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Application of Integrated Modeling and Simulation Capabilities for Full Scale Multiphysics Simulation of Microreactor Concepts

Piyush Sabharwall, Ching-Sheng Lin, Joshua Hansel, Vincent Laboure, David Andrs, William Hoffman, Stephen Novascone, Andrew Slaughter and Rich Martineau

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SUMMARY

Microreactors are small mobile transportable nuclear reactors with thermal power less than 20 MWt that are designed to meet the needs of remote areas, military installations, emergency operations, and disaster relief zones. These reactor are concepts that are intended to be factory-manufacturable, easily transportable, and will allow for semi- or full-autonomous operation. To assist with development of microreactors, modeling and experimentation need to be performed with verification and validation to gain confidence in the models and tools. The objective of this study is apply advanced modeling and simulation capabilities being developed by the DOE Office of Nuclear Energy Nuclear Energy Advanced Modeling and Simulation (NEAMS) program to perform integrated modeling and simulation capability for multiphysics simulation of the microreactor concepts. This activity will provide an opportunity to exercise the codes to provide both gain experience and to provide feedback to the developers.

An integrated microreactor capability is being developed by NEAMS using an advanced MOOSE-based multiphysics modeling and simulation capability for heat pipe-cooled microreactor concepts. This modeling capability is provided by an application called DireWolf, which is composed of the following MOOSE-based applications as submodules, coupled together using MOOSE MultiApps and Transfers and executed as a single application: MAMMOTH (reactor physics), BISON (nuclear fuel performance), GRIZZLY (structural mechanics), Sockeye (heat pipe technology), and RELAP-7 (open-air and super-critical CO_2 Brayton cycle).

Two different microreactor heat-pipe concepts were considered for the analysis to allow demonstration on a range of design features that are currently being considered by microreactor developers. Simulations performed model the steady-state operation and startup of the microreactor concepts with full integrated physics including neutronics, thermo-mechanics, heat transfer and structural behavior. Results from this study demonstrate the current capabilities for the integrated modeling and simulation capability for multiphysics simulation of microreactor concepts. Key observations include:

- The integrated capabilities have been successfully applied to perform steady-state simulations across a range of microreactor test cases.
- The detailed results from the simulations can be effectively visualized to communicate results and support analyst needs.

While these tools are still under active development, the current capability is promising. Additional needs and future work include:

- Continued development of Sockeye for simulation of heat simulations including development of closure relationships for common heat-pipe working fluids.
- Comparison of results with previously calculated values from the reactor design activities.
- Completion of the development of the ability to simulate microreactor power conversion systems and coupling with the integrated reactor models using RELAP-7.

- Development of a validation plan for the individual components and integrated simulation capabilities that can be used by NEAMS and the Microreactor Program to guide experimental work.
- Expanded assessment of capabilites that include increased physics fidelity to understand impact of modeling assumptions, determination of mesh and solution parameters. This includes comparisons of neutronics solutions with higher-fidelity Monte Carlo simulations.
- Expanded application of the capabilities for a range of normal operating conditions (startup, shutdown, and load following) and off-normal transient conditions.
- Application of the capability to an expanded range of designs including specifically gas-cooled microreactor.

ACKNOWLEDGEMENTS

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ACRONYMS

DOE	Department of Energy
DOF	Degree of freedom
INL	Idaho National Laboratory
JFNK	Jacobian-Free Newton Krylov
LANL	Los Alamos National Laboratory
MOOSE	Multiphysics Object Oriented Simulation Environment
NNSA	National Nuclear Security Administration
TRISO	Tristructural isotropic

Application of Integrated Modeling and Simulation Capabilities for Full Scale Multiphysics Simulation of Microreactor Concepts

1. INTRODUCTION

Microreactors are small mobile transportable nuclear reactors with thermal power less than 20 MWt and are designed to meet the needs of remote areas, military installations, emergency operations, and disaster relief zones. These reactor concepts are intended to be factory-manufacturable, and easily transportable, and will allow for semi- or full-autonomous operation. To assist with development of microreactors, modeling and experimentation needs to be performed with verification and validation to gain confidence in the models and tools. While several concepts are under development, none of them have been constructed. There is a desire to begin operation of a first-of-a-kind demonstration microreactor in the early 2020s [1].

This aggressive goal will require the use of high-technology readiness-level components and additional maturation of integration and control technologies and strategies to enable semi- or full-autonomous operation. The microreactor development can be divided in three branches: materials, thermal-hydraulics, and neutronics, which are intimately coupled. For materials, the primary development efforts necessary to deploy a microreactor include testing, qualification, code case development, and manufacturability of individual components. Thermal-hydraulics and neutronics analyses are coupled with each other due to fuel and coolant thermal response interactions [1]. To perform fully integrated system analysis modeling, various information from subsystems and testing is required to perform verification and validation of design and modeling assumptions. Thus, to perform a detailed system analysis for a microreactor, having information on all three categories is critical. Furthermore, some high-fidelity methods (e.g., Monte Carlo transport) challenge implementation within multiphysics simulation frameworks.

To provide information about potential benefits and challenges of microreactor concepts and support microreactor design and analysis, a preliminary evaluation of modeling and simulation tools for microreactor concepts has been performed [2]. The evaluation is focused on assessing the available codes and potential toolsets for heat-pipe-cooled microreactors modeling, identifying the assessment problem, and selecting toolsets that are designed and developed to succeed for the future demonstration of the self-regulation behaviors of heat-pipe-cooled microreactors. Three simulation spaces (thermal-mechanical, neutronics, and heat pipe), along with codes, have been evaluated, which include [2–8]:

- Thermo-mechanical codes: BISON and ANSYS/ABAQUS
- Neutronics codes: MCNP, SERPENT, OpenMC, MAMMOTH, and PROTEUS
- Heat pipe codes: Sockeye, HTPIPE, and HPAPPX.

The recommended toolset for the future modeling of the identified assessment problem is the MOOSE-based tool-suite being developed by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, which shows great promise in simulating the feedback mechanism between thermal-hydraulics, neutronics, and material behavior. The specific tools being used for this study are described in Section 2. The objective of this study is to apply advanced modeling and simulation capabilities being developed by the DOE Office of Nuclear Energy Nuclear Energy Advanced Modeling and Simulation (NEAMS) program to perform integrated modeling and simulation capability for multiphysics simulation of the microreactor concepts. This activity will provide an opportunity to exercise the codes to provide both gain experience and to provide feedback to the developers.

2. MICROREACTOR MODELING AND SIMULATION CAPABILITIES

For the past few years, the NEAMS program has invested in development of advanced modeling and simulation capabilities to support the design and analysis of advanced reactor concepts including microreactors. Many of these tools are based on the Multiphysics Object Oriented Simulation Environment (MOOSE) framework that provides for the solution of multiphysics systems that involve multiple physical models on widely varying space and time scales. An integrated microreactor capability is being developed by NEAMS using an advanced multiphysics modeling and simulation capability for heat pipe-cooled microreactor concepts. This modeling capability is provided by an application called **DireWolf**, which is composed of a number of MOOSE-based applications as submodules, coupled together using MOOSE MultiApps and Transfers, and executed as a single application.

The DireWolf software framework and physics modeling and simulation capabilities proposed for the heat pipe-cooled reactor modeling and simulation are described below.

Software and Multiphysics Coupling Framework: MOOSE provides the software infrastructure for developing the integrated modeling capability. Within MOOSE, the Jacobian-Free Newton Krylov (JFNK) method is implemented as a parallel nonlinear solver that naturally supports effective coupling between physics equation systems.

The MOOSE is a C++ finite element framework for building modular and flexible applications [3]. Each application is a set of building blocks, that build on tools within MOOSE as well as other applications to create a suite of capability. An application can focus on a single set of physics, a complex system of equations, or any combination. All applications leverage the Portable, Extensible Toolkit for Scientific Computation (PETSc) library for efficient and scalable nonlinear solvers, which allows all systems within a simulation to be solved in a fully coupled manner.

An application is itself a library of building blocks, which can be combined with other applications to create large cross-discipline simulations. Using building blocks within MOOSE, multiple teams, with minimal code, can tightly connect fully coupled systems together with varying spatial and time domains to create complete simulations of real physical systems. Additionally, a modular toolset exists to couple with legacy codes, thus allowing non-MOOSE-based applications to operate in a similar manner.

