

NEAMS Model Contributions in 2023 to the National Reactor Innovation Center Virtual Test Bed for Use by Industry and Other Stakeholders

Nuclear Science and Engineering Division

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NEAMS Model Contributions in 2023 to the National Reactor Innovation Center Virtual Test Bed for Use by Industry and Other Stakeholders

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Abstract

The U.S. Department of Energy (DOE) Office of Nuclear Energy's Advanced Modeling and Simulation (NEAMS) Program develops models of advanced reactor phenomena to demonstrate code applicability to challenging physics problems, drive code development through user assessment, and perform code verification and validation. Meanwhile, the U.S. DOE's National Reactor Innovation Center (NRIC) hosts an open-source website and associated GitHub repository called the Virtual Test Bed (VTB) on which computational models for advanced reactors are documented and shared with the reactor community.

This work documents NEAMS efforts to support industry adoption of advanced modeling tools through contribution of 10 NEAMS models to the NRIC Virtual Test Bed including models for the High Temperature Test Facility (HTTF), TRISO fuel failure in a microreactor, and multiphysics models of a molten chloride fast reactor, among others. The open sharing of these models benefits the reactor community by providing "best practice" examples using NEAMS tools for advanced reactor physics problems. In particular, the HTTF model is being used for code validation and benchmarking activities. The microreactor and molten chloride fast reactor models are representative of analysis that may be useful for current candidates of DOME and LOTUS, NRIC's physical testbeds. This report summarizes and provides links to these new models and highlights their importance in developing and demonstrating advanced nuclear reactor systems.

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1 Overview

The U.S. Department of Energy (DOE) Office of Nuclear Energy's Advanced Modeling and Simulation (NEAMS) Program [1] develops software tools based on the Multiphysics Object Oriented Simulation Environment ([MOOSE](#)) [2] and applies these tools to advanced reactor phenomena to demonstrate code applicability to challenging physics problems, drive code development through user assessment, and perform code verification and validation. Meanwhile, the U.S. DOE's National Reactor Innovation Center (NRIC) hosts an open-source [website](#) and associated [GitHub repository](#) called the Virtual Test Bed (VTB) [3] on which computational models for advanced reactors are documented and shared with the reactor community.

One important way NEAMS supports industry adoption of advanced modeling tools is by making NEAMS-funded models openly available to the reactor community through the NRIC VTB. This year, NEAMS contributed 10 models including systems and computational fluid dynamics (CFD) models for the High Temperature Test Facility, a TRISO fuel failure analysis model in a microreactor, and a molten chloride fast reactor model relevant to NRIC's LOTUS testbed. Prior to release on the VTB, each model is cleared by DOE laboratory export control offices and reviewed by VTB staff to ensure quality. Industry, regulatory bodies, academia, and other Department of Energy partners can freely access these models which are kept up to date as the software evolves through a rigorous continuous testing process.

2 NEAMS Models Added to the Virtual Test Bed in 2023

Table 1 lists ten NEAMS-developed models contributed to the VTB during January to December 2023. The models are categorized by reactor type: high temperature gas-cooled reactor (HTGR), molten salt reactor (MSR), microreactor (MR), and liquid metal cooled fast reactor (LMFR). The breadth of models contributed is reflective of the NEAMS program mission to support advanced modeling and simulations for a wide range of industry reactor concepts.

The newly contributed models leverage a variety of NEAMS applications and physics phenomena: MOOSE (open-source physics modules, meshing, and framework), Griffin [4] (reactor physics), Pronghorn [5] (engineering scale fluids), SAM [6] (systems scale fluids), Nek5000 [7] (computational fluid dynamics), NekRS (GPU-enabled CFD solver) [8], Sockeye [9] (heat pipe analysis), and Bison [10] (fuel performance and heat conduction).

The development of each model was fully or partially funded by the NEAMS program and is the result of multiple contributors' efforts. NRIC provided support to port each existing model to the VTB, including creation of documentation, peer review of models, and setting up testing. For more information on the model development work and contributors, see related publications on each model's documentation page. The development and contribution of these models to the VTB constitutes a significant programmatic investment by NEAMS and commitment to sharing gained knowledge with the reactor community.

Table 1. Summary of 2023 NEAMS model contributions to the VTB (Jan – Dec 2023)

Reactor Type	Description	Contact	Status
HTGR	High Temperature Test Facility (HTTF) systems-level thermal fluids model using SAM	Thanh Hua (ANL)	Available
HTGR	High Temperature Test Facility (HTTF) lower plenum CFD mixing model using Nek5000 & NekRS	Jun Fang (ANL)	Available
MSR	LOTUS Molten Chloride Reactor (LMCR) multiphysics model using Griffin & Pronghorn	Mauricio Tano (INL)	Available
MSR	Molten Salt Reactor Experiment (MSRE) multiphysics model using Griffin & Pronghorn	Mauricio Tano (INL)	Submitted
MSR	Molten Salt Reactor Experiment (MSRE) lower plenum CFD mixing model using NekRS	Jun Fang (ANL)	Available
MSR	Molten Salt Fast Reactor (MSFR) spatially-resolved thermochemistry using Thermochemica	Samuel Walker (INL)	Submitted
MSR	Molten Salt Fast Reactor (MSFR) system model transient updates using SAM	Jun Fang (ANL)	Available
MR	Heat pipe-cooled microreactor core multiphysics transients using Griffin, Bison, and Sockeye	Nicolas Stauff (ANL)	Available
MR	Heat pipe-cooled microreactor TRISO fuel failure analysis using Bison	Yinbin Miao (ANL)	Available
LMFR	Effect of Partial Blockages in Simulated LMFBR Fuel Assemblies at THORS facility with Pronghorn-SC	Vasileios Kyriakopoulos (INL)	Available

