Exploring Effects of Homogenization on an OpenMC Depletion Analysis of a TRISO Fueled, Helium Cooled Microreactor

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Outline

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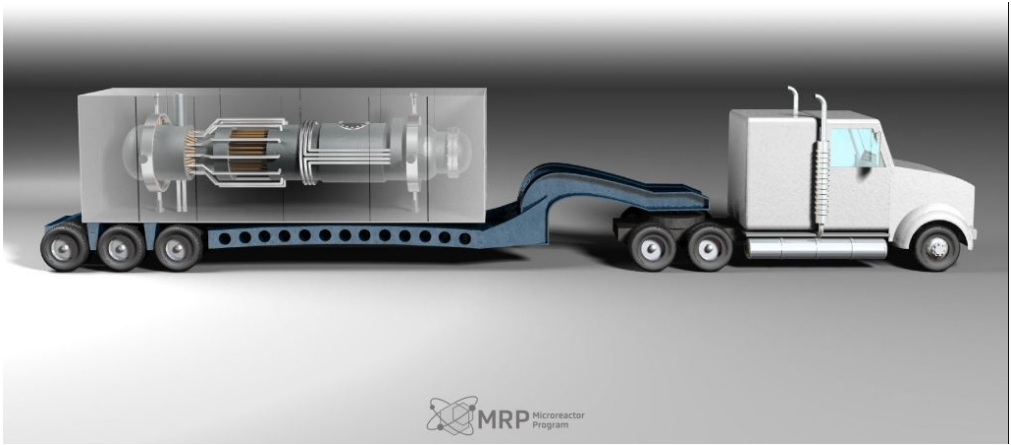
Virtual Test Bed [1]

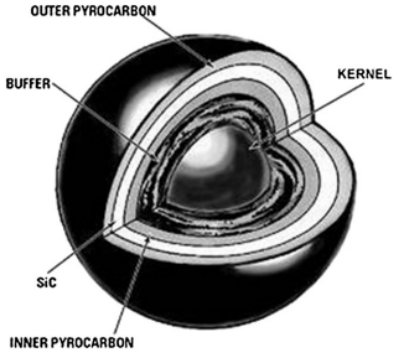
NRIC National Reactor Innovation Center

NEAMS

Microreactors [2]



TRISO Fuel

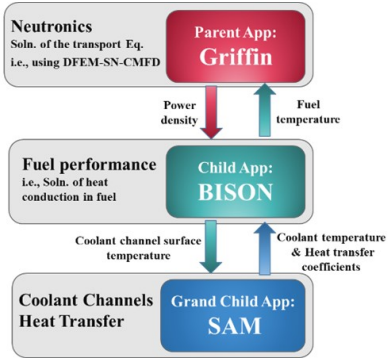


Layers from innermost to outermost: fuel kernel, buffer, Inner PyC, SiC,Outer PyC [3].

- Common fuel for HTGRs
- UCO fuel kernel radius 212.5 microns
- Outer PyC radius 427.5 microns
- Melting temperature significantly higher than operational temperatures [3]
- Designed to contain fission products [3]
- Typically packed into graphite compacts or into spherical pebbles for PBRs
- TRISO modeling challenges
  - Five surfaces per TRISO
  - Many TRISOs per reactor

Virtual Test Bed Gas Cooled Microreactor (VTB GCMR)

- Existing VTB GCMR simulations
  - Preliminary multiphysics models: Griffin-BISON-SAM [4, 5, 6]
  - Dynamic multiphysics simulations: flow blockage and Reactivity Insertion Accident [7]
  - Balance of plant 1D thermal hydraulic simulation [8]
- This work presents the first published OpenMC Model of the VTB GCMR
  - Plans to add this work's model to the VTB this summer
- For a full core model, it will be prohibitively expensive to model every TRISO explicitly



MultiApp hierarchy of preliminary GCMR models. Image from [6].

Research Goal

- **What degree of explicitness is required to represent TRISO for a full-core GCMR model?**
- To answer this question, varying degrees of homogenization were used in an infinite-assembly depletion model, computing k_{inf} as a function of burnup up to 29 GWd/tonne-U.
- Since this reactor is intended for load-following, a burnup simulation was conducted at 100%, 50%, and 10% of full power (225 KWt).
- Two homogenization strategies: "**kernel only**" and "**full volume**"
- Kernel only homogenizes all non-fuel TRISO layers by volume fraction into the background graphite.
- It then packs UCO kernels with the same original positions as in the fully explicit case.
- Full volume homogenizes all material within a compact by their volume fraction into a single material.
- Comparing both homogenizations to the fully explicit case can be used as a basis for deciding how proceed with a full core model.