MOOSE provides a comprehensive set of finite element support capabilities (libMesh) and provides for mesh adaptation and parallel execution. The framework heavily leverages software libraries from DOE's Office of Science and National Nuclear Security Administration (NNSA), such as the nonlinear solver capabilities in the PETSc project from Argonne National Laboratory and Hypre from Lawrence Livermore National Laboratory for advanced multigrid preconditioning. In MOOSE, all "computer science," parallelization, spatial and temporal discretization, and dimensionality are hidden from the user while allowing the user to focus on the physics and multiphysics coupling. MOOSE provides a wide variety of capabilities to assist in development of MOOSE-based applications, such as thermo-mechanics, phase-field operators, multibody contact, multimesh fields, etc.

MOOSE contains a novel approach to code coupling, for both MOOSE-based applications and external codes. The approach uses the MultiApp system, which allows multiple MOOSE-based (or external) applications to run simultaneously in parallel. Multiple codes are compiled into one executable, can efficiently exchange data in memory, and effectively converge all coefficients in an implicit iterative manner (Picard iteration). External codes can be coupled using a "MOOSE wrapped" application.

Finally, MOOSE includes aids for testing, documentation, and visualization, and when combined, provide the basis for a development process that meets NQA-1 standards. More importantly, applications using the tools included within the framework can also follow the same process and minimize the resources required to meet a similar standard.

Fuel Performance: BISON is the very first application developed under the MOOSE framework and is a nuclear fuel performance code applicable to a variety of fuel forms including light-water reactor fuels, tristructural isotropic (TRISO) particle fuel, and metallic rod and plate fuels.

BISON is a finite element-based engineering scale fuel performance code [4]. It solves the fully coupled thermo-mechanics and species diffusion equations in 1-D, 1.5-D, 2-D axisymmetric or plane-strain, or full 3-D. Historically, BISON has been used for best-estimate calculations of light-water reactor, gas-cooled (TRISO) and advanced technology fuel where the emphasis is using all the relevant physics and material models without tuning to any one set of experiment measurements. BISON has also been extended to metallic and mixed-oxide fast reactor fuel. BISON is applicable to both steady and transient operations. Examples of LOCA and RIA capability in light-water reactor fuel are readily available in the open literature. Additionally, BISON can be coupled to lower length scale material models, is designed for efficient use on parallel computers, and its development follows NQA-1 process. An example of using BISON for the thermo-mechanics analysis of microreactor is presented in Subsection 3.1.

It solves the fully coupled equations of thermo-mechanics and species diffusion for either two-dimensional axisymmetric or three-dimensional 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. BISON has been coupled to the mesoscale fuel performance code MARMOT, demonstrating fully coupled multiscale fuel performance capability.

Neutronics: Rattlesnake [9] is a multilevel, multiscale radiation transport code capable of performing time dependent transport calculations with multiple transport schemes, including multigroup diffusion, spherical harmonics, and first- and second-order S_n (also known as discrete ordinates). The overall simulation design goal of Rattlesnake is to take advantage of the multiphysics simulation capability inherent in MOOSE to tightly couple radiation transport to multiscale nuclear fuel performance physics in INL's BISON and MARMOT multiscale fuels performance capability and RELAP-7's thermal fluids conjugate heat transfer capability. This uniquely coupled capability will allow resolution of nonlinear dependencies associated with burnup and temperature feedback, as well as strong reactor transients requiring highly nonlinear coupling.

Reactor Physics: MAMMOTH [5] provides a reactor physics application coupling neutronics (Rattlesnake), fuels behavior (BISON) and isotopic transmutation and decay. It extends beyond traditional reactor physics simulation capabilities by applying radiation-induced material evolution to nuclear reactor materials issues. Here the radiation material evolution is defined as the change of material microstructure and isotopic content exposed to nuclear radiation as a function of fission, isotope production and migration, and atomic displacement. MAMMOTH is designed to support different multiphysics analysis for different types of nuclear reactors and nuclear radiation driven systems.

MAMMOTH is a general reactor physics tool primarily designed for multiphysics applications MOOSE framework and developed at INL. It relies on the radiation transport solver Rattlesnake to determine the neutron flux distribution throughout the core and the corresponding power density. It can solve for steady-state, transient and eigenvalue problems using many different numerical discretization schemes. These range from diffusion schemes to transport schemes using discrete-ordinate (S_N) and spherical harmonics (P_N) for angular discretization. Both continuous and discontinuous finite elements are available.

Currently, MAMMOTH relies on the use Monte Carlo capabiltes to provide the nuclear cross sections needed for the neutron transport simulation. The typical workflow; therefore, it consists of first creating a Monte-Carlo model (usually Serpent [10]) to compute macroscopic cross sections. This is done by determining the key variables upon which the cross sections depend on (fuel temperature, boron concentration, control rod position, etc.) and generating libraries for different values of these variables.

For practical problems, two approaches can be alternatively selected: (1) a high-fidelity heterogeneous model solved using transport or (2) a coarser model with transport-corrected cross sections using MAMMOTH built-in homogenization equivalence capabilities, such as the Super Homogenization method, to preserve key reference quantities of interest [11]. The latter can be particularly efficient for multiphysics coupling where a fully heterogeneous for all physics may not be tractable. Another unique feature offered by MAMMOTH is the so-called multischeme capability, where various parts of the domain can be discretized with a different numerical scheme [12]. This allows to focus the computational resources towards the regions of the problem where precision is most desired.

A typical transient simulation in MAMMOTH requires two steps. First the multiplication factor of the reactor needs to be determined so that the initial condition can be self-sustained until the transient initiating event is started (e.g., control rod withdrawal). This is necessary in practice even though the actual reactor may be critical because the numerical discretization does affect the multiplication factor and the reactor would not start in a critical state. Once it is determined, the fission cross sections are scaled to make it exactly critical and the transient calculation can be started without introducing numerical bias. For multiphysics calculations, the same is true, which implies that a multiphysics initial condition must be established.

From a coupling point of view, MAMMOTH couples to other physics by providing the power density as a heat source to the heat transfer equation and possibly the local burnup and fast flux for fuel performance in BISON. The other physics are coupled back to MAMMOTH through the variables the cross sections depend on and through the thermal expansion induced displacement.

Materials Behavior: Grizzly [13] is being developed for simulating component aging and damage evolution events specific for nuclear power plant structures experience over its lifetime, including thermal and mechanical loading and degradation due to aging and irradiation effects. Like BISON, Grizzly heavily leverages the thermo-mechanics physics found in MOOSE modules as a starting point. Grizzly provides capabilities to both calculate the degraded properties of material and the loading applied to a component that has experienced degradation.

Thermal-Fluid Analysis and Power Generation: RELAP-7 (Reactor Excursion and Leak Analysis Program) [14] is the next generation nuclear reactor system safety analysis tool. The overall design goal of RELAP-7 is to take advantage of the previous thirty years of advancements in computer architecture, software design, numerical integration methods, and physical models. The four major RELAP-7 advancements are (1) A well-posed seven-equation two-phase flow model (liquid, gas, and interface pressures); (2) Improved numerical approximations resulting in first or second-order accuracy in both space and time; (3) Implicit tightly coupled time integration for long duration transients, such as providing plant behavior for full life fuel cycle evaluations; (4) the ability to tightly couple to higher fidelity physics through advanced multiphysics algorithms. This multiphysics coupling capability includes both MOOSE-based software applications, such as BISON/MARMOT multiscale nuclear fuels performance capability and the MAMMOTH/Rattlesnake reactor physics and radiation transport capability, and non-native applications such OpenMC, Serpent, and Nek5000. Future multiphysics additions to RELAP-7 will be coupling to the MOOSE-based Pronghorn for three-dimensional subchannel flow. A super critical CO_2 Brayton power generation loop implementation is planned for near future.

In the context of microreactor simulations, RELAP-7 will be used to model open and closed Brayton cycles power conversion systems that remove heat from the heat pipes and performs work via a turbine. To create a Brayton cycle loop, various components (pipes, valves, pumps, and turbines) are pieced together at the user level. RELAP-7 has both single-phase and two-phase flow capabilities, but for the application of microreactor modeling, single-phase flow is appropriate. Pipes in RELAP-7 are modeled with 1-D, compressible Euler equations, supplemented by several closure relations such as friction factors and heat transfer coefficients. Flow models are fluid-independent; users are free to plug in their own equations of state. Examples of relevant fluid properties already available include air and carbon dioxide.

