OpenMC Depletion Analysis of the Virtual Test Bed Gas-Cooled Microreactor

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ABSTRACT

OpenMC is a state-of-the art, Open-Source (OS) Monte Carlo transport code. This work uses OpenMC for depletion analysis of an infinite-assembly model of the Virtual Test Bed (VTB) Gas-Cooled Microreactor (GCMR). This microreactor is prismatic, Tri-structural Isotropic (TRISO)-fueled, and helium gas cooled. Since the GCMR is intended for load-following, a depletion analysis was run at 100%, 50%, and 10% of the rated power (225 kWt) for both explicitly represented TRISO and volume-homogenized fuel cases. The time steps used were twice as long and ten times as long for the lower power cases, respectively, to ensure the same total burnup occurred at each time step. The system eigenvalue k_{inf} was plotted versus the burnup at each time step. The isotopics after one year of operation at steady-state were compared at each power between both fidelities. **missing anything here?**

Keywords: OpenMC, TRISO, depletion, microreactor, gas-cooled

1. INTRODUCTION

For advanced reactors, especially those early in the design stage, sufficient Modeling and Simulation (M&S) is required to ensure the success of the design concept. The VTB [1] is a repository of reactor models used for research and demonstration of current tools in the nuclear industry as a part of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) initiative. Various types of reactors are available on the VTB. Microreactors are one viable class of next generation systems with ongoing efforts to model them using NEAMS tools [2, 3]. One key advantage of microreactors is the ability to supply power to lower demand areas that may not be able to consume power on the order of a GW reactor or to areas needing temporary power, e.g. natural disaster relief efforts. While microreactors can be very diverse in fuel, coolant, and general design, there is interest in combining High-Temperature Gas Reactor (HTGR) and microreactor technologies. HTGRs have the benefits of higher electricity conversion efficiency due to the high temperature coolant and the desirable melting properties of TRISO fuel. Adding these benefits to a microreactor bring many attractive features together. Previous work on the VTB GCMR includes analysis of the system for a two day load-following transient [4]. This work coupled Griffin [5], BISON [6], and SAM [7] using the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework. Griffin is a deterministic transport solver that was used for neutronics. BISON is a fuel performance code that can compute heat conduction in the solid parts of the system. SAM is a system analysis code that was used for 1-D fluid flow of the coolant channels. **add more?** While previous works used Griffin for neutron transport, this work chose OpenMC as an alternative to Griffin due to the OS status of the software, as well as to take advantage of Monte Carlo and depletion capabilities in OpenMC.

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The rest of this paper will be organized as follows. Section 2 will provide some background theory on depletion. Section 3 will detail the VTB GCMR and its components. Section 4 will explain the OpenMC model of the system and the simulations' depletion schemes. Section 5 will present results for the system. Section 6 will interpret those results and discuss the plans forward for more M&S.

2. DEPLETION THEORY

Tracking the isotopic composition of nuclear reactors is a highly important task, as nuclide number density directly influences the solution of the transport equation. Isotopes exposed to neutron flux will transmute into radioisotopes that have various modes of decay, creating new isotopes that did not exist at the start of operation, as well as decaying into other isotopes already in the system. The rate at which isotopes transmute and decay into each other depends on the transport solution via the reaction rates, which depend directly on the neutron flux. This relationship causes the coupling between transport and depletion to behave non-linearly [8].

Certain isotopes have more influence on the system than others. For example, Xenon-135 has an extremely high neutron absorption cross section. It is so high that its negative reactivity insertion influences the positioning of the control elements. Xenon-135 is particularly important in load-following contexts, in which the power changes once or twice per day, as it's concentration increases when power decreases, and it is burned off when power increases again. This matters more in load-following contexts because the Xenon-135 half-life is on the order of 9 hours [9]. For context, the load following schedule in Abdelhameed et al. has high power for 12 hours, lower power for 7 hours, and 2.5 hour ramps between them [4]. Considering these rates, the transient behavior for load-following will be more interesting since the power, and neutron flux, changes on a similar timescale as the Xenon-135 half-life.

