INL/CON-16-37597
PREPRINT

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Top Fuel 2016

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September 2016

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Frederick Gleicher,[1] Javier Ortensi,[1] Mark DeHart, [1] Yaqi Wang,[2] Sebastian Schunert,[2] Stephen Novascone,[3] Jason Hales,[3] Rich Williamson,[3] Andrew Slaughter,[4] Cody Permann, [4] David Andrs, [4] and Richard Martineau[4]

[1]Reactor Physics Design and Analysis, Idaho National Laboratory, Idaho Falls, Idaho, 83415
[2]Nuclear Engineering Methods Development, Idaho National Laboratory, Idaho Falls, Idaho, 83415
[3]Fuel Modeling and Simulation, Idaho National Laboratory, Idaho Falls, Idaho, 83415
[4]Modeling and Simulation, Idaho National Laboratory, Idaho Falls, Idaho, 83415
1-(208)-526-6896 and Frederick.Gleicher@inl.gov

Abstract. The accurate calculation of desired quantities to predict fuel behavior in a nuclear reactor requires the solution of interlinked equations representing different physics phenomena. Traditional fuels performance codes often rely on internal empirical models for the pin power density and a simplified boundary condition on the cladding outer surface. These simplifications are performed because of the difficulty of coupling applications or codes on differing domains and mapping the required data. In this work the MAMMOTH application is employed in the demonstration of an approach that more consistent with first principles, in a simulation that couples the neutronics application Rattlesnake, the thermal fluids application RELAP-7 and the fuels performance application BISON. A single fuel pin was modeled based on the dimensions of a fuel rod from a Westinghouse 17x17 optimized fuel assembly. The simulation consisted of a depletion period of 1343 days, representing three full operating cycles, followed by a station blackout (SBO) event. The fuel rod was depleted with a total pin power of 65.81 kW. After 1343 days the fission power was reduced to zero (simulating a reactor shutdown). Decay heat calculations provided the time-varying energy source after this time. For this problem, Rattlesnake, BISON, and RELAP-7 are coupled under MAMMOTH in a tightly coupled approach. Each system solves its physics on a separate mesh and, for RELAP-7 and BISON, on only a subset of the full problem domain. Rattlesnake solves the neutronics over the whole domain, which includes the fuel, cladding, gaps, water, and top and bottom rod holders. Here BISON is applied to the fuel and cladding with a 2-D axisymmetric domain, and RELAP-7 is applied to the flow of the circular outer water channel with a set of 1-D flow equations. For this work, the mesh on the Rattlesnake side is either be 3-D (for low order P_N transport or diffusion) or 2-D axisymmetric (for diffusion). BISON has a matching ring structure mesh for the fuel so both the power density and local burnup are transferred accurately from Rattlesnake. At each depletion time step, Rattlesnake calculates a power density, fission density rate, burnup distribution and fast flux based on the current water density and fuel temperature. These are then mapped to the BISON mesh to perform a fuels performance solution. BISON calculates the fuel temperature and cladding surface temperature based upon the current power density and bulk fluid temperature. RELAP-7 then calculates the fluid temperature, water density fraction and water phase velocity based upon the cladding surface temperature. The fuel temperature and the fluid density are then passed back to Rattlesnake for another neutronics calculation.

For this paper, sets of results from the detailed calculation are provided for both depletion and the SBO event. We demonstrate that a detailed simulation akin to first principles can be achieved using MAMMOTH and the various MOOSE application on differing domains.

Keywords: Multiphysics, Neutronics, Fuel Performance, Thermal-Hydraulics.

INTRODUCTION

Computational analysis and modeling are applied to nuclear fuels to better predict and understand fuel and cladding behavior and interactions during different conditions in a nuclear reactor. The modeling of nuclear fuels in a radiation environment with thermal-hydraulic feedback is a computational challenge and involves complex physics that depend on many interlinked physical phenomena [1,2].

