

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

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April 24, 2024



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① Virtual Test Bed Gas-Cooled Microreactor

② OpenMC Model

③ Results and Discussion

④ Next Steps



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Virtual Test Bed [1]

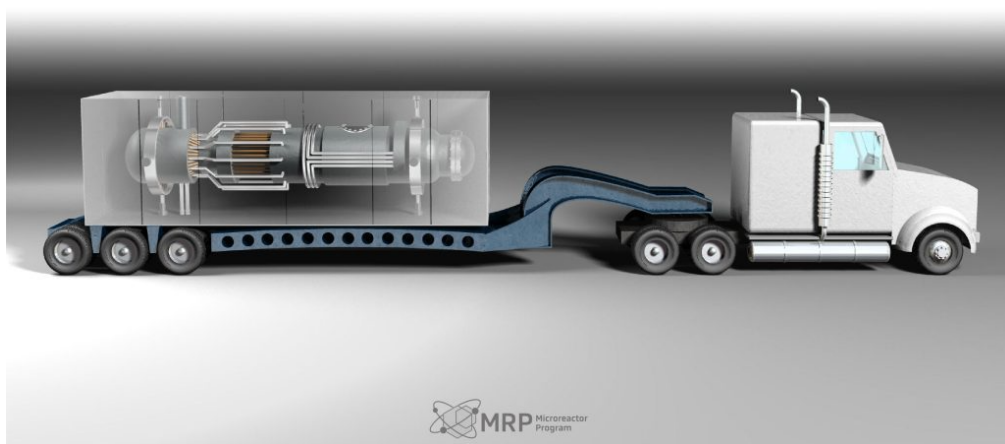


NRIC National Reactor
Innovation Center

NEAMS



Microreactors [2]

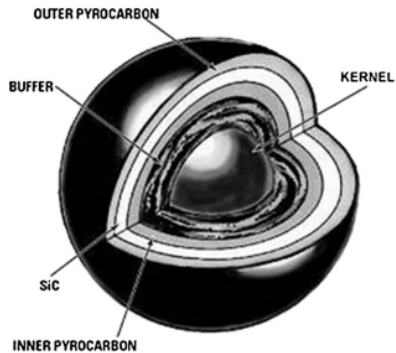


TRISO Fuel





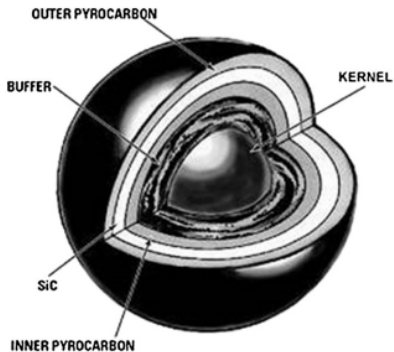
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Layers from innermost to outermost: fuel kernel, buffer, Inner PyC, SiC, Outer PyC [3].



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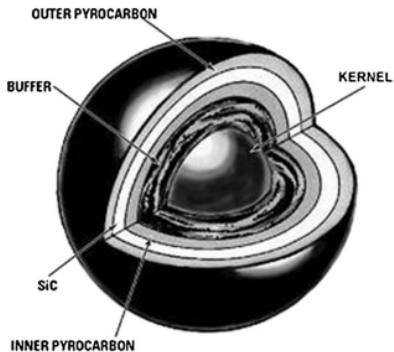


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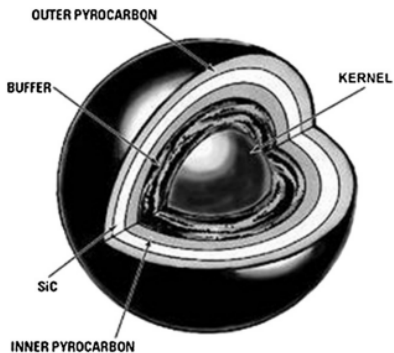


