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Refining NEAMS MARVEL Reactor Model Accuracy

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eling and Simulation (NEAMS)

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SUMMARY

This report outlines the progress Idaho National Laboratory made in improving the fidelity of the multiphysics Microreactor Applications Research Validation and Evaluation (MARVEL) reactor model, developed in Fiscal Year 2024. The MARVEL reactor is a Department of Energy Microreactor Program–funded reactor development project.

The multiphysics model first developed in Fiscal Year 2024 leverages three single-physics models coupled via the Multiphysics Object-Oriented Simulation Environment (MOOSE) MultiApps and Transfer systems. The first single-physics model, which functions as the driver application, leverages Griffin to model neutron transport in the core through the discontinuous finite element discrete ordinates solver (SN). The second single-physics model uses BISON to compute the solid temperature in the reactor. Finally, the System Analysis Module (SAM) was used to model the flow of the sodium-potassium eutectic in the primary loop. In this report, we detail the following improvements:

- An updated mesh leveraging the latest feature in the reactor module (Section 3.1.)
- A verification of NEAMS neutronic models against reference Monte Carlo N-particle benchmarks (Section 3.2.)
- An enhanced representation of material properties in the solid heat transfer model (Section 3.3.)
- The development of a thermal-hydraulic subchannel model to capture NaK temperature distributions (Section 3.4.).

Future work will focus on leveraging these improvements to simulate selected transient scenarios, including a reactivity insertion accident.

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Specific contributions:

1. Dr. Stefano Terlizzi—Conceptualization, Mesh, Neutronic model, Solid heat transfer model, Formal analysis, Investigation, Writing, Review & editing, Visualization.
2. Dr. Jan Vermaak—Sub-channel model integration, Writing, Review & editing, Visualization, Supervision and Management.
3. Dr. Lise Charlot—Thermal hydraulic model development and analysis, Visualization, Supervision and Management.

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ACRONYMS

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MARVEL Microreactor Applications Research Validation and Evaluation

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Refining NEAMS MARVEL Reactor Model Accuracy

1. INTRODUCTION

The Microreactor Applications Research Validation and Evaluation design is an 85 kWth microreactor nuclear test bed funded under the Department of Energy Microreactor Program (MRP) projected to start operations at Idaho National Laboratory in 2028 [3]. Once operational, MARVEL is planned to demonstrate several operating features of microreactors, including the investigation of diverse electrical and thermal applications and the evaluation of autonomous controls. The MARVEL design will employ uranium zirconium hydride (UZrH) for fuel and sodium-potassium eutectic (NaK) for coolant. Reactivity control is performed through four boron carbide (B₄C) control drums. The reactor will utilize a power conversion system to generate up to approximately 20 kWe.

It should be noted that the MRP maintains an ensemble of physics models to support the licensing of the reactor. These models are separate from those developed under the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, which aims to assemble a computational model using NEAMS tools. This report details the progress made in improving the accuracy and performance of the full-core multiphysics model of MARVEL that was initially developed in Fiscal Year (FY) 2023–2024 [1]. During this FY25, we focused on enhancing the fidelity of this model by improving several aspects, including the mesh, performing additional verification for the neutronics, and developing a novel subchannel model to capture the nonhomogeneous temperature field in the coolant. The remainder of the report is structured as follows. Section 2. summarizes the characteristics of the model developed in FY24, while the work performed in FY25 is detailed in Section 3.. Finally, a summary and future work are addressed in Section 4..

2. FY24 MULTIPHYSICS MODEL

The MARVEL model developed in FY24 coupled three single-physics models using the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework [4].

1. A full-core neutronic model developed in Griffin, in which the angular flux was computed using the discontinuous finite elements, discrete ordinates solver (DFEM-SN) [5],
2. a full-core heat transfer model in BISON [6], and
3. a system-level System Analysis Module (SAM) model for thermal hydraulics as fully described in Reference [7]. The full coupling scheme is reported in Figure 1, while the transfers used are shown in Table 1.

