Pebble Database for PBR MC&A – NEUP

Advanced Reactor Safeguards & Security Spring Working Group Meeting, May 14 – May 16, 2024

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Project Team

Core VCU team

- Braden Goddard (PI)
- Zeyun Wu (co-PI)
- Kashminder Mehta (Ph.D. student)
- Ben Impson (undergrad)
- Holden Walker (undergrad)

External advisory team

- Claudio Gariazzo (ANL)
- Yonggang Cui (BNL)
- Philip Gibbs (ORNL)
- Donny Hartanto (ORNL)

- Project duration: Oct. 2022 – Sept. 2024
  - Requesting 3 month no cost extension
- Funding amount: $400k

The Challenge

- Knowing the nuclear and radiological material content in used pebbles is important for:
  - Safeguards
  - Facility operations
  - Waste management
  - Etc.

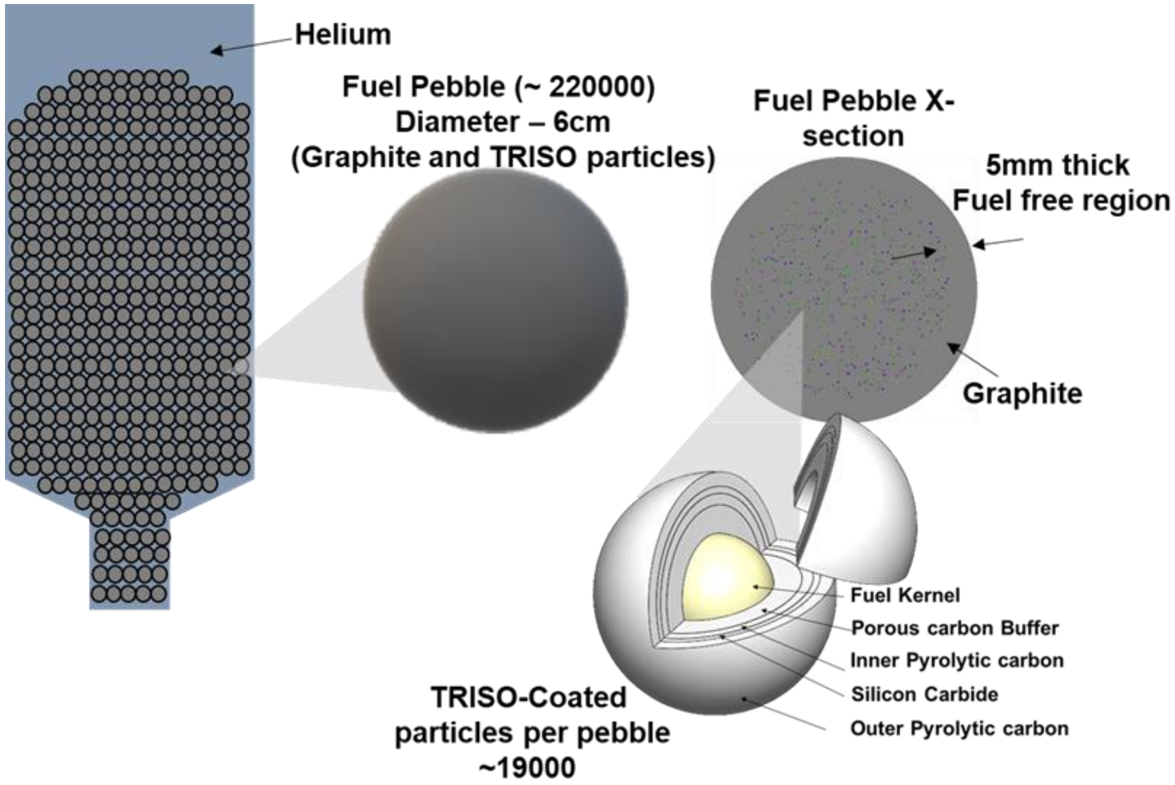
- Used pebbles are measured relatively quickly after discharge and there path through the reactor can vary between pebbles
  - Traditional LWR gamma and neutron NDA correlations may not be applicable

