s, and reflood was not modeled.

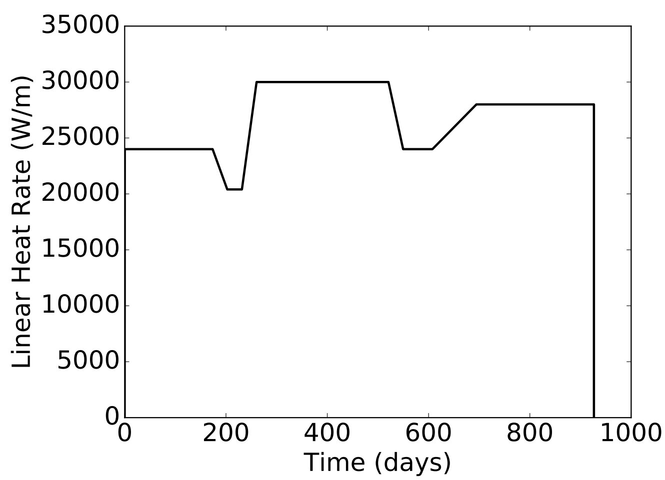
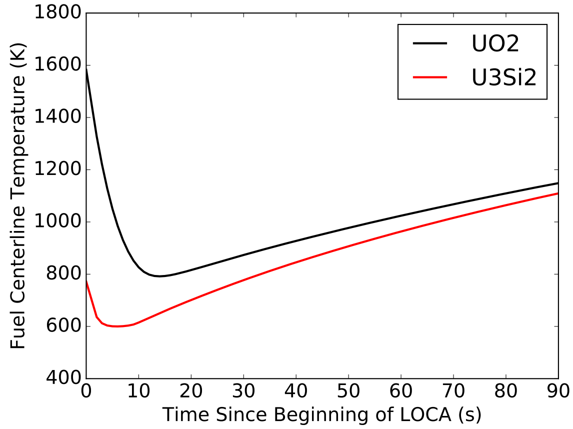
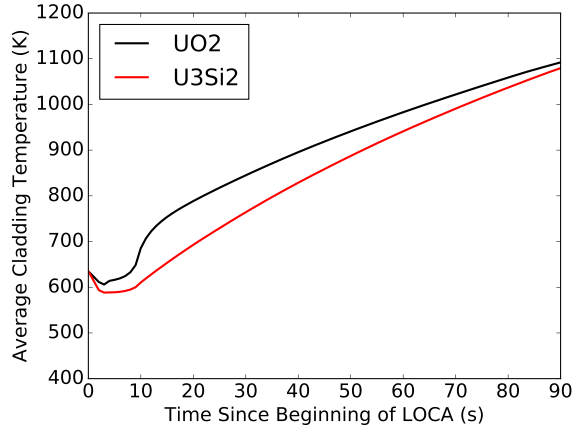


Figure 3: Representative base irradiation power history used for the LOCA transient.

Selected comparative results during the LOCA transient are shown in Figure 4. The results shown are the fuel centerline temperature and the average cladding temperature. It is observed that the U_3Si_2/Zircaloy-4 rodlet achieves lower temperatures than the UO_2/Zircaloy-4 rod. Determining the peak cladding temperature is an important criteria for Emergency Core Cooling Systems (ECCS) outlined in the NRC regulation 10 CFR 50.46. During the LOCA the average cladding temperature is close to the peak as the thermal conductivity is high through the cladding thickness essentially bringing the entire cladding to the coolant temperature. Improvements in areas of interest for the ECCS criteria indicate that based upon these preliminary calculations U_3Si_2 may have superior response to a LOCA transient than UO_2 fuel. Further investigation is required to determine definitively if U_3Si_2 is in fact superior to UO_2 under LOCA conditions.