Table 1. Transferred quantities within the coupling scheme. The transfer numbers refer back to the labels used in Figure 1 from Reference [1].

Transfer Number	Transferred Quantities
a ₁	$P_d; T_f; h_f$
a ₂	$T_c; h_c; \rho_c$
b ₁	P_d
b ₂	T_s

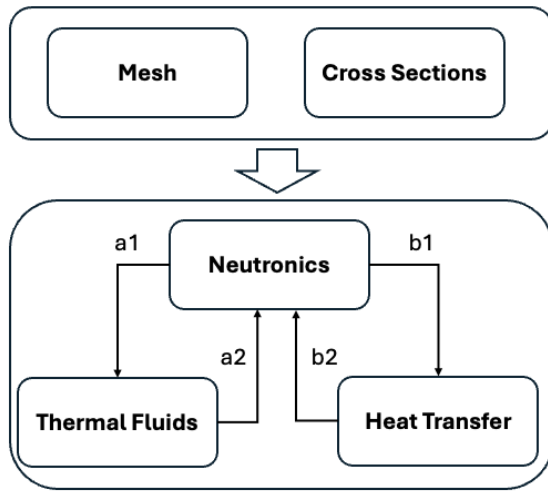


Figure 1. Multiphysics coupling scheme for steady-state calculations from Reference [1].

The model was leveraged to compute the power density and temperature distributions in steady state as shown in Figure 2. The full description of the model is reported in Reference [1].

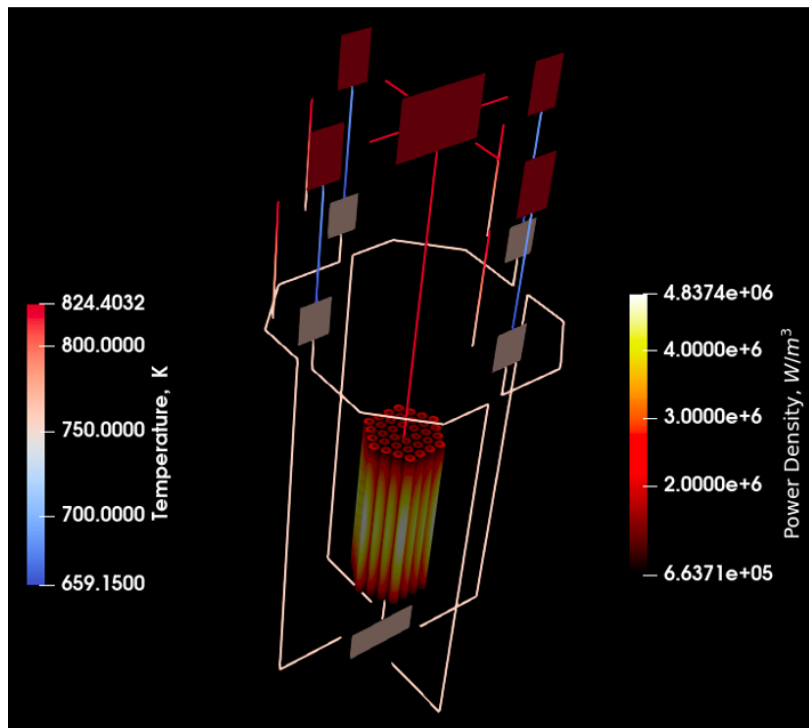


Figure 2. Power density and coolant temperature distribution for the FY24 model [1].

3. MULTIPHYSICS MODEL IMPROVEMENTS

The model developed in FY24, although representing the first NEAMS-based multiphysics model of MARVEL, exhibited several limitations. These included a reliance on multiple geometric simplifications, the absence of neutronic verification against reference Monte Carlo N-particle (MCNP) design calculations, and a limited spatial resolution of coolant temperature resulting from the use of the thermal-hydraulic SAM model.