Junctions, valves, pumps, and turbines are 0-D models that connect two or more pipes. Valves can be controlled with logic defined by the user, using MOOSE's "Controls" system. Pumps and turbines use performance data curves to determine shaft power input and extracted from the flow. For open-air Brayton cycle simulation, inlet and outlet components are available, which are 0-D components connected to one end of a pipe. Heat conduction through solids is achieved using 2-D "heat structure" components, which can be used for pipe walls or heat exchangers, for example. These can be coupled to the fluid in the pipes to perform heat exchange with the fluid.

RELAP-7 couples to other MOOSE-based applications via the following interfaces:

- Wall temperature: Temperature from other applications (typically MAMMOTH, BISON, and Sockeye) can be transferred onto a pipe, to be used to compute a convective heat flux.
- Thermal power: A power profile, such as one that MAMMOTH might generate, can be applied directly to the fluid in a pipe.

Heat Pipe Performance: Sockeye [6] is a MOOSE-based heat pipe application model developed based on Los Alamos National Laboratory's (LANL's) experience with the development of heat pipe technologies. Sockeye is a derivative of RELAP-7 using the pipe component of RELAP-7 to develop concentric annular cylinders to approximate heat pipe geometry.

Sockeye adapts the 1-D, two-phase, compressible flow model used in RELAP-7 to the two-phase flow of the working fluid in a heat pipe. A virtual wick separates the vapor core from the liquid annulus. Curvature of the menisci along the wick surface is estimated from the void fraction solution and used to determine the capillary pressure difference between the phases. This capillary pressure difference is then used in stiff relaxation terms to drive the system toward the equilibrium pressure condition.

Sockeye uses the same components system as RELAP-7 and provides some new components related to heat pipe modeling. The main component is the heat pipe flow channel itself, which can be broken into axial sections for convenience of boundary conditions and coupling.

Modeling startup of heat pipes is very complex and is a large project itself. Sockeye currently only offers a very simple, aggregate heat transfer model for melting. Currently, this requires a two-step approach, where the first phase performs heat transfer until the working fluid is saturated, and the second phase, the fluid phase, uses the first phase's output as initial conditions. This melting model is not expected to be accurate, other than an overall energy balance. To truly capture startup behavior, some degree of 3-phase modeling would be necessary.

Heat pipe operation is subject to several limits on the ability to remove heat. Some of the most prominent limits that have been identified are as follows:

- Sonic limit: speed of the flow in the vapor core reaches sonic conditions (often during startup), which means that pressure changes in the condenser do not propagate to the evaporator.
- Entrainment limit: liquid can be entrained in the core region due to shear forces, which can lead to dry out of the evaporator.
- Wicking limit: lack of capillary forces in the wick can prevent fluid circulation.
- Boiling limit: vapor bubbles can create hotspots and impair wick action.

The lumped capacitance model in Sockeye directly computes some of these operation limits analytically and uses them in the solution process. The two-phase flow model in Sockeye has not yet implemented any of these limits. The sonic limit should need no explicit model, since it should already be captured by the compressible flow formulation. However, since the sonic limit often comes into play during the startup phase, startup modeling needs to include this type of compressible flow model to capture the limit. The entrainment limit will require extending the model to allow liquid in the core and vapor in the annulus, as well as some terms to perform the shearing. The wicking limit should already be captured by the current model via the capillary pressure model. The boiling limit will require some boiling closures to be added, as well as possibly enhancing the capillary pressure model.

Sockeye's coupling interfaces are the same as those in RELAP-7: wall temperature can be applied via convective heat transfer, and power can be applied directly to the working fluid.

Thus, Sockeye is identical in structure to RELAP-7 and will provide cohesive coupling with RELAP-7. Sockeye has been prototyped and demonstrated and benchmarked against a LANL code employing simplified models. Sockeye has also been tightly coupled to the BISON nuclear fuels performance application.

3. APPLICATION AND ASSESSMENT OF INTEGRATED SIMULATION CAPABILITES

The modeling and simulation capabilities discussed in Section 2 have been applied to a series of microreactor configurations to perform an initial demonstration of integrated capabilities. These cases include microreactor segments used to understand the performance of single physics codes, such as mesh refinement for the structural mechanics capability, and simulations of single heat pipes. Full-scale simulations of two heat-pipe cooled microreactor concepts were performed to demonstrate ability to model different geometry configurations and steady state and transient startup conditions. These simulations are intended to initial exercising of the codes to establish the current state of functionality of the tools and suitability for microreactor design and analysis.

3.1 Single Microreactor Assembly (BISON)

In this case, BISON is used for thermo-mechanics calculations of a segment of a microreactor conceptual designs. One such design consists of a monolith structure, which encloses heat pipes, neutron reflectors, and fuel. A simple 2-D solid mechanics model was developed to better understand the required mesh density for microreactor core structure analysis. As shown in Figure 1, the model created for this study is a small cutout hexagonal section of a microreactor assembly that contains central hole where a single heat pipe resides. That hole is surrounded by core structural material and sections of control rods and fuel rods at each corner of the hexagon. For this study, the core structure, fuel, and control rods have similar mechanical properties, which serve the purpose for demonstrating mesh refinement for stress resolution. The bottom surface is fixed in both directions and the top surface is given a prescribed vertical displacement to induce stress in the materials. Stress values are obtained over a line spanning the thickness of the webbing in three locations, as shown in the figure below.

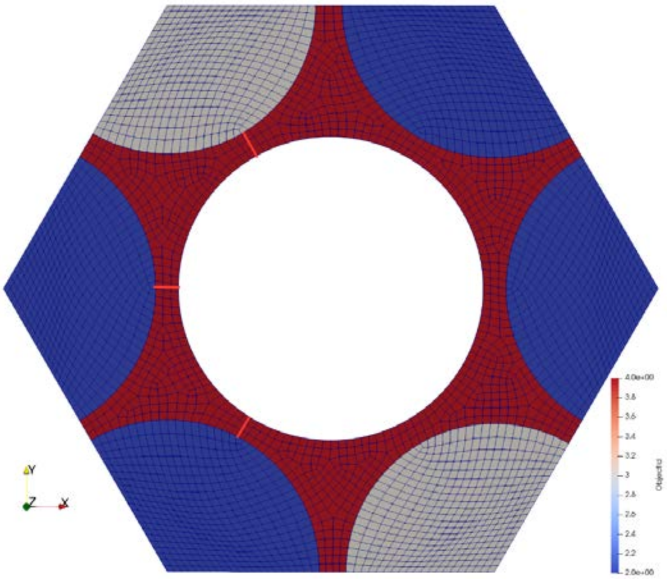

Figure 1. Illustration of a hexagonal section of microreactor assembly. Here, red indicates the core structural material, grey is fuel, and blue represents control rods. The red lines drawn through the core structure indicate where stress calculations are reported.

The model was created using six levels of mesh refinement (using linear elements), with Level 1 being the coarsest and Level 6 being the finest. Careful consideration was given to the mesh refinement in the webbing consisting of the metallic structure that exists between the fuel and heat pipe channels in the core structural block that separates the various reactor components, as these are the areas of particular interest under thermomechanical loads. Table 1 provides a summary of the various mesh refinement levels with the increasing number of elements and degrees of freedom

(DOF) representing refinement of the mesh. Figures 2 and 3 show the actual simulation mesh for refinement Levels 1 and 6, respectively.

Table 1. The number of elements and degree of freedom (DOF) in various meshes.

