INL/RPT-23-74793

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Idaho National Laboratory

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SUMMARY

Efforts are currently underway to deploy microreactor modeling and simulation tools to better support vendors and regulatory authorities in submitting and reviewing licensing applications. In particular, the Nuclear Regulatory Commission is expected to rely on the Comprehensive Reactor Analysis Bundle (BlueCRAB) multiphysics toolset in performing design- and beyond-design-basis accident analyses. In addition, the Nuclear Regulatory Commission has been using the MELCOR code to estimate mechanistic source terms during accidents. As MELCOR relies on isotopic inventory and reactor temperature/power evolution profiles during accident conditions—all of which can theoretically be obtained from BlueCRAB—the ultimate goal of this activity is to establish a common BlueCRAB-MELCOR framework. However, prior to the present research, BlueCRAB had never been used to calculate such quantities of interest at the full-core level. While there are many Monte Carlo (MC) codes capable of computing such quantities of interest, they are unable to readily account for multiphysics feedback. BlueCRAB allows for the coupling of different physics codes together to perform multiphysics-informed calculations. Therefore, the purpose of this fiscal year 2023 work is to investigate the feasibility and challenges of performing such calculations within BlueCRAB so as to generate the data that MELCOR relies on.

To demonstrate the methodology, the proposed workflow was applied to a prototypical heat pipe-cooled microreactor model. To predict isotopic concentrations (taking into account the accumulation of fission products during operation), the necessary microscopic cross sections were generated via OpenMC and tabulated with respect to temperature and burnup. Next, a recently developed capability in Griffin (the reactor physics application in BlueCRAB) was used to convert the OpenMC output format into the ISOXML format used by Griffin. A multiphysics microscopic depletion calculation that involved performing a coupled full-core, heterogeneous neutron transport and thermal calculation at each depletion step was conducted to deplete the core to end of life (EOL) conditions so as to provide both isotopics and the initial condition for the transient calculation. Following a brief null-transient to verify that the initial condition had been properly restarted and was indeed in thermal equilibrium, a heat pipe failure transient was simulated.

Thus, the entire workflow of using BlueCRAB to generate MELCOR inputs, from cross-section generation to producing isotopic inventory and power/temperature evolution profiles during transients, is demonstrated. This report also details the identified gaps in the workflow and how they were (for the most part) addressed. Future work should focus on directly including MELCOR into the workflow by performing a MELCOR calculation using the BlueCRAB-generated input data. In addition, the heat pipe reactor design should be improved so as to reflect more prototypical burnup characteristics at EOL.

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CONTENTS

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ACRONYMS

BlueCRAB Comprehensive Reactor Analysis Bundle

CMFD Coarse-Mesh Finite Difference

DFEM discontinuous finite element method

EOL end of life

HP heat pipe

HPs heat pipes

INL Idaho National Laboratory

MC Monte Carlo

MOOSE Multiphysics Object-Oriented Simulation Environment

SiMBA Simplified Microreactor Benchmark Assessment

Sn discrete ordinates

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1 INTRODUCTION

MELCOR plays a pivotal role in reactor safety analysis, serving as a specialized tool centered around analyses of severe accidents that lead to radiological release. Developed at Sandia National Laboratories in the early 1980s for use in modeling light-water reactors, MELCOR has since evolved into a comprehensive severe accident code. Its versatility has been expanded to encompass advanced reactor types such as high-temperature gas-cooled reactors and sodium fast reactors [1]. To perform accident analyses, MELCOR relies on input full-core isotopic inventory and power/temperature evolution profiles throughout the postulated accident. Though MELCOR is capable of producing such input via simplified models, these internal models are potentially not as accurate as external models. These quantities of interest can be computed using a high-fidelity multiphysics code such as the Comprehensive Reactor Analysis Bundle (BlueCRAB), which is comprised of an array of codes designed to simulate various aspects of reactor behavior, including system thermal hydraulics, neutronics, core thermal hydraulics, and fuel performance. BlueCRAB relies on the Multiphysics Object-Oriented Simulation Environment (MOOSE), which was developed at Idaho National Laboratory (INL).

As MELCOR relies on isotopic inventory and reactor temperature/power evolution profiles during accident conditions—all of which can theoretically be obtained from BlueCRAB—the overarching goal of this work is to establish a streamlined workflow for conducting BlueCRAB-informed MELCOR simulations of advanced microreactor technology. In particular, this report focuses on work performed using BlueCRAB to generate the mechanistic source term (i.e., isotopic inventory) and time-dependent power/temperature spatial distributions during accident scenarios under end of life (EOL) conditions, when the source term is largest. This information is intended to be passed on to MELCOR when performing release calculations for advanced microreactor technology. The main advantage of BlueCRAB over Monte Carlo (MC) methods is that it accounts for multiphysics feedback and can be used to obtain the thermal system response (while MC codes may be leveraged to perform similar calculations, this is a very computationally expensive process to perform on full-core models). However, BlueCRAB has never been used to successively generate isotopics for dynamically simulating full-core microreactor transients under EOL conditions. To test the workflow, a prototypical microreactor was defined based on the Simplified Microreactor Benchmark Assessment (SiMBA) problem presented in Ref. [2]. Feeding time-dependent temperature distributions—computed using BlueCRAB's high-fidelity multi-dimensional models—to MELCOR's release models should enable analysts to improve the accuracy of their results.

The remainder of this report is organized as follows. Section 2 describes the problem used to test the BlueCRAB workflow. Section 3 discusses the BlueCRAB-MELCOR workflow. Section 4 shows and discusses the results of the BlueCRAB-MELCOR workflow, as applied to the microreactor model, and discusses the workflow gaps addressed. Finally, Section 5 presents the conclusion reached over the course of this research, and describes future work aimed at fully deploying a BlueCRAB-MELCOR framework.

2 MODEL DESCRIPTION

To establish a workflow between BlueCRAB and MELCOR, a problem derived from the SiMBA problem was leveraged. The SiMBA fuel assembly is a modification of the Empire reactor's fuel assembly [3] obtained by switching the positions of the moderator and fuel rods. Small adjustments to the rod diameters were also made. These modifications were performed to obtain a negative temperature reactivity coefficient. In fact, the original Empire reactor concept is characterized by a moderator temperature coefficient of 5 pcm/K, against a fuel temperature coefficient of -1.2 pcm/K. The design was made generic enough to avoid any proprietary concerns, but specific enough to capture the primary design characteristics of envisioned heat pipe (HP)-cooled monolithic microreactors [2].

2.1 Model Description at Beginning of Life

The SiMBA problem is a 2 MW microreactor composed of 18 hexagonal assemblies arranged into two rings. The tops and bottoms of these 160-cm-high assemblies are surrounded by 20-cm-high axial beryllium reflectors. Each assembly contains 96 fuel pins that are 1 cm in radius, 60 YH_x pins that are 0.975 cm in radius, and 61 1-cm-radius sodium HPs drilled into a graphite monolith. The HPs penetrate only into the top axial reflector, making the reactor axially asymmetric. The central shutdown rod slot is empty. The core is surrounded by 12 control drums, with boron carbide employed as the absorbing material. To enable a simplified mesh, the beryllium radial reflector is hexagonal. Figure 1 shows an axial and radial view of the reactor, as produced using OpenMC [4]. The material and geometry specifications are reported in Tables 1 and 2, respectively.