Project Goal

- Create a data library of used pebble NDA signatures
  - Gamma spectra (HPGe)
  - Neutron counts
- Validate data library using an independent code
  - MCNP, OpenMC, Serpent
  - INDEPTH (ORIGEN)
- Document methodology used to create the data library
  - Focus is Xe-100

Introduction of PBR

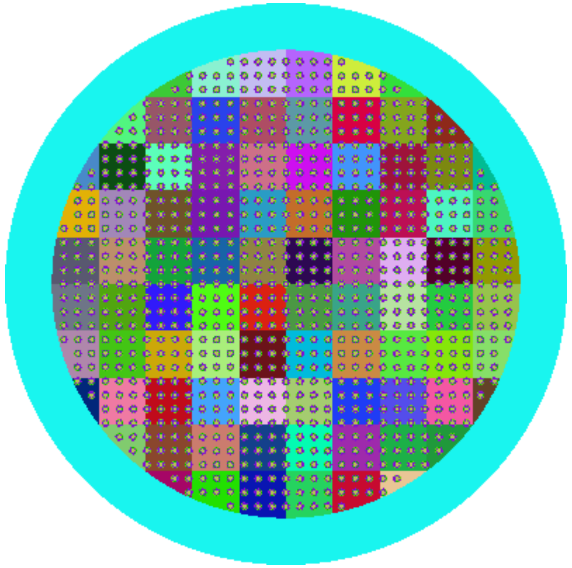
- PBR is an emerging as a next generation (Gen-IV) reactor
- Thousands of pebbles used as fuel
- Each pebble is spherical and filled with thousands of TRISO particles
- Helium is used as the coolant
- Pebbles circulates continuously through the reactor core throughout operational lifespan



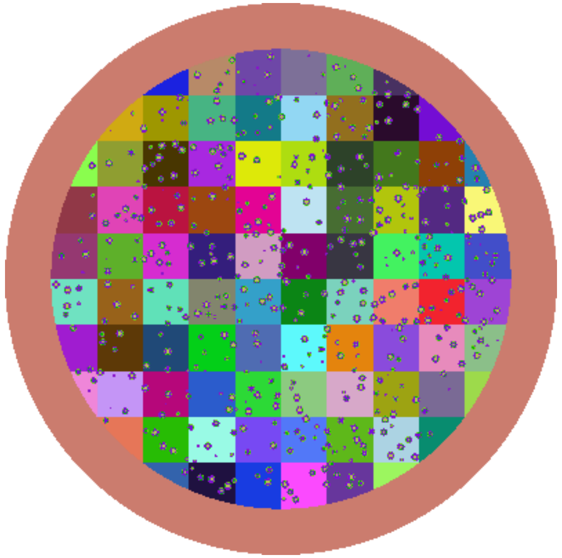
Single Pebble Model

Single Pebble Model – Code Verification

- Code to Code verification of k_∞ in a single pebble with different Monte Carlo code: OpenMC and MCNP (and Serpent)



Uniform TRISO distribution



Random TRISO distribution

Pebble material composition

Material	Density (g/cm³)	Composition (atomic fraction)	Dimension (μm)
UCO Fuel	10.9	^{235}U: 0.05232 ^{238}U: 0.28101 ^{16}O: 0.49982 ^{17}O: 0.00019 C: 0.16667	425 (diameter)
Carbon Buffer	1.0	C: 1.0	100 (thickness)
PyC1	1.9	C: 1.0	40 (thickness)
PyC2	1.9	C: 1.0	40 (thickness)
SiC	3.2	C: 0.5 Si: 0.5	35 (thickness)
Graphite	1.75	C: 1.0	6 cm diameter with a 0.5 cm thickness non-fuel shell