This section summarizes the improvements made in FY25 to the single physics models. Specifically, the following updates have been incorporated:

1. An updated mesh leveraging the latest features in the MOOSE Reactor Module (Section 3.1.).
2. The neutronic model was updated to reflect the most recent MRP-provided MARVEL geometry and initial verification of NEAMS neutronic models against reference MCNP benchmarks provided by the MRP (Section 3.2.).
3. Enhanced representation of material properties and geometry in the solid heat transfer model (Section 3.3.).
4. Development of a thermal-hydraulic subchannel model to capture the NaK nonhomogeneous temperature distribution in the core (Section 3.4.).

3.1. Neutronic and Heat Transfer Mesh

A new mesh was developed to more accurately represent the reactor geometry. Special emphasis was posed on the beryllium inner reflector that features a curved profile following the outer ring of fuel pins. In FY24, the curved reflector surfaces were approximated using a polygonal line, which introduced artificial temperature peaks at the geometric edges, see Figure 3.

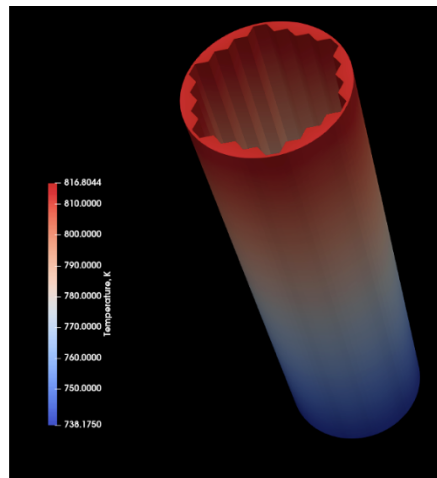


Figure 3. A picture of numerical artifacts due to the polygonal line profile.

To mitigate the numerical artifacts caused by approximating the curved profile with curved polygonal lines, we decided to employ the `PolyLineMeshGenerator` capability of the MOOSE reactor module [8]. The curve was defined using a custom Python utility that generated 100 discrete points along the inner surface

of the beryllium inner reflector. The points generated by the custom Python script are shown in Figure 4, while Figure 5 compares the FY24 inner reflector mesh with the updated version adopted in FY25.

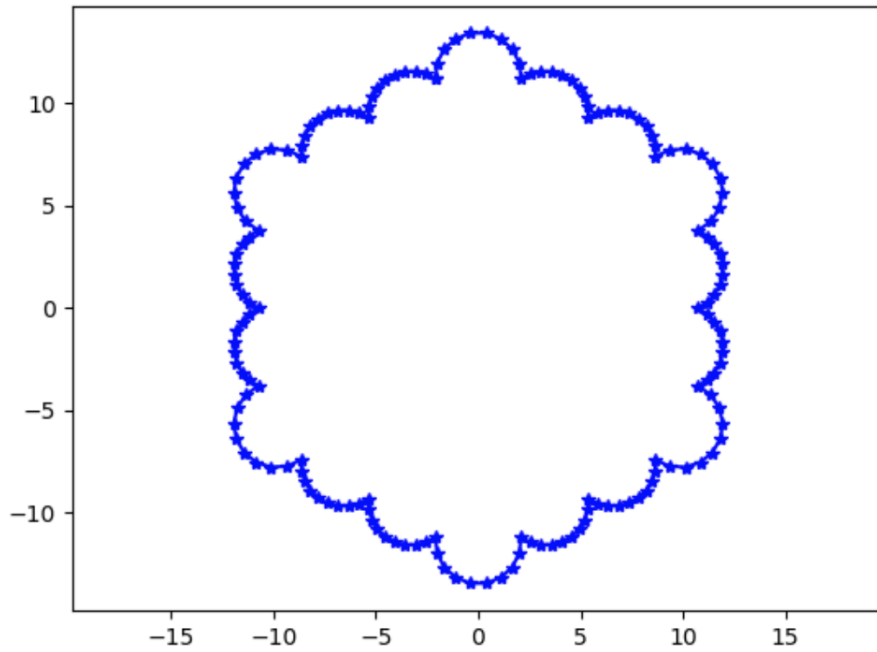


Figure 4. Points generated with a custom Python script for PolyLineMeshGenerator.