	Elements	DOFs	Simulation time (sec)
Level 1	81	218	0.24
Level 2	418	972	0.46
Level 3	3466	7326	2.54
Level 4	14074	28934	10.4
Level 5	39255	79818	37.97
Level 6	156811	316224	197.8

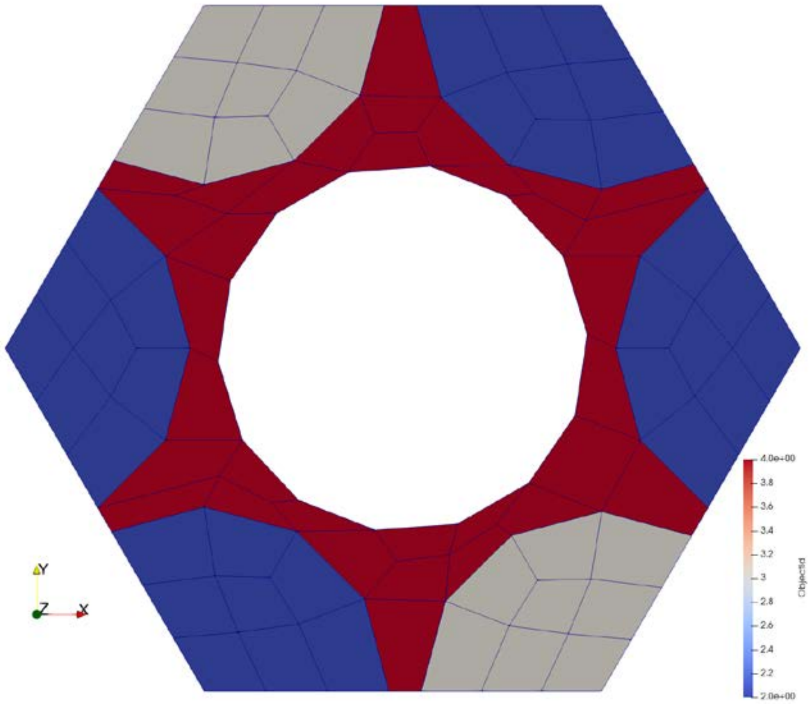

Figure 2. Illustration of mesh refinement Level 1.

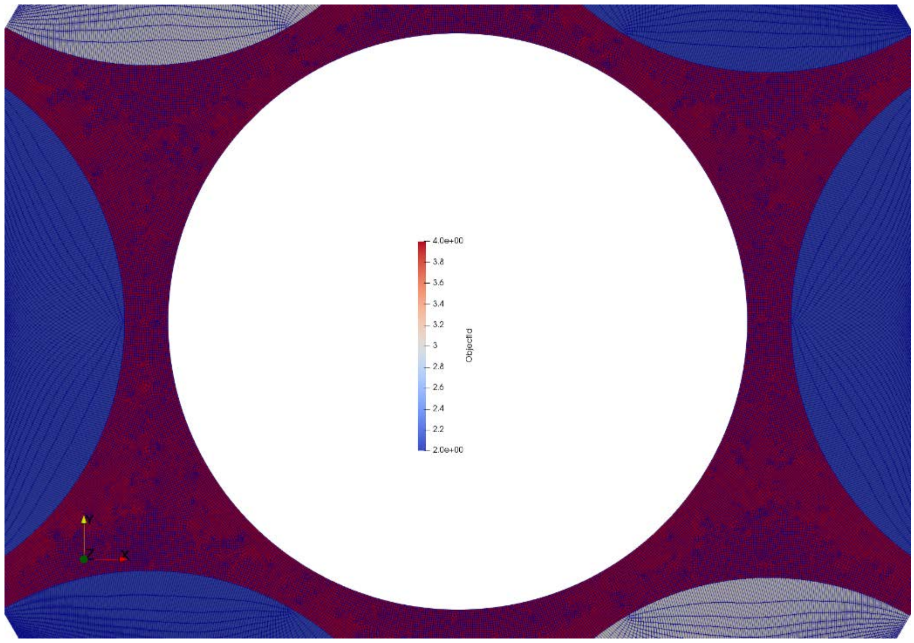

Figure 3. Illustration of mesh refinement Level 6.

The von Mises stress was obtained over the three lines shown in Figure 1 for each of the six mesh refinement models and are presented in Figures 4–6 for Line 1, Line 2, and Line 3 respectively. These lines are at the point of the minimum core structure thickness where the most limiting stresses are likely to occur. The x-axis on Figures 4–6 represents a normalized location value representing the relative distance along the line.

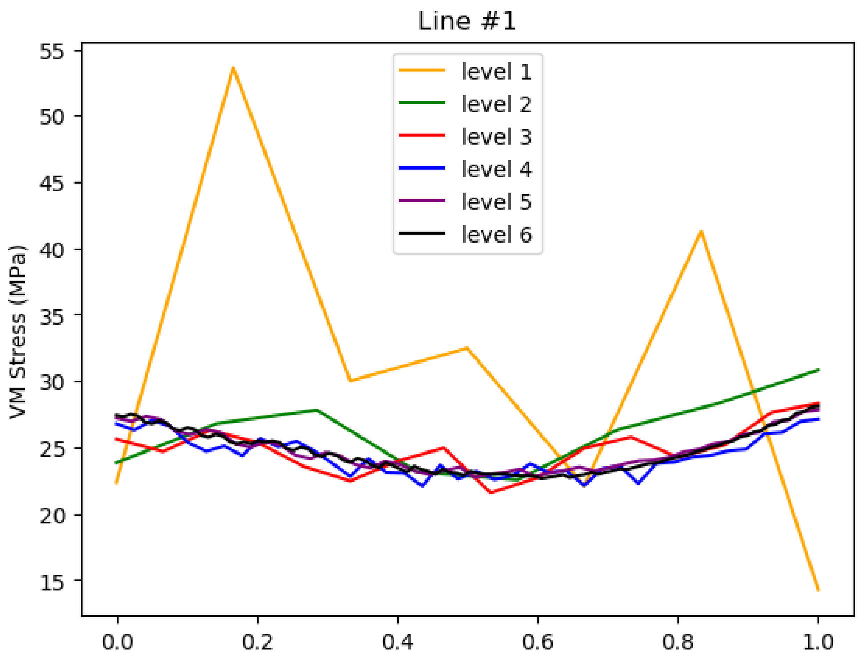

Figure 4. Von Mises stress of Line 1 for six levels of mesh refinement.

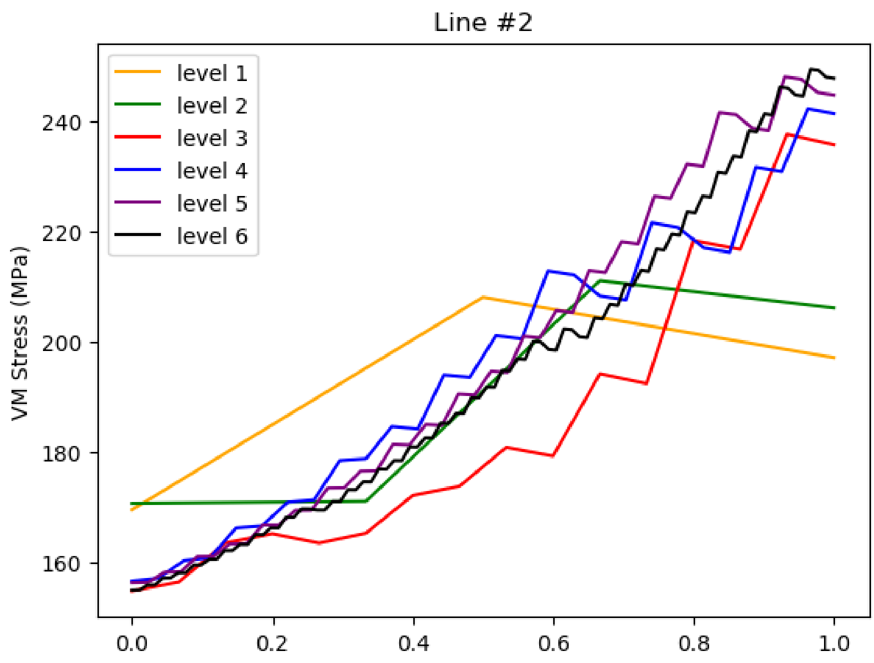

Figure 5. Von Mises stress of Line 2 for six levels of mesh refinement.

