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Changing the World's Energy Future

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Recent Advanced Reactor Multiphysics Model Highlights in the Virtual Test Bed (VTB)

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ABSTRACT

The Virtual Test Bed (VTB) host over 30 distinct simulations that showcase state-of-the art capabilities across the national lab complex. An update on the status of models on the VTB is summarized here, along with a more detailed overview of select recent new capabilities to showcase. All of the major advanced reactor types are represented in the VTB. The first example consists of a multiphysics simulation to track the transport of species in Molten Salt Reactors using depletion, advection, and thermochemical calculations. The second consists of a coupled neutronic and thermal hydraulic simulation to validate a gas cooled reactor. The third consist of pebble-bed equilibrium model for a fluoride high-temperature reactor. The fourth is a high-fidelity neutronic and thermal hydraulic model of a liquid metal reactor assembly. And lastly the fifth consists of transient multiphysics simulations of heat pipe microreactors.

Keywords: multiphysics; simulations; advanced reactors; repository

1. INTRODUCTION TO THE VTB REPOSITORY

1.1. Background on the Virtual Test Bed

The Department of Energy's National Reactor Innovation Center (NRIC) mission is to accelerate the deployment of novel reactor concepts by providing both physical and virtual spaces for building and testing various components, systems, and complete pilot plants. The Virtual Test Bed (VTB) represents the virtual arm of NRIC [1]. It is being developed in collaboration with U.S. Department of Energy's (DOE) Nuclear Energy Advanced Modeling and Simulation (NEAMS) program.

The mission of the VTB is to accelerate the deployment of advanced reactors by facilitating the adoption of cutting-edge DOE advanced modeling and simulation (M&S) tools to design, evaluate, and license reactors. This is primarily achieved by making available the inputs and descriptions of example challenge problems for various advanced reactor types in a public repository and by developing models to fill the potential demonstrator's M&S gaps. The end goal is to provide an open forum for various stakeholders to leverage and develop cutting-edge M&S capabilities. Industry users can leverage these capabilities to further mature their concepts, while reviewers can use them as a starting point for regulatory/confirmatory evaluations. As a result, the VTB is expected to help accelerate timelines for reactor demonstrations. Models being developed are already being used for the confirmatory analysis of demonstration reactors at Idaho National Laboratory (INL).

1.2. Using the Virtual Test Bed

The Virtual Test Bed is first a public-facing GitHub repository hosted under the idaholab organization. The repository contains the inputs files for each model, the cross sections, meshes and reference outputs for testing. These files are organized in folders, sorted first by reactor category (molten salt reactor, liquid metal fast reactor, etc) then by the actual reactor (HTR-10, MSRE, etc), or the generic part (air-jacket, assembly, etc) modeled. The repository can be consulted online or be downloaded to the user's machine following the instructions on the website.

The Virtual Test Bed also comprises a website, at https://mooseframework.inl.gov/virtual_test_bed/, that hosts the model documentation as well as an index of the models and modeling-specific trainings. For most models, the documentation consists of a description of the reactor modeled, of the system modeled within that reactor, of the inputs and finally presents sample results. The inputs are not all documented to the same level of detail, but all should remain understandable to the reader unfamiliar with the tools. The models are indexed based on reactor type, codes used, modeling features and computational cost. A dynamic search engine has been recently added to the repository. The website also hosts a tutorial for multiphysics modeling and tutorials for modeling certain classes of reactors with the NEAMS tools. To this date, the Virtual Test Bed contains upwards of 30 advanced reactor models.

1.3. Codes Represented

The VTB primarily contains models which leverage the Multiphysics Object Oriented Simulation Environment (MOOSE) [2], an open-source, parallel finite element framework for constructing physics applications (e.g. reactor physics, systems analysis, fuel performance). MOOSE also offers built-in physics modules, meshing capabilities, and coupling methods for performing multi-physics problems. MOOSE-based applications (and MOOSE-wrapped external codes) may be coupled together in-memory via specifications in the input file using MOOSE's MultiApp [3] system, without requiring code updates to transfer information. This flexibility allows tools in the MOOSE ecosystem to communicate with each other for virtually any advanced reactor concept (molten salt reactor, high temperature gas cooled reactor, microreactor, liquid metal fast reactor). MOOSE's Reactor Module [4] is frequently leveraged for meshing reactor geometries.

