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NEAMS PSU Subcontract: Development of Macroscale Models of UO_2 Fuel Sintering and Densification using Multiscale Modeling and Simulation

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1 Summary

The overall goal of this three year project is to develop a mechanistic model of fuel densification for use in the BISON fuel performance code. The development of this model is being informed by MARMOT simulations of sintering, that will consider the impact of irradiation. During the first year, our effort has been focused on developing a sintering model in MARMOT for UO_2.

2 Introduction

Light water reactor fuel pellets are fabricated using sintering to final densities of 95% or greater. During reactor operation, the porosity remaining in the fuel after fabrication decreases further due to irradiation-assisted densification. While empirical models have been developed to describe this densification process, a mechanistic model is needed as part of the ongoing work by the NEAMS program to develop a more predictive fuel performance code. In this work we will develop a phase field model of sintering of UO_2 in the MARMOT code, and validate it by comparing to published sintering data. We will then add the capability to capture irradiation effects into the model, and use it to develop a mechanistic model of densification that will go into the BISON code and add another essential piece to the microstructure-based materials models. The final step will be to add the effects of applied fields, to model field-assisted sintering of UO_2. The results of the phase field model will be validated by comparing to data from field-assisted sintering.

Tasks over three years:

1. Develop a sintering model for UO_2 in MARMOT
2. Expand model to account for irradiation effects
3. Develop a mechanistic macroscale model of densification for BISON

3 Work during FY 2016

In the first twelve months of this project, we have focused on task 1, developing a sintering model for UO_2 in MARMOT. The majority of the work was completed by first year graduate student Ian Greenquist.

To understand the context of the project, a large literature review of dimensional changes in UO_2 was completed, including sintering and densification. We are currently writing a review paper on the theories and common computer-modeling techniques for the dimensional changes.

Another important step was for Ian to learn to use the computational tools for the project. He has learned a great deal about the MOOSE framework by completing example problems (including participating in the 2016 ChiMaD Phase Field Methods Hackathon), studying the Rigid Body Motion (RBM) tools in MOOSE that account for particle motion, learning C++, and studying the code structures in MOOSE objects.

The existing sintering model in MOOSE had never been applied to UO_2 and could only feasibly model a small number of particles. Therefore, we have improved the capabilities in MOOSE to facilitate larger sized simulations. Custom syntax was created in MOOSE that automatically creates all of the necessary objects needed for a sintering simulation. Another critical step was adding the capability to generate the initial structure of particle compacts. To ensure high code quality, we have created robust tests for all our new additions that are run every time changes to the code are made. Finally, we have added materials models that specifically account for the properties of UO_2.

Using the new capabilities, we conducted test sintering simulations starting from a compact containing 15 UO_2 particles. The results of one simulation are shown in Fig. 1.

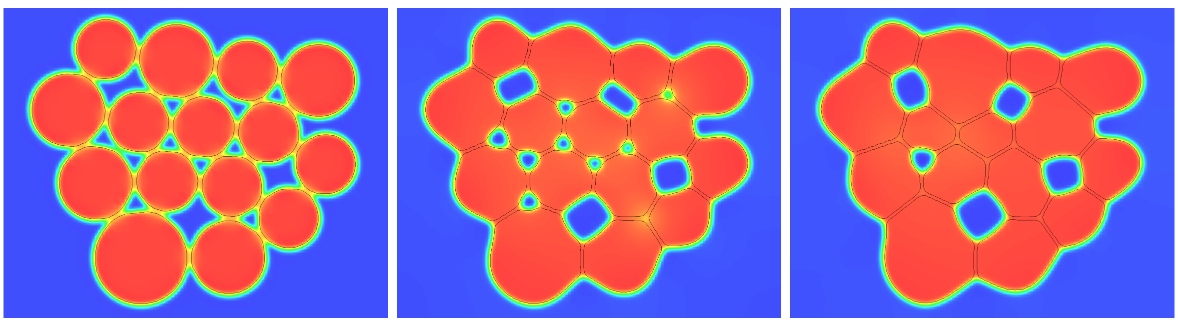

Figure 1: Example of a UO_2 sintering simulation with fifteen initial particles, where the red color represents the solid particles, the blue empty space, and the black lines are grain boundaries.

4 Future work

In the second year of the project, we will complete development of the UO_2 sintering model in MARMOT and we will run 2D and 3D simulations using large numbers of particles. These results will be compared against published sintering data for UO_2. We will also begin to implement irradiation effects into the model.

In the third year we will complete the implementation of irradiation effects, and use the MARMOT results to implement the development of a mechanistic model of densification for the BISON fuel performance tool.