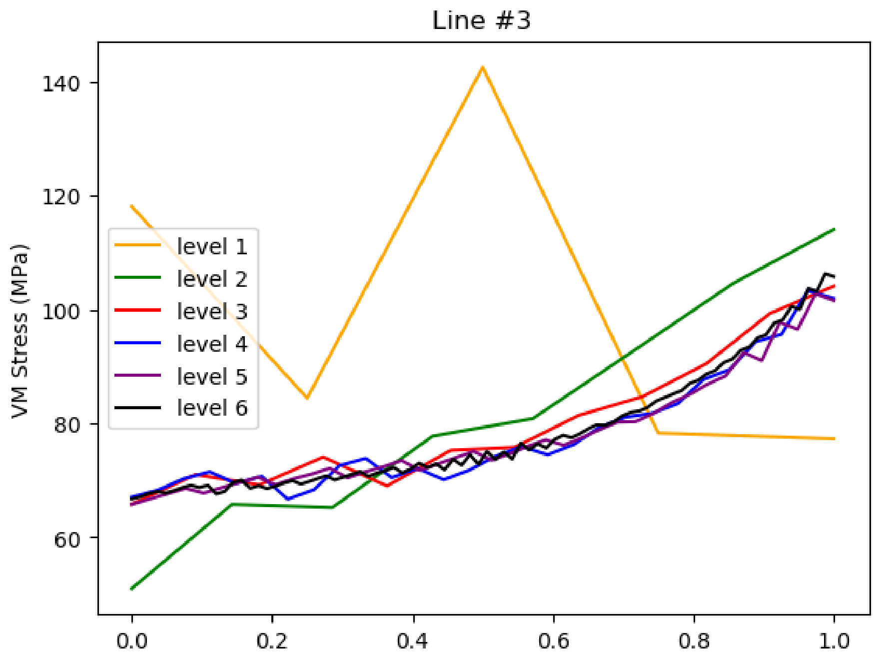

Figure 6. Von Mises stress of Line 3 for six levels of mesh refinement.

The information shown in the plots can and should be considered for future modeling efforts regarding monolithic microreactor structures to determine suitable mesh refinement. It appears that meshing Levels 4–6 have converged, meaning Level 4 mesh refinement is adequate. This model is simplified to the extent that it excludes thermal effects and non-linear material phenomena, the heat pipe is not included in the simulation and there is no contact modeling between the differing materials; it is meant to demonstrate the mesh resolution necessary to resolve stress in the thin section of the monolith and the corresponding computation cost. For instance, a model with 100 heat pipes and the same approximate element size shown in Level 5 would require roughly 4 million elements for 2-D. Then, multiply by the number of layers desired for 3-D. This study shows that a full-size or near full-size 3-D and even 2-D simulation quickly becomes very computationally expensive.

3.2 Single Heat Pipe (Sockeye)

To gain experience with Sockeye and understand its capabilities and performance, a test problem was developed and modeled with an established code HTPIPE [7] and Sockeye. A test problem was modeled using a 1.2-m annular-screen heat pipe with a heat source at 1000 K and heat sink at 300 K, with a 0.2-m adiabatic section separating the evaporator and condenser sections, each 0.5 m in length. The working fluid in the heat pipe was potassium. The problem was analyzed with both codes to steady conditions and then compared. For a more detailed information on the HTPIPE code, see Appendix A.

Figure 7 compares HTPIPE's temperature profile with Sockeye's liquid and vapor temperature profiles. Sockeye's temperatures are lower than HTPIPE's temperatures by 1–5 K in the evaporator region, up to roughly 15 K in the adiabatic section. Given that the wall heat transfer coefficients were taken to be the same in each code, these temperature differences are likely attributed to differences in the equations of state of the working fluid between the two codes and further study is under way to understand the differences.

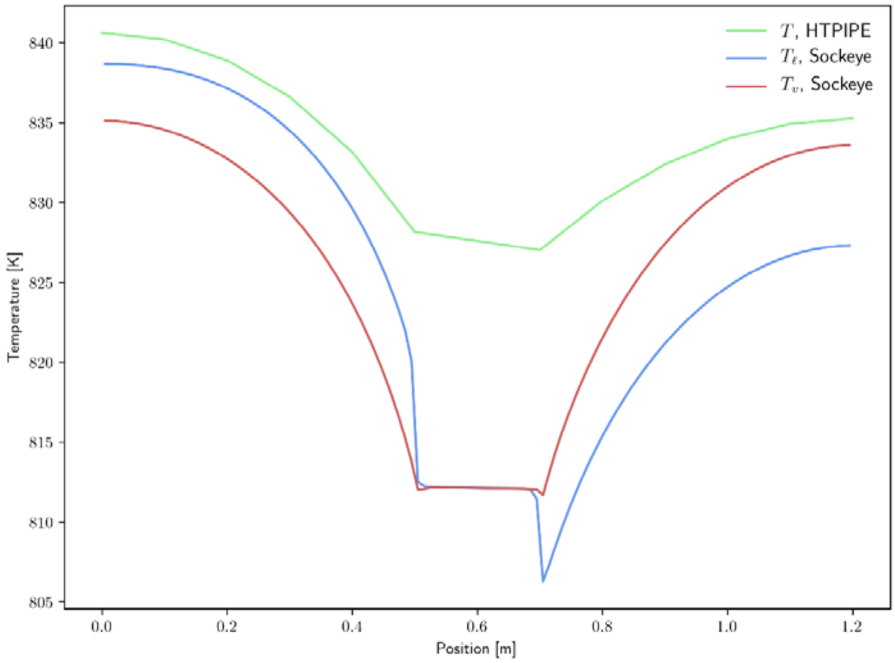

Figure 7. Comparison of temperature profile of HTPIPE and Sockeye.

The heat-pipe internal pressure differences between the two codes are shown in Figure 8. Some of the pressure changes follow the temperature differences that are thought to be due to variances in equations of state and filling level of the wick. Additionally, pressure changes arise due to differences in the capillary pressure model. Sockeye currently assumes that the wick is nearly perfectly saturated with working fluid and thus does not allow for "flooding" of the wick, such as what often happens in the condenser region. HTPIPE's pressure solutions illustrate that flooding occurs since the pressure difference between the phases is zero in this region. In Sockeye, since no flooding occurs, the interfaces between the phases are curved and yield capillary pressure differences between the phases.

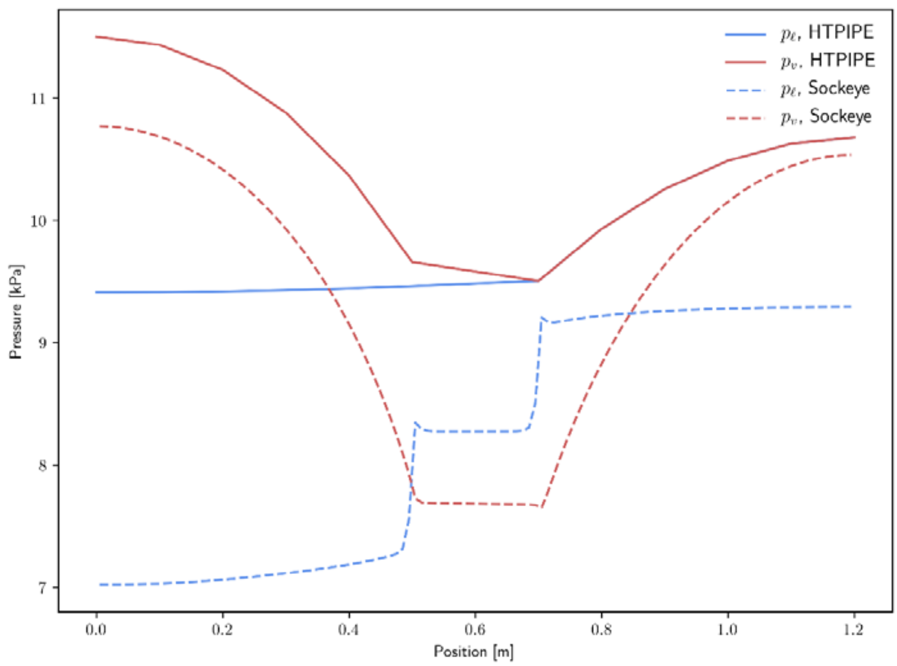

Figure 8. Comparison of pressure profile of HTPIPE and Sockeye.

Sockeye's models are still in their infancy and will continue to develop as validation efforts are made. Several closures still need to be implemented, such as friction factors for the tube and wick and interfacial and wall heat transfer coefficients. Additionally, refinements will be made to the capillary pressure model, which infers interface curvature from the void fraction and assigns a corresponding capillary pressure.

3.3 Empire Microreactor Core (MAMMOTH/BISON)

The MOOSE toolset was also selected by the MEITNER eVinci Resource Team to study the self-regulating behavior of the Los Alamos National Laboratory empire design. Figure 9 shows the layouts of the LANL empire unit assembly and core design [2]. The reactor core is a stainless-steel block that features cylindrical holes for fuel, moderator and heat pipes, which are arranged in a hexagonal pattern. A MAMMOTH/BISON model to simulate various safety transients at the pin and assembly level was developed in collaboration with LANL staff [15]: (1) sudden change in the heat pipe wall temperature, (2) sudden change in the heat flux removed by the heat pipe, and (3) heat pipe failures. Neutronics, heat transfer and thermal expansion effects were studied.