The NEAMS program has developed a suite of physics applications based on the MOOSE framework: Griffin [5] for deterministic reactor physics, Bison [6] for fuel performance, SAM [7] for systems analysis, Pronghorn [8] for engineering scale fluid dynamics, and Sockeye [9]for heat pipe modeling. In addition, the non-MOOSE computational fluid dynamics code NekRS [10] is MOOSE-wrapped via the Cardinal [11] application for connection to MOOSE-framework based codes. These codes, among a few others not highlighted here, can be combined into multiphysics coupling schemes for analysis of steady state and transient scenarios for various reactor types. The coupling flexibility enabled by MOOSE ensures that investments in developing the common set of physics applications are applicable for multiple reactor types.

1.4. Continuous Integration

The Virtual Test Bed benefits from the continuous integration infrastructure developed for the NEAMS program tools. Once uploaded, the inputs are maintained by the VTB team, with help and permission from the original contributors when required. A full suite of syntax and regression tests is included and covers nearly all the models contributed. Syntax tests make sure the input syntax remains correct and is relatively inexpensive. Regression tests make sure the results do not vary with new versions of the tools. They can be expensive for large models and generally only a few times steps or decoupled models are run for expensive simulations. Continuous integration is then performed in two parallel and complementary ways. Every model change request made to the repository is tested automatically using the CIVET platform. Model change requests include new contributions or modifications / improvements to existing models. Similarly, even change request made to the NEAMS tools is also tested against the models hosted on the Virtual Test Bed for the tool concerned. If the changes made to the code break the model, because the syntax changed or because the results are affected, a patch must be created either by the VTB team or the NEAMS tool developer. Until the patch is made, a new version of the NEAMS tool may not be released. In summary, continuous integration enforces that all inputs on the Virtual Test Bed are compatible with the current main branch of each of the NEAMS tools.

1.5. Library of Current Models

A plethora of advanced reactor models are currently available on the VTB. Table I provides a high-level overview of the different types of simulations represented. Additional informationon thevariou modls can be obtained using the filter at: https://mooseframework.inl.gov/virtual_test_bed/resources/filter/index.html. Section 2 will highlight specific new M&S capabilities in each reactor category: (1) species tracking multiphysics for MSRs, (2) multiphysics validation problem for HTGR, (3) multiphysics pebble equilibrium tracking for FHR, (4) high-fidelity multiphysics model for LMFR, and (5) multiphysics transient simulations for microreactors.

Table I. Overview of all reactor models hosted on the VTB. Core multiphysics simulations are highlighted in blue.

Type	Designs Represented	No. of models	Codes Represented
MSR	MSFR, MSRE, LOTUS	9	Griffin; Pronghorn; SAM; Nek5000; Thermochimica
HTGR	PBRM, MHTGR, HTTF, HTR10, HTTR, TREAT	13	Griffin; Pronghorn; SAM; Nek5000; Bison; Cardinal
FHR	Mk1, gFHR	5	Griffin; Pronghorn; SAM; Nek5000; Cardinal
LMFR	Assembly; VTR; ABTR; LFR	7	Griffin; Pronghorn; SAM; Bison
Microreactor	Heat pipe; gas-cooled; SNAP8	5	Griffin; Sockeye; SAM; Bison

2. OVERVIEW OF REACTOR PHYSICS MODELS

The VTB contains a wide variety of single and multiphysics reactor models including, Molten Salt Reactors (MSRs), High Temperature Gas Reactors (HTGRs), Fluoride-salt-cooled High-temperature Reactors (FHRs), Liquid Metal Fast Reactors (LMFRs), and Micro Reactors (MRs). The open-source repository has become quite prolific, offering external users the option to plug and play, taking the various physics modeling capabilities demonstrated in the hosted models and coupling or altering them for their own reactor design and research.

The VTB allows to showcase the most cutting-edge modeling capabilities developed by the NEAMS program for the various advanced reactor types listed above. This section takes one example from each of the five advanced reactor types and showcases novel M&S capabilities. The multiphysics models here are selected due to their novelty and their expected relevance for future demonstrations.