Results at Hot Operation Condition

- k_∞ of a single pebble with TRISO particles uniformly and randomly distributed at **1200 K** temperature

Pebble Model		k_∞ (White B.C.)	k_∞ (Mirror B.C.)
Uniform	MCNP	1.50821 +/- 0.00007	1.51774 +/- 0.00007
	OpenMC	1.50789 +/- 0.00012	1.51757 +/- 0.00012
	deviation	0.00031	0.00017
Random	MCNP	1.51203 +/- 0.00008	1.52111 +/- 0.00006
	OpenMC	1.51071 +/- 0.00012	1.51980 +/- 0.00012
	deviation	-0.00132	0.00131

Results at Cold Operation Condition

- k_∞ of a single pebble with TRISO particles uniformly and randomly distributed at **room temperature**

Pebble Model		k_∞ (White B.C.)	k_∞ (Mirror B.C.)
Uniform	MCNP	1.60743 +/-0.00008	1.61471+/-0.00004
	OpenMC	1.60818 +/- 0.00011	1.61560 +/- 0.00012
	deviation	-0.00067	-0.00089
Random	MCNP	1.61017 +/-0.00007	1.61723 +/-0.00006
	OpenMC	1.61025 +/-0.00011	1.61739 +/- 0.00012
	deviation	0.00008	0.00016

Full Core Model

Approach

- Integrate the open-source CFD-DEM and OpenMC codes for the full reactor model
- To analyze the neutronic behavior, including spatial and temporal pebble depletion, as well as conduct thermal and fluid flow analysis within the reactor core

Computational Models (CFD-DEM)

cfdemSolverPiso

- LIGGGHTS → DEM
- OpenFOAM 5.0 → CFD

DEM:

$$m_i \frac{d\mathbf{U}_i}{dt} = \sum_{j=1}^{n_j^c} \boldsymbol{F}_{i,j}^{c} + \boldsymbol{F}_i^{g} + \left(\boldsymbol{F}_i^{b} + \boldsymbol{F}_i^{d}\right)^{f} + \boldsymbol{F}_{\mathbf{i,b}}$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{n_j^c} \boldsymbol{M}_{i,j}^{c}$$

CFD:

$$\frac{\partial \varepsilon\rho_f}{\partial t} + \nabla\cdot\left(\varepsilon\rho_f \boldsymbol{u}\right) = 0,$$

$$\frac{\partial \varepsilon\rho_f \boldsymbol{u}}{\partial t} + \nabla\cdot\left(\varepsilon\rho_f \boldsymbol{uu}\right) - \varepsilon\nabla\cdot\left(\mu\nabla\boldsymbol{u}\right) = -\nabla p - \boldsymbol{F}^{pf} + \varepsilon\rho_f \boldsymbol{g},$$

$$\varepsilon\rho_f C_{p,f}\frac{\partial T_f}{\partial t} + \varepsilon\rho_f C_{p,f}\nabla\cdot\mathbf{u}(\mathrm{T}_f) - \nabla\cdot(\varepsilon k_f'\nabla \mathrm{T}_f) + \alpha\left(T_f - T_s\right) = \dot{q}_f''',$$

$$\left(1-\varepsilon\right)\rho_s C_{p,s}\frac{\partial T_s}{\partial t} - \nabla\cdot(\varepsilon k_s'\nabla \mathrm{T}_s) + \alpha\left(T_s - T_f\right) = \dot{q}_s'''$$

DEM: discrete element method
CFD: computational fluid dynamics

Computational Models (OpenMC)