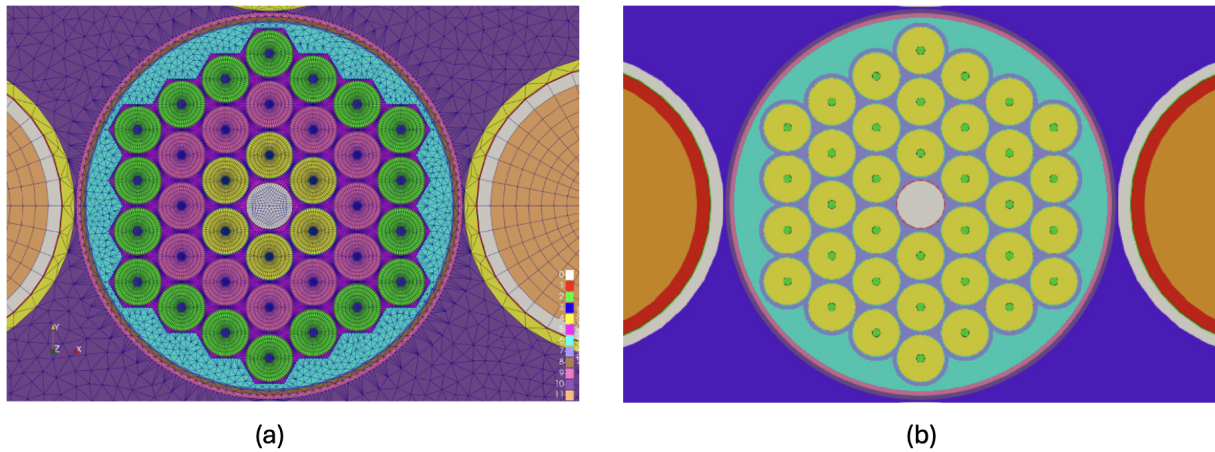


Figure 5. Zoom-in at the mid-plane for the (a) FY24 mesh from Reference [1] and (b) the FY25 mesh used in this work.

An additional modification was introduced for the control drum geometry in the thermal mesh. In the previous model, the absorber and structural materials were homogenized, resulting in a simplified representation. To more accurately capture the temperature and flux distributions in these distinct regions, the `AzimuthalBlockSplitGenerator` capability was employed to explicitly define the beryllium carbide poison segment. The control drums in their updated form can be seen in the full-core representation shown in

Figure 6. The control drums are still idealized with respect to the original MCNP model. However, cross sections were averaged over the heterogeneous geometry to conserve reaction rates despite the geometrical simplifications.

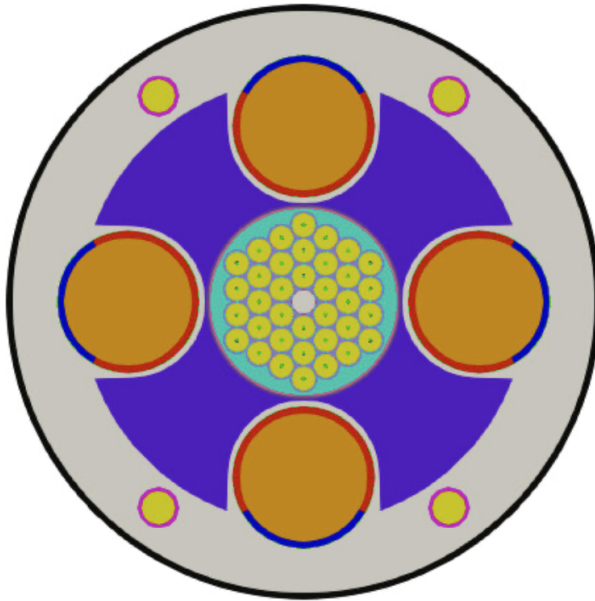


Figure 6. Full-core geometry for the MARVEL reactor neutronic mesh.