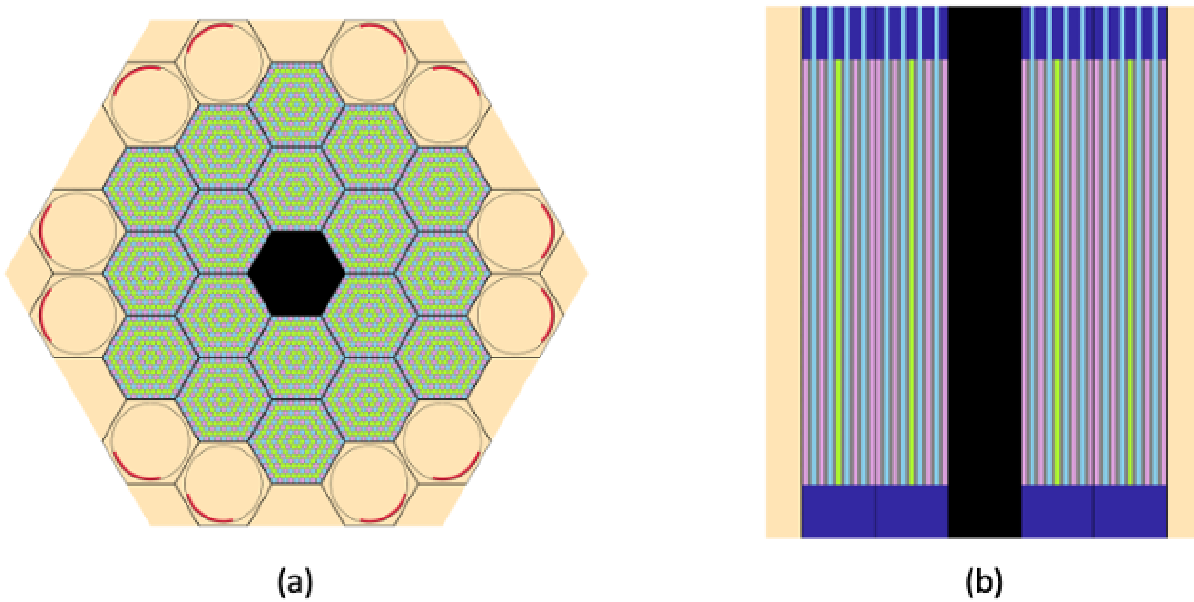

Figure 1: (a) Radial and (b) axial view of the OpenMC model geometry.

Table 1: Materials of each component and their corresponding densities (Table courtesy of [2]).

Component	Material	Density, g/cm^3	Conductivity, W/(m $\cdot$ K)
Fuel	UN	14.3	300
Moderator	$YH_{1.8}$	4.30	500
Monolith	Graphite	1.80	1830
Heat Pipe	SS-316+Sodium	2.27	N/A
Absorber	B_4C	2.52	20
Reflector	Be	1.85	200

2.2 Heat-Pipe Failure Accident Progression at End of Life

To reduce the computational resources required for the simulation, a 2D slice of the SiMBA core was modeled. Additionally, planes of symmetry were identified that divide the core into 12 sections. Reflective boundary conditions were imposed on the reflection boundaries, and all simulations were performed on a 1/12th section of the core. The microreactor was depleted for 10 years to EOL by using BlueCRAB (the temperature feedback was accounted for during this calculation). Shortly after that 10-year period, an accident was postulated in which 2 HPs simultaneously failed

Table 2: Geometrical specifications of the SiMBA reactor assembly (Table courtesy of [2]).

Property	**Value**
Fuel Radius, cm	1.0
Moderator Radius, cm	0.975
Heat Pipe External Radius, cm	1.0
Monolith Pitch, cm	2.15
Unit Assembly Flat-to-Flat, cm	32
Assembly Height, cm	160
Core Flat-to-Flat, cm	195.3
Poison Strip Internal Radius, cm	14.8
Arc Width for Poison Strip, deg	120
Control Drum External Radius, cm	15.0
Axial Reflector Thickness, cm	20.0
Enrichment, wt%	19.75

in the simulation domain (there being 24 failed HPs over the full core). Although simultaneously failing this many HPs is not necessarily realistic, this number was arbitrarily chosen to test and demonstrate the capabilities of BlueCRAB. Figure 6 shows 2 failed HPs on a 1/12th slice of the core. Note that, though three HPs (green circles) appear in the figure, the domain slice excludes half of two of them. The accident sequence of events is summarized in Table 3.

Table 3: Accident sequence of events.

Time Range	Event	BlueCRAB Simulation Type
$0 \rightarrow 10$ yr	Depletion at full power	Depletion
10 yr $\rightarrow$ 10 yr + 60 s	Full-power operation at steady-state	Transient
10 yr + 60 s $\rightarrow$ 10 yr + 2000 s	HP failure accident	Transient

3 ENVISIONED BLUECRAB-MELCOR WORKFLOW

The codes utilized in the workflow are described in Section 3.1. Section 3.2 describes how they were integrated into the workflow.

3.1 Code Description

Here, a brief overview of each code is given, along with a description of how it was used in this work.

3.1.1 OpenMC

OpenMC is a MC particle transport simulation code primarily designed for neutron transport calculations in nuclear reactor physics and radiation shielding applications. Developed and maintained by a collaborative community of scientists and engineers, OpenMC leverages the MC method to simulate the behavior of neutrons for various materials and geometries. OpenMC can perform fixed-source, k-eigenvalue, and subcritical multiplication calculations and can generate flux-weighted cross sections for multigroup transport problems. [4]

In this work, OpenMC was used to generate multigroup microscopic cross sections for BlueCRAB's transport and depletion solver, Griffin. OpenMC was chosen over other MC codes (e.g., Serpent) for its ability to easily and seamlessly generate multigroup microscopic cross sections (including the group-to-group scattering cross sections).

3.1.2 MOOSE

The INL-developed MOOSE framework [5], on which BlueCRAB relies, is a versatile open-source platform for solving complex coupled multiphysics problems. Developed with a focus on flexibility and extensibility, MOOSE provides an environment in which researchers and engineers can construct and analyze simulations involving a wide range of physical phenomena such as fluid dynamics, heat transfer, and structural mechanics. MOOSE is distinguished by its object-oriented design, which enables users to define and seamlessly link together multiple physics models. This framework facilitates the development of custom simulations, making it invaluable for addressing diverse engineering and scientific challenges. With its active user community and open-source codebase, MOOSE continues to adapt to meet the evolving demands for multiphysics simulations across various disciplines.

This work utilized MOOSE to couple the neutronics code Griffin to the fuel performance code BISON in order to produce a coupled neutronics-heat conduction simulation that incorporates the effects of thermal feedback. This coupling was accomplished using MOOSE's Multiapp and Transfer systems [6].

3.1.3 Griffin

Griffin [7], a reactor physics analysis tool (found in the BlueCRAB code suite) now in collaborative development at both INL and Argonne National Laboratory, was built on the MOOSE framework. Griffin stands as an application for examining advanced reactor designs, thereby accommodating steady-state and transient (kinetics) simulations. Its capabilities are structured into three components: radiation transport for various solvers, reactor analysis for specific tasks such as depletion, and ISOXML for handling multigroup cross sections and decay transmutation data.