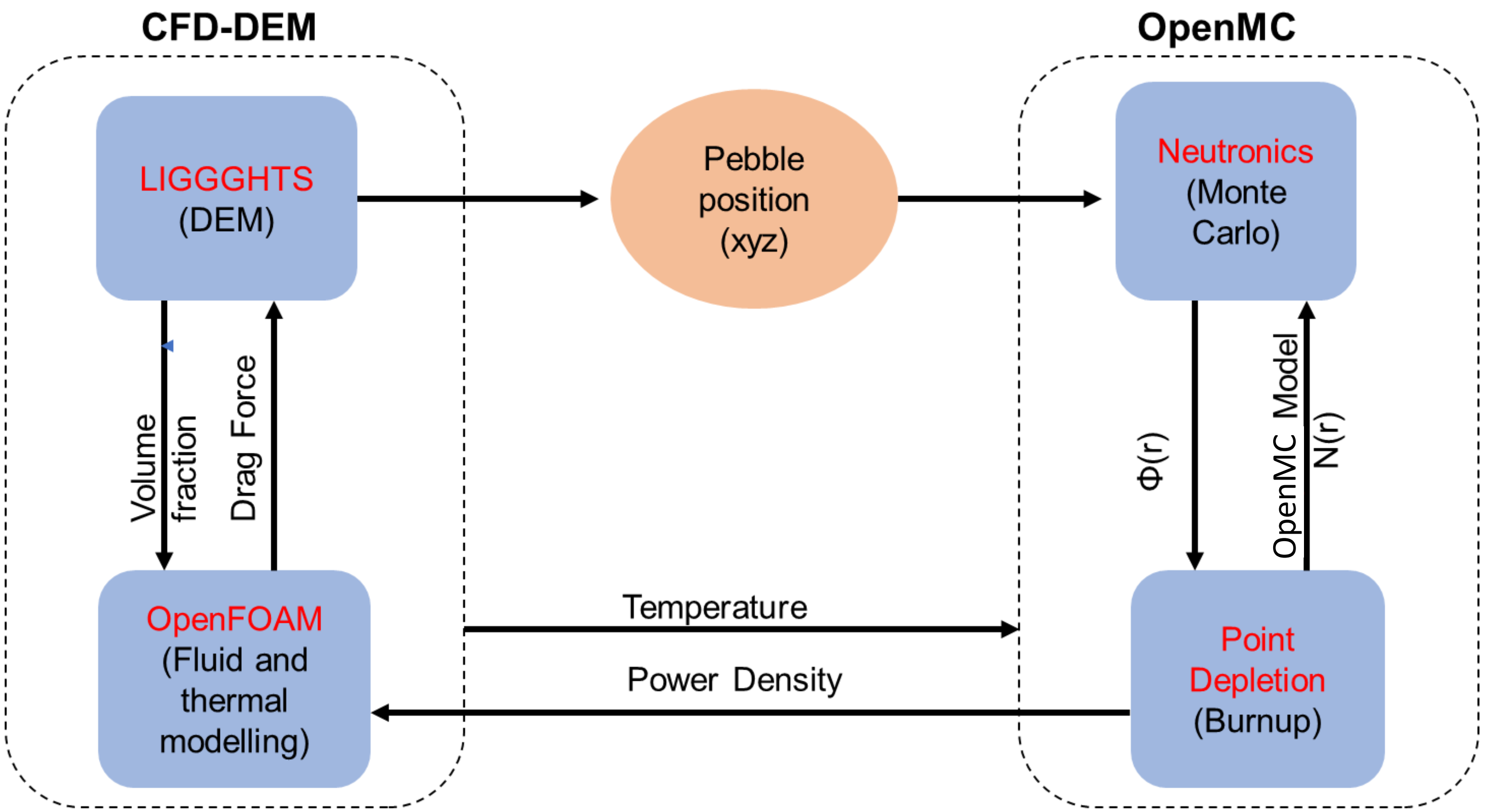
- OpenMC – Monte Carlo based 3D neutron transport code, analyzing neutronic behavior in reactors

$$\Sigma_t(\vec{r},E)\psi(\vec{r},E,\vec{\Omega})+\vec{\Omega}\cdot\nabla\psi(\vec{r},E,\vec{\Omega})-\int_0^\infty dE'\int_{4\pi}d\Omega'\Sigma_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\psi(\vec{r},E',\vec{\Omega}')$$
$$=\frac{1}{k_{\text{eff}}}\frac{\chi(E)}{4\pi}\int_0^\infty dE'\nu(E')\Sigma_f(\vec{r},E')\phi(\vec{r},E')$$