2.1 High Temperature Test Facility (HTTF) Systems-Level Thermal Fluids Model using SAM

POC: Thanh Hua (ANL)

Code(s): SAM

Status: [Available](#)

The High Temperature Test Facility (HTTF) [11] is an integral helium-cooled test facility located at Oregon State University. It was based on the General Atomics MHTGR design which uses prismatic graphite blocks in the core and reflectors. Compared to the MHTGR, the HTTF was scaled $\frac{1}{4}$ in length and diameter and operated at prototypical temperature but at reduced pressure. The HTTF was primarily designed to study depressurized conduction cooldown and pressurized conduction cooldown transients in HTGR. A variety of tests were performed in the HTTF, providing experimental data to reflect system-level response, which are suitable for code benchmark of system analysis codes like SAM. The SAM model of the HTTF uses a “ring model” approach to approximate a 3D geometry in 2D (Figures 1b, 1c). In this approach, the structures are homogenized and rearranged in concentric rings (annuli). In the core a coolant or heater ring represents one hexagonal array of coolant channels or heater rods, and a ceramic ring represents the matrix material that provides the heat conduction path connecting coolant channels to heater rods. There are multiple rings in the core to capture the localized heat transfer and ring-to-ring radial conduction captures core-wise heat conduction. This model is used to simulate two of three benchmark problems within the scope of the Organization for Economic Co-operation and Development Nuclear Energy Agency (OECD NEA) International HTTF Benchmark.

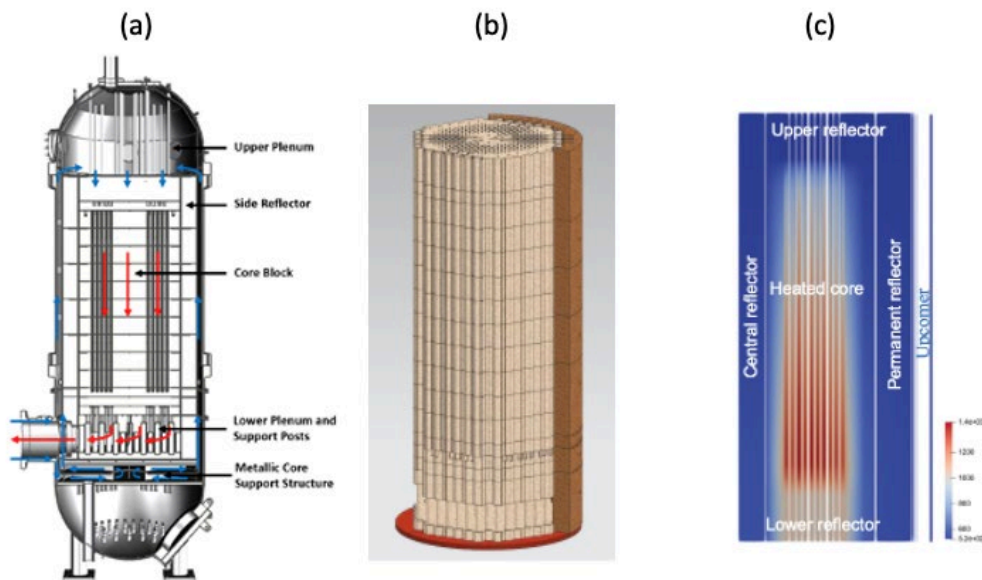


Figure 1. (a) HTTF reactor pressure vessel with flow path, (b) schematic of the 3D core, and (c) 2D ring model.

2.2 High Temperature Test Facility (HTTF) Lower Plenum CFD Mixing Model using Nek5000 & NekRS

POC: *Jun Fang (ANL)*

Code(s): *Nek5000 and NekRS*

Status: [Available](#)

The High-Temperature Test Facility (HTTF) [11] serves as a crucial test facility for exploring thermal fluid behavior in high-temperature gas-cooled nuclear reactors (HTGR), and it offers invaluable data for benchmarking simulation codes. Given the need for precise simulation in HTGR development, a significant knowledge gap has been identified in understanding the flow distribution in the lower plenum. This study employs advanced Computational Fluid Dynamics (CFD) modeling, focusing on the lower plenum of the HTTF, where heated coolant gas from the core region mixes and interacts. The non-uniform temperature of coolant jets entering the lower plenum poses risks, including high cycling thermal stresses, negative pressure gradients opposing flow ingress, and hot streaking. Traditional 1-D system codes fall short in accurately capturing these phenomena. By leveraging high-fidelity turbulence modeling provided by NEAMS CFD codes Nek5000 and NekRS, this simulation campaign examines velocity and temperature patterns to deepen our comprehension of thermal-fluid dynamics in the HTTF lower plenum. Notably, the nekRS code has been developed to fully exploit the unprecedented computing power of GPU-based supercomputers. The resulting insights, critical for advancing gas-cooled reactor research, will also facilitate code-to-code and code-to-data comparisons under the OECD/NEA international benchmark campaign, driving the integration of CFD applications in reactor innovation.