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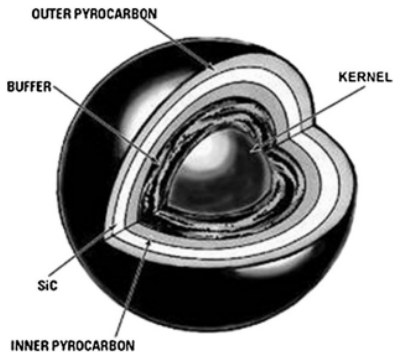


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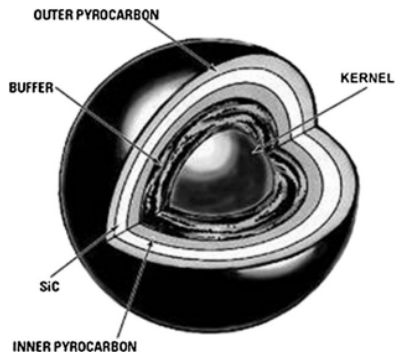


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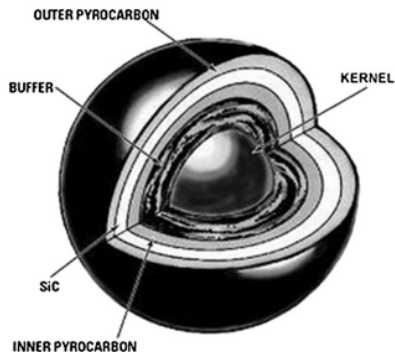


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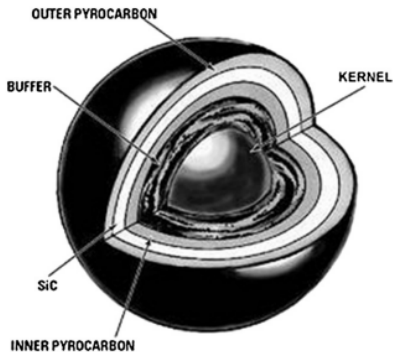


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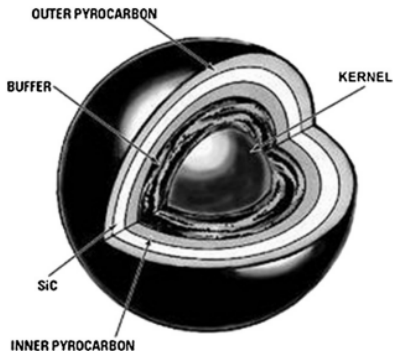


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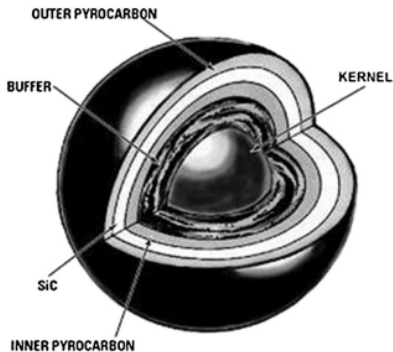


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 - Many TRISOs per reactor



Virtual Test Bed Gas Cooled Microreactor (VTB GCMR)



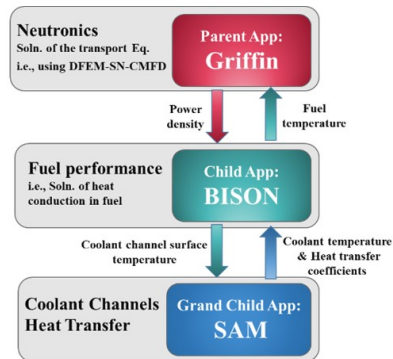
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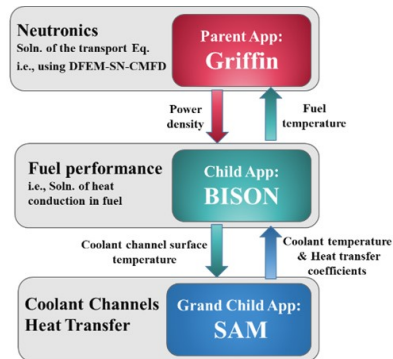


MultiApp hierarchy of preliminary GCMR models. Image from [6].