2.1. Spatially Resolved Depletion-Driven Thermochemistry of Molten Salt Reactors

MSR behavior is dictated by the interaction between neutronics, thermal-hydraulics, and chemistry. Recent modeling multiphysics coupling methodologies for simulating MSRs have made great strides for integral

MSR system analysis [12]. A new NEAMS based multiphysics and multiscale framework for MSR analysis is shown in Figure 1. By incorporating equilibrium thermochemistry via the Gibbs Energy Minimizer (GEM) Thermochimica [13] in MOOSE and the Molten Salt Thermodynamic Database: Thermochemical (MSTDB-TC) [14], the integral effect that reactor thermal-hydraulics, fuel depletion, and chemistry control has on the thermochemistry of the MSR can be determined.

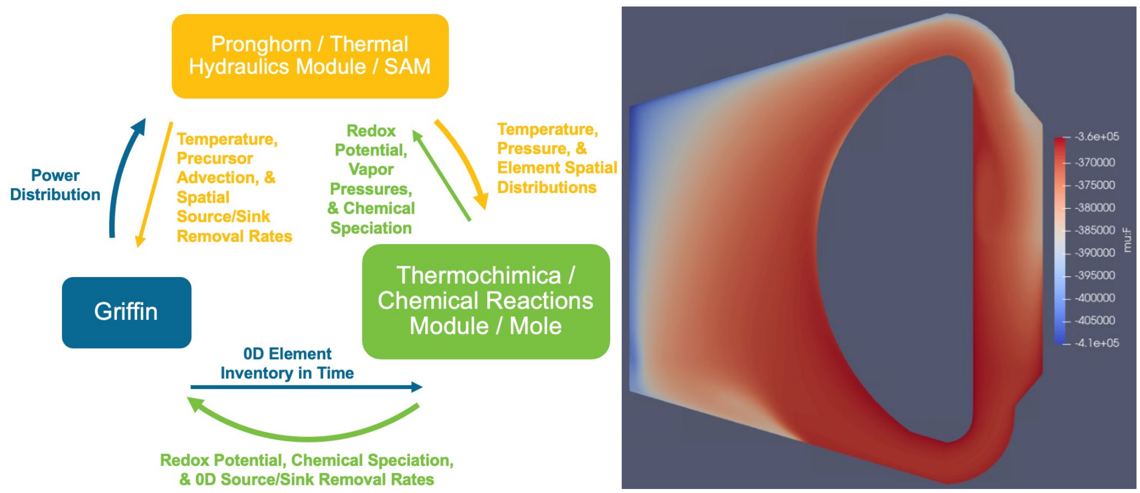

Figure 1. (left) multiphysics framework for MSR analysis and (right) [redox] Fluoride (F-) potential [J/mol] at 2.07 MWd/Kg-U burnup with no redox potential control from [12].

Coined as spatially-resolved, depletion-driven thermochemistry – the new modeling capability incorporates the effect that reactor physics has on altering reactor chemistry, and in turn the effect that altering reactor chemistry has on reactor dynamics, safeguards, source term, and reactor safety among other important analyses. An example of source term analysis is shown in Figure 1, where the change in fluoride (F^-) potential due to depletion, temperature, and pressure, directly effects the volatility of iodine in the fluoride salt in the Molten Salt Fast Reactor (MSFR) [15]. Redox chemistry control can then be modeled to reduce the fluorine or chlorine potential of the fuel salt and the effect this has on corrosion and volatilization of chemical species can be determined.

Table 2 summarizes the effect that redox control on source term. Iodine is partially stable in the MSFR fuel salt when the fluoride salt is kept reduced but becomes more volatile as the fluorine potential increases. The amount of ^{131}I accumulating in an off-gas system of the MSFR used for extracting noble gases with and without chemistry control demonstrates this phenomenon. Current work is ongoing to validate this new capability against Molten Salt Reactor Experiment (MSRE) [16] data.

Table 2. ^{131}I in OGS of MSFR after 2.07 MWd/Kg-U burnup with and without redox potential control from [12].