To model burnup, transmutation and decay cross sections of the isotopes are combined with the computed flux to determine production and destruction rates for each isotope. These formulate a system of differential equations for the nuclide densities. For isotope i with number density $N_i(t)$, the Bateman or burnup equations describe the time dependent isotopic composition, given by

$$\frac{dN_i}{dt} = \sum_j \left[f_{j\to i} \int_0^\infty \sigma_j(E,t)\phi(E,t)dE + \lambda_{j\to i} \right] N_j(t) - \left[\int_0^\infty \sigma_i(E,t)\phi(E,t)dE + \sum_j \lambda_{i\to j} \right] N_i(t), \quad (1)$$

where $\sigma_j(E)$ is the transmutation cross section of isotope j at energy E, $f_{j\to i}$ is the fraction of transmutation reactions for nuclide j that produce nuclide i, and $\lambda_{j\to i}$ are the decay constants for decay modes in nuclide j that produce nuclide i. The system of equations for isotopes $i \in [1, n]$ can be expressed in matrix notation using the nuclide vector $\mathbf{n} \in \mathbb{R}^n$

$$\frac{d\mathbf{n}}{dt} = \mathbf{A}(\mathbf{n}, t)\mathbf{n} \qquad \text{WITH} \qquad \mathbf{n}(0) = \mathbf{n}_0, \quad (2)$$

where $\mathbf{A} \in \mathbb{R}^{n\times n}$ is the burnup matrix. Since the transport equation depends on number density and $\mathbf{A}$ depends on the solution to the transport equation, $\mathbf{A}$ then also depends on number density. Because "the timescale over which material compositions change is sufficiently long ... the transport equation can be solved as a steady-state equation" [8]. Taking the burnup equations as steady-state allows the earlier

non-separable equation to be solved via separation solution

$$\frac{d\mathbf{n}}{dt} = \mathbf{A}(\mathbf{n})\mathbf{n} \qquad \text{WITH} \qquad \mathbf{n}(0) = \mathbf{n}_0, \tag{3}$$

The solution to which is

$$\mathbf{n}(t) = \exp(\mathbf{A}t)\mathbf{n}_0 \tag{4}$$

Solving Equation (3) and Equation (4) involves two separate components [8]:

1. Using a numerical method to integrate the matrix **A** in Equation (3) forward in time. This usually involves taking one or more matrix exponential.
2. Evaluating the matrix exponential $\exp(\mathbf{A}t)$ or the action of the matrix exponential on a vector of nuclide concentrations.

The key to correctly representing $\mathbf{n}(t)$ is to use small enough time steps that **A** remains *constant enough* to get the new nuclide concentrations, then updating **A** forward in time to account for the fact that **A** *does* have time dependence.

3. SYSTEM DESCRIPTION

The system analyzed is the VTB GCMR. Figure 1 shows a diagram of the system. The overall structural material of the assembly is graphite with cylindrical holes for various compacts: burnable poison, a central control rod, moderator, coolant, and fuel. The fuel kernel uses a U235 enrichment of 19.95% inside the center of the TRISO particles. The TRISO has a 40% packing fraction. The moderator uses YH_2 encased in a FeCrAl envelope. The poison compacts contain B_4C burnable absorber sphere, which have a 25% packing fraction. The coolant uses helium and the control rod chamber has a B_4C rod, where helium fills the space when the control rod is not fully injected; this helium is not circulating like the coolant. There is a top and bottom reflector made of BeO. Since the goal of this simulation is to determine excess reactivity in the assembly, the control rod is not inserted into the active core region, resting in the central compact of the upper reflector region [4].