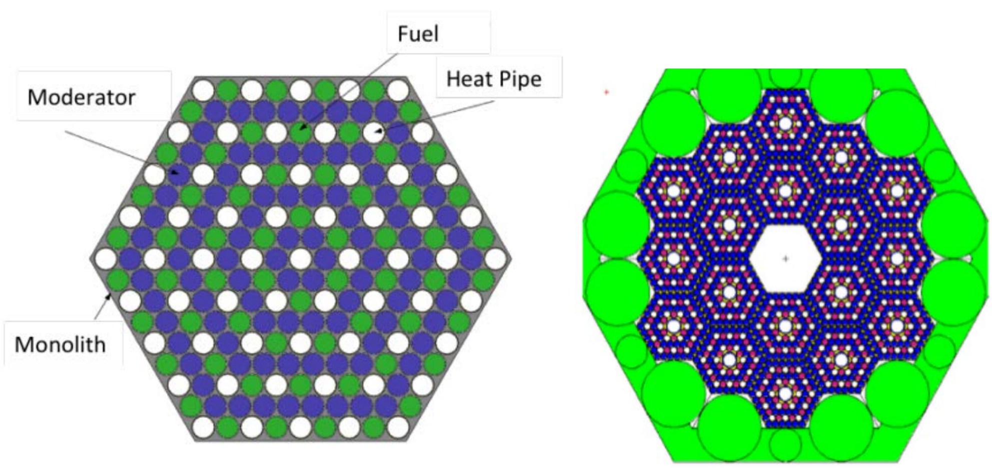

Figure 9. LANL empire unit assembly and core design [2].

Each transient followed the aforementioned pattern: a multiphysics steady-state solution was established to provide the initial condition and then the transient initiating event was started. Figure 10 illustrates some of the results from Matthews et al.'s 2019 report, which shows the temperature, power density, and stresses obtained over a 2-D assembly when the heat removed by the heat pipe is dropped to remove 90% of the nominal power at the initial time [15]. The fuel temperature rapidly increases, in turn decreasing the reactor power to a stable value.

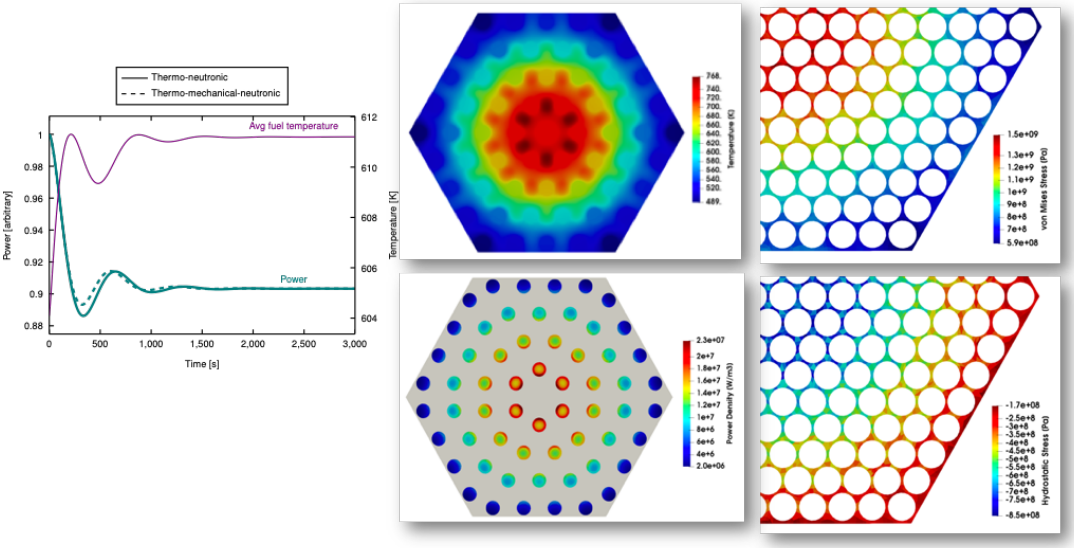

Figure 10. Visualization of the temperature, power density, and stress distribution over a transient simulation.

3.4 Design A Microreactor Core (MAMMOTH/BISON/Sockeye)

Design A is a 5-MWt microreactor concept developed at INL, which is an alternative proposed in lieu of the LANL's Megapower core concept [16]. Figure 11 shows the layouts of the core and the fuel element of Design A. The core consists of an array of hexagonally shaped fuel elements, where the centrally located cylindrical heat pipe is surrounded by hexagonal fuel, cladding, and duct. A total of 1,134 fuel elements were used in Design A, and each heat pipe needs to transport an average of 4.4 kWt of power for the core operating at 5 MWt.

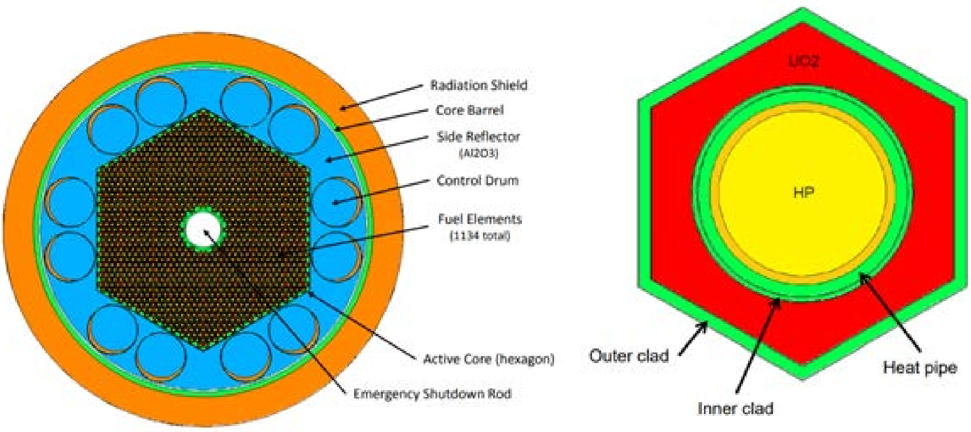

Figure 11. Radial core layout of Design A and its fuel element [16].

3.4.1 Single Pin Simulation

The first calculation performed on Design A was a steady-state calculation on a 3-D pin model with MAMMOTH, BISON, and Sockeye coupled. Figure 12 illustrates the coupling between these codes. With the given geometry and cross section data, the MAMMOTH code provides the fission source term and then used by the BISON code to determine heat generated in the fuel, heat transfer and the temperature distributions. The cladding temperature is then pass to the Sockeye code that captures the thermal behavior of the heat pipe and the calculated heat removal rate can be used by the BISON and MAMMOTH codes to determine the thermo-mechanical and neutronic responses to thermal transients.

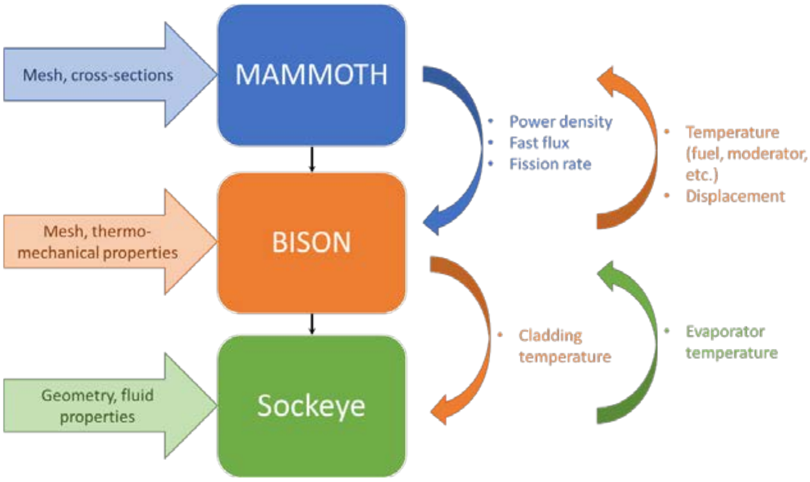

Figure 12. Coupling of MAMMOTH, BISON, and Sockeye.