3.2. Neutronic Model Update and Verification vs. MCNP Reference Results

The neutronic model geometry was updated to match the geometry of the MARVEL reactor by modifying the existing pseudo-MARVEL concept, which, as illustrated in References [1]–[9], was a simplified geometrical representation. The results obtained with the updated geometry were verified for selected conditions against reference calculations performed with MCNP and reported in ECAR-6099-Rev. 1 [2].

3.2.1. Control Drum Reactivity Worth Curve

The control drum reactivity curves were evaluated under cold zero power (CZP) conditions, where an isothermal temperature of 294 K was imposed throughout the model. The effective multiplication factor, denoted by k_{eff} , calculated with the Griffin DFEM-SN solver was compared to reference results obtained using MCNP. The comparison, summarized in Table 2, shows discrepancies ranging between 164 and 557 pcm across all cases. This order of magnitude is consistent with expectations for microreactors employing a nonoptimized energy structure [10].

The observed bias is likely not solely attributable to the nonoptimized energy structure. It may also be partially influenced by the combined effects of:

1. **Anisotropic scattering treatment**—The cross sections generated in SERPENT for Be and BeO reflectors do not fully capture anisotropic scattering, as they are weighted by the angular flux rather than by higher-order flux moments.

2. **Geometric simplifications**—Approximations in the modeled geometry of the Be and BeO reflectors, as well as the control drums, introduce additional error.

Ongoing work aims to reduce this bias by addressing these limitations.

Table 2. Comparison of MCNP and Griffin k_{eff} .

θ	MCNP	Griffin	Error
0	0.91319	0.90889	-470
30	0.92108	0.91745	-394
60	0.95376	0.95045	-347
90	0.99585	0.99011	-576
120	1.02193	1.01623	-557
150	1.03259	1.03089	-164
180	1.03486	1.03201	-275

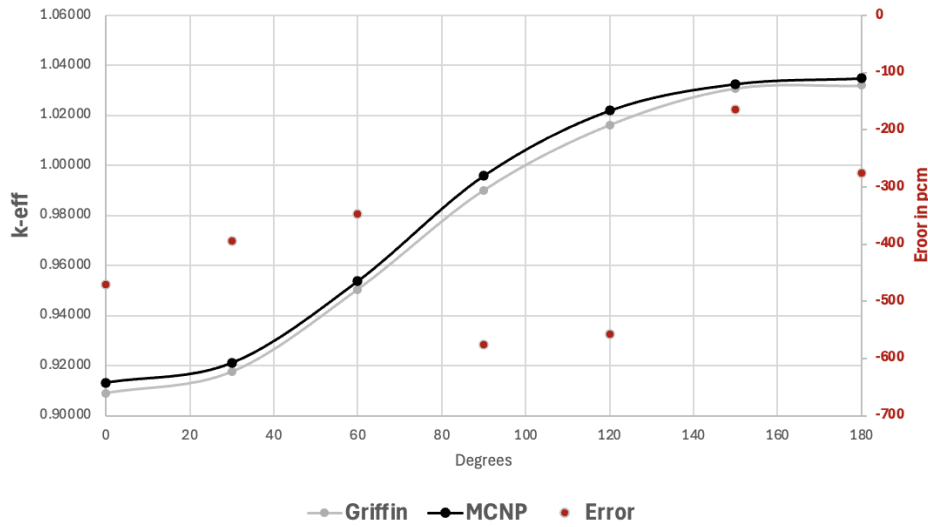


Figure 7. k_{eff} vs. angle of insertion of the control drums and relative error. The MCNP values are taken from Reference [2].