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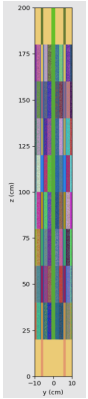
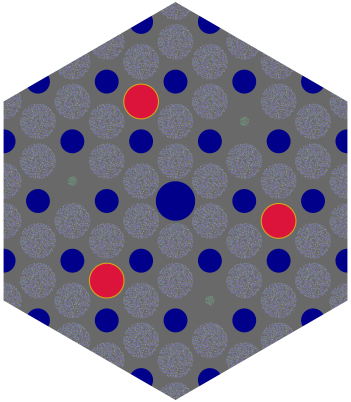
OpenMC Model



YZ slice of reactor



XY slice of reactor

- materials in XY slice
  - gray = graphite
  - blue = helium
  - red = YH2 moderator
  - gold = FeCrAL envelope
  - green = B4C poison spheres
  - purple dots = TRISO
- 8 axial layers in the core
- 2 axial layers per reflector
- pin pitch = 2cm
- periodic BC on hexagonal boundary
- vacuum BC at z = 0, z = 200 cm
- 3-way symmetry cloning scheme
- images via openmc-plotter

System Parameters

geometric parameters		
fuel compact radius 0.90 cm	poison compact radius 0.25 cm	moderator compact radius 0.843 cm
control compact radius 0.99 cm	coolant compact radius 0.60 cm	FeCrAl thickness 0.05 cm
Cr coating thickness	reflector heights	core height
0.007 cm	20 cm	160 cm

operation and design parameters		
fuel packing fraction	poison packing fraction	enrichment
0.4 -	0.25 -	19.95%
inlet temperature	outlet temperature	outlet pressure
873.15 K	1133.65 K	7 MPa

Depletion Theory

- Depletion simulations numerically solve the Bateman equations for the number densities $N_i(t)$:

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

  - $\sigma_{j\to i}(E,t)$ = transmutation cross section of isotope j that produces isotope i at energy E at time t
  - $\phi(E,t)$ = energy and time dependent flux
  - $\lambda_{j\to i}$ = decay constants for decay modes in nuclide j that produce nuclide i
- We can represent the system of equations in matrix form to solve for a nuclide vector $\mathbf{N}(t) \in \mathbb{R}^n$

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

where $\mathbf{A} \in \mathbb{R}^{n\times n}$ is commonly referred to as the burnup matrix.

Depletion Theory

- Assuming $\mathbf{A}(\mathbf{N}, t)$ changes slowly enough over time that it can be approximated as constant within a timestep (quasi steady-state assumption) gives

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

- The solution to which is

$$\mathbf{N}(t) = e^{\mathbf{A}t}\mathbf{N}_0. \tag{4}$$

- Since $\mathbf{A}$ technically does change in time (via $\mathbf{N}(t)$ changing), it needs to be updated accordingly.

- Solving (3) numerically involves two components [9]:
  1. Using a numerical method to integrate the matrix $\mathbf{A}$ in (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.

OpenMC Depletion Settings

- Predictor-Corrector time integration scheme
  - requires two transport solves per time step
  - Constant Extrapolation/Constant Midpoint scheme from Isotalo et al. [10]
  - k-eigenvalue simulations used 25 inactive and 75 active batches with 10000 particles per batch
  - continuous energy cross sections from ENDF-B-VII.1
- Chain XML file
  - contains transmutation and decay data necessary to compute the burnup matrix
  - based on the CASL project [11], which uses a thermal spectrum to compute the burnup matrix
  - provided by OpenMC [12]
- Time Steps - kept total burnup the same at each step in the simulation
  - Full power time steps: `[1]*5 + [5]*3 + [15]*3 + [60]*17` (days)
  - Half power time steps: `[2]*5 + [10]*3 + [30]*3 + [120]*17` (days)
  - Tenth power time steps: `[10]*5 + [50]*3 + [150]*3 + [600]*17` (days)

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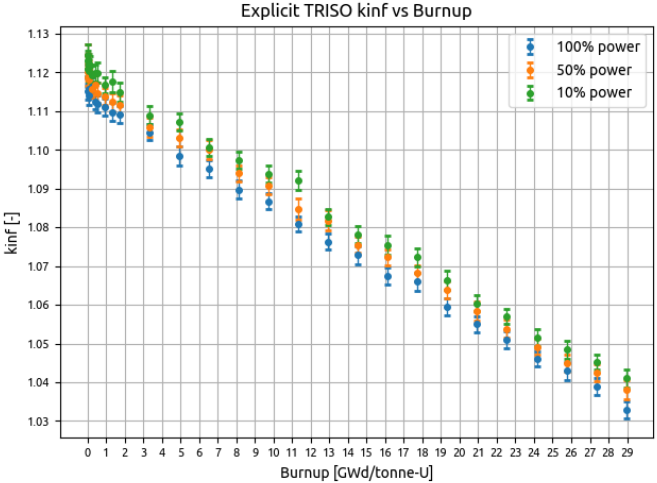
Fully-explicit k_{inf} versus burnup with 2σ error bars up to ~29 GWd/tonne-U