For this work, Griffin was utilized to deplete the core (via successive eigenvalue calculations) and then conduct transient neutron transport calculations. Specifically, the multigroup discontinuous finite element method (DFEM) discrete ordinates (Sn) numerical scheme was employed to discretize the transport equation, while Coarse-Mesh Finite Difference (CMFD) acceleration was used to speed up the solution convergence [8]. The core depletion was performed using microscopic cross sections, thus enabling explicit computation of decay heat. The computed power distribution was used as a source term to solve the heat conduction equation in BISON.

3.1.4 BISON

BISON [9], a MOOSE-based nuclear fuel performance code in the BlueCRAB code suite, utilizes a finite element methodology. BISON offers versatility across diverse fuel types such as light-water reactor fuel rods, TRi-structural ISOtropic (TRISO) particle fuel, and metallic rod/-plate fuel. In this work, BISON was used to perform thermal analyses for obtaining transient temperature distributions throughout the core. It uses the Griffin-provided spatial power distribution as a source term. The resulting temperature distributions affect the cross-section values, in turn affecting the neutronics solutions.

3.2 Workflow Description

For this work, the SiMBA problem referenced in Section 2 was used as a test problem for assessing gaps in the BlueCRAB workflow so as to inform the release model in MELCOR.

3.2.1 Complete Workflow

Figure 2 depicts the complete envisioned BlueCRAB-MELCOR workflow. A detailed explanation of each block in the workflow is given below.

1. Multigroup microscopic cross sections are generated using OpenMC. The cross sections are tabulated with respect to burnup, fuel temperature, and non-fuel (i.e., moderator, reflector, HP, and monolith) temperature.

2. The cross-section library generated via OpenMC in ISOTXS format is converted to ISOXML by leveraging a new converter tool specifically prepared for this work scope.

3. The ISOXML microscopic cross-section library generated in the previous step is input to a coupled neutronics-heat transfer multiphysics depletion calculation in BlueCRAB. The full-core neutron fluxes, temperature, and nuclide spatial distributions at EOL are written to a binary file for use in restarting the transient simulation modeling the accident scenario.

4. A coupled neutronics-heat transfer multiphysics transient accident scenario is simulated in BlueCRAB, using the EOL binary files to establish the initial conditions and depleted fuel compositions.

5. The nuclide inventory from the depletion calculation and the power/temperature profiles from the transient calculation—as computed via BlueCRAB—are used to inform the MELCOR release model, which serves as the basis for calculating the nuclide dispersion in the environment.

The present report focuses on testing and addressing the gaps in the BlueCRAB workflow so as to produce the mechanistic source term and time-dependent temperature distributions for a prototypical microreactor, for use in MELCOR. The full workflow (i.e., including MELCOR simulations) is planned to be completed and fully tested in fiscal year 2024.

3.2.2 BlueCRAB Workflow

We now discuss the process of solving the depletion and transient problems in BlueCRAB. The neutron transport and Bateman (nuclide depletion) [10, 11] equations are solved using Griffin. The

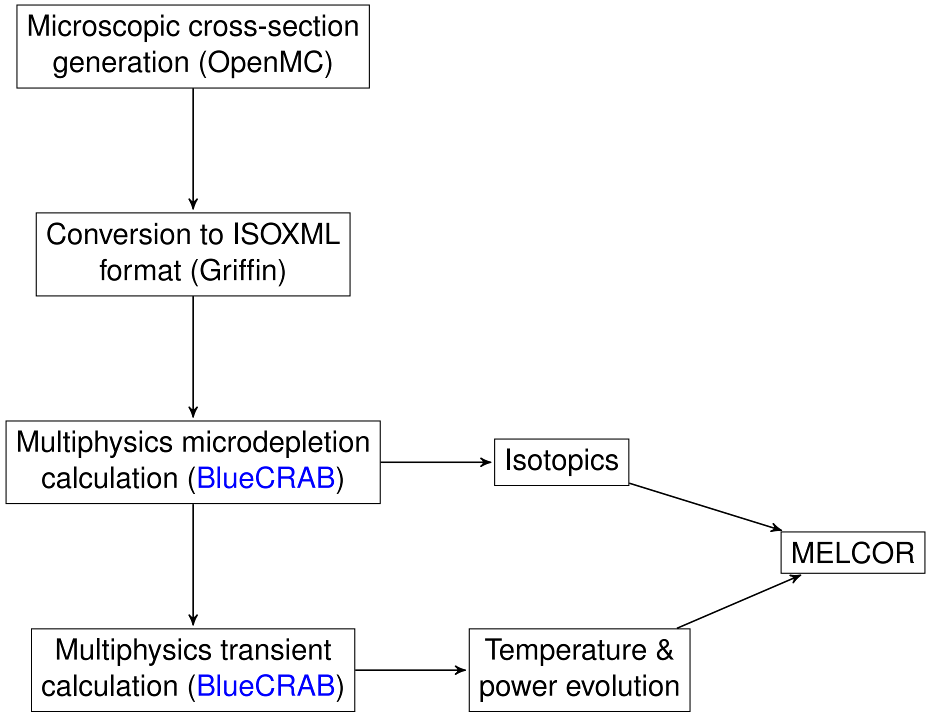

Figure 2: Envisioned BlueCRAB-MELCOR workflow.

thermal solve is performed using BISON. Because cross sections are temperature-dependent, the neutronics and thermal equations must be solved in a coupled fashion, utilizing a fixed-point iteration solution procedure that iterates over different physics until convergence is achieved. Figure 3 illustrates this solution process.

4 ACHIEVEMENTS AND RESULTS

Having described the microreactor model and the envisioned workflow, this section presents the results of the workflow as applied to that model. Section 4.1 describes the simulations performed, and analyzes the numerical results. Section 4.2 discusses gaps discovered in the workflow, in addition to the actions taken to address them. Section 4.3 discusses additional observations made during the course of the work.

4.1 Multiphysics Analysis Results

The cross-section generation procedure is explained in Section 4.1.1, whereas the depletion calculation and HP failure scenario results are reported in Sections 4.1.2–4.1.4.