3.2.2. Temperature Reactivity Coefficients

The temperature reactivity coefficients were computed at 300–600 K, 600–900 K, and 900–1200 K, consistently with the neutronic engineering calculations and analysis report for MARVEL [2]. The reactivity coefficients were computed by varying the temperature of the material of interest, while keeping the remainder of the core at the environmental condition of 294 K. The results for the calculations are reported in Table 3 and show a good agreement for all the scenarios. The coefficients were computed using the following equation:

$$\alpha = \frac{1}{k} \frac{\Delta k}{\Delta T}, \quad (1)$$

where k denotes the effective multiplication factor and T the temperature.

Table 3. Temperature reactivity feedback coefficients in pcm/K.

Material	Temperature, K	MCNP	Griffin
UZrH	300–600	-5.46E-05	-5.33E-05
	600–900	-5.20E-05	-5.16E-05
	900–1200	-4.76E-05	-4.73E-05
BeO	300–600	1.74E-05	1.68E-05
	600–900	1.08E-05	1.10E-05
	900–1200	8.37E-06	8.86E-06
Be	300–600	4.15E-06	4.32E-06
	600–900	2.51E-06	2.48E-06
	900–1200	1.94E-06	2.01E-06

The table shows the predominance of the fuel temperature feedback that accounts for the Doppler effect and scattering libraries change. The coefficients computed with MCNP also account for axial thermal expansion that is not included in Griffin. Both the Be and BeO thermal feedback account for thermal scattering and Doppler effects.

3.2.3. Power Distribution

The axial peaking factor was computed at CZP and the critical drum position. The power distribution is obtained with a user object for 10 equally spaced points along the axial direction (i.e., z-axis). The profile is sinusoidal and near-symmetrical with respect to the center of the reactor. This is due to the weak neutron reflection provided by the graphite axial reflectors. In fact, despite having a top and bottom reflector of different thicknesses (i.e., the bottom reflector is 5 cm thicker), this does not result in tilting of the power distribution. This is comparable to Figure 7-3 in Reference [2] where the normalized maximum axial power peak is just above 1.2 and the minimum is equal to 0.6.

The radial peaking was also calculated for the CPZ configuration, showing the same radial pattern observed in Figure 7-4 of Reference [2] with the maximum value in the external ring due to neutrons reflected from the beryllium and beryllium oxide reflectors. No numerical comparison is performed between the two distributions in this case since the distribution in the engineering calculations and analysis report was obtained at hot full-power conditions. Figure 7-4 of Reference [2] also corroborates the observation on the importance of capturing the effect of the reflectors on the neutronics.

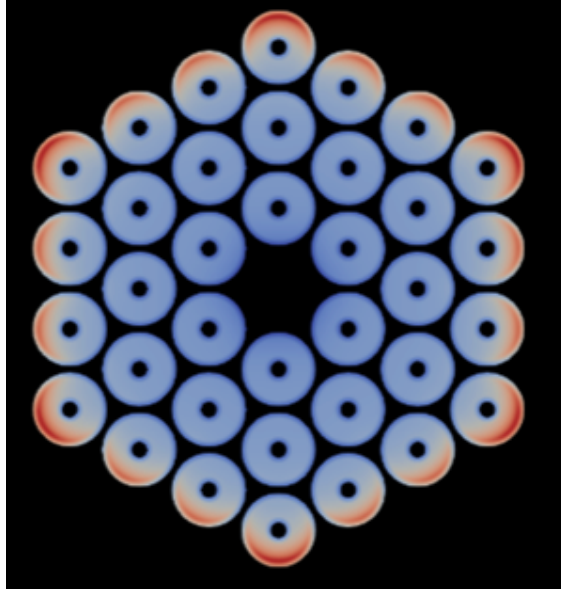


Figure 8. Radial power profile of the MARVEL reactor core.

3.3. Improving the Solid Heat Transfer Model

In addition to updating the mesh as described in Section 3.1., the material definitions were updated to use the most accurate material properties implemented in BISON [6] rather than constant properties as in FY24. The properties are dependent on temperature and burnup. For all the calculations we assumed zero burnup and, therefore, fresh fuel.

The temperature profile for the whole core at the axial mid-plane is reported in Figure 9. The temperature is relatively flat in the solid materials due to the high conductivity of the beryllium and beryllium oxide that are employed for the MARVEL inner and external reflector, respectively.