Traditionally fuels performance codes have applied either internal surrogate or simplified models for the different physics that allow a single fuel rod to be modeled. An example of such a surrogate is the internal model for determining the fuel rod power density. These models are traditionally either derived from experimental data or external (uncoupled) neutronics calculation [3-5] and are often limited to a single fuel type and lack thermal feedback for neutron cross sections.

To overcome these challenges a number of code systems have either coupled together different code or application packages or incorporated simplified fuel performance models. Examples include combining codes for fuel performance and thermal fluids, fuel performance and neutronics [6-8], and fuel performance, thermal fluids and neutronics [9-11]. There are additional challenges for coupling two or more codes [12]. Often, there is the need for communication of information across dissimilar spatial grids [13,14], the resolution of the time scheme [15,16] and resolution of the nonlinear coupling to some tolerance value. To resolve these issues for explicit coupling, the original codes are sometimes modified, which can introduce unanticipated errors. There is also the ongoing challenge of maintaining the combined code packages while additional physics are added to one or more of the various coupled codes.

The fuels performance application BISON overcomes many of these challenges. BISON is built upon the Multi-physics Object Oriented Simulation Environment (MOOSE) and an expanded multi-physics interface allows different applications to combine and run with BISON [17-19] without code modification. Since BISON is built on the MOOSE framework, extension of current or new capabilities in the framework allows BISON to seamlessly incorporate these features.

In addition since MAMMOTH is built with BISON, additional models added to BISON are incorporated into MAMMOTH. To demonstrate an approach closer to first principles, the master application MAMMOTH couples the neutronics application Rattlesnake, the thermal hydraulics application RELAP-7, and the fuels performance application BISON.

A single fuel pin was modeled based on the dimensions of a fuel rod from a Westinghouse 17x17 optimized fuel assembly. The simulation consisted of a depletion period of 1343 days, representing three full operating cycles, followed by a station blackout (SBO) event. The fuel rod was depleted with a total pin power of 65.81 kW. After 1343 days the fission power was reduced to zero (simulating a reactor shut-down). Decay heat calculations provided the time-varying energy source after this time.

The paper is organized as follows. Brief descriptions of each application are given. Next, a detailed description of the problem and mesh transfer mechanism is discussed. Results are then examined followed by brief concluding remarks.

APPLICATION DESCRIPTIONS

A number of applications built on the MOOSE framework have been developed at Idaho National Laboratory (INL) to solve challenging multi-physics problems. The three relevant applications in the work described here are the neutronics application Rattlesnake, the fuels performance application BISON, and the system analysis application RELAP-7. These three applications use finite element methods (FEM) and are compiled and linked into the core simulation application called MAMMOTH. A description of each MOOSE application is given in the subsections below.

Rattlesnake

Rattlesnake is the radiation transport application built with MOOSE for modern multi-physics simulations [20]. Rattlesnake solves steady-state (forward and adjoint), transient and k-eigenvalue problems for the linear Boltzmann equation discretized with the multigroup approximation for the energy independent variable. There are a number of different transport schemes available in Rattlesnake. One can choose between self-adjoint angular flux (SAAF) formulation, the least squares formulation (LS), the first order (FiS_N) transport formulation and diffusion. For transport Rattlesnake has the angular discretization schemes spherical harmonics expansion (P_N), and discrete ordinates (S_N). There are continuous and discontinuous finite element methods for solving the S_N, P_N, and diffusion angular representation. The SAAF has weaknesses for void or near void regions but this can be resolved using a special void treatment. SAAF has global particle conservation making it a good choice for k-eigenvalue calculations. The LS method does not have global particle conservation but can be used for k-eigenvalue calculations with the S_N scheme and nonlinear diffusion acceleration (NDA).