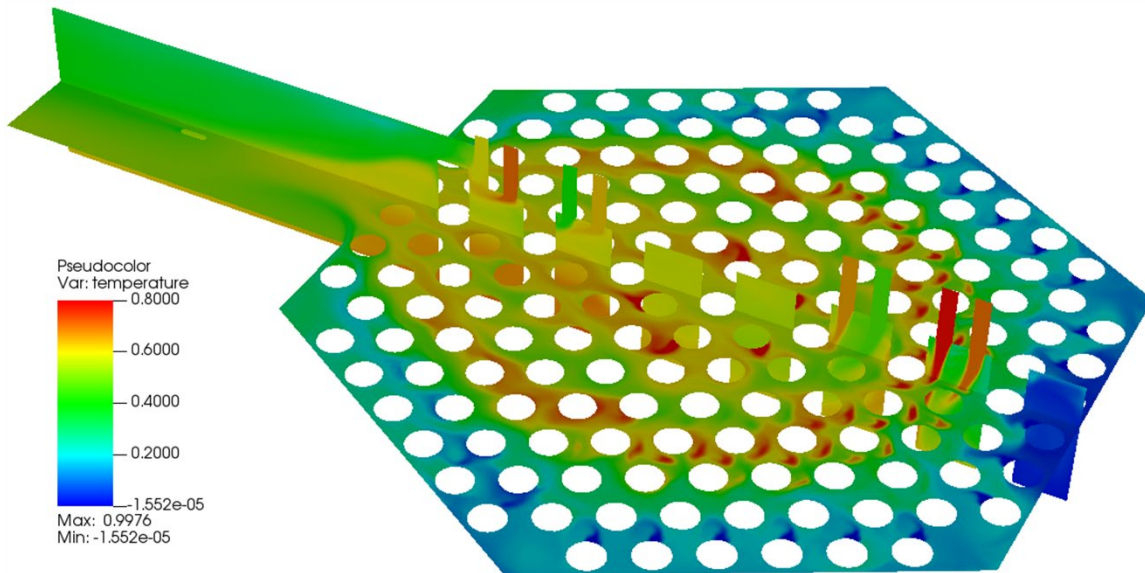


Figure 2. Time-averaged non-dimensional temperature distribution in the HTTF lower plenum predicted by nekRS simulation. The hot streaking and lower plenum temperature mixing are both identified from the CFD calculations.

2.3 LOTUS Molten Chloride Reactor (LMCR) Multiphysics Model

POC: *Mauricio Tano (INL)*

Code(s): *Griffin, Pronghorn*

Status: [Available](#)

The NRIC Laboratory for Operation and Testing in the U.S. (LOTUS) Molten Chloride Reactor (LMCR) is an open-source generic chloride fuel salt reactor [12]. Although this open-source model is similar to the Molten Chloride Reactor Experiment (MCRE) scheduled to be built at Idaho National Laboratory, readers should note that these two reactors are not the same. The model is a tightly-coupled, 3D Griffin-Pronghorn multiphysics analysis at steady state modeling the flow of liquid fuel through the reactor core and piping. Development of this model was co-funded by both NEAMS and NRIC program.

The steady-state velocity field during reactor operation is depicted in Figure 3. Liquid nuclear fuel exits the reactor core through the upper elbow connected to the pump. As the fuel passes through the pump region, the superficial velocity homogenizes due to the porous friction forces. The fuel salt then circulates through the return pipe.

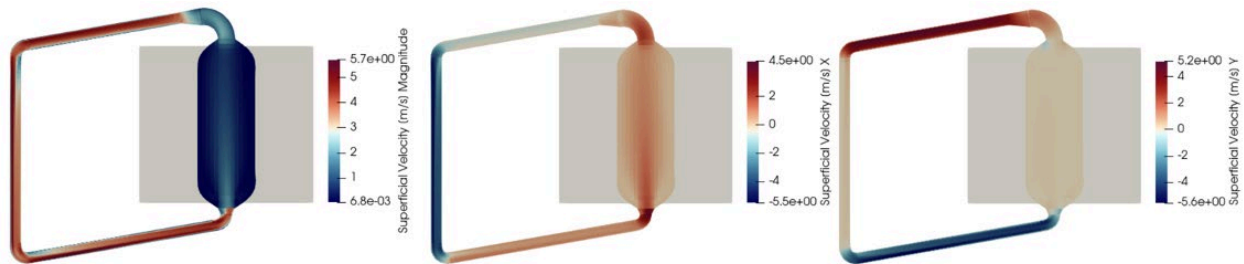


Figure 3. Velocity fields during steady-state reactor operation for LMCR. (left) Velocity magnitude, (center) velocity in vertical direction, (right) velocity in horizontal direction [13].

At the elbows, the flow follows the expected flow profile, characterized by centripetal flow acceleration. Specifically, the flow accelerates towards the closed edge of the elbow and then deflects towards the open edge downstream. Achieving this correct behavior was possible through the calibration of the turbulent mixing length in the turbulence model. It should be noted that using a suggested mixing length model of 7% of the hydraulic diameter of the pipe would result in over-diffusive and incorrect results.

2.4 Molten Salt Reactor Experiment (MSRE) Multiphysics Model

POC: *Mauricio Tano (INL)*

Code(s): *Griffin, Pronghorn*

Status: *[Submitted](#)*

This model of the Molten Salt Reactor Experiment (MSRE) [14] couples Griffin and Pronghorn to simulate both the steady state reactor behavior, and a reactivity insertion experiment. MOOSE is leveraged to create a 2D RZ (cylindrical coordinates) mesh of the MSRE. Griffin computes neutronics and resulting normalized power source [15]. Pronghorn perform medium-fidelity, coarse mesh thermal-hydraulics analysis of the core, upper plenum, pump, downcomer, and lower plenum [16] (Schunert et al., 2023). Griffin and Pronghorn are then coupled via the MultiApp system to perform tightly coupled multiphysics analyses.