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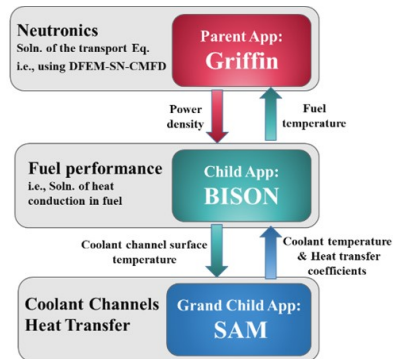


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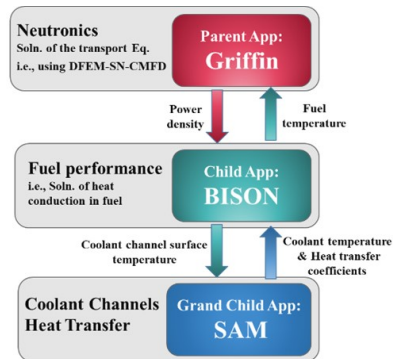


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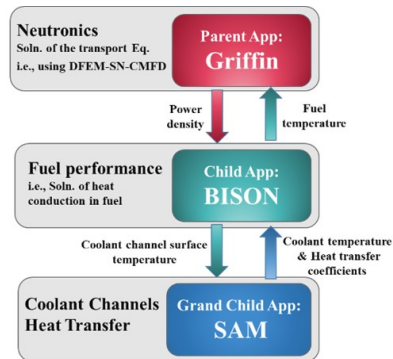


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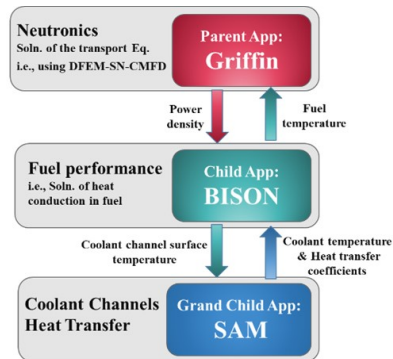


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- For a full core model, it will be prohibitively expensive to model every TRISO explicitly



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- 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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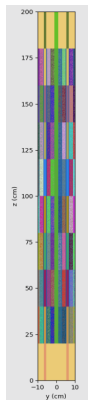
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OpenMC Model





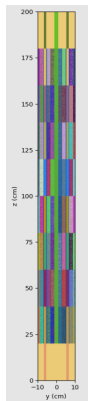
OpenMC Model



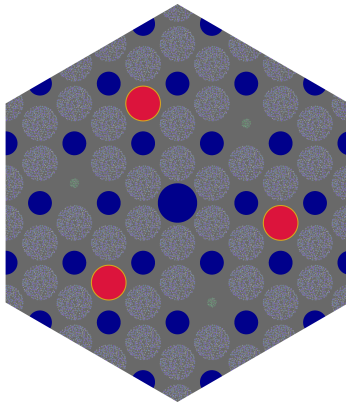
YZ slice of reactor



OpenMC Model



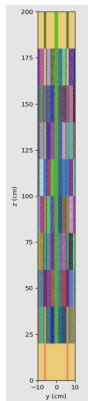
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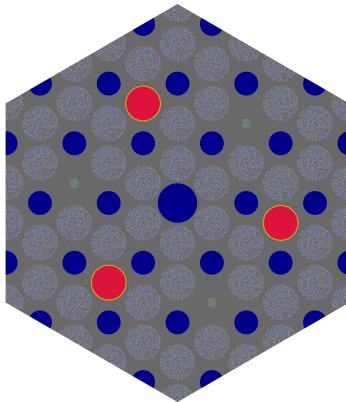
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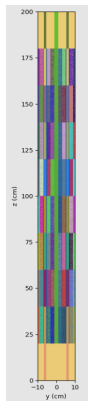