BISON

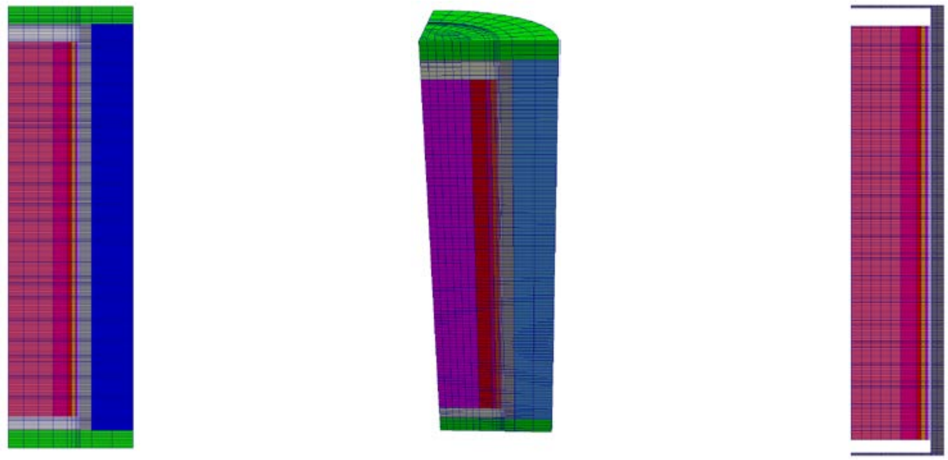
BISON is a nuclear fuel performance application built on the MOOSE framework and is suitable to a variety of fuel forms including light water reactor fuel rods, TRISO particle fuels, and metallic rod and plate fuel types [21]. It solves the fully coupled equations of thermo-mechanics and species diffusion, for either 1-D spherical, 2-D axisymmetric or 3-D geometries. Fuel models are included to describe temperature and burnup dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. Plasticity, irradiation growth, and thermal and irradiation creep models are implemented for clad materials. Models are also available to simulate gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, gas temperature, and fission gas addition. Because BISON is based on the MOOSE framework it can efficiently solve problems using standard workstations or very large high-performance computers.

RELAP-7

The RELAP-7 application is being developed as the next generation nuclear reactor system safety analysis tool, based on the industry standard RELAP5 code [22]. RELAP-7 utilizes well-posed governing equations for compressible two-phase flow, which can be strictly verified in a modern verification and validation effort. Both the homogeneous equilibrium two-phase flow model and the seven-equation two-phase flow model have been implemented into RELAP-7. A number of physical components with two-phase flow capability have been developed to support the simplified boiling water reactor (BWR) station blackout (SBO) analyses. The ability to use realistic fluid properties based on the IAPWS-95 formulation for water/steam [23], using a numerically efficient Spline-Based Table Look-up (libSBTL) approach, have been incorporated into RELAP-7. Also integrated into this approach was an extension to include the metastable states of boiling liquids needed by the 7-equation non-equilibrium two-phase model used by RELAP-7. An improved entropy viscosity method was implemented for solution stabilization. New and improved boundary conditions for both single-phase and non-equilibrium, 7-equation, two-phase flows, consistent with the method of characteristics, are included. Constitutive equations were added which depend upon the phase's topological sizes and arrangements, e.g. interfacial area concentration and its effects, wall friction and heat transfer, interface v friction and heat transfer, etc. Currently, the topology-dependent closures are limited to pre-CHF, vertical flows, but extensions to CHF and to horizontal flows are ongoing.

PROBLEM DESCRIPTION

A single fuel rod has been modeled in detail with the parameters listed in Table 1. This fuel pin design is based on the Takahama-3 pin [24][25] with the exception that the fuel stack height is taller and the presence of both lower and upper plena, which are a fuel characteristic of newer fuel rod designs [26]. Power conditions for the Takahama-3 SF97-3 fuel sample were selected because they represent the average behavior in the core.



(a) The axisymmetric mesh used by the Rattlesnake diffusion solver

(b) The 3-D quarter fuel pin mesh used by the Rattlesnake P_N transport solver

(c) The axisymmetric mesh used by the BISON

FIGURE 1. The neutronics and fuel performance meshes used for the coupled calculation (scaled).