Radionuclide	Concentration in Core [atoms/b-cm]	Concentration in OG System [atoms/b-cm]	Percentage in OG System
^{131}I – redox control	**1.75e-07**	**~0.0**	**~0.00%**
^{131}I – no control	**1.74e-07**	**5.46e-11**	**0.03%**

2.2. Multiphysics Validation with High Temperature Engineering Test Reactor (HTTR)

The High Temperature Engineering Test Reactor (HTTR) is a graphite moderated and helium cooled prismatic reactor developed and operated by the Japan Atomic Energy Agency (JAEA) [17]. INL recently performed model development against experimental data for validation of the HTTR model [18].

The multiphysics HTTR model on VTB (shown in Figure 2) combines 3-D full core super homogenization-corrected neutronics, macroscale 3-D full core homogenized heat transfer, 2-D axisymmetric pin-scale fuel rod heat transfer, and distributed 1-D thermal-hydraulics channel. Here Griffin solves the eigenvalue problem and provides the power density to the thermal model which contains both pin-level heat transfer in BISON and thermal-hydraulics via RELAP-7. This model utilizes the MOOSE framework's MultiApps and Transfers systems to couple the individual physics models until they converge via Picard iterations.

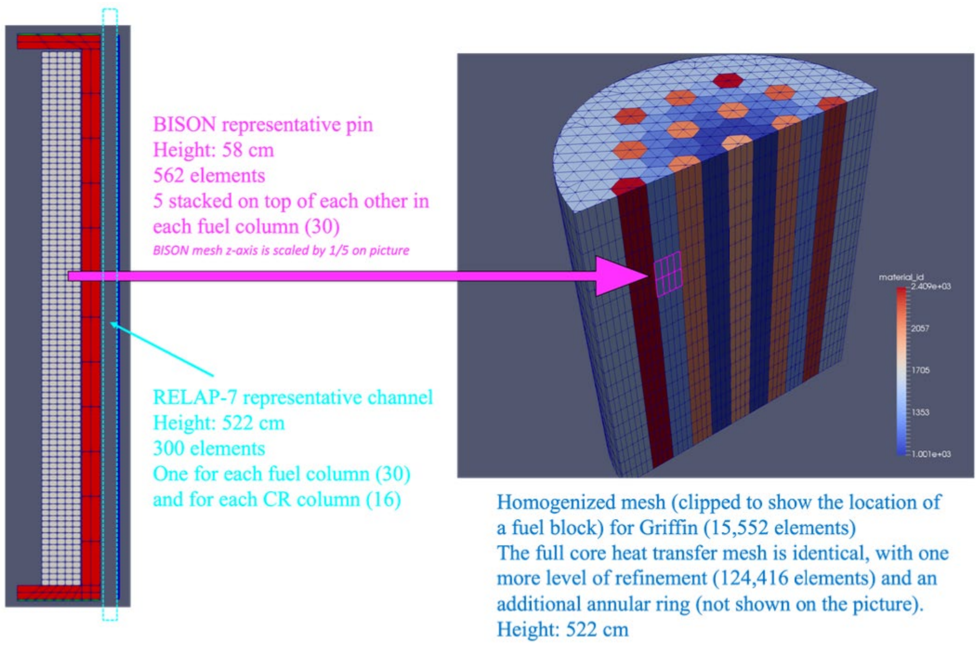

Figure 2. Relationship between various sub-models, from [17].

The HTTR model successfully reproduces the measured experimental data of excess reactivity, axial flux distribution, shutdown margin, and axial and radial power distribution within acceptable tolerances [16]. The multiplication factor of this model was calculated to be 1.0123, which is acceptable given the uncertainties in the graphite composition are very high. Additionally, when global energy conservation is considered, the outlet temperature measured by the experiment and predicted by the model is shown in Table 3. The indicate a discrepancy under 2% between the reference output temperature measured in the HTTR and the output temperature predicted by the model. This within the range of the absolute error of ~15 K or ~5% in the measurement [17].

Table 3. Summary of key performance parameters of the HTTR model.