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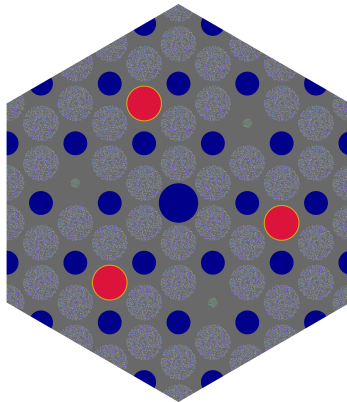
- materials in XY slice



OpenMC Model



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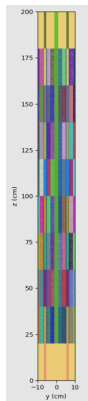


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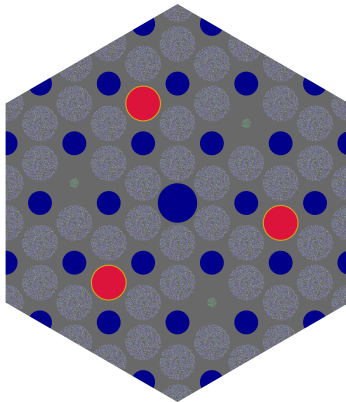
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OpenMC Model



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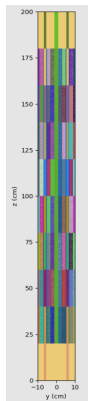


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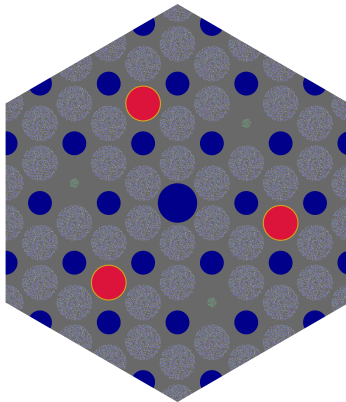
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OpenMC Model



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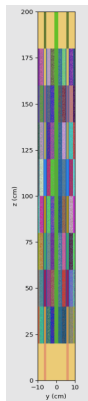


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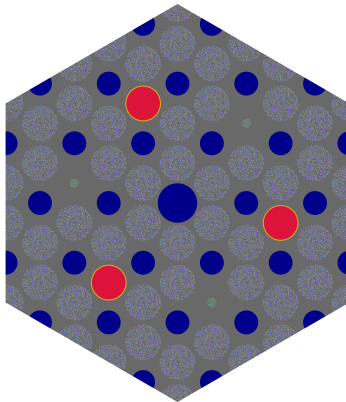
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OpenMC Model



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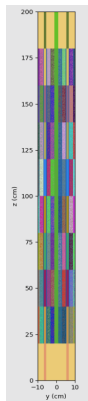


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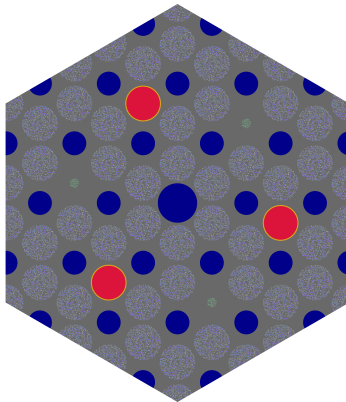
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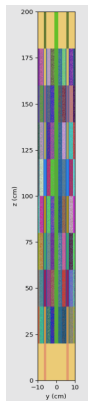