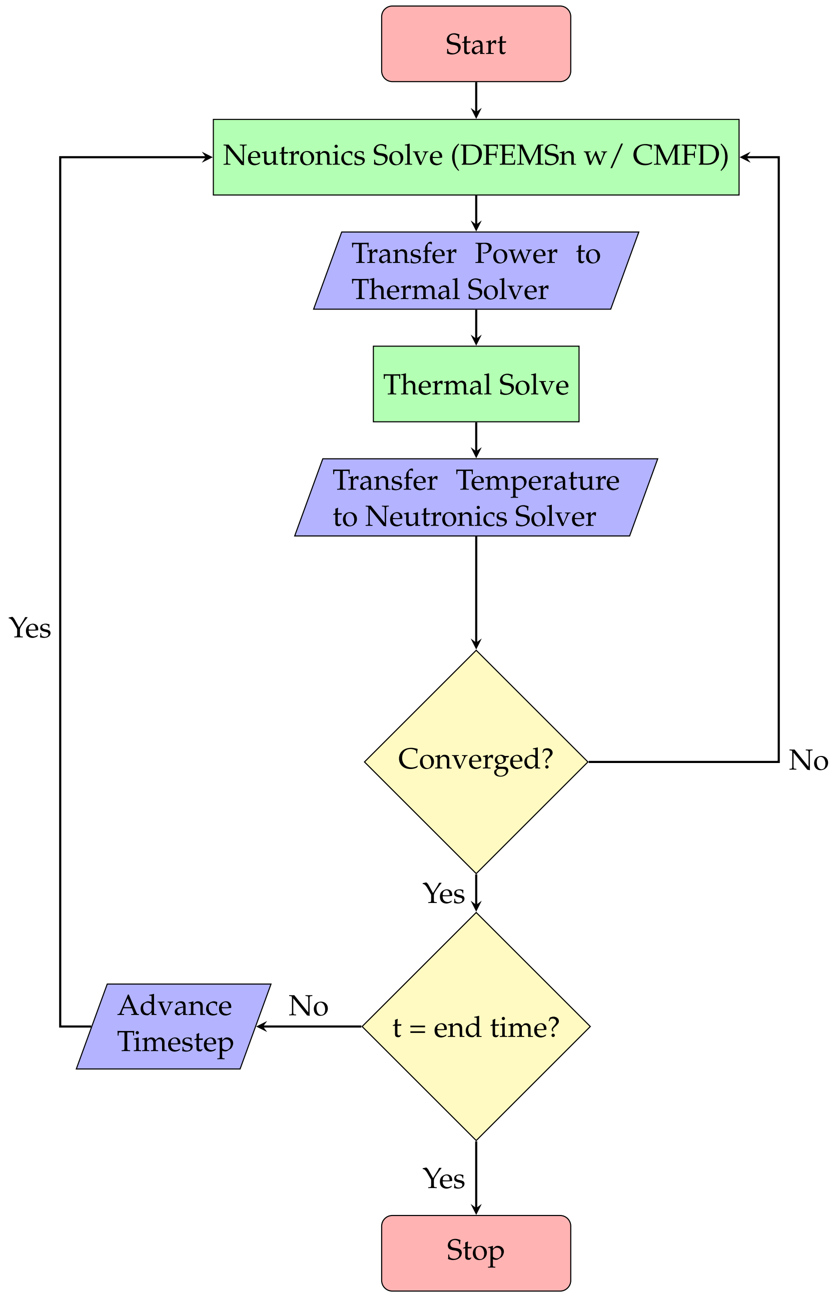

Figure 3: Flowchart for the logic of the coupled neutronics-heat conduction solve.

4.1.1 Multigroup Microscopic Cross-Section Generation

In this work, the OpenMC code [4] was used to generate microscopic cross sections in the multigroup format. This format was required for the deterministic neutron transport calculation and micro-depletion calculation to determine the isotopic composition of the burned fuel in the SiMBA microreactor.

A full core model of the SiMBA microreactor was developed to generate multigroup microscopic cross sections for each material used by BlueCRAB, and to enable parametric neutronics studies of the core. The microscopic cross sections were generated for 233 isotopes in an 11 energy group structure, then tabulated with respect to burnup, fuel temperature, and non-fuel (moderator, reflector, HP, and monolith) temperature in order to account for spectral effects in the cross-section generation stage. The decay chain used to perform depletion calculations with Griffin includes data for 295 nuclides. However, the generated cross sections were only for 233 isotopes, as the fact that some of these nuclides had too-low concentrations resulted in poor statistics when tallied using OpenMC; thus, they were eliminated from the isotopes list. The energy group structure and the cross-section tabulation points are provided in Tables 4 and 5, respectively. The group structure coincides with that reported in Ref. [2]. The cross sections generated by OpenMC are not directly compatible with the BlueCRAB neutronics solver, Griffin; thus, they were directly converted into ISOXML format by using the Griffin code's newly developed capability to process OpenMC output files. The OpenMC model was used to calculate the temperature coefficients for the initial core and the burned core (1.5, 5.0, and 10.0 years of operation at full power, respectively), as listed in Table 6. Because 233 isotopes is too few for an accurate decay heat calculation, the approach of Ref. [11] was utilized, in which pseudo-isotopes were added to the decay chain to enable Griffin to accurately model decay heat.

Table 4: Neutron energy group boundaries for the 11 group structure.

Group	Upper Energy [eV]	Lower Energy [eV]
1	4.000E+07	8.210E+05
2	8.210E+05	1.830E+05
3	1.830E+05	4.900E+04
4	4.900E+04	4.540E+02
5	4.540E+02	4.810E+01
6	4.810E+01	9.880E+00
7	9.880E+00	4.000E+00
8	4.000E+00	1.000E+00
9	1.000E+00	3.200E-01
10	3.200E-01	6.700E-02
11	6.700E-02	1.000E-05

Table 5: Microscopic cross-section tabulation parameters of the SiMBA microreactor.

Parameter	Value
Number of isotopes	233
Burnup tabulation [days]	0.0, 500, 1700, 3650
Burnup tabulation [MWd/kg]	0.0, 0.0853, 0.2899, 0.62238
Fuel temperature tabulation [K]	800.0, 1000.0, 1200.0, 1400.0
Non-fuel temperature tabulation [K]	800.0, 1000.0, 1200.0

Table 6: Temperature feedback coefficients, calculated using OpenMC.

Feedback Coef.	Time [days]			
$[pcm/K]$	0.0	500.0	1700.0	3650
Isothermal	-0.873 $\pm$ 0.031	-0.862 $\pm$ 0.030	-0.860 $\pm$ 0.034	-0.864 $\pm$ 0.034
Fuel	-1.426 $\pm$ 0.021	-1.436 $\pm$ 0.021	-1.415 $\pm$ 0.023	-1.406 $\pm$ 0.023
Others	0.527 $\pm$ 0.031	0.564 $\pm$ 0.031	0.566 $\pm$ 0.034	0.527 $\pm$ 0.034

4.1.2 Depletion Calculation

To account for temperature and material distribution changes due to depletion during operation, a depletion calculation was performed for the SiMBA microreactor. Using the cross sections from OpenMC, a 2D slice of the core was depleted for 10 years at a linear power density of 1.250 MW/m. This power density was based on a total power of 2 MW and an active core height of 1.6 m, as detailed in Section 2. In the BlueCRAB steps of the workflow, the SiMBA problem was modeled as a 2D reactor so as to decrease the computational resources required to perform the simulations. The problem will be extended to 3D in future work.

Eleven energy groups and 96 directions were used for the discrete ordinates calculation. The final burnup spatial distribution for each unique assembly is presented in Figure 4. Note that the burnup values are small for this reactor design. The design will be modified in future work to increase burnup. Figure 5 shows the corresponding effective multiplication factor as a function of time. Note that while a linear relationship between multiplication factor and time is expected, an oscillation occurs around the one year mark. This behavior is consistent with that observed in the OpenMC simulation to generate burnup-dependent (and thus time-dependent) cross sections. OpenMC reported oscillations in multiplication factor with standard deviations on the order of the variation between two time steps. Future work will be devoted to further investigate uncertainty propagation from OpenMC-generated microscopic cross sections to griffin. Note that the effective multiplication factor only changes by 404 pcm over 10 years of depletion. This is due to the low burnup of the reactor design. Table 7 gives the concentration of some isotopes important to dose for each assembly at 10 years. Each of these concentrations will be provided as a source term to MELCOR. Although only a few isotopes are presented here, all relevant isotopes are available as output from BlueCRAB. The purpose here is solely to demonstrate the workflow.