P (MW)	P_{VCS} (MW)	T^{in} (K)	$T^{ref,out}$ (K)	T^{out} (K)	Δ
9	**0.055**	**453.15**	**592.01**	**594.40**	**-1.7%**
30	**0.241**	**668.15**	**1130.12**	**1134.65**	**-1.0%**

2.3. Equilibrium Pebble Bed Core Modeling in Generic Fluoride-salt-cooled High-temperature Reactor (gFHR)

A generic FHR design based on published material by Kairos Power [19] was developed and uploaded to the VTB. The reactor geometry is shown in Figure 3, including the active core, reflector, core barrel, salt downcomer, and reactor vessel regions [20].

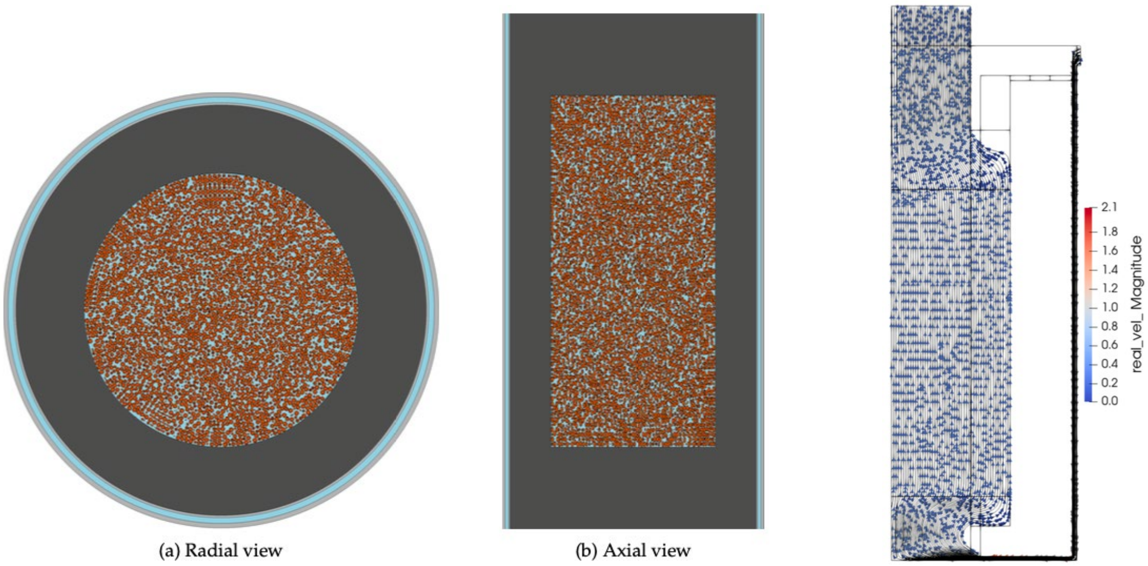

Figure 3. (left and center) gFHR conceptual design and (right) velocity field stream lines from

This design uses pebbles containing TRISO fuel which float in the fluoride salt coolant. The model uses a multi-pass strategy where the pebbles are discharged at the top of the core and then uniformly reintroduced at the bottom of the core. On average the pebbles are slowly cycled upwards through the core for eight passes before they are discharged. This pebble transport during depletion problem is simulated in this model and the effect this has on neutronics is determined. Here, Griffin calculates the spatial flux and eigenvalue solution of the problem and passes this information to Pronghorn, which determines the TRISO fuel heat conduction, temperature distribution and flow field. Griffin creates one pebble and TRISO sub application for each burnup group and determines the graphite and fuel temperature field in the pebble-bed core.

The equilibrium core is then attained via a streamline depletion method developed in Griffin for FHR pebble bed cycling depletion. This depletion approach utilizes both the 2D and 3D core flux solution and maps them to a set of 1D axial streamlines to capture the effect of pebble cycling. The resulting set of 1D steady-state advection-transmutation equations for all isotopes is then solved in each streamline. The model includes nine burnup groups that detail the unique fuel and moderator temperatures in each core mesh zone. This method is then used to obtain the final equilibrium core solution. The parameters of the final equilibrium core solution can be seen in Table 4.