For this single pin simulation, MAMMOTH used diffusion theory with 20 energy groups with the power normalized to the average pin power of 4.4 kWt. The BISON model used a finite strain model to simulate stress and thermal expansion. At the time, the Sockeye model was using its lumped capacitance model. For numerical stability, BISON and Sockeye were solved using a pseudo-transient to reach a time-independent solution. Picard iterations between MAMMOTH and BISON were used to enforce a multiphysics tightly coupled approach. Figure 13 shows the mesh used for the MAMMOTH calculation. Figure 14 shows the power density obtained on the MAMMOTH side (non-zero only in fuel regions). Figure 15 shows the mesh used for the BISON calculation with the steady-state temperature and von Mises stresses shown on Figure 16 and Figure 17, respectively.

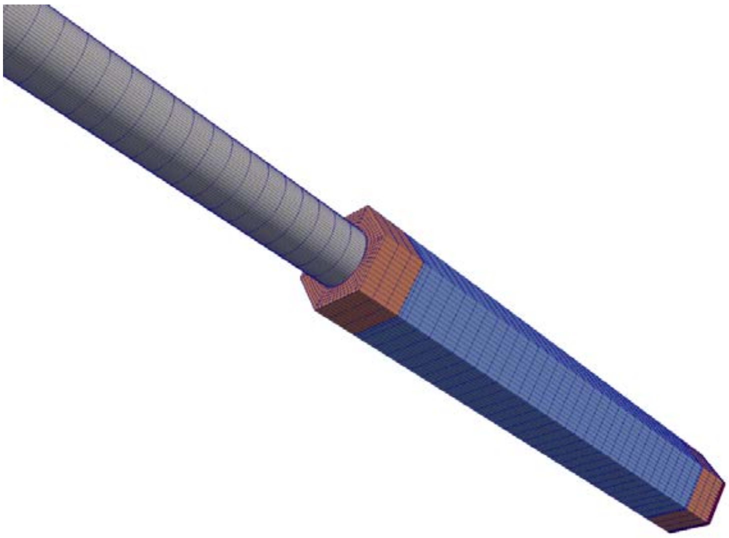

Figure 13. Mesh used in MAMMOTH calculation of a single heat pipe and fuel structure.

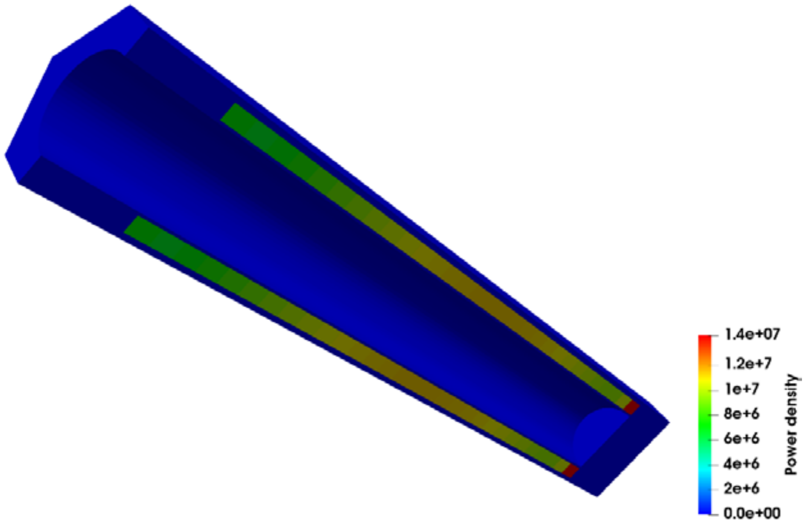

Figure 14. Power density [W/m^3] obtained from MAMMOTH calculation (heat pipe not shown).

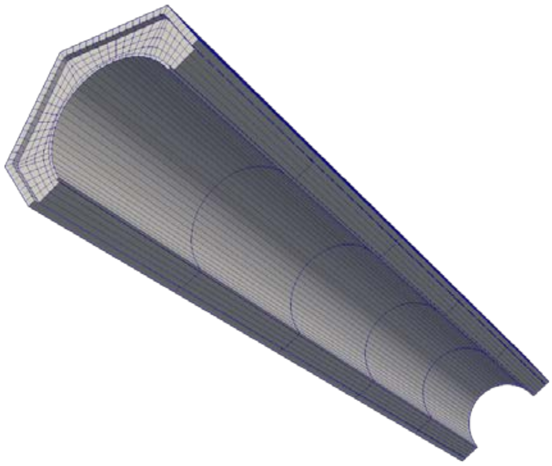

Figure 15. Mesh used in BISON calculation of the fuel structure.

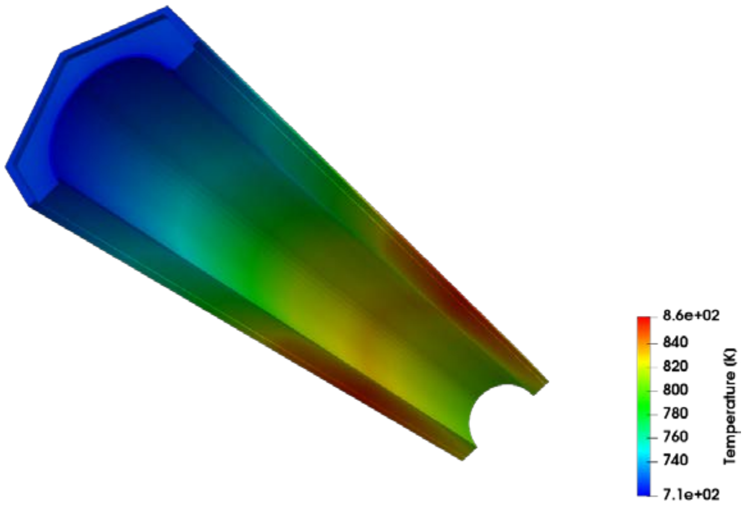

Figure 16. Fuel temperature distribution obtained from BISON calculation.

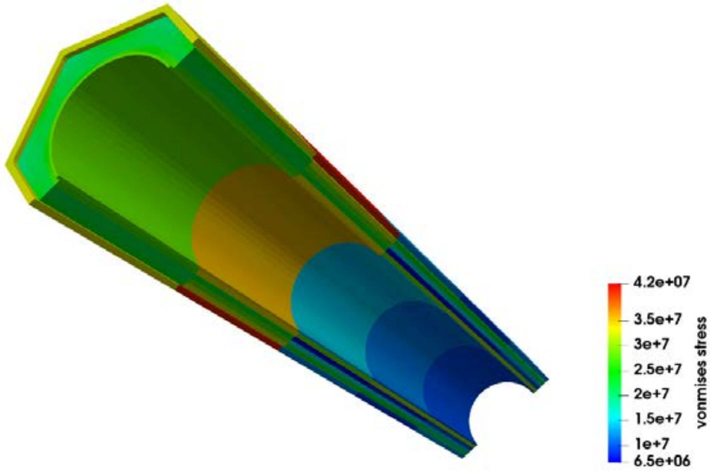

Figure 17. Fuel Von Mises stress [Pa] obtained from BISON calculation.

3.4.2 Full-core Simulation

A full-core calculation of Design A was also demonstrated using MAMMOTH, BISON, and Sockeye during start-up with the core going from 5% to 100% power (5 MWt) over the course of 7.25 hours, as shown in Figure 18. Due to the large size of the problem, the BISON input file was limited to a heat conduction within the core with heat convection with the boundary of the core and the wall of each of the 1134 heat pipes. Figure 19 shows the temperature and fast neutron flux at full power.

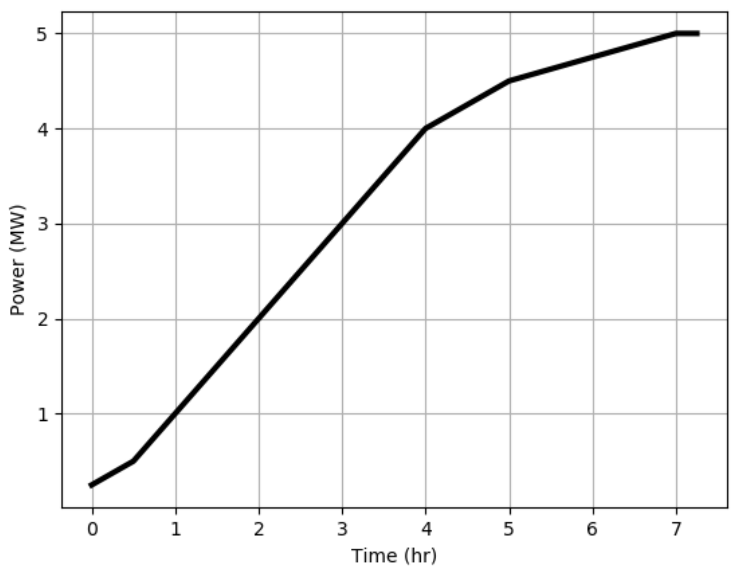

Figure 18. Power profile versus time for the start-up transient.