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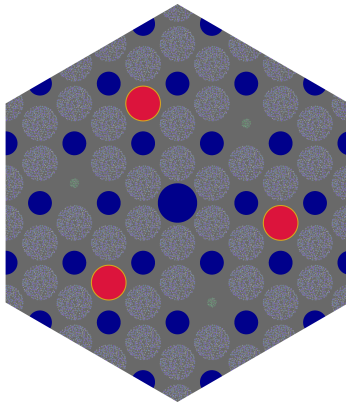
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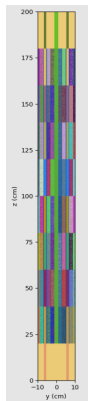


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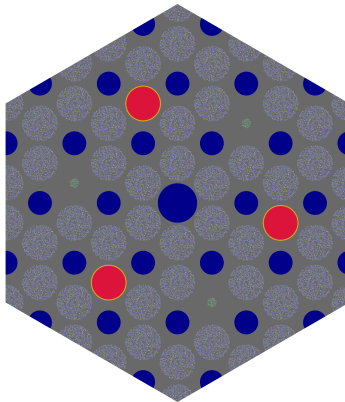
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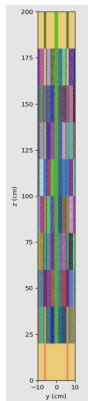


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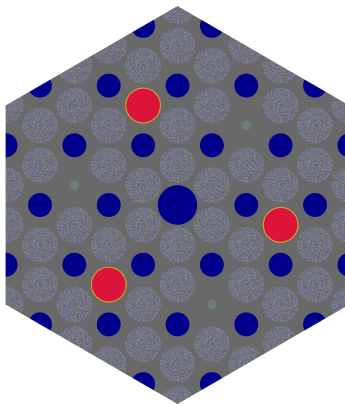
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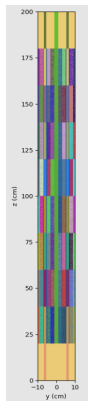


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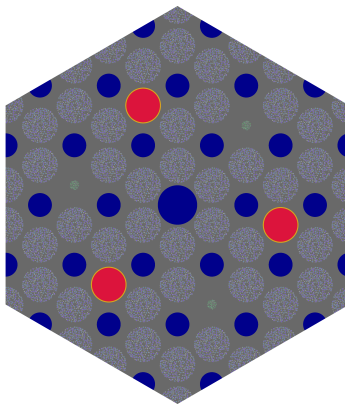
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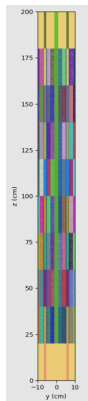


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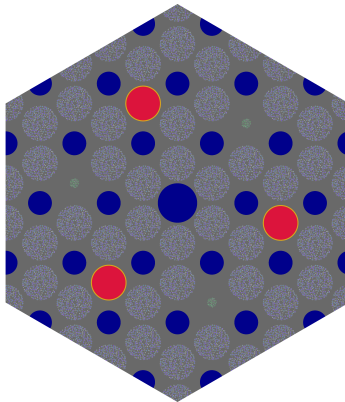
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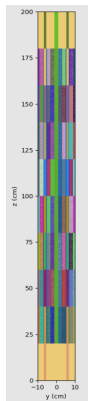


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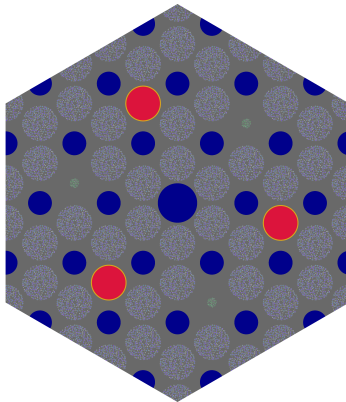
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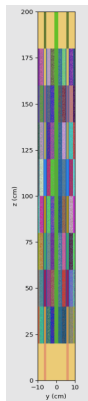