Table 4. Coupled equilibrium core results from [20].

k_{eff}	Discharge burnup [EFPD]	Discharge burnup [MWd/kg]	FLiBe av. density [kg/m^3]	T^{fuel} [K]	T^{mod} [K]	T^{ref} [K]
1.01	**468.2**	**153.8**	**1982.5**	**953.6**	**928.9**	**858.9**

2.4. Griffin-MOOSE-Cardinal Coupling for Heterogeneous Liquid Metal Fast Reactor Analysis

Motivated by the need for "hot channel factor" calculations where input parameters such as thermal conductivity or coolant density can be perturbed to investigate the impact on peak temperatures, a high-fidelity coupling scheme using Griffin, MOOSE Heat Conduction (HC) module, and NekRS (via Cardinal) has been developed by the NEAMS program and tested on a 7-pin 3D mini-assembly [21][22]. This scaled-down toy problem, based on a lead-cooled fast reactor concept developed by Westinghouse Electric Company [23], reduces computational requirements while still performing all of the fundamental operations needed for the full-scale problem. The mini-assembly includes 7 explicitly modeled annular MOX fuel pins, lead coolant, and an assembly duct (also called a wrapper). The active fuel zone is surrounded on the top and bottom by an upper and lower reflector region. Explicit geometry modeling is important in this problem as local effects will be considered in future hot channel factor calculations.

The mesh for Griffin and MOOSE Heat Conduction is generated using the MOOSE Reactor Module. Griffin's discontinuous finite element method with discrete ordinates (DFEM-SN) with coarse mesh finite difference (CMFD) acceleration is leveraged due to the highly heterogeneous mesh which requires an accurate and efficient transport method. Griffin computes the flux and power distribution in the entire spatial domain and passes it to HC, which then calculates the heat transfer within the solid fuel and duct, and heat flux on solid-fluid interfaces. Finally, NekRS (via Cardinal) is sub-cycled within heat conduction solves to develop the lead coolant flow heat transfer behavior. The fluid and solid temperatures computed by HC and NekRS are transferred back to reactor physics to incorporate feedback in cross sections. However, neutronics and thermal fluids are weakly coupled for this problem so neutronics converges fairly quickly. Prior to performing the Griffin – HC – NekRS(Cardinal) coupled simulation, NekRS is run in standalone mode to develop the flow velocity and temperature profile to be used as initial conditions for the multi-physics case. This improves the computational efficiency of the multi-physics simulation by starting iterations at a converged flow velocity profile. Detailed heat flux distribution transferred at the fluid-solid interfaces as well as rod, duct, and coolant temperatures are shown in Figure 4. This is the first known coupling demonstration between Griffin and NekRS (via Cardinal).

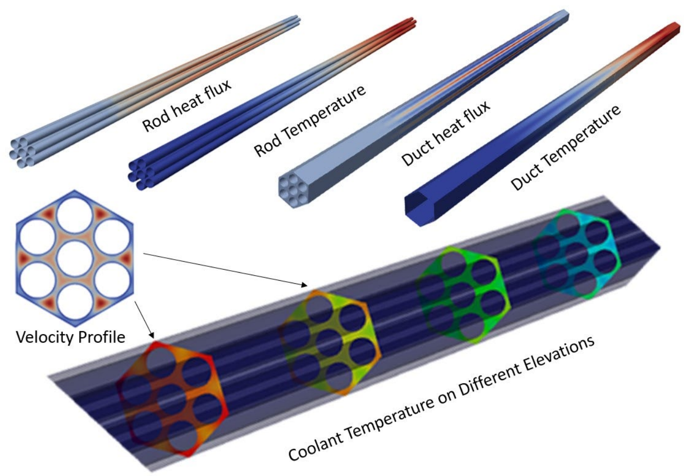

Figure 4. Detailed heat flux and temperature in a 7-pin lead-cooled fast reactor mini-assembly computed using Griffin + MOOSE Heat Conduction + NekRS (via Cardinal).

2.5. Multiphysics Transients in a Heat Pipe-Cooled Microreactor Core

A 2 MW thermal spectrum heat pipe-cooled microreactor (HP-MR) core design [24] is shown in Figure 5. The HP-MR uses 9.95 at% Low-Enriched Uranium (LEU) TRISO fuel in a hexagonal graphite matrix. Thirty fuel assemblies are surrounded by one ring of beryllium reflector and 12 control drums. This concept employs heat pipes with stainless-steel envelope and potassium as the working fluid. Yttrium-hydride (YH_2) pins are employed to provide efficient neutron slowing-down capability enabling the design of a compact core.