For the transient results, we tested a reactivity insertion of 19 percent-mili (pcm) at 5 MW, from ORNL (Oak Ridge National Laboratory) reports [17]. The multiphysics model successfully captured the thermal oscillations induced by the density-Doppler power-temperature relationship. The method converges reliably and efficiently, with a maximum of 15 iterations but usually less than ten iterations in the tested case. This coupling method converges faster than comparable methods, achieving less error than the domain-segregated method or a standalone SAM model as seen in Figure 4. The increased accuracy of Griffin-Pronghorn is likely due to the improved temperature resolution in the core, and shows good agreement with the experimental results.

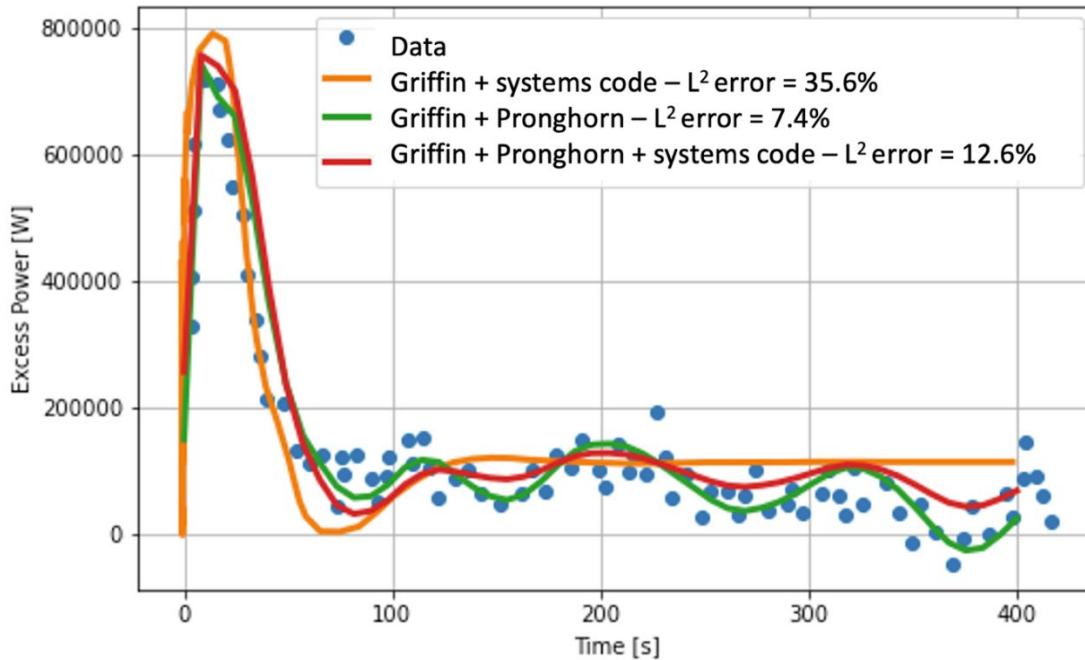


Figure 4. MSRE calculations compared to experimental data (Schunert et al., 2023)

2.5 Molten Salt Reactor Experiment (MSRE) Lower Plenum CFD Mixing Model

POC: *Jun Fang (ANL)*

Code(s): *NekRS*

Status: [*Available*](#)

Detailed inflow conditions are essential for accurately modeling the three-dimensional reactor physics and thermal fluid behavior within the core region of the Molten Salt Reactor Experiment (MSRE) [14]. However, this task is hindered by the lack of comprehensive information about the MSRE's lower plenum. In the MSRE, molten salt flowed from the downcomer into the lower plenum of the reactor core, an area characterized by complex geometries and poorly understood flow patterns. This CFD study focused on addressing the complex flow mixing problem within the MSRE lower plenum. This critical area of the reactor presented challenges in accurately modeling the fluid behavior. The study [18] aimed to bridge the knowledge gap by developing a representative CFD model that incorporates detailed geometric features such as anti-swirl fans, the main support grid, and horizontal plates within the MSRE lower plenum. Leveraging advanced meshing techniques and NekRS, the NEAMS GPU-enabled CFD code, detailed simulations were performed to better understand flow distribution in this region. The primary goal is to improve the accuracy of inflow boundary conditions for multiphysics simulations within the core, enhancing our understanding and modeling capabilities for the MSRE reactor and its crucial lower plenum region.

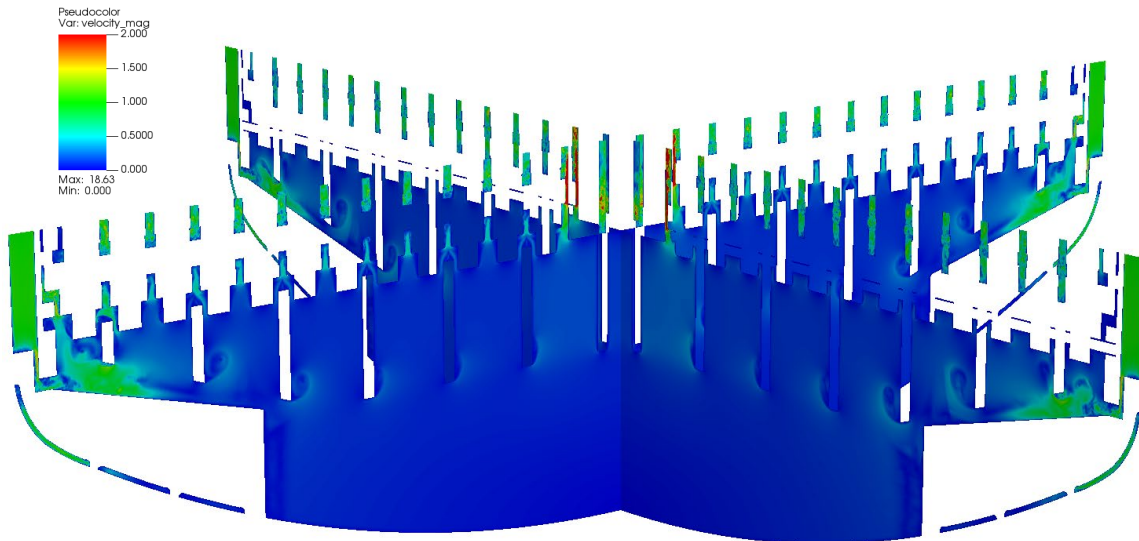


Figure 5. Instantaneous velocity distribution in MSRE lower plenum predicted by nekRS simulation, and the variation of outlet velocities.