In this work Rattlesnake uses either a 2-D axisymmetric pin cell pitch model for diffusion or a 3-D round channel quarter pin cell pitch model for low order P_N transport. Figure 1 (a) and (b) show the scaled down mesh applied to diffusion and P_N transport respectively. In the figure the fuel is colored purple, red and orange, the clad is colored grey, and the pure water is colored blue. The homogenized water-water nozzle is colored green. In both models the fuel pin has a top and bottom plenum gas gap and cladding caps. The assembly nozzles are located above and below the cladding fuel rod caps are the assembly nozzles. Leakage neutronic boundary conditions (void) are set on the top and bottom nozzles, and reflective boundary conditions are set on the outer radial boundaries. The fuel is divided into six radial spectral regions for accurate mapping of the radial power density distribution. BISON employs a 2-D axisymmetric fuel pin mesh that consists of the fuel and clad, and is shown scaled down in Figure 1 (c). The fuel rod is colored red, pink, purple and orange and the outer clad is colored grey. The outer temperature boundary condition for the clad in BISON is imposed by RELAP-7. RELAP-7 does a 1-D axial calculation for flow conditions. The top and bottom water reflectors include additional (artificial) neutron poison material in order to prevent a sharp increase in the power density in these locations, which lead to power oscillations during the depletion calculations. These oscillations are attributed to the physical constraint imposed on the fuel burnup distribution, which limits the redistribution of the power in an infinite domain composed of the same fuel pin with the same burnup distribution.

TABLE 1. Parameters for the fuel rod geometry

PARAMETER	VALUE
Fuel Stack Height	426.720 cm
Cladding Top and Bottom Cap Thickness	2.3191 cm
Top Plenum Height	18.5530 cm
Bottom Plenum Height	13.9148 cm
Top and Bottom Assembly Nozzle	20.0000 cm
Fuel Pellet Radius	0.4025 cm
Radial Gap Thickness	0.0085 cm
Radial Cladding Thickness	0.0640 cm
Fuel Pin Pitch	1.4206 cm
UO_2 wt%	4.11 wt%
UO_2 Fuel Pellet Density	10.42 g/cc
Initial Fuel Temperature	552.6 K
Inlet Water Velocity	484.6 cm/sec
Coolant Channel Pressure	15.51 MPa

MAMMOTH does not include a cross section development capability at this point, and thus cross sections must be computed with a lattice physics code. Weighted multigroup neutron cross sections for the problem were prepared with DRAGON5 [27] and tabulated as a function of burnup, fuel temperature, moderator density, and soluble boron concentration for each of the six radial regions in the fuel, the clad, and the radial water region. Axial reflector cross sections were obtained from an axial 1-D homogenized calculation with DRAGON5. The fine group energy structure from the lattice calculation was condensed to two, four, and eight coarse energy groups to leverage run time and accuracy during the various calculations. The fine group energy structure consisted of the SHEM 361 based on ENDF/B-VII.r1 libraries [28].

MAMMOTH performs the macroscopic depletion calculation for 1343 consecutive effective full power days in ten day increments. MAMMOTH also computes the decay heat based on the ANS Decay Heat Standard [29] with the local burnup conditions and isotopic power fractions from a pre-tabulated file as a function of local burnup for each radial fuel ring, based on the DRAGON5 calculations. Rattlesnake ramps from 0 initial power to 65.81 kW full in 12 hours. After 437.5 days of running at 65.81 kW the power is linearly increased to 70.2 kW over 464 days. At 937 effective full power days the total power is maintained at 70.2 kW for 12 hours and then it is decreased linearly back down to 65.81 kW over 405.5 days. At 1343 effective full power days the simulation of a station black begins. In a postulated SBO event, the reactor station undergoes a complete loss of power. This results in an immediate reactor scram, and pumps coast down to zero flow. After this point cooling is via natural convection.

For fuel rod deformation only the thermal expansion and fission gas release models were used in the BISON calculation. At the start of the blackout the neutron transport calculation is turned off and the scalar flux is set to zero. MAMMOTH then maps only the decay heat power corresponding to the burnup at the time of the station blackout to the fuels performance mesh. Starting at the station blackout, RELAP-7 decreases the water velocity and density linearly for 60 seconds to 0.04846 m/s. This simulates the spin down of the pumps and the restriction of water that occurs.