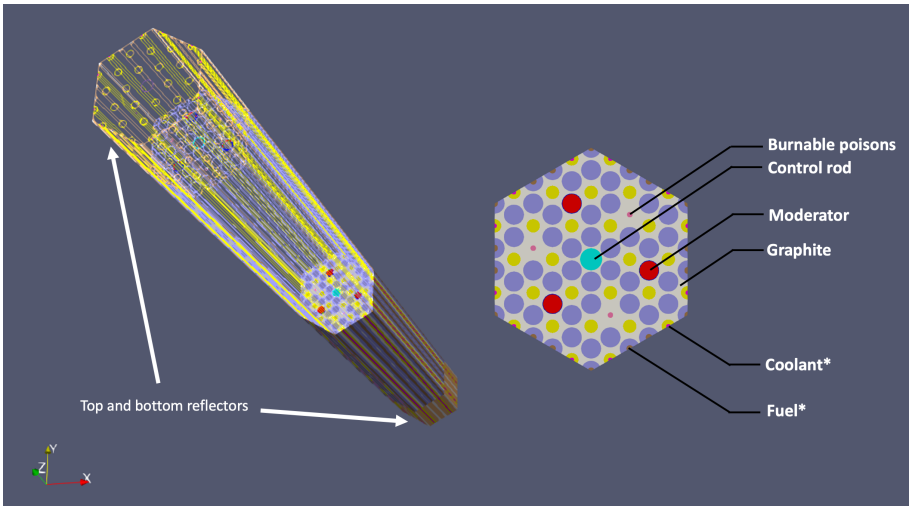


Figure 1. An image of the VTB GCMR along with a cross section of the fuel containing section of the system.

4. OPENMC MODEL

There are two aspects to the OpenMC model that will each be described. The first is assembling the geometry, material, and tally definitions. In OpenMC, a python script is used to generate XML files that will be used by a neutronics simulation. After that, the depletion simulation settings are defined in a separate script that take the XML files generated and use them to set up everything needed to iterate between transport and depletion steps using the correct time integration method and time steps.

4.1. Model Definition

In order to allow for axial variation in the flux, the system is divided into axial layers. This allows a more accurate flux to be computed, which is a primary input to depletion. The axial division used matched exactly the choice of [4], which was to have two regions per reflector and 16 regions in the active region of the assembly. The dimensions are 20 cm for each reflector and 160 cm for the fuel, which corresponds to each axial layer modeling 10 cm of the reactor. Figure 2 shows a radial slice of the fuel portion of the reactor. Figure 3 shows a radial slice of each reflector region.

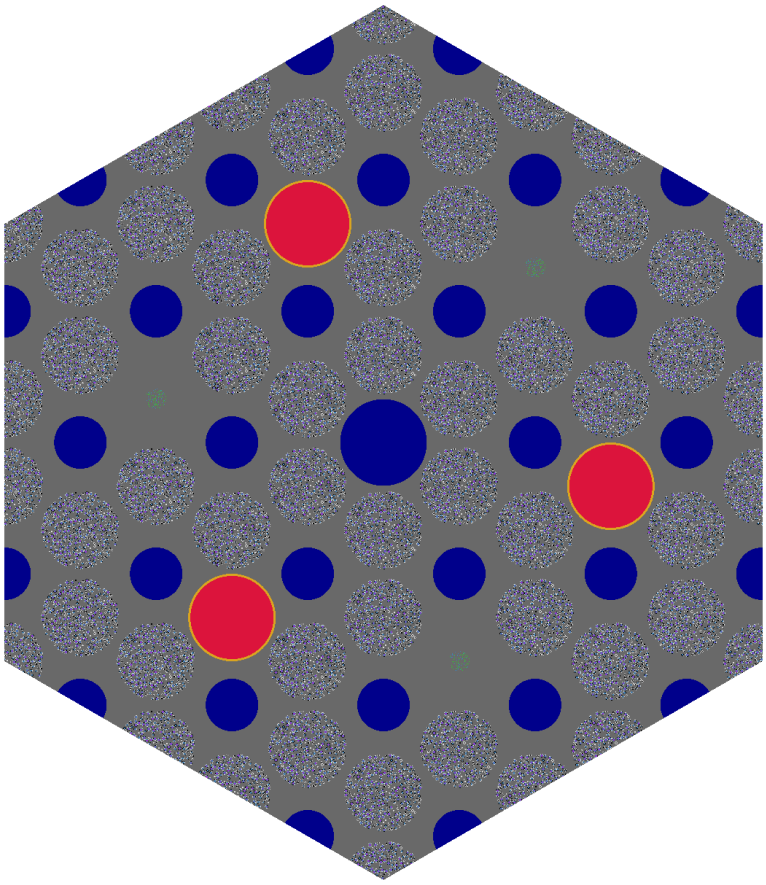
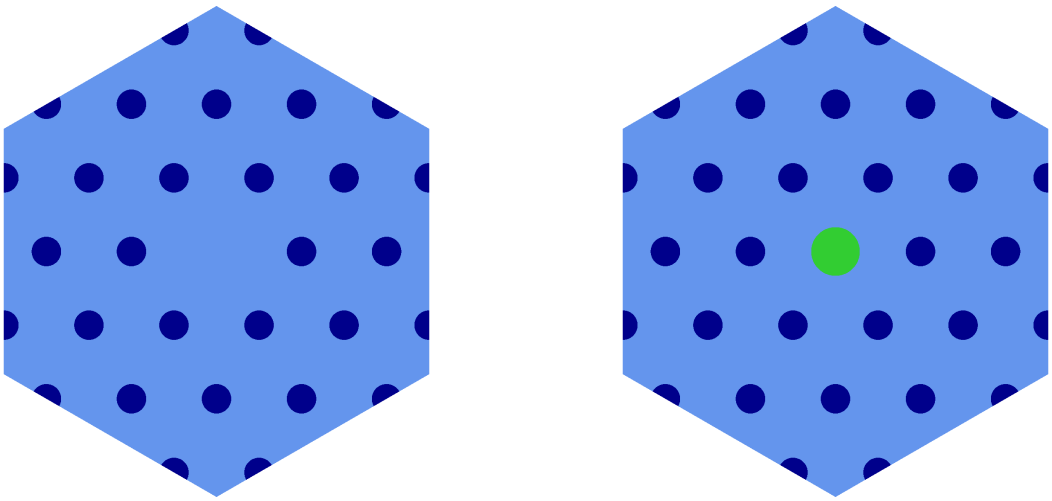