- OpenMC utilizes the Bateman equation for pebble fuel depletion

$$\frac{dN_i(t)}{dt}=\lambda_{i-1}N_{i-1}(t)-\lambda_i N_i(t)$$

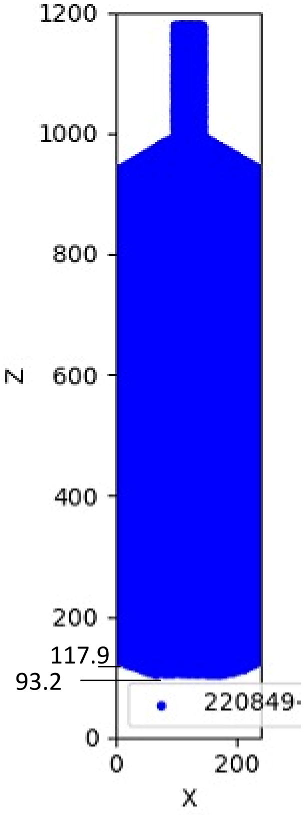
Coupling CFD-DEM and OpenMC



PBR Model – OpenMC (Static Core)

Pebbles positions imported from DEM to OpenMC

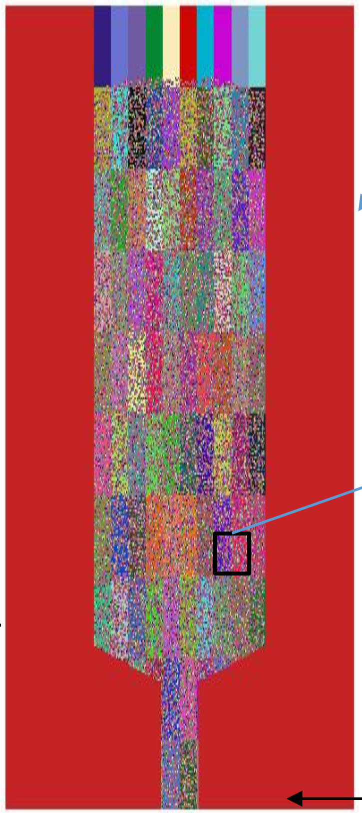
pf ~60.5%



Modelling of reactor Core and RPV in OpenMC

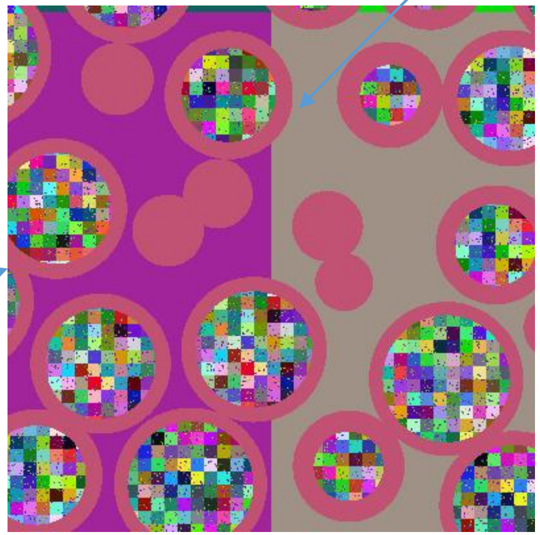
RPV – dia. 4.88 m (Graphite Material)

Reflective Top B.C.