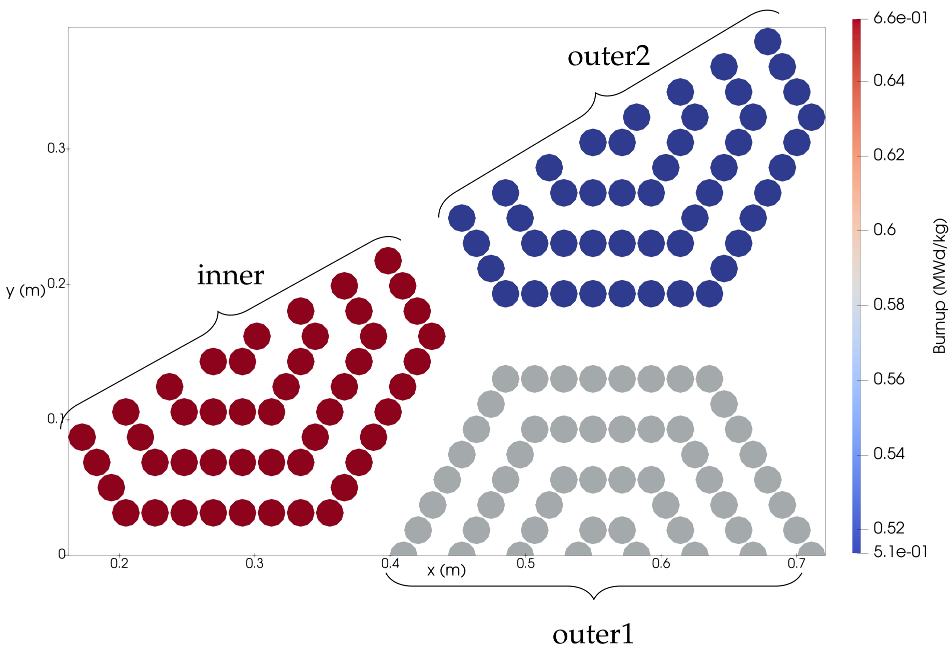

Figure 4: Burnup spatial distribution for 1/12th of the core after 10 years of depletion, reported per labeled assembly.

4.1.3 Null-Transient Test

After performing the depletion calculation to obtain the full-core isotopic inventory, the results could then be used to perform a transient simulation of a HP failure accident so as to obtain the power and temperature evolutions during the accident. To do this, the restart system in Blue-CRAB (the binary system in Griffin and the checkpoint system in MOOSE) was used to load the results from the depletion calculation as initial conditions and material definitions for the transient problem.

Before simulating a HP failure, it was crucial to test that the restart system functioned as in-

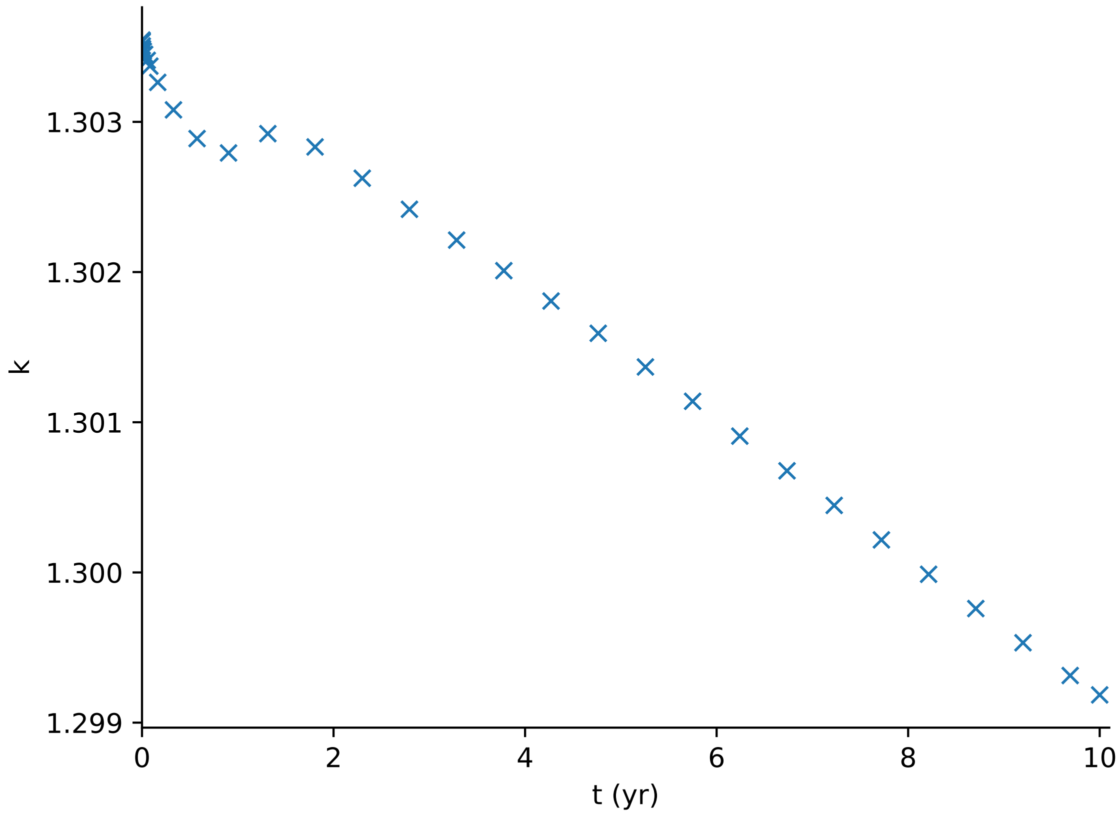

Figure 5: Effective multiplication factor as a function of time.

tended. A null-transient (steady-state) problem was simulated to test this. To model this, the fundamental mode from the eigenvalue problem at 10 years was used as the initial condition for a transient neutronics problem. BlueCRAB's restart system loads the fundamental mode as the initial condition, along with the depleted isotopics for the material definitions. The restart system divides the fission cross sections by the effective multiplication factor to ensure that the transient begins in a steady state. Although this effectively changes the fuel material, it is a convenient way to simulate a steady-state problem. For practical applications, the reactor will operate with $k_{\text{eff}} = 1$, except during power level adjustments or when offline. In such a case, dividing the fission cross section by unity does not artificially modify the material properties. For a more realistic future simulation, a criticality search could be performed to find the critical drum position at each depletion timestep. When starting a subsequent transient calculation, the initial condition would be a true steady-state condition (depletion effects can be ignored on short timescales), without needing

Table 7: Concentrations of important dose-contributing isotopes in the 10-year-depleted fuel (nuclides/b-cm), reported per fuel assembly.

Isotope	Assembly ID		
	inner	outer1	outer2
Xe-133	3.427e-09	3.027e-09	2.684e-09
Kr-85	3.984e-08	3.536e-08	3.141e-08
I-131	2.318e-09	2.043e-09	1.810e-09
Te-132	1.374e-09	1.211e-09	1.073e-09
Cs-137	1.349e-06	1.191e-06	1.055e-06
Cs-134	1.033e-09	7.616e-10	5.874e-10
Sr-90	1.202e-06	1.065e-06	9.453e-07
Ag-111	2.671e-11	2.261e-11	1.969e-11
Sb-125	4.880e-09	4.184e-09	3.667e-09
Ru-103	1.269e-08	1.113e-08	9.843e-09
Ce-144	1.492e-07	1.320e-07	1.172e-07
La-140	1.004e-09	8.876e-10	7.875e-10
Pu-239	9.804e-06	8.001e-06	6.888e-06

to alter fission cross sections.