MESH TRANSFER

Rattlesnake, BISON and RELAP-7 are coupled under (and co-exist within) the master application MAMMOTH. Each application is compiled as an individual library and linked into MAMMOTH, and each application reads its individual input file, mesh, and other external files, as needed [18]. For this simulation MAMMOTH uses Rattlesnake as the top application and begins by initializing all three applications. BISON is a sub-application called by Rattlesnake, and RELAP-7 is a sub-application called by BISON. Each sub-application is allowed to take smaller time steps within the bounds of the time step taken by the calling application. For this work we refer to this process as sub-cycling in time. To step through time before the station blackout, Rattlesnake performs a series of macroscopic depletion calculations. Six one-second macroscopic depletion calculations are performed at each depletion time step to help resolve the nonlinearities of the multi-physics system. No error control for the nonlinearities is performed during the six one-second depletion steps; improved linkage for depletion iterations is planned in the near future.

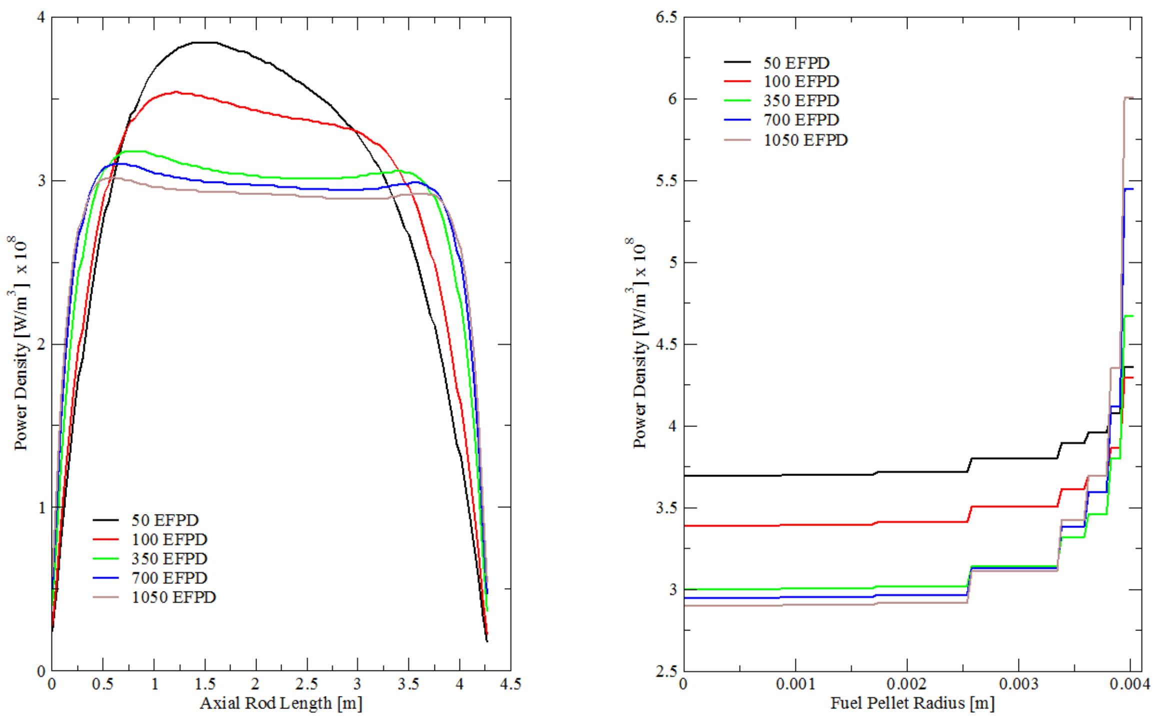
The fuel and cladding portion of the 2-D axisymmetric mesh domain used by the Rattlesnake calculation is overlapped with the fuel and cladding mesh domain used by BISON. For the Rattlesnake 3-D transport calculation the fuel and cladding portion of the mesh domain on a reflective boundary is overlapped with fuel and cladding mesh domain used by BISON. Domain deformation is allowed to happen on the BISON mesh, but the Rattlesnake mesh is kept un-deformed. Data is mapped between the un-deformed Rattlesnake mesh and the equivalent un-deformed fuel performance mesh.