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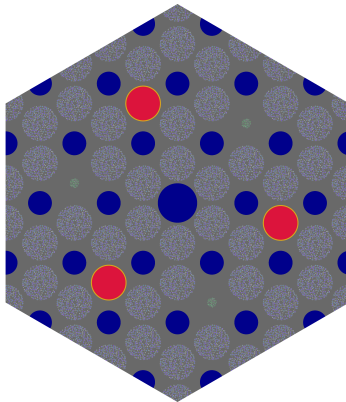
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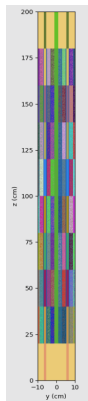


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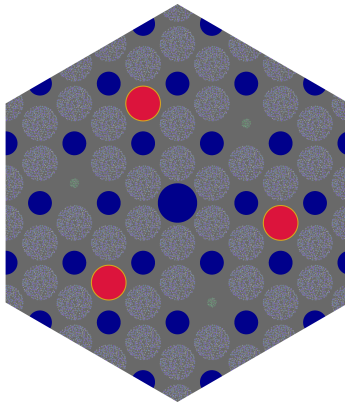
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- 3-way symmetry cloning scheme
- images via openmc-plotter



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 0.007 cm	reflector heights 20 cm	core height 160 cm

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

Depletion Theory





Depletion Theory

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

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



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 - $\phi(E, t)$ = energy and time dependent flux
 - $\lambda_{j \rightarrow i}$ = 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 $\mathbf{N}(t) \in \mathbb{R}^n$

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

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

Depletion Theory





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

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 - Evaluating the matrix exponential $\exp(\mathbf{A}t)$ or the action of the matrix exponential on a vector of nuclide concentrations.

OpenMC Depletion Settings





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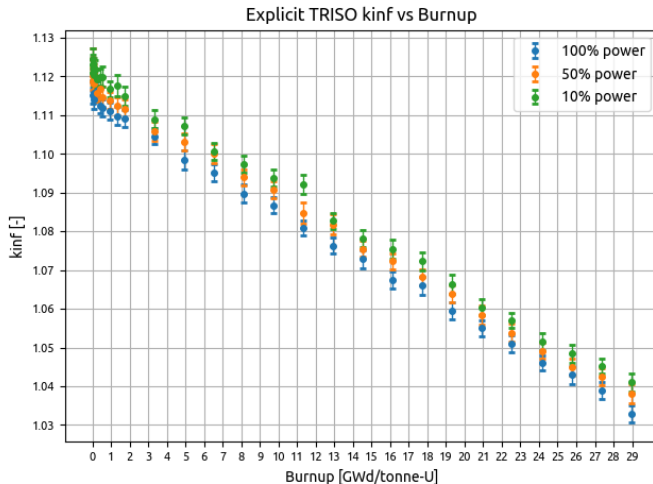
② OpenMC Model

③ Results and Discussion

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



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$\overline{\Delta\rho}$	explicit - homogenized	explicit - kernel only
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- 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 ~ 29 GWd/tonne-U

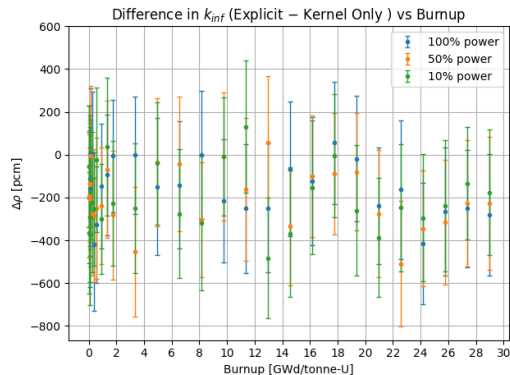
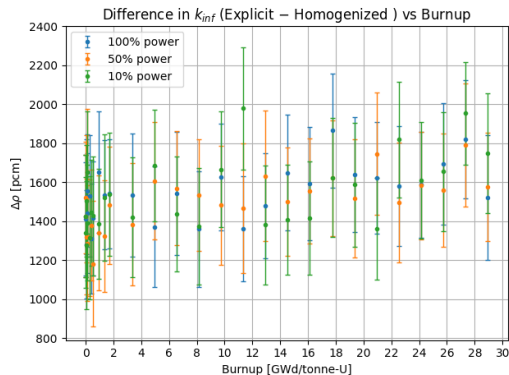




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Two-layer TRISO Homogenization



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 - 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.