It was confirmed that the null-transient gave the expected steady-state results (i.e., results equal to the initial conditions), proving that BlueCRAB's restart system functions as intended. While functioning correctly, the restart system is being improved to use a single checkpoint file to restart all aspects of a given multiphysics simulation.

4.1.4 Heat-Pipe Failure Transient Calculation

At the end of the 10 years of depletion, a HP failure accident was simulated. Starting at t = 60 seconds, 2 HPs in the 1/12th core (corresponding to 24 HPs in the entire core) were failed by instantaneously setting the HP heat transfer coefficient to zero, as shown in Figure 6. Although 24 simultaneously failing HPs was not meant to reflect a realistic scenario, the problem demonstrates the capabilities of the BlueCRAB tool. The transient was run for an arbitrary 2000 seconds—sufficient time for the core to stabilize to a new equilibrium. Figures 6–8 show the temperature distribution at various times in the transient. Figure 9 shows the power and temperature responses as a function of time for the HP failure simulation. When the HPs failed, they stopped removing heat from the core. This caused a buildup of heat in the region of the failed HPs, resulting in increased local temperature. The temperature increase affected the neutron cross sections through negative thermal feedback, causing power to drop. As power drops, temperature outside the failed HP region decreased, causing positive thermal feedback. The power oscillated about the new equilibrium value until negative and positive thermal feedback balanced each other, resulting in a new equilibrium at a power level lower than the initial condition.

From Figure 9, note that although the equilibrium maximum fuel temperature exceeded its initial value, the average fuel temperature was lower than its initial value. Though counter-intuitive, inspection of the spatial temperature distribution and assembly-wise average fuel temperatures in Figures 8 and 9, respectively, reveal this feature to be a property of the location of the failed HPs. When the maximum fuel temperature increases near the failed HPs in the *inner* assembly, it depresses the power in all assemblies. Because the central assembly has higher neutronics importance, the temperature decrease in the peripheral assemblies is not enough to bring the power above its nominal value. The end result is that the average fuel temperatures of the *outer*1 and *outer*2 assemblies are lower than the assemblies' initial conditions, with the *inner* assembly having a higher average temperature due to the HP failure. These conditions result in an overall average fuel temperature that is lower than its initial value.

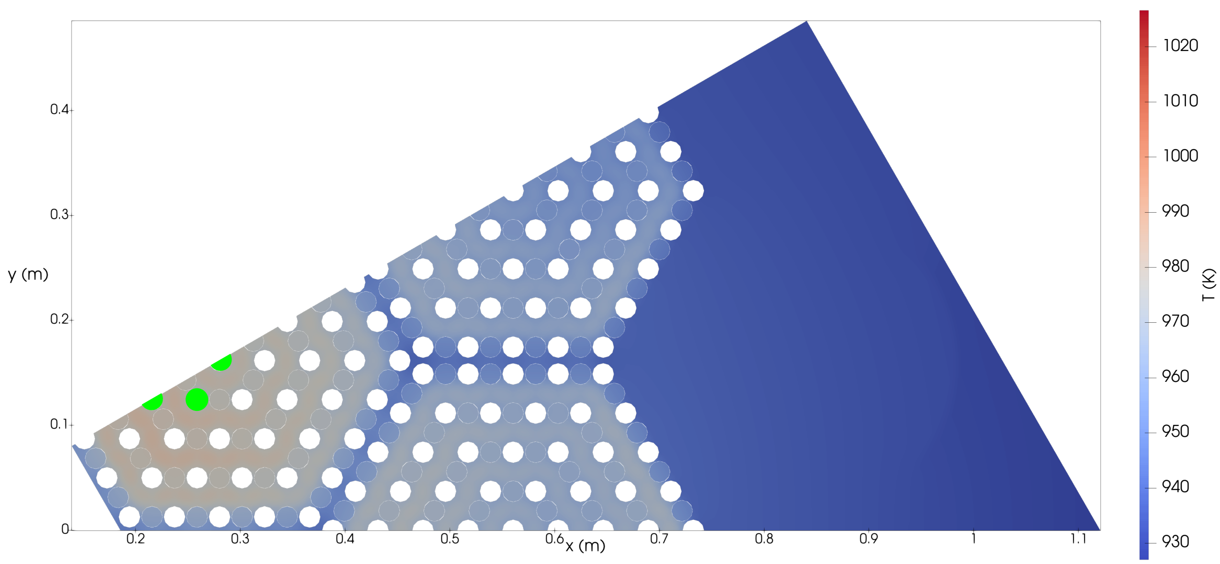

Figure 6: The 1/12th core geometry, in which the 2 failed HPs are indicated by green circles. Note one full HP and 2 half HPs are failed, for a total of 24 failed HPs in the full core. The temperature distribution at $t = 0$ s is also shown.

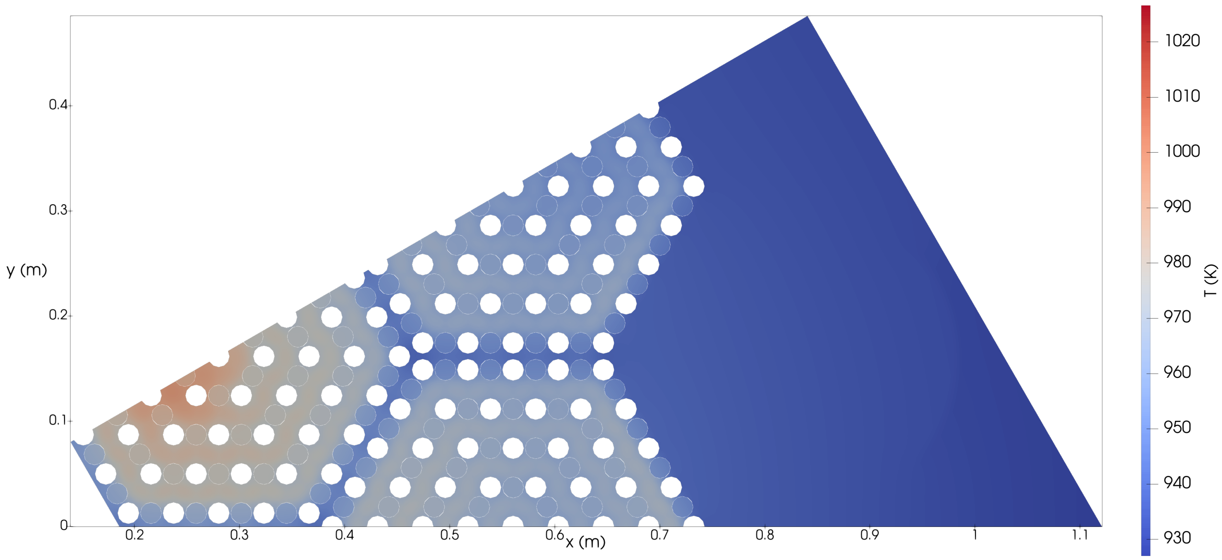

Figure 7: Heat pipe failure transient at t = 120 s.