Comparing Eigenvalues

- Denote the first set of eigenvalues k_1 and the second set k_2, the $\Delta\rho$ between them is given by

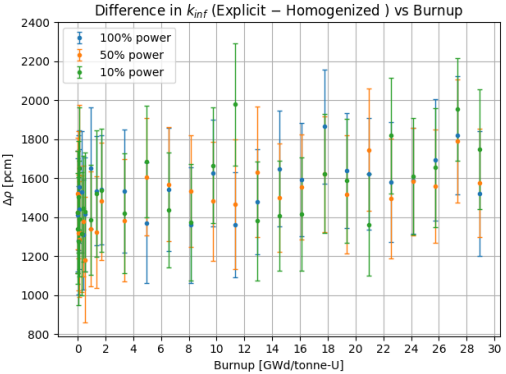
$$\Delta\rho \equiv \rho_1 - \rho_2 = \frac{k_1 - 1}{k_1} - \frac{k_2 - 1}{k_2} = \frac{1}{k_2} - \frac{1}{k_1} \tag{5}$$

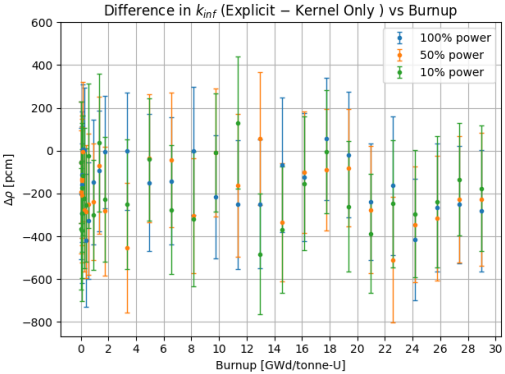
- Average $\Delta\rho$ compared with the explicit reference at every power with 2σ uncertainties

$\overline{\Delta\rho}$	explicit - homogenized	explicit - kernel only
100% power	1533 $\pm$ 55 pcm	-158 $\pm$ 55 pcm
50% power	1495 $\pm$ 56 pcm	-193 $\pm$ 55 pcm
10% power	1529 $\pm$ 56 pcm	-203 $\pm$ 55 pcm

- Kernel only $\Delta\rho$ on average performs about 1 order of magnitude better than full homogenization.

$\Delta\rho$ with 2σ error as a function of burnup up to $\sim$29 GWd/tonne-U





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Two-layer TRISO Homogenization

- While the kernel only eigenvalue computation outperforms the fully homogenized in terms of accuracy, it would be desirable to lower $\Delta\rho$ below 100 pcm.
- One potential source of error in the kernel only model is the effect of moving SiC.
- The kernel only model moves SiC further from the fuel than it exists in the explicit model.
  - Typically, SiC is located in a spherical region 175 - 215 microns away from fuel.
- Si has a much higher $\alpha = (\frac{A-1}{A+1})^2$ than C, so moving it away from fuel and replacing it with more graphite than in the explicit case increases the thermalization of neutrons near the fuel.
  - Accordingly, more neutrons will escape the resonance region than should.
  - This explains why $\Delta\rho$ is negative for explicit minus kernel
- A next iteration on fuel homogenization would be to leave the graphite background alone and only homogenize within a TRISO to create a **two layer** homogenization that packs TRISO fuel particles with a UCO fuel kernel at the center and all other layers homogenized together.

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- Co-authors: Patrick Shriwise, Benjamin Lindley, and Paul P.H. Wilson.

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Open Source Projects

- OpenMC website: https://openmc.org/
- OpenMC repository: https://github.com/openmc-dev/openmc
- VTB: https://mooseframework.inl.gov/virtual_test_bed/
- VTB repository: https://github.com/idaholab/virtual_test_bed
- Add me on LinkedIn (lewisgross1296) and GitHub (lewisgross1296)!

Equilibrium Xenon-135 Number Densities

Table: All units are atom per cubic centimeter. Since the first five time steps are used to converge xenon, the numbers below are the average of the fifth to the last value for xenon number density.

representation	explicit	kernel only	homogenized
100% power	2.43127×10^{16}	2.41845×10^{16}	1.19125×10^{15}
50% power	1.31047×10^{16}	1.30864×10^{16}	6.45668×10^{14}
10% power	2.82398×10^{15}	2.81919×10^{15}	1.38810×10^{14}

- These equilibrium values explain the observed trend at fresh fuel – and for much of the simulation – that lower power with the same total burnup has more excess Reactivity.
- The higher the power, the more Xenon-135 is produced during the initial jump to steady state, contributing to a larger negative reactivity insertion.

Plutonium 241 at Each Power for the Fully Explicit Case