Vacuum

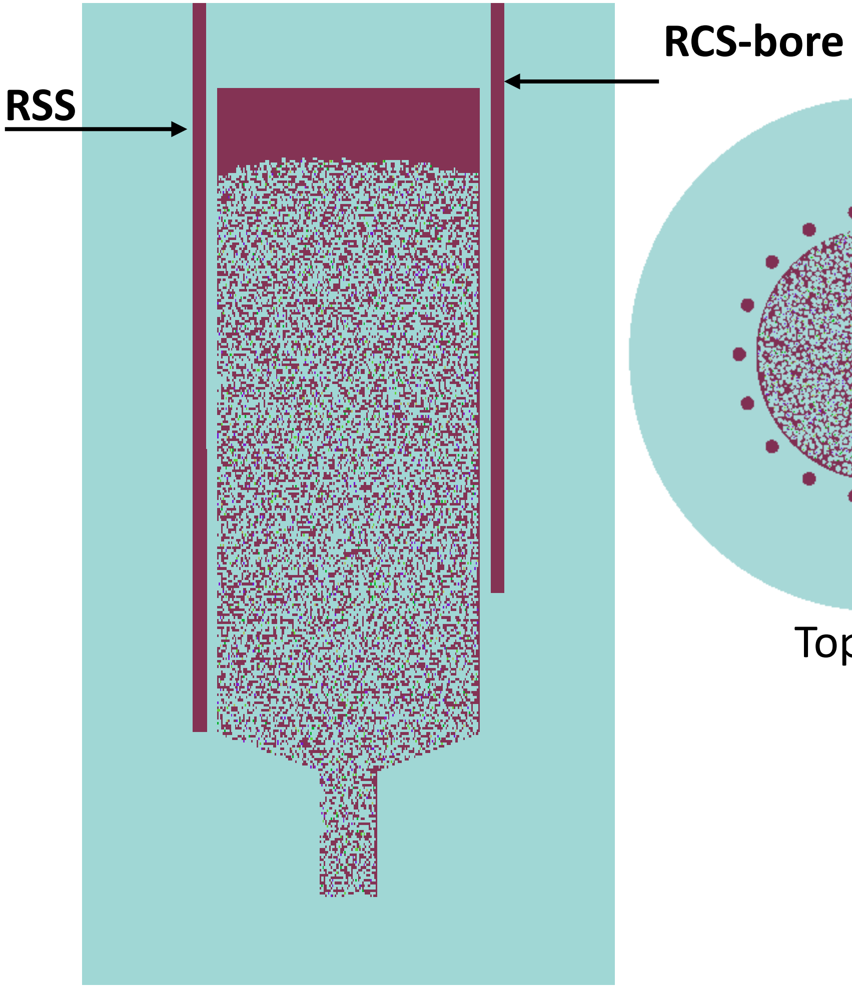
Helium gas 0.00286 g/cm3



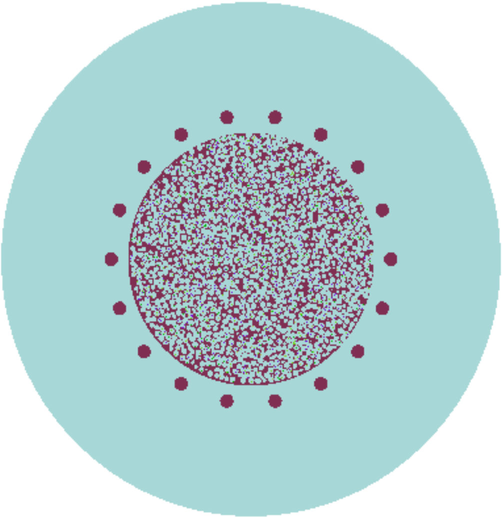
Bottom Reflector

Lattice Acceleration in reactor and pebble

OpenMC PBR – Modeling Control Rods



Front View



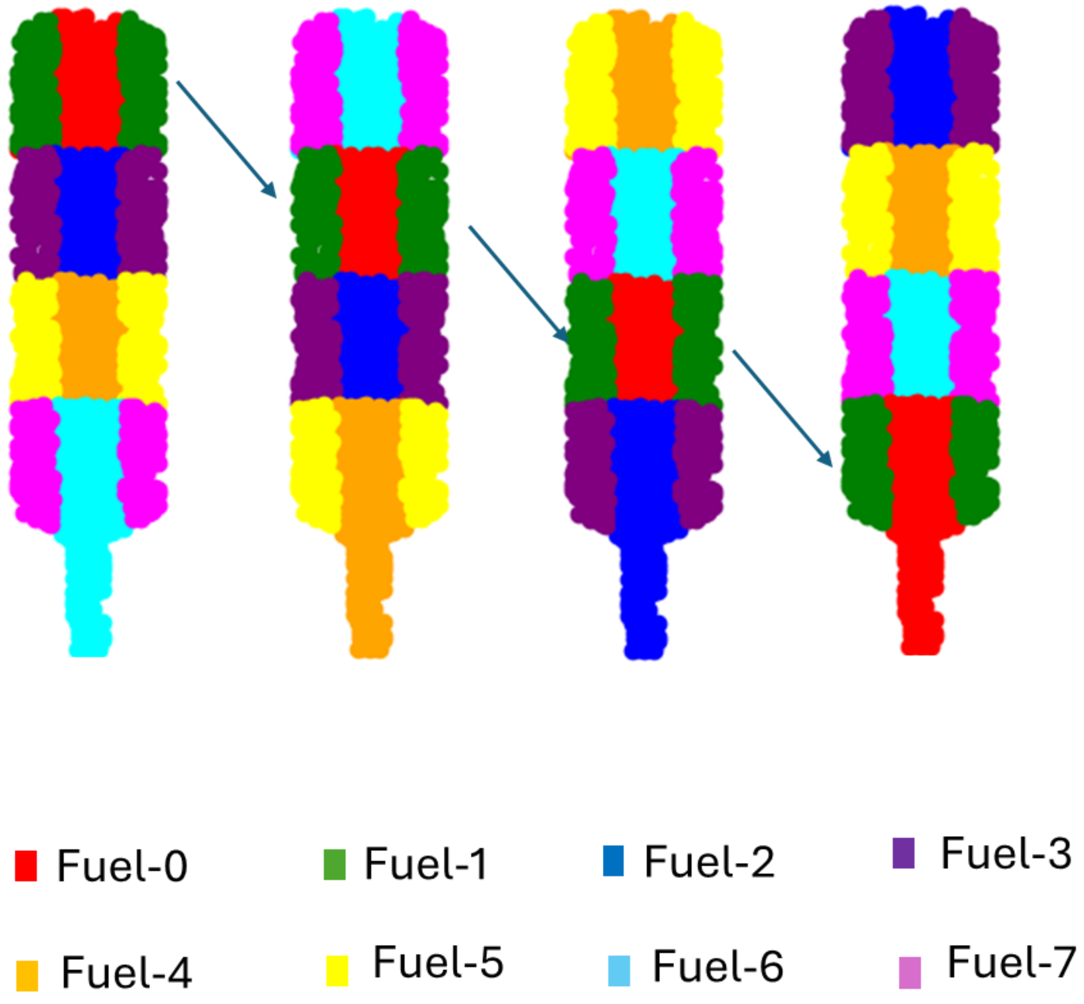
Top View

	Radius	**Layers**	**Material**	**Inner Radius**	**Outer radius**	
RCS /RSS	6.5cm	Layer 1	Incoloy800	4.15 cm	4.2 cm	0.5 mm
		Layer 2	B4C	4.2 cm	5 cm	8 mm
		Layer 3	Incoloy800	5	5.25	2.5 mm

Type	Total number	Inserted length (in present case)	Total insertion length
RCS	9	330 cm	660 cm
RSS	9	124 cm	860 cm

OpenMC PBR – Region Circulation

- The reactor core is divided into four axial and two radial regions
- Currently, there is no radial mixing of pebbles