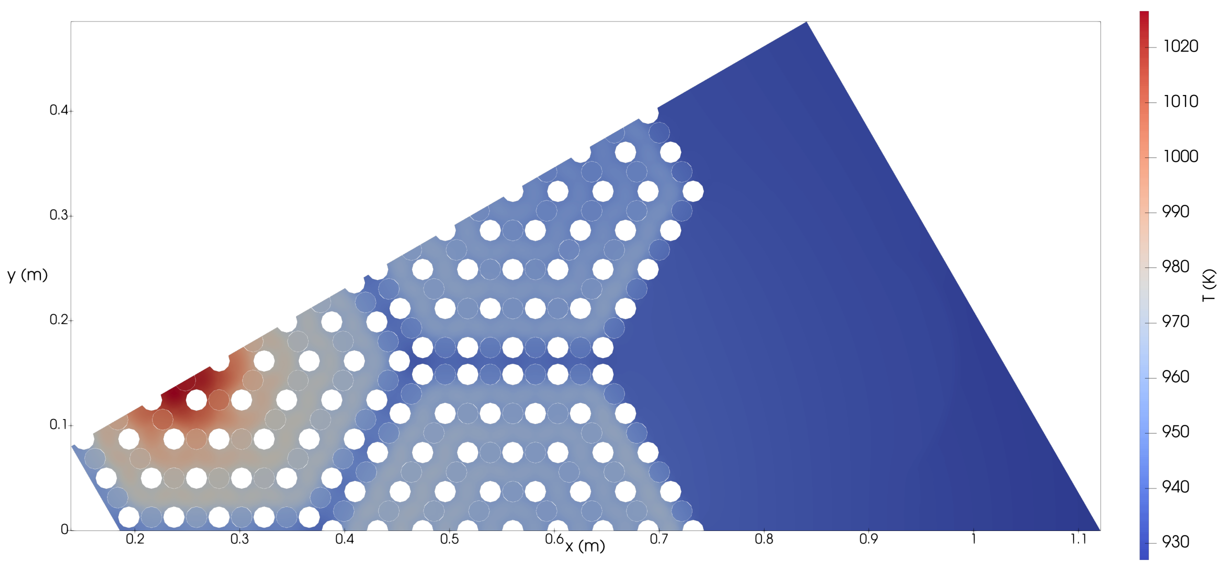

Figure 8: Heat pipe failure transient at t = 2000 s.

4.2 Addressing Workflow Gaps

Several gaps in the BlueCRAB workflow were identified while modeling the SiMBA reactor. Table 8 lists these gaps and their associated pull request numbers. Each gap will now be discussed in greater detail.

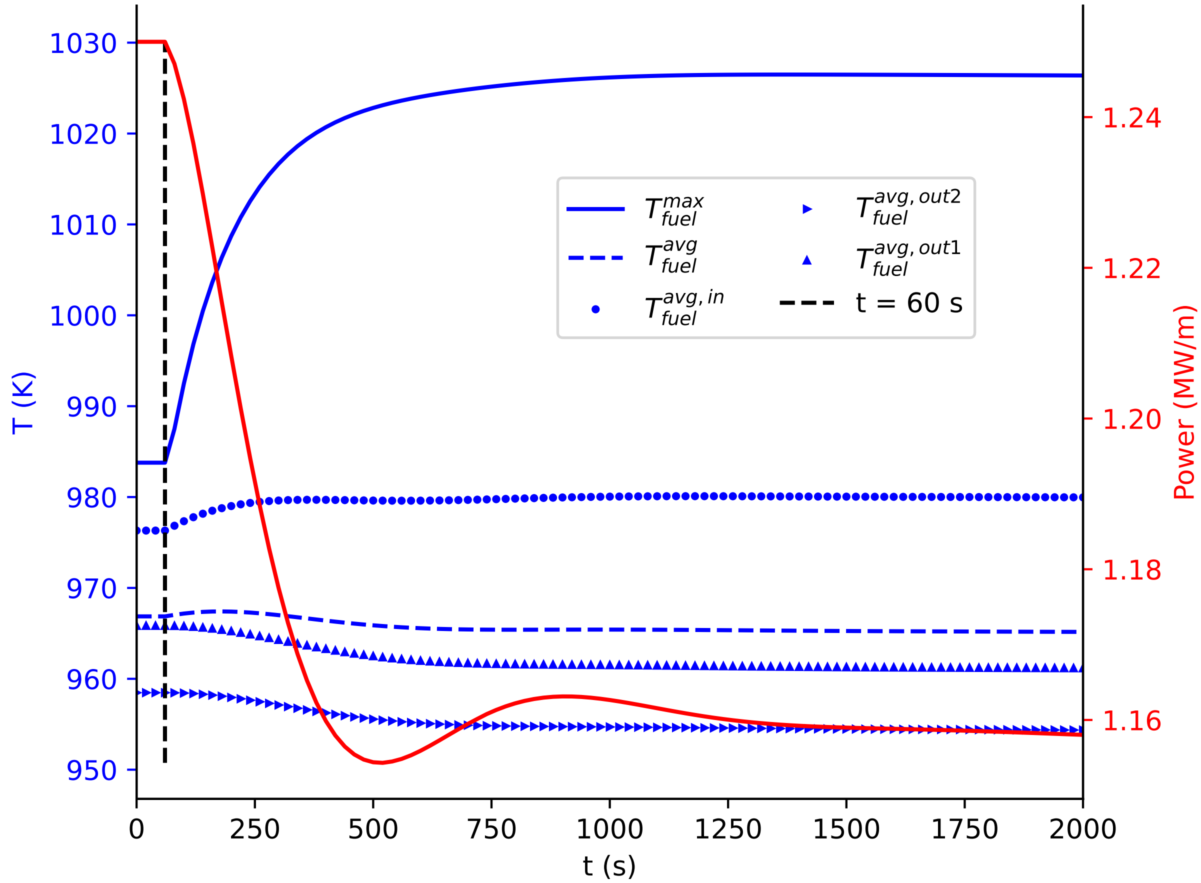

Figure 9: Power and fuel temperature response to HP failure as a function of time. The *in*, *out*1, and *out*2 superscripts indicate the inner, outer1, and outer2 fuel assemblies, as defined in Figure 4 and Table 7.

4.2.1 Parallel Execution Issues

Because the depletion feature in Griffin was implemented fairly recently, some code bugs were discovered and patched. In particular, two parallel execution bugs were found in Griffin that prevented depletion models from being run on a large number of processors. Griffin issues 1168 and 1230 pertained to a simulation crash when trying to use more processors. The solutions provided in Griffin pull requests 1183 and 1233 modified how cross-section libraries are loaded into Griffin when conducting parallel simulations, resulting in a more robust system capable of running depletion simulations on higher numbers of processors. These high-impact issues have been satisfactorily resolved and closed.

Table 8: Summary of the workflow gaps identified. The gaps are listed from high- to low-impact with regard to the workflow.

Issue Title	Issue Number	Pull Request Number	Issue Status
Depletion error thrown only on some MPI configurations	Griffin 1168	Griffin 1183	resolved
Inconsistent MPI behavior for delayed neutron data in `DepletionNeutronicsMaterial`	Griffin 1230	Griffin 1233	resolved
One-step conversion from the OpenMC state point file to ISOXML	Griffin 1405	Griffin 1406	resolved
Binary restart does not include `DepletionNeutronicsMaterial`	Griffin 1347	Griffin 1348	partially resolved, workaround in place
Duplicate thermal postprocessors in CSV output for coupled transport/thermal transient problems	Griffin 1410	N/A	unresolved, workaround in place
Subapp of type `FullSolveMultiapp` does not output checkpoint when enabled in subapp input file	MOOSE 24777	N/A	unresolved, workaround in place
`CoupledFeedbackNeutronicsMaterial` does not work without block parameter	Griffin 1412	N/A	unresolved, workaround in place

4.2.2 Cross-Section Converter

After running OpenMC to compute the multigroup cross sections, the results had to be formulated into a BlueCRAB-compatible format. Specifically, the Griffin neutronics code requires cross sections to be in the ISOXML format, necessitating an OpenMC-to-ISOXML cross-section converter. To meet this need, Griffin issue 1405 was opened to develop a robust and streamlined cross-section converter that reads an OpenMC state point file in HDF5 format and converts it into Griffin's native ISOXML format. Griffin pull request 1406 was opened to address this high-impact issue. Although the pull request has not yet been merged as of this writing, the resulting cross-section converter is functioning satisfactorily. Thus, this issue is considered resolved.