The multi-physics HP-MR model [25] adopts a three-level Griffin-BISON-Sockeye MultiApp hierarchy. The main Griffin application calculates power based on the temperature feedback from the BISON child application using a DFEM-SN(1,3) neutronics solver with CMFD acceleration. The BISON child application computes the solid temperatures based on the power profile and interacts with the Sockeye grandchild application that governs heat pipe performance using the effective conduction model. A 1/6th core mesh utilizing symmetry was constructed for both Griffin and BISON applications by the MOOSE Reactor Module. For the BISON mesh, boundary layer and biased meshing features were used to create a finer mesh with a focus on the external/interface boundaries to improve the accuracy of the predicted heat flux over these boundaries and thus ensure the energy balance of the system.

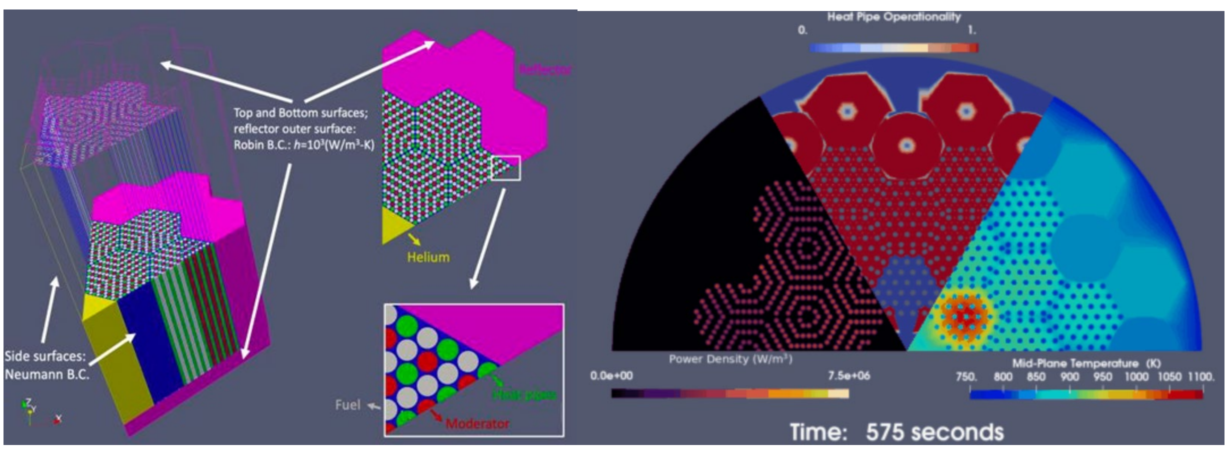

Figure 5. Mesh (left), power and temperature (right) performance of the heat pipe MR during a transient simulation using Griffin + Sockeye + Bison.

The load following transient is initiated by introducing a drop in the heat removal capability of the secondary coolant loop that transfers the heat from the condenser regions of the heat pipes to either a heat exchanger or directly to the energy conversion component. The heat removal capacity of all the heat pipes is reduced by artificially reducing the condenser side heat transfer coefficient by 10^{-4} of its original value. The heat pipe failure transient is initiated by the inactivation of a single heat pipe at the center of the inner-most assembly in the core. Depending on the power level, a single heat pipe failure is either localized or leads to cascade failures.

3. SUMMARY

The NRIC Virtual Test Bed (VTB) showcases a breadth of M&S capabilities for advanced nuclear reactors. The repository currently hosts over 30 simulations, across 5 reactor types, and using 8 codes. Key recent new highlights were summarized in this paper. This includes novel species tracking capabilities for MSRs, validation of an HTGR, a pebble-equilibrium model for FHR, a high-fidelity assembly of a LMFR, and a multiphysics transient of a heat pipe microreactor. These state-of-the art capabilities can be leveraged in a plug-and-play manner to specific vendor/licensor evaluation needs. This is expected to help accelerate timelines for advanced reactor demonstration by providing the foundation for safety and confirmatory evaluations for these new concepts.

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