Figure 2. A radial slice of the active region. Gray corresponds to graphite in the matrix or pyrolitic carbon, dark blue corresponds to helium coolant, red corresponds to YH_2 moderator, gold corresponds to FeCrAl, green corresponds to the B_4C poison particles (packed at 25 percent in graphite), and purple corresponds to the fuel kernel in the TRISO particles (packed at 40 percent in graphite).



(a) A slice of the lower reflector, colored by material. **(b) A slice of the upper reflector, colored by material.**

Figure 3. A radial slice of the lower reflector (left) and the upper reflector (right). The difference between the upper and lower reflectors is that the upper reflector has an extra compact for the B_4C control rod. Dark blue corresponds to helium coolant and light blue corresponds to BeO, while the B_4C control rod is shown in green.

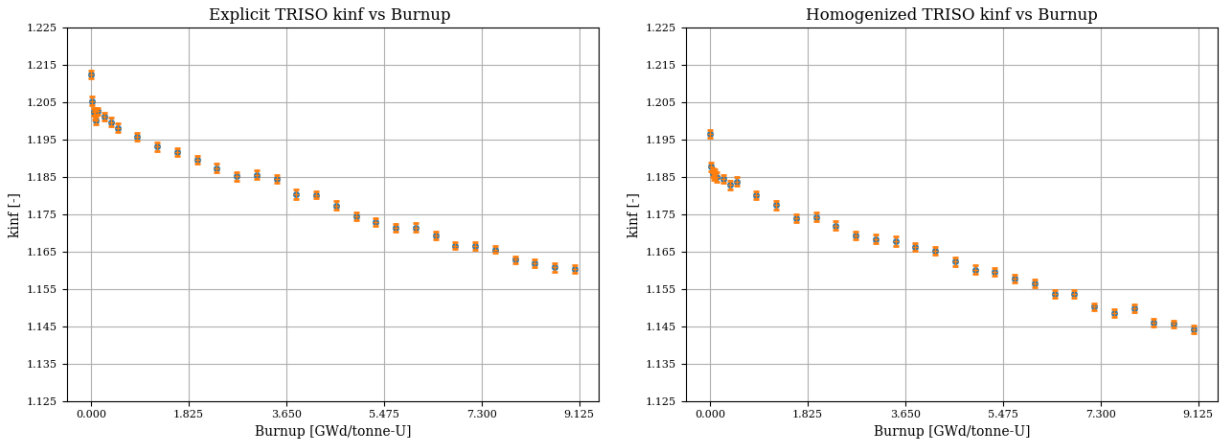
The cross-sections used for transport are continuous energy from ENDF-B-VII.1. The chain file, a file used for depletion in OpenMC, contains transmutation and decay data to solve for the burnup matrix and each depletion time step. The chain file used in this simulation is based off the Consortium for Advanced Simulation of LWRs (CASL) project. While the chain is used for a Light Water Reactor (LWR), it is really the spectrum that is the key to validity of the chain file. Since this system has a thermal specturm, it is appropriate to use the CASL chain. The CASL chain can be found on OpenMC's website, specifically the portion that provides data for users to download.