Describes the recirculation of fuel in the reactor core

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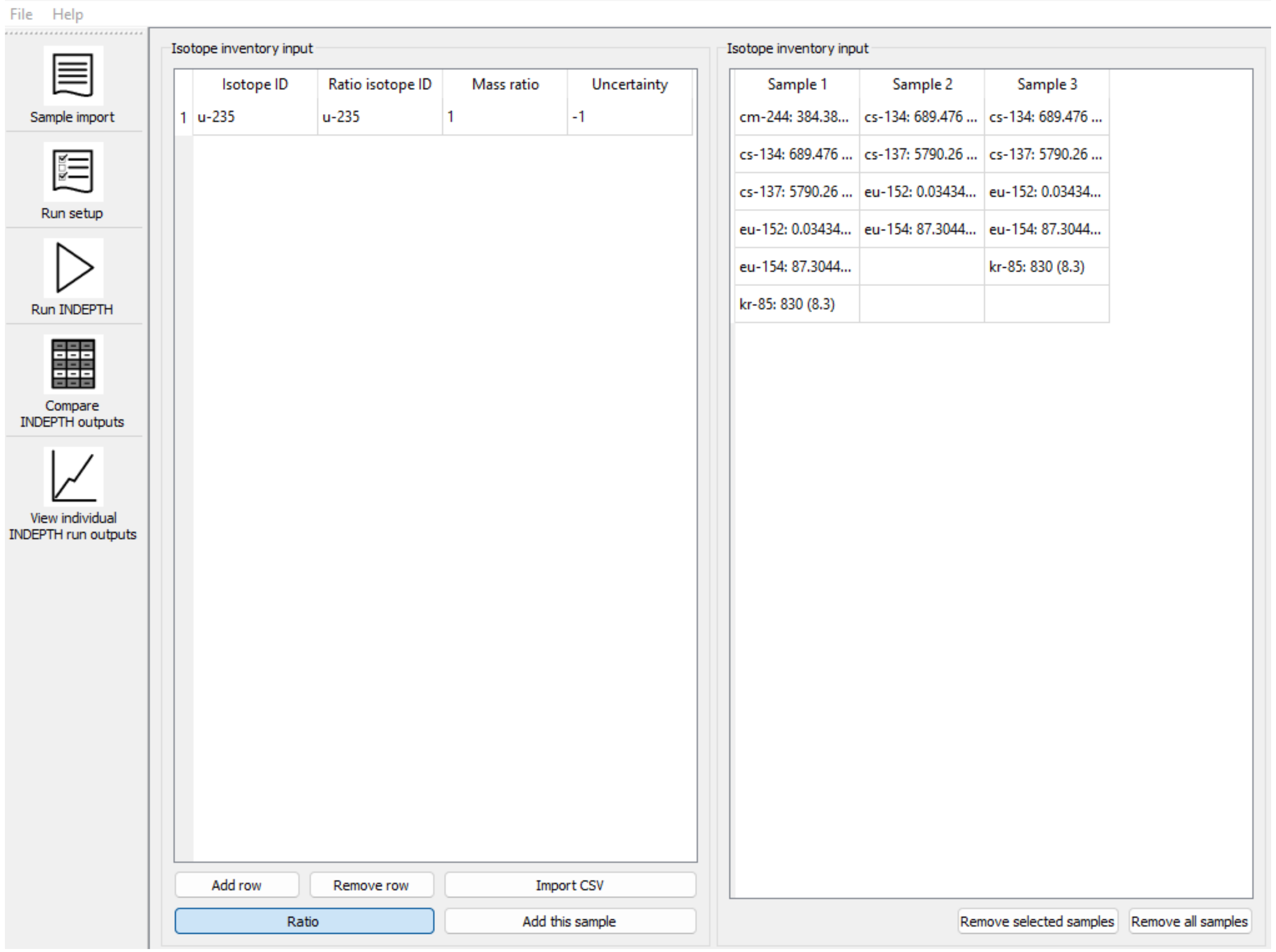