2.6 Molten Salt Fast Reactor (MSFR) Spatially-Resolved Thermochemistry Model

POC: *Samuel Walker (INL)*

Code(s): *Griffin, Pronghorn, Thermochemica*

Status: *Submitted*

This model development effort was co-funded by NEAMS (thermochemistry modeling capability development) and DOE's ART-Molten Salt Reactor Campaign (model application). The NEAMS program has recently supported the wrapping of the Gibbs Energy Minimizer Thermochemica [19] within the MOOSE framework [20]. The purpose of Thermochemica is to determine the thermochemical equilibrium of a system by minimizing the internal Gibbs Energy of the system through the use of the CALculation of PHase Diagrams (CALPHAD) method with the Molten Salt Thermal Properties Database - Thermochemical (MSTDB-TC) [21]. With Thermochemica wrapped within MOOSE, the ability to perform various thermochemical analyses of MSRs with other multiphysics analyses now exists.

The Molten Salt Fast Reactor (MSFR) developed under the Euratom EVOL project [22,23] was modeled with Griffin-Pronghorn-Thermochemica to showcase what has been coined 'Depletion driven thermochemistry' [24], meaning the effect that neutronic fuel depletion has on altering the thermochemistry of the fuel salt. Figure 6 showcases this effect. Here the fluorine potential increases due to the consumption of Uranium fuel and the generation of less thermodynamically stable fission products (i.e. noble gases and noble metals). Accordingly, the volatilization of iodine also increases by a minimum of four orders of magnitude as seen in the right of the figure. Therefore, iodine gas will begin to be extracted to the off-gas system along with the noble gases. These results showcase the importance of chemistry control for both corrosion and source term mitigation in MSR systems.

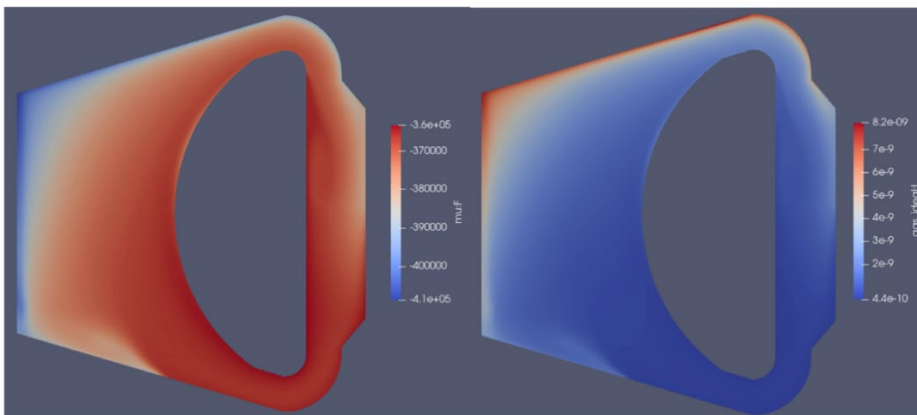


Figure 6. (left) Fluoride (F-) potential [J/mol] and (right) corresponding iodine in stable gas phase [mol] at 2.07 MWd/Kg-U burnup without chemistry control – i.e. oxidizing.

2.7 Molten Salt Fast Reactor (MSFR) Systems Model Transient Updates

POC: *Jun Fang (ANL)*

Code(s): *SAM*

Status: [Available](#)

The Molten Salt Fast Reactor (MSFR) design developed under the Euratom EVOL project [22,23] is a 3000 MW fast-spectrum reactor with three different circuits: the fuel circuit, the intermediate circuit, and the power conversion circuit. Based upon the design specifications of EVOL MSFR, representative 1-D system models were created using the NEAMS system modeling code, SAM. The system modeling covers both the fuel and intermediate circuit, whereas only the heat exchanger is modeled for the energy conversion circuit. The 16 ex-core loops are lumped together, which means only one loop is considered for both fuel and intermediate circuit. In addition to the steady-state modeling, transient scenarios that involve pump head changes were also simulated to study the MSFR system responses under possible accident conditions including the influence of possible head changes of the primary pump. The neutronics response is modeled by the Point Kinetics Equations (PKE). The evolution of the mass flow rates for each transient is computed as well as time-dependent behavior of core inlet and outlet temperatures, and reactor power.