In addition, Rattlesnake calculates the local power density, fission rate density, integral fast neutron flux (above 1 MeV), and the local burnup, and then maps these quantities to the BISON sub-application in the fuel domain of the mesh [18]. The local power density is applied to the heat equation solved in BISON, and the fission rate density, integral neutron flux and local burnup are applied to physics material models in BISON. The fuel domain in the BISON mesh has the same radial spectral regions and preserves these quantities in the mapping transfer. BISON calculates the clad surface temperature and maps that temperature directly onto the 1-D nodes of the RELAP-7 mesh. RELAP-7 calculates the cladding heat transfer coefficients of liquid and vapor and the coolant density of liquid, and these are mapped onto the cladding surface of the BISON mesh. Axial layered radial averages are calculated for the fuel temperature and water density, and mapped onto the Rattlesnake mesh. The fuel temperature is restricted to the fuel portion of the Rattlesnake domain, but the water density is mapped to the entire Rattlesnake domain for tabular cross section interpolation.

During the station blackout simulation Rattlesnake continues marching through time but the neutronics calculation is stopped. The scalar fluxes are set to zero at the beginning of the station blackout, and the power density is set to the calculated decay power derived from the ANS standard. The sub-application BISON is called from Rattlesnake, and the sub-application of RELAP-7 is called from BISON.

RESULTS

A set of results is presented from each of the different MOOSE applications. Rattlesnake generates the fuel pin power densities at different burnup times. BISON generates fuel centerline and outer coolant side cladding temperatures, and the volume fractions at different axial locations are generated by RELAP-7. The pin cell domain is constrained such that power density generated by Rattlesnake is similar for the different angular approximations. Here a set of diffusion results is shown but similar results have been generated with spherical harmonics (P_N). The similarity of the results gives confidence in the lower order diffusion solution.