4.2. Depletion Simulation Definition

In this work, the system is held at constant power for each case. This has some implications for the time stepping scheme chosen. To correctly account for the rapid build up of strong neutron absorbers, a few short initial time steps are included to increase those nuclides' accuracy. Since the simulations are constant power, the time steps can be lengthened after this initial transient behavior, after allowing these important isotopes to reach a steady-state. The time steps for the full power case, in days, were as follows: three one-day time steps, three five-day time steps, and 23 fifteen-day timee steps. This adds up to one year, while allowing some fine time steps initially to account for rapidly changing isotopes, including some strong absorbers, which affect the flux notably, e.g. Xenon-135.

5. RESULTS

Figure 4 shows results for the full power case of k_{inf} versus burnup for the time steps mentioned above. The full paper will show comparison for each lower power case as well.



(a) Explicit **(b) Homogenized**

Figure 4. Pictured above is results for k_{inf} versus burnup, both for the explicit TRISO representation and homogenized fuel cases.

6. CONCLUSIONS

The above results are in line with previous work measuring the effects of TRISO homogenization. The explicit case has a notably higher eigenvalue. This is due to the difference of neutrons interacting with the fuel. When the TRISO is explicitly represented, neutrons slow down significantly more before hitting fuel atoms, meaning they thermalize and are more likely to cause fissions. In the homogenized case, the neutrons encounter uranium at higher energies, and thus are more likely to be absorbed in a resonance reaction. **todo add citations for other homogenization?**

This paper simulated the VTB GCMR for some preliminary depletion analysis of an infinite assembly model. Since the reactor is intended to load follow, it depleted the system at 100%, 500% and 10% power. The k_{inf} versus burnup showed that after one year, the reactor still has excess reactivity for both cases.

This work extends modeling on the VTB GCMR. Depletion analysis is new for this system, and is important for a reactor intended to load follow. The software selected for future analyses will rely on Cardinal [10]. The Cardinal simulation will couple OpenMC for neutron transport, MOOSE's Heat Conduction Module (HCM) for heat conduction, and Thermal Hydraulics Module (THM) for 1-D thermal hydraulics. After standalone multiphysics work is completed, the future goal is to couple depletion into the multiphysics algorithm to see the impact of depletion on high-fidelity multiphysics.

NOTE TO ORGANIZERS

Between now and the final deadline in January, there will be sufficient time to expand this analysis to hit the other power cases for each fidelity. Some results that are intended to be included are

- Longer depletion simulations (to find out when reactor goes subcritical)

- Isotopic comparison of important nuclides (U235,U238,Xe135) at the end of cycle

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ACRONYMS

CASL Consortium for Advanced Simulation of LWRs
GCMR Gas-Cooled Microreactor
HCM Heat Conduction Module
HTGR High-Temperature Gas Reactor
LWR Light Water Reactor
M&S Modeling and Simulation
MOOSE Multiphysics Object-Oriented Simulation Environment
NEAMS Nuclear Energy Advanced Modeling and Simulation
OS Open-Source
THM Thermal Hydraulics Module
TRISO Tri-structural Isotropic
VTB Virtual Test Bed

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