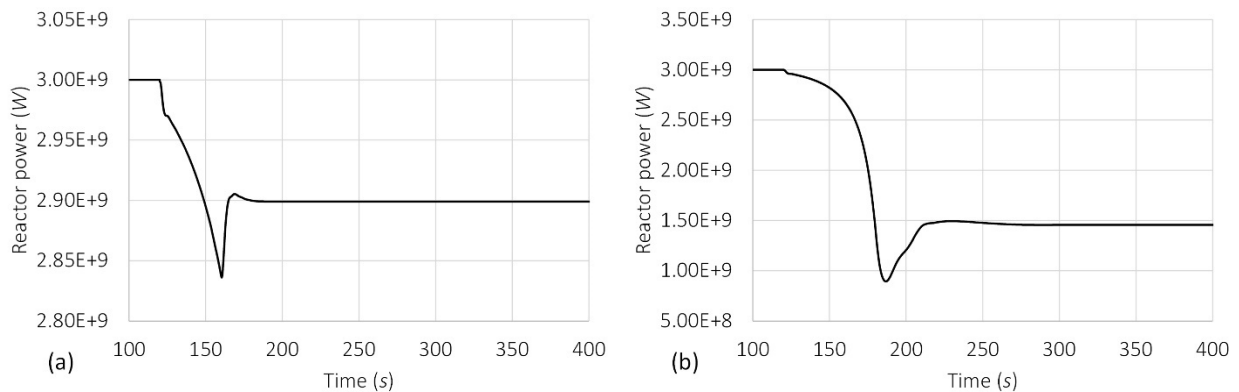


Figure 7. Evolution of reactor power during postulated pump transient scenarios in MSFR: (a) 50% pump head loss, (b) pump trip.

2.8 Heat Pipe-Cooled Microreactor Multiphysics Models including Heat Pipe Failure and Load Following

POC: *Nicolas Stauff (ANL)*

Code(s): *Griffin, Bison, Sockeye*

Status: [Available](#)

This heat pipe microreactor model (HP-MR) [25,26] gathers some of the most pressing modeling challenges faced by the microreactor industry: a) the use of heat pipe technologies to remove the thermal energy; b) the use of TRi-structural ISOtropic (TRISO) fuel to enable operations at very high temperatures; c) the use of rotating control drums in the radial reflectors.

This 1/6 full-core HP-MR model demonstrates multiphysics transient simulations performed through coupling of the Griffin DFEM-SN neutronic solver, BISON for thermal physics, and Sockeye for heat transfer and operational limits within each heat-pipe. Two different scenarios are modelled including a load following transient and a scenario initiated by the forced failure of a single heat-pipe. The load following transient is initiated by a significant reduction in the heat removal capacity of the secondary coolant loop, which causes the temperature of the heat pipe and core temperature to increase, and then the power drops due to negative temperature reactivity feedback. The heat pipe failure transient is induced by setting the central heat pipe of the innermost assembly to fail. The simulation predicts that nearby heat pipes remove the excess heat effectively and keep the heat pipe failure localized.

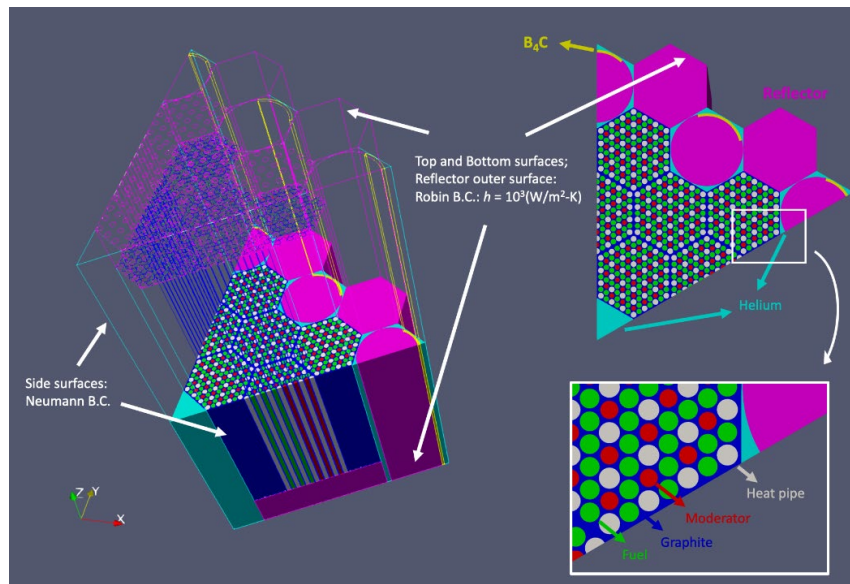


Figure 8. Heat pipe-cooled microreactor geometry showing fuel, graphite, moderator, and heat pipes, control drums, and reflectors

2.9 Heat Pipe-Cooled Microreactor TRISO Fuel Failure Analysis

POC: Yinbin Miao (ANL)

Code(s): Bison and MOOSE Stochastic Tools Module

Status: [Available](#)

This heat pipe microreactor (HP-MR) Tri-structural ISOTropic (TRISO) fuel failure model provides an example for evaluating TRISO particle fuel performance based on multiphysics simulation of a specific reactor design [27,28]. This TRISO fuel failure model is based on the simplified unit-cell HP-MR model [25], shown in Figure 9 (left). The multiphysics model includes neutronics, heat transfer, tensor mechanics, and heat pipe performance applications coupled using the hierarchy shown in Figure 9 (right).

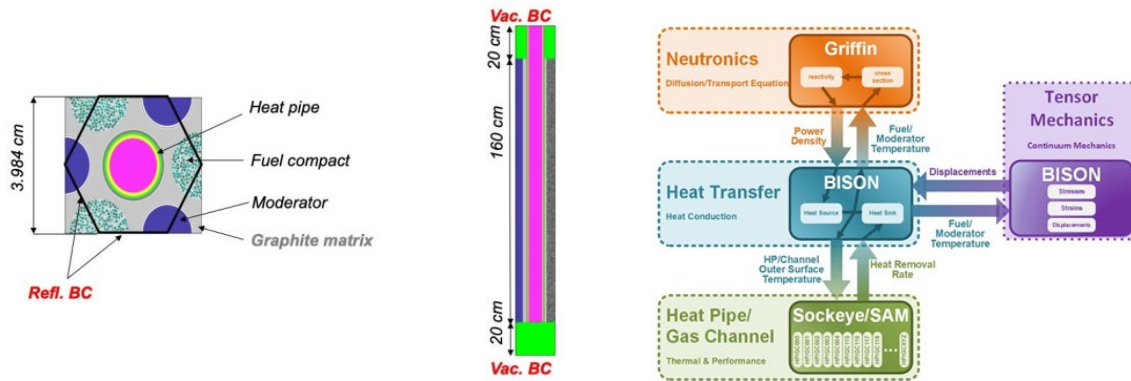


Figure 9. (left) HP-MR unit cell radial and axial layout, (right) HP-MR multiphysics simulation hierarchy.