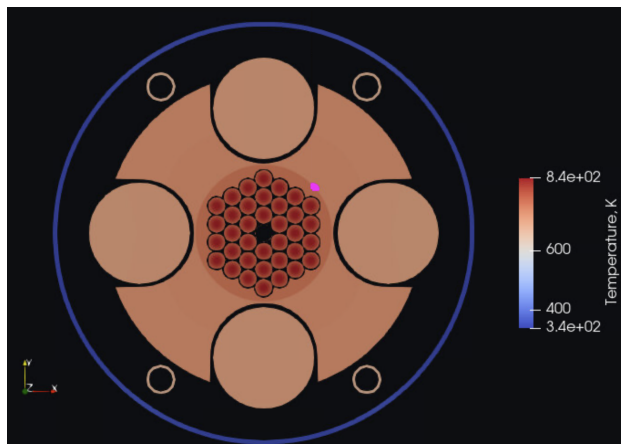


Figure 9. Temperature distribution in the mid-plane for the full reactor.

Importantly, the geometry fidelity improvement due to the updated mesh together with the use of correct conductivities leads to a decreased temperature gradient across the space dividing the inner and outer reflectors,

from 100 K to about 30 K, see Figure 10. The latter temperature difference is much closer to the value reported in Reference [11], where the temperature difference is below 10 K. Ongoing work is focused on adding nonlocal power deposition to match more closely the results from Reference [11]. It is expected the nonlocal energy deposition, accounting for 2% of the thermal energy, will contribute to further reducing the temperature difference between the outer surface of the inner reflector and outer reflector.

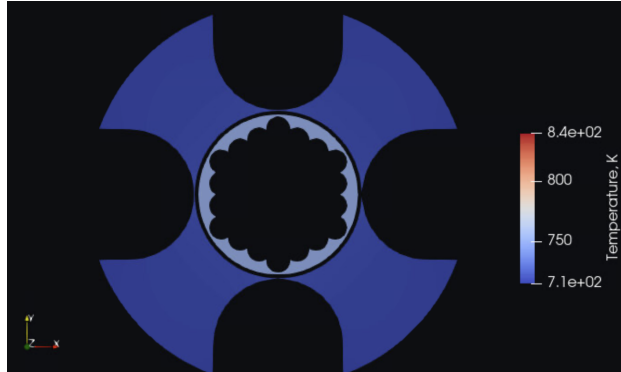


Figure 10. Temperature distribution in the mid-plane of the two reflectors rescaled to the maximum temperature in the inner reflector.

3.4. Subchannel T/H Model Development

The system-level thermal hydraulics of the MARVEL model is simulated using SAM, which is a MOOSE-based thermal-hydraulics code developed by Argonne National Laboratory [7]. The SAM model includes the flow paths in and around the core with a simplified in-core model.

To enhance the in-core fidelity, a subchannel model is employed using the Sub-Channel Module (SCM), which is MOOSE-based module with specific features suited to the MARVEL core [12]. The SCM code was developed in collaboration with the Thermal Hydraulics Technical Area and is fully described in Reference [13]. The SCM model includes fuel pin and subchannel geometries with one-dimensional (1D) representations as shown in Figure 11. The 3D mesh elements in the figure shows the mesh used by the solid heat transfer model. The mesh from FY24 was used for this initial coupling to minimize dependencies between the work performed at INL and Penn State. The “lines” in the figure are the 1D mesh representations from SCM.