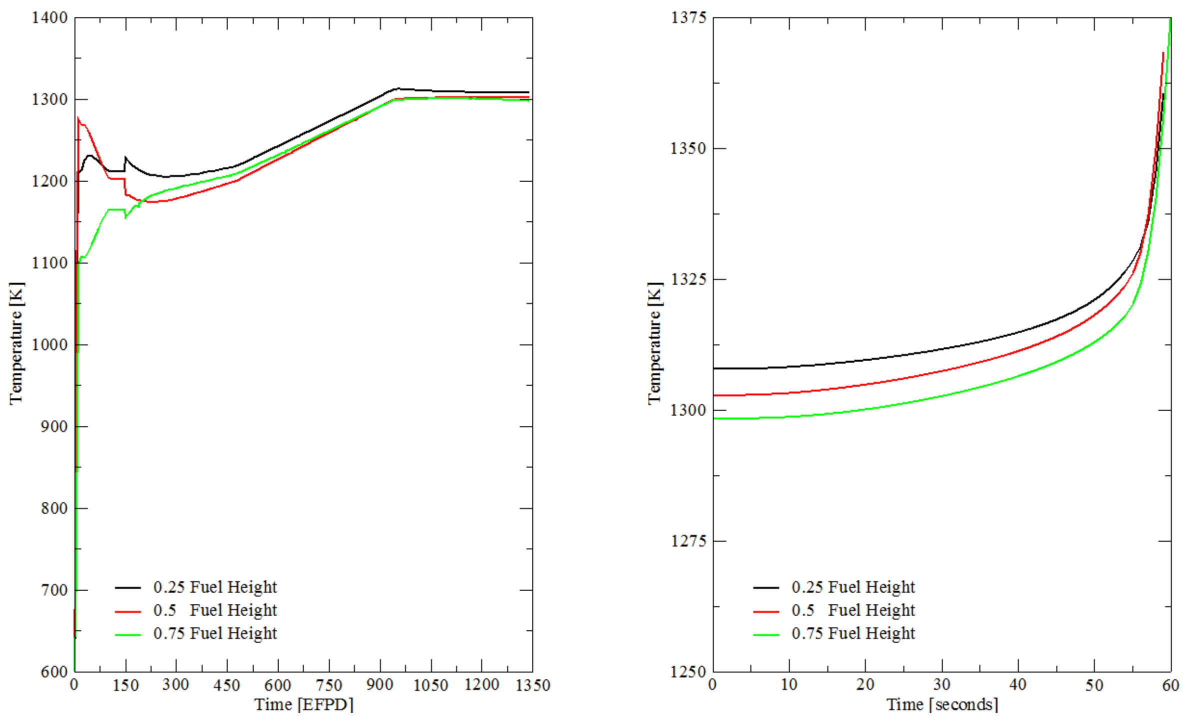


(a) Axial Power Distribution (b) Radial Power Distribution

FIGURE 2: Axial and radial power density profiles plotted vs. fuel height and radius respectively. The depletion units are given in effective full power days (EFPD).

Figure 2 shows the axial and radial power profiles along the respective centerlines. The axial power density starts with a bottom-shifted cosine shape, which is due to the moderator density and temperature difference between the bottom and top of the active fuel region. As the fuel is consumed at the axially central regions, the central power density is reduced and becomes more pronounced towards the axial edges of the active core. The radial power density in Figure 2 (b) shows the effect from the production of plutonium and subsequent fission from ^{238}U resonance capture. As the fuel is depleted the plutonium content increases and creates a higher power density at the radial periphery of the fuel rod. To maintain the assigned power level the inner fuel power density decreases. The radial power density is computed from radial reaction rates and is flat across each radial fuel region, because it is stored using shape functions that are constant in each element.

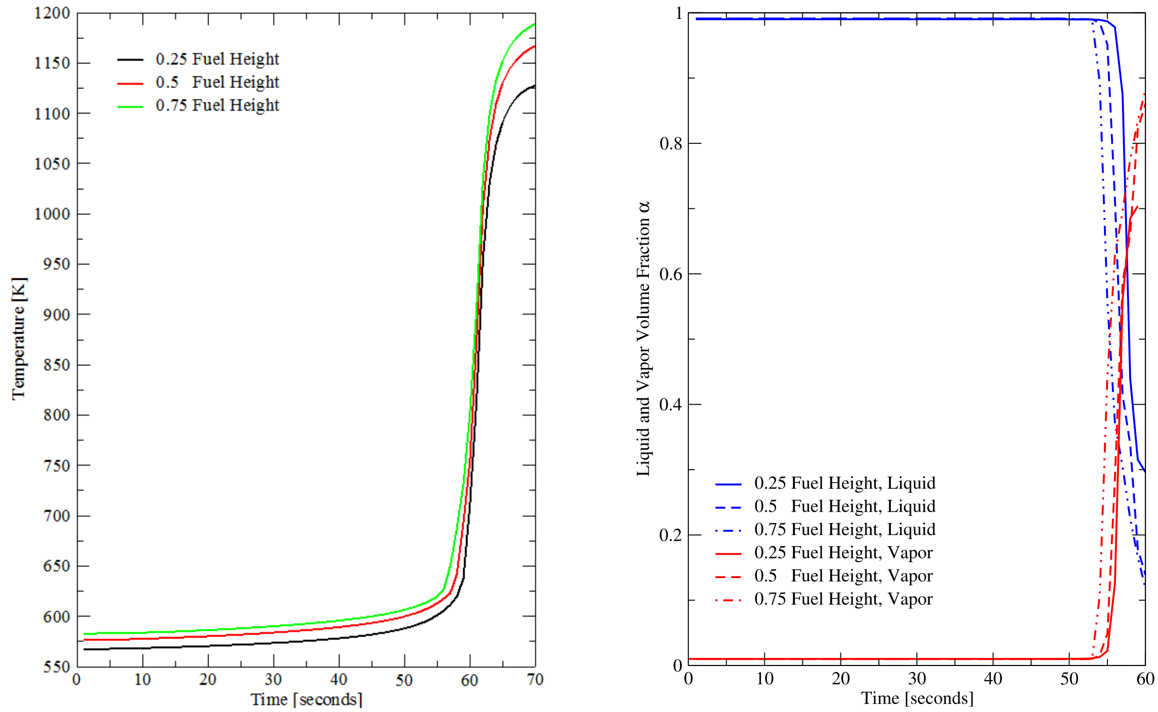
Centerline fuel temperatures are shown in Figure 3, where the three axial locations are given as a decimal percentage of fuel height. The results shown in Figure 3 (a) are observed immediately before the station blackout and show a linear increase in the centerline temperature as the pin power is ramped up during the depletion history. Subsequently, we observe a decrease of the temperature at the bottom axial and center and increase in the top axial quarter as the temperature changes from the bottom-shifted cosine shape to a flatter distribution as shown in Figure 2 (a). The temperature remains constant for the 50 EFPD time step between depletion steps starting at 100 EFPD. Thereafter, an update of the power distribution from Rattlesnake causes a slight jump in the temperature at the bottom quarter and the middle and top quarter to fall. After the correction, the radial rim effect generates more power at the fuel pin edge than in the center causing the slight decrease in fuel centerline temperature. The additional power ramp and degradation of fuel thermal conductivity, as computed by BISON) then cause an increase in the fuel centerline temperature and the fuel pin top centerline quarter temperature increases beyond the middle centerline as the fuel burns at the center and the power distribution spreads towards the fuel ends. The fuel temperature reaches a maximum and begins declining slightly as the total power is decreased.