Fuel failure is considered after a ten-year steady-state operation. A load-following transient was also investigated but was found not to significantly affect the failure rates of the HP-MR TRISO fuel particles. The fuel temperature, power density, and hydrostatic stress calculated by the multiphysics unit-cell model are used by the BISON TRISO failure model as input data.

A Monte Carlo scheme is used to calculate failure probability of TRISO particles in BISON. The MOOSE Stochastic Tools Module samples and computes statistics of many one-dimensional TRISO particles. For computational efficiency, a one-dimensional TRISO particle model is used for the Monte Carlo sampling scheme, with a multi-dimensional stress correlation to help describe the multi-dimensional TRISO phenomena, such as particle cracking and asphericity.

Based on the irradiation conditions predicted by the unit-cell model, the axial distribution of IPyC layer failure rate for the TRISO particles during the 10-year steady-state HP-MR operation is shown in Figure 10. The axial variation in the crack rate of IPyC layer is due to the combined variations of principal stresses and strength of the IPyC layer across the unit-cell. Meanwhile, the

crack rate of the SiC layer is zero across the axial profile of the unit-cell. As a TRISO particle is regarded as failed only when the SiC layer fails, the overall TRISO failure rate is also zero.

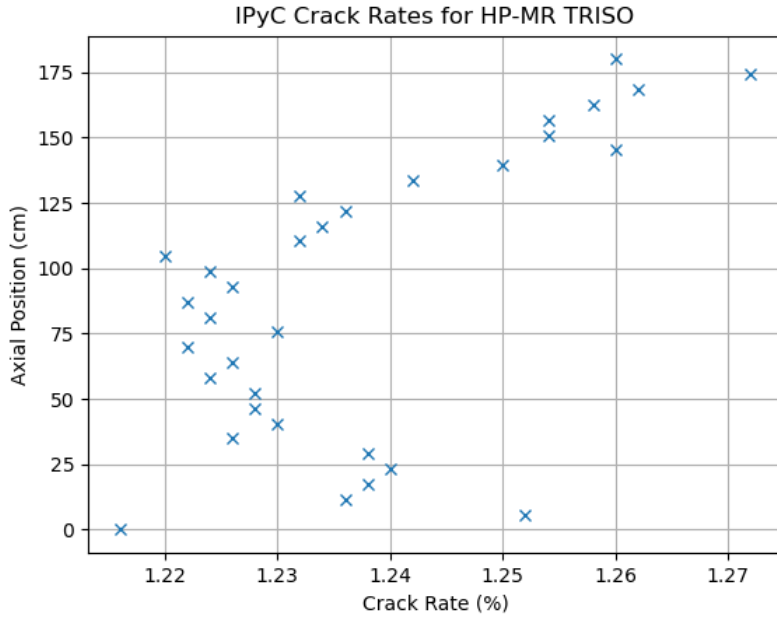


Figure 10. Axial distribution of spatially-averaged IPyC crack rate in HP-MR TRISO fuel.

2.10 Effect of Partial Blockages in Simulated LMFBR Fuel Assemblies at THORS facility

POC: *Vasileios Kyriakopoulos*

Code(s): *Pronghorn-SC (Subchannel)*

Status: [Available](#)

The effect of partial blockages in simulated Liquid Metal Fast Breeder Reactor (LMFBR) fuel assemblies at the Thermal Hydraulic Out-of-Reactor Safety (THORS) facility was modeled using Pronghorn-SC (subchannel) under the NEAMS Thermal Fluids Technical Area. Information on the THORS facility and experiments can be found in [29,30,31].

THORS bundle 5B has the same fuel configuration as bundle 2B, except that 0.0711-cm-diameter wire-wrap spacers are used to separate the peripheral pins from the duct wall. The half-size spacers used in this configuration serve to reduce the flow in the peripheral flow channels and to cause a flatter radial temperature profile across the bundle. The flat-to-flat distance is reduced accordingly. The pins have a heated length of 45.7 cm. A 0.3175 cm thick stainless steel blockage plate is located 10.2 cm above the start of the heated zone to block several (14) edge and internal channels along the left duct wall. The blocked cross-sectional area is illustrated with a thick gray outline in Figure 11 (left). The Pronghorn-SC model's geometry and subchannel/rod index notation is shown in Figure 11 (right). Pronghorn-SC modeled the blockage with a 92% area reduction on the affected subchannels and a local form loss coefficient of 6.

The subchannel index mapping between the Pronghorn-SC model and the experimental convention as follows: 34(39), 33(38), 18(20), 9(19), 3(4), 0(1), 12(11) and 25(30). The number outside the parentheses refers to the Pronghorn-SC model and the number inside the parentheses refers to the experimental convention.

Both a high flow and low flow case are modeled, and results are compared against the thermocouple measurements in the middle of the exit region on the channels (Figure 12). The code calculations exhibit good agreement with the experimental measurements.