- The first author was supported in part by the US Nuclear Regulatory Commission's Graduate Fellowship Program administered by the University of Wisconsin-Madison.
- The OpenMC team!
- The Center for High Throughput Computing at the University of Wisconsin - Madison
- Co-authors: Patrick Shriwise, Benjamin Lindley, and Paul P.H. Wilson.



- [1] Guillaume L. Giudicelli et al. "The Virtual Test Bed (VTB) Repository: A Library of Reference Reactor Models Using NEAMS Tools". In: *Nuclear Science and Engineering* 0.0 (2023), pp. 1–17. URL: <https://doi.org/10.1080/00295639.2022.2142440>.
- [2] Joel Hiller. *Microreactors*. Idaho National Lab, Aug. 2023. URL: <https://inl.gov/trending-topics/microreactors/> (visited on 04/09/2024).
- [3] X.W. Zhou and C.H. Tang. "Current status and future development of coated fuel particles for high temperature gas-cooled reactors". In: *Progress in Nuclear Energy* 53.2 (2011), pp. 182–188. ISSN: 0149-1970. DOI: <https://doi.org/10.1016/j.pnucene.2010.10.003>. URL: <https://www.sciencedirect.com/science/article/pii/S0149197010001587>.
- [4] Nicolas E. Stauff et al. "Preliminary Applications of NEAMS Codes for Multiphysics Modeling of a Heat Pipe Microreactor". In: *Proceedings of the American Nuclear Society Annual 2021 Meeting* (2021).
- [5] Nicolas E. Stauff et al. "Applications of NEAMS Codes for Multiphysics Modeling of Several Microreactors Problems". In: *Proceedings of the American Nuclear Society Winter Conference*. 2022.

- [6] Ahmed Amin Abdelhameed et al. “High-Fidelity Multiphysics Modeling of Load Following for 3-D Gas-Cooled Microreactor Assembly using NEAMS Codes”. In: *Proceedings of the American Nuclear Society Winter Conference*. 2022.
- [7] N. Stauff et al. *High-fidelity multiphysics load following and accidental transient modeling of microreactors using NEAMS tools*. Tech. rep. Argonne National Laboratory, Sept. 2023.
- [8] Edward M. Duchnowski et al. “Pre-conceptual high temperature gas-cooled microreactor design utilizing two-phase composite moderators. Part I: Microreactor design and reactor performance”. In: *Progress in Nuclear Energy* (2022).
- [9] Paul K. Romano et al. “Depletion capabilities in the OpenMC Monte Carlo particle transport code”. en. In: *Annals of Nuclear Energy* 152 (Mar. 2021). ISSN: 03064549. URL: [10.1016/j.anucene.2020.107989](https://doi.org/10.1016/j.anucene.2020.107989) (visited on 11/18/2022).
- [10] Aarno Isotalo and Ville Sahlberg. “Comparison of Neutronics-Depletion Coupling Schemes for Burnup Calculations”. en. In: *Nuclear Science and Engineering* 179.4 (Apr. 2015), pp. 434–459. ISSN: 0029-5639, 1943-748X. URL: [10.13182/NSE14-35](https://doi.org/10.13182/NSE14-35) (visited on 04/13/2023).
- [11] Kang Seog Kim. “Specification for the VERA Depletion Benchmark Suite”. In: (Dec. 2015). URL: [10.2172/1256820](https://doi.org/10.2172/1256820).



- [12] *Depletion Chains*. URL: <https://openmc.org/depletion-chains/>.



- 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