4.2.3 Depletion to Transient Binary Restart

As has been discussed, once cross sections were obtained from OpenMC, running the SiMBA problem using BlueCRAB consisted of two actions: (1) running a depletion calculation to 10 years in order to determine the EOL composition of the fuel, and (2) running a transient calculation using EOL fuel to simulate a HP failure. After solving the depletion problem, the fundamental mode and corresponding temperature field at 10 years were used as the initial conditions for the HP failure transient calculation. Additionally, the fuel isotopic composition at 10 years was used for the fuel material definition in the transient calculation. To port data fields from the depletion problem into the transient problem, several "restart" capabilities of BlueCRAB were utilized. MOOSE's built-in checkpoint system was employed to restart the thermal solution as the initial condition in BISON. Restarting the neutronics data, however, was not so straightforward. To load the neutronics solution as the initial condition in Griffin, a `TransportSolutionVectorFile` `UserObject` must be defined in the input files for the depletion and transient problems. This simply writes the neutronics solution to a binary file after the depletion solve, then reads it in to the transient problem as an initial condition. While this in itself does not add a significant burden to the workflow, the depleted material definitions are not included in these binary files. To successfully restart the depleted fuel material in the transient calculation, the nuclide number densities initially had to be obtained from the output file, then manually entered into the transient input file. Griffin issue 1347 was opened to alleviate the burden of manual entry. The Griffin team added Boolean flags (`save_binary` and `load_binary`) to the `DepletionNeutronicsMaterial` object to toggle the binary writing/reading of depleted nuclide number densities between transport problems, thus eliminating the manual entry requirement. This capability was introduced via Griffin pull request 1348. In the future, everything required to load the depletion results into the transient problem will be incorporated into MOOSE's checkpoint system so as to enable a more streamlined restart approach. Until these future plans are implemented, this high-impact issue is considered partially resolved, as the current `save_binary` / `load_binary` workaround is deemed satisfactory.

4.2.4 Low-Impact Issues

The remaining identified workflow gaps are described below. Griffin issue 1410 delineates the process by which multiple postprocessor values are output for each timestep when only a single value is requested. When running a coupled transient transport-heat conduction problem with thermal postprocessors, unconverged thermal postprocessor values are written to a CSV file at each fixed point iteration. The end result is a thermal CSV postprocessor file that lists many postprocessor values at each time step. The current workaround to this issue is to use a script that parses out the last (converged) postprocessor value listed for each time step. Though unresolved, this significant issue has been communicated to the Griffin team.

MOOSE issue 24777 refers to an issue with MOOSE's restart/recover system. When running a `FullSolveMultiapp` subapp after each time step of a transient parent app, subapp checkpoints are not written when `Outputs/checkpoint = true` is set in the subapp input file. However, this issue can be circumvented by setting `Outputs/checkpoint/additional_execute_on = 'FINAL'`. Though unresolved, this issue is considered low priority thanks to this workaround.

Griffin issue 1412 refers to the fact that a simulation using a `CoupledFeedbackNeutronicsMaterial` will crash if the optional `block` parameter is not specified. The workaround to this issue is to always explicitly specify the `block` parameter in all simulations. Though unresolved, this issue is considered low priority thanks to this workaround.

4.3 Additional Observations

To solve the neutron transport equation for practical applications—without an excessive number of linear iterations—some means of diffusion acceleration is often required. Griffin utilizes CMFD acceleration [12–15], a method that solves a low-order neutron transport equation for a correction in flux. A significant observation that arose from utilizing CMFD was that the convergence tolerance for the depletion problem had to be set tighter than the tolerance for the transient problem. When using the depletion solution as the initial condition to the transient problem, it is important to ensure that, prior to solving the transient problem, the depletion solution is sufficiently converged. If it is not, an incorrect solution may be obtained for the transient problem. For example, if the depletion tolerance is set too loosely, the transient solver cannot maintain a null transient when the depletion solution is used as the initial condition. Although the general rule of thumb is to set the depletion convergence tolerance two orders of magnitude tighter than the transient convergence tolerance, this topic could benefit from greater investigation.

5 CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

This report presented the development of a BlueCRAB-MELCOR framework usable to help streamline microreactor modeling and simulation tools so as to better support vendors and regulatory authorities in submitting and reviewing licensing applications. The Nuclear Regulatory Commission uses MELCOR to estimate mechanistic source terms during accident conditions. Such estimations require knowledge of the full-core isotopic inventory and power/temperature evolution profiles during postulated accidents. As BlueCRAB is a suite of codes that can compute this information for use in MELCOR, the Nuclear Regulatory Commission is expected to use it in conjunction with MELCOR to perform design- and beyond-design-basis accident analyses. However, prior to this report, BlueCRAB had never been used to produce the required MELCOR inputs at the full-core level.

By applying the proposed framework to the SiMBA problem, which is a prototypical microreactor, this work demonstrates the feasibility of a BlueCRAB-MELCOR framework. To perform the microscopic depletion simulation so as to compute the core isotopic inventory, OpenMC was used to generate burnup- and temperature-dependent microscopic cross sections. After converting these cross sections into the ISOXML format appropriate for use in BlueCRAB's Griffin, BlueCRAB performed a multiphysics microdepletion calculation that solves the coupled neutron transport, nuclide depletion, and heat conduction equations in order to calculate the core isotopic inventory. After depleting the core to EOL, a HP failure accident was simulated, setting the depleiton solution as the initial condition. In addition to the core inventory from the depletion calculation, this yielded the power and temperature evolutions required by MELCOR to compute a mechanistic source term.

Thus, the entire workflow of using BlueCRAB to generate MELCOR inputs, from cross-section generation to producing isotopic inventory and power/temperature evolution profiles during a transient, was demonstrated. This report also detailed the identified gaps in the workflow, along with how they were (for the most part) addressed. Any issues not fully addressed were submitted to the BlueCRAB development teams. These are not high-priority issues, as there are ways of circumventing them. As of this writing, the BlueCRAB-MELCOR workflow is now fairly mature.

5.2 Future Work

At this point, the BlueCRAB-MELCOR framework has been proven up to the moment of running MELCOR to compute a mechanistic source term. This next step will complete the workflow and address any remaining gaps. In particular, the fiscal year 2024 scope will include demonstrating an example case of the full workflow encompassing both BlueCRAB and MELCOR.

Furthermore, the microreactor model for this exercise will be improved to (1) yield higher burnup at EOL—in line with the envisioned vendor design—and (2) include explicit thermal-hydraulic modeling of the HPs. Additionally, a more thorough testing, including adding more depletion zones to the workflow and the verification of the decay heat calculation, will be considered.

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