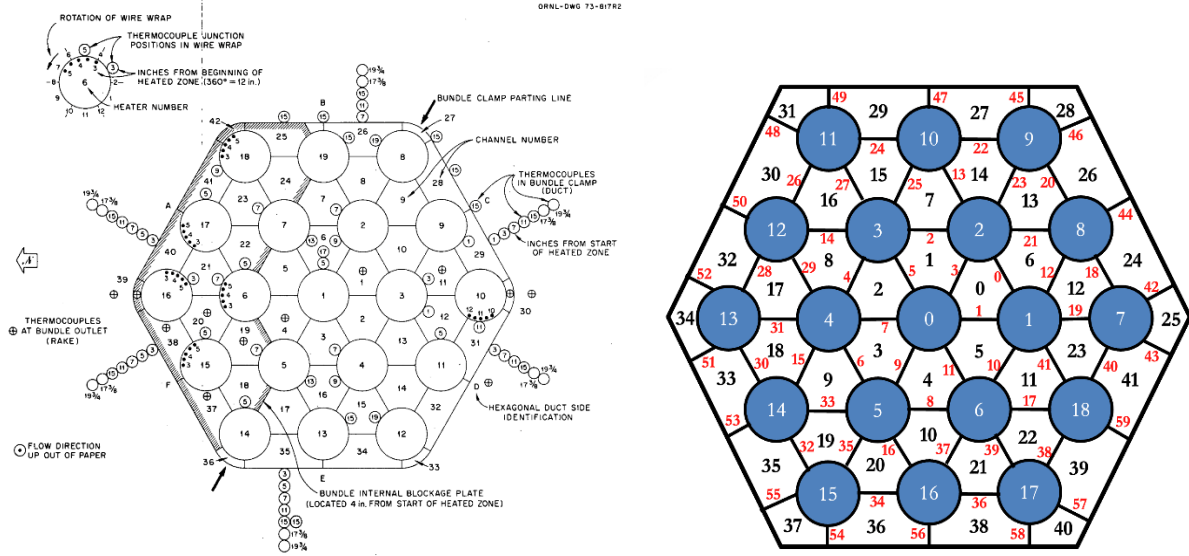


Figure 11. THORS bundle 5B (cross-section) showing (left) blockage area outlined in gray, and (right) Pronghorn-SC model geometry and subchannel/rod notation (white: fuel pin index; black: subchannel index; red: gap index).

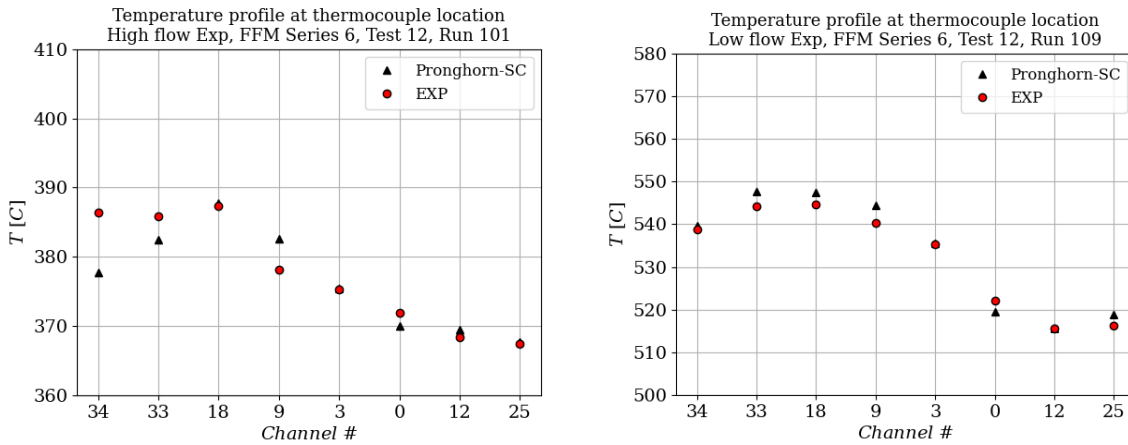


Figure 12. Exit temperature profile for THORS bundle 5B (left) high flow case and (right) low flow case.

3 Summary

Computational models for several advanced reactor concepts have been developed under the NEAMS program and shared openly with the reactor community on the NRIC Virtual Test Bed website and Github repository. The contributed models span various phenomena present in a wider range of advanced reactor concepts. Specifically, new models of experimental configurations were shared including HTTF (HTGR), MSRE (MSR), and THORS (LMFR). Models for MSR concepts were also shared including a model for LOTUS-MCFR and MSFR. Finally, models studying multiphysics transients and fuel performance in a hypothetical HP-MR were contributed.

These models demonstrate the use and best practices of various NEAMS codes on advanced reactor concepts. The open sharing of these models on the VTB permits interested parties to pick up these public models for academic purposes, collaboration opportunities, and for conversion to proprietary models. Open access to working, best practices models lowers the barrier to entry for adoption of advanced modeling and simulation tools by industry, regulators, academia, and other Department of Energy collaborators. The NEAMS program will continue to contribute advanced reactor models to the nuclear community via the NRIC VTB in the future.

4 Acknowledgements

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Model development was funded by the NEAMS program unless otherwise noted, and in most cases, the National Reactor Innovation Center (NRIC) funded the porting of models to the Virtual Test Bed including the generation of detailed documentation. NRIC also supported the model peer review process as well as maintenance of the VTB site. We thank both NEAMS and NRIC for their support in making the sharing of these models possible.

Large teams were involved in the initial creation of these models under the NEAMS program. These teams are acknowledged in reports listed in the VTB documentation for each model. The porting of these models, which is the focus of this technical report, was made possible by the points of contact listed in this report.

5 References

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