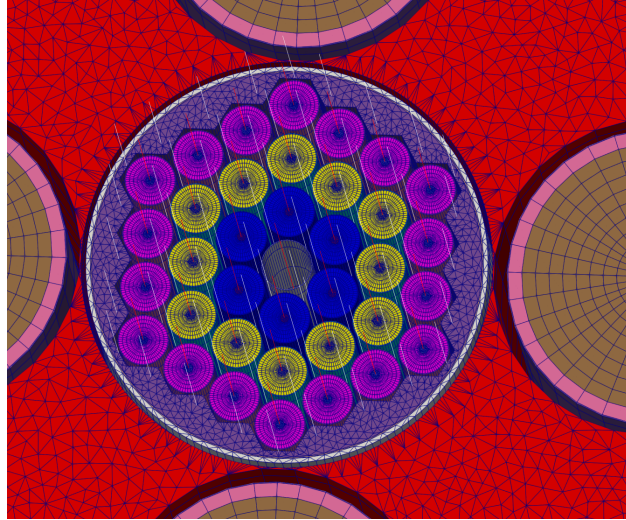


Figure 11. Visualization of the 1D SCM mesh elements superimposed onto the mesh used by the solid heat transfer model.

Preliminary results for the SCM model show a core temperature rise of 63.2 K, which is not quite close enough to the published value of 69 K [14]. This could be a difference in thermal properties and is still being investigated.

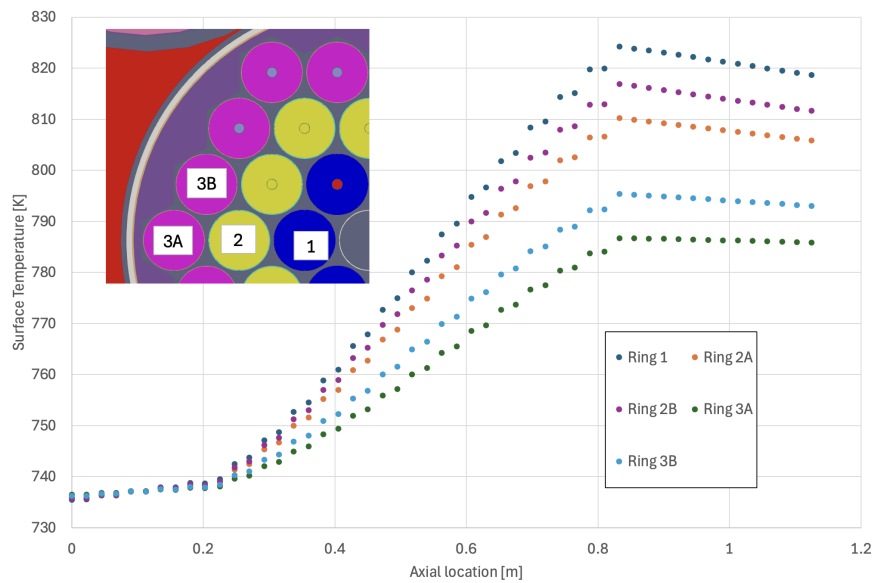


Figure 12. Preliminary results for fuel pin surface temperature (circumferential-average) obtained from the SCM model.

4. SUMMARY AND FUTURE WORK

The current fiscal year was focused on improving the single physics models developed in FY24. In particular, the following improvements were made:

- An updated mesh leveraging the latest feature in the reactor module (Section 3.1.).
- The ongoing verification of NEAMS neutronic models against reference MCNP benchmarks (Section 3.2.).
- An enhanced representation of material properties and geometry in the solid heat transfer model (Section 3.3.).
- The development of a thermal-hydraulic subchannel model to capture NaK radial temperature distribution in the core (Section 3.4.).

Ongoing work will generally be focused on leveraging the improved single-physics models to perform steady-state and transient multiphysics analysis. In particular, the following future work is planned for FY26:

- By coupling together the MOOSE-based thermal-hydraulics codes, steady-state and transient simulation results can be compared to the MRP RELAP5-3D model or at least a surrogate model of the MRP model if the MRP program chooses not to share their latest model.
- The MARVEL thermal-hydraulics experiment called the Primary Coolant Apparatus Test has collected experimental data that can be used to validate thermal-hydraulic models. Comparing the results of a RELAP5-3D model to that of MOOSE-based models is planned.
- The control drum cusping effect needs improvement and will be addressed.

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