The simulation used one instance of MAMMOTH with 2,287,656 FEs, one instance of BISON with 1,506,168 FEs, and 1134 instances of Sockeye, with 732,042 FEs. For BISON, 256 MPIs were used, and for MAMMOTH, 1080 MPIs were used. The run time was approximately 3 hours.

While the calculation itself was reasonably fast, the many approximations in the model show that obtaining a full-core solution with all relevant physics modeled will require further work. In particular, unlike the pin and assembly calculations of the Empire model (see previous section), this simulation did not include any mechanics effects, which are likely to be a significant challenge on problems of that size, both for resolving the stress fields and properly accounting for the thermal expansion induced displacement. In addition, the neutronics calculation – though currently a small fraction of the computational effort – uses a fairly coarse diffusion approximation. This may not be extremely challenging as both transport and transport-corrected diffusion are readily available in MAMMOTH but it is clear that further neutronics studies would be required to fully understand the important parameters to consider for cross-section interpolation. This would obviously be design dependent.

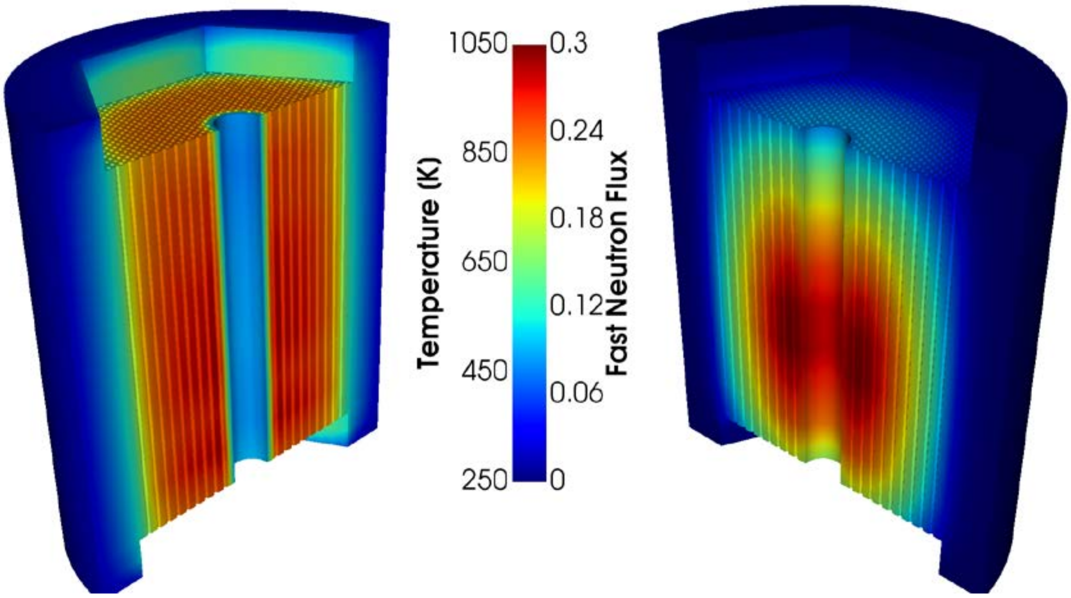

Figure 19. Full-core temperature and fast neutron flux distributions.

3.5 Open-Air Brayton Power Generation Loop (RELAP-7/Sockeye)

Simulation of the full microreactor system will require the addition of the capability to model the power conversion system. Development of an open-air Brayton cycle capability in RELAP-7 is scheduled for completion in FY 2019. The model, shown in Figure 20, consists of inlet and outlet boundary conditions, a pump and turbine operating on a common shaft, and a heat exchanger section.

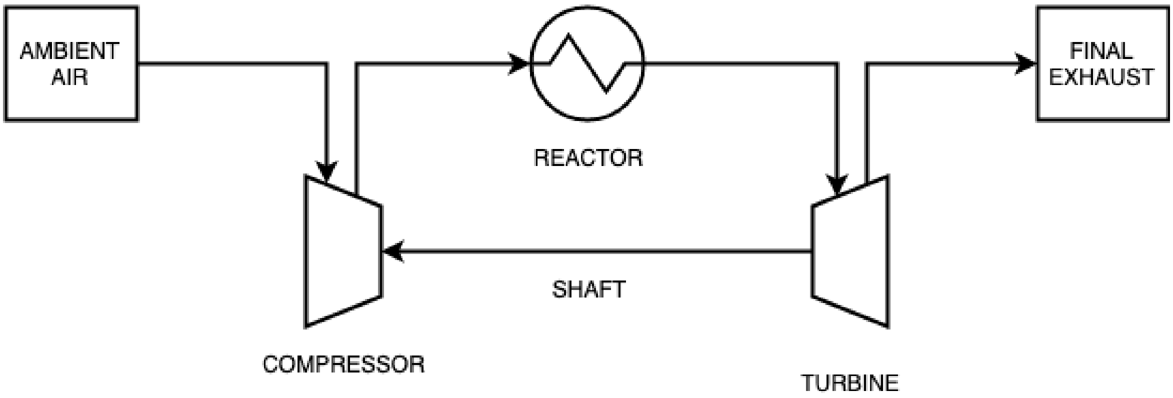

Figure 20. Open air Brayton cycle.

In an open-air Brayton cycle, ambient air is taken into the system and then compressed and convected over the heat pipes (modeled using Sockeye) that are connected to the reactor core. After the air is heated, it expands through the turbine, which performs shaft work for driving the compressor and electric generator. The exhaust of the system of the system exits the turbine and is returned into the environment [17].

This capability will be considered for future applications and evaluation when available.

4. CONCLUSION

The NEAMS program is developing capabilities to model a range of advanced reactor concepts including microreactor designs. Recent advances provide capabilities to model the heat pipe cooled microreactors. The results of preliminary analysis of microreactor concepts using MOOSE based tool-suite presented in this report include:

- Mesh refinement analysis of the thermo-mechanics performance of a microreactor assembly with BISON
- Thermal analysis of heat pipe with Sockeye and comparisons with HTPIPE
- Coupled simulation for LANL empire core design with MAMMOTH and BISON
- Coupled simulation for INL Design A with MAMMOTH, BISON and Sockeye.

Two different microreactor heat-pipe concepts were considered for the analysis to allow demonstration on a range of design features that are currently being considered by microreactor developers. Simulations performed model the steady-state operation and startup of the microreactor concepts with full integrated physics including neutronics, thermo-mechanics, heat transfer and structural behavior. Results from this study demonstrate the current capabilities for the integrated modeling and simulation capability for multiphysics simulation of microreactor concepts. It is shown that the MOOSE-based tool-suite is capable of applying different multiphysics solvers to predict the behavior of heat-pipe-cooled microreactor. Key observations include:

- The integrated capabilities have been successfully applied to perform steady-state simulations across a range of microreactor test cases.
- The detailed results from the simulations can be effectively visualized to communicate results and support analyst needs.

While these tools are still under active development, the current capability is promising. Additional needs and future work include:

- Continued development of Sockeye for simulation of heat simulations including development of closure relationships for common heat-pipe working fluids.
- Comparison of results with previously calculated values from the reactor design activities.
- Completion of the development of the ability to simulate microreactor power conversion systems and coupling with the integrated reactor models using RELAP-7.
- Development of a validation plan for the individual components and integrated simulation capabilities that can be used by NEAMS and the Microreactor Program to guide experimental work.
- Expanded assessment of capabilities that include increased physics fidelity to understand impact of modeling assumptions, determination of mesh and solution parameters. This includes comparisons of neutronics solutions with higher-fidelity Monte Carlo simulations.
- Expanded application of the capabilities for a range of normal operating conditions (startup, shutdown, and load following) and off-normal transient conditions.
- Application of the capability to an expanded range of designs including specifically gas-cooled microreactor.

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