(a) Fuel center line temperature before station blackout (b) Fuel center line temperature after station blackout

FIGURE 3: Fuel centerline temperatures at different axial locations before and after station blackout.

In addition, the centerline temperatures for fuel and cladding after the station blackout are shown in Figures 3 (b) and 4 (a) respectively. The fuel centerline temperature increases rapidly as the water flow from the system reduced during pump coastdown during the blackout, following by boiling due to lack of cooling, as illustrated by the decrease in water volume fraction in Figure 4 (b) between 50 and 60 seconds after the initiating event.



(a) Outer wall clad temperature after station blackout

(b) Liquid and vapor volume fraction after station blackout

FIGURE 4: Cladding temperature and volume fractions at different axial locations.

The outer wall clad temperature at different fuel heights are shown in Figure 4 (a) for the first sixty seconds after the start of the station blackout. After sixty seconds the cladding temperature increases significantly due to the vaporization of the coolant with the top of the fuel rod showing the greatest temperature jump. The volume fractions at different fuel heights are shown in Figure 4 (b). The fluid and vapor velocity are linearly decreased during the station blackout, and at about fifty five seconds the vapor fraction increases and the fluid fraction decreases. During the vapor and fluid transition the bottom portion of the fuel rod retains greatest amount of liquid and thus has better heat transfer properties and gives the smallest increase in the outer cladding temperature.

CONCLUSION

The MOOSE applications Rattlesnake, BISON and RELAP-7 were successfully coupled under MAMMOTH to perform a simulation more consistent with first principles of a single fuel pin under irradiation and station blackout conditions. Only basic features of the fuel performance model were applied in the simulation. The results from the simulation are consistent with previous work and with the expected physical phenomena that govern depletion and the voiding of a fuel channel. The presented coupling under MAMMOTH shows the suitability of the MOOSE framework for performing tightly-coupled, high-resolution simulations of complex multi-physics problems. Future work will include extending the simulation such that more detailed material models and physics are included in the fuels performance application. Additional work will include improving the neutronics model such as improving the rounded reflective boundary conditions by replacing with the actual square fuel pin pitch, and increasing the angular discretization representation. Additional future work will include leveraging the tight coupling system that is now in MOOSE and doing Picard iterations between the three applications.

ACKNOWLEDGMENTS

We would like to than Derek Gaston, John Peterson, Jason Miller, and Benjamin Spencer for their support and dedication on the MOOSE framework and on the BISON application. The submitted manuscript has been authored

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