(a)



(b)

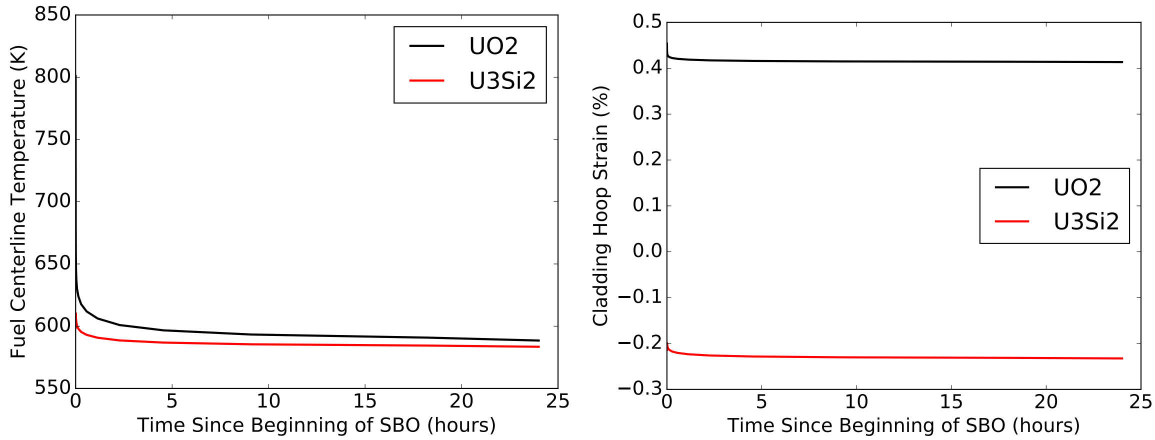
Figure 4: Temporal comparison of (a) centerline temperature and (b) cladding temperature during the LOCA transient for the UO_2 and U_3Si_2 fueled rods.

Application to a Station Blackout

Investigation of the response of U_3Si_2 to postulated station blackout conditions was completed using the same 10 pellet rodlet in the LOCA case. The SBO scenario is modeled similarly to the LOCA except the coolant pressure remains at 15.5 MPa while the coolant flow is decreased to 100 kg m^{-2} s^{-1} to simulate the minimal flow provided by the backup cooling system. As per the LOCA scenario the power is shut off over 2 s and decay heat is turned on as a heat source. Select comparative results for the SBO scenario are shown in Figure 5. The fuel centerline temperature and cladding hoop strain is presented. 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 two systems during a station blackout event. It should be noted that the reduced flow does decrease the rate of cooling from full power.

Publications

Throughout this FY, three conference publications have been produced on this work. These publications are a full paper presented at the Enlarged Halden Programme Group (EHPG) meeting in Norway (May 8-13, 2016), a full paper accepted to the TopFuel 2016 conference in Boise (September 11-16, 2016), and an ANS Transactions summary presented as a poster at the ANS Annual meeting in New Orleans (June 12-16, 2016). The EHPG paper and ANS summary focused normal operating conditions and preliminary LOCA simulations. Both comparative and sensitivity analyses were completed. The TopFuel paper extends the LOCA analysis to longer exposure times, higher burnups



(a) **(b)**

Figure 5: Temporal comparison of (a) centerline temperature and (b) cladding hoop strain during the SBO transient for the UO_2 and U_3Si_2 fueled rods.

and investigates a modified set of sensitive input parameters. In addition, the TopFuel paper covers the preliminary investigations of station blackouts. A journal paper is currently in preparation.

Conclusion

This report documents recent work in the development and validation of accident capabilities for U_3Si_2 fuel including:

- Standard material model options have been chosen for U_3Si_2 under accident conditions.
- Verification of the material models have been completed.
- Qualitative comparisons between U_3Si_2 and UO_2 fueled rods indicates superior performance of U_3Si_2 under accident conditions.

Although significant insight into the behavior of U_3Si_2 fuel under accident conditions has been completed, development and testing of accident models is far from complete. As additional experimental data is obtained and new lower length scale models are developed, new and improved material models will be added to the BISON fuel performance code. Future goals include:

- Inclusion of irradiation damage degradation to thermal conductivity in the Zhang thermal conductivity model and the Miao gaseous swelling model.
- Development of a fission gas release model.
- Implementation of the radial power profile for U_3Si_2 currently being obtained from neutronics calculations.
- Apply the Zhang and Miao models to the accident scenarios and compare the results.
- Investigate the accident response of U_3Si_2 on full length rods for LOCA and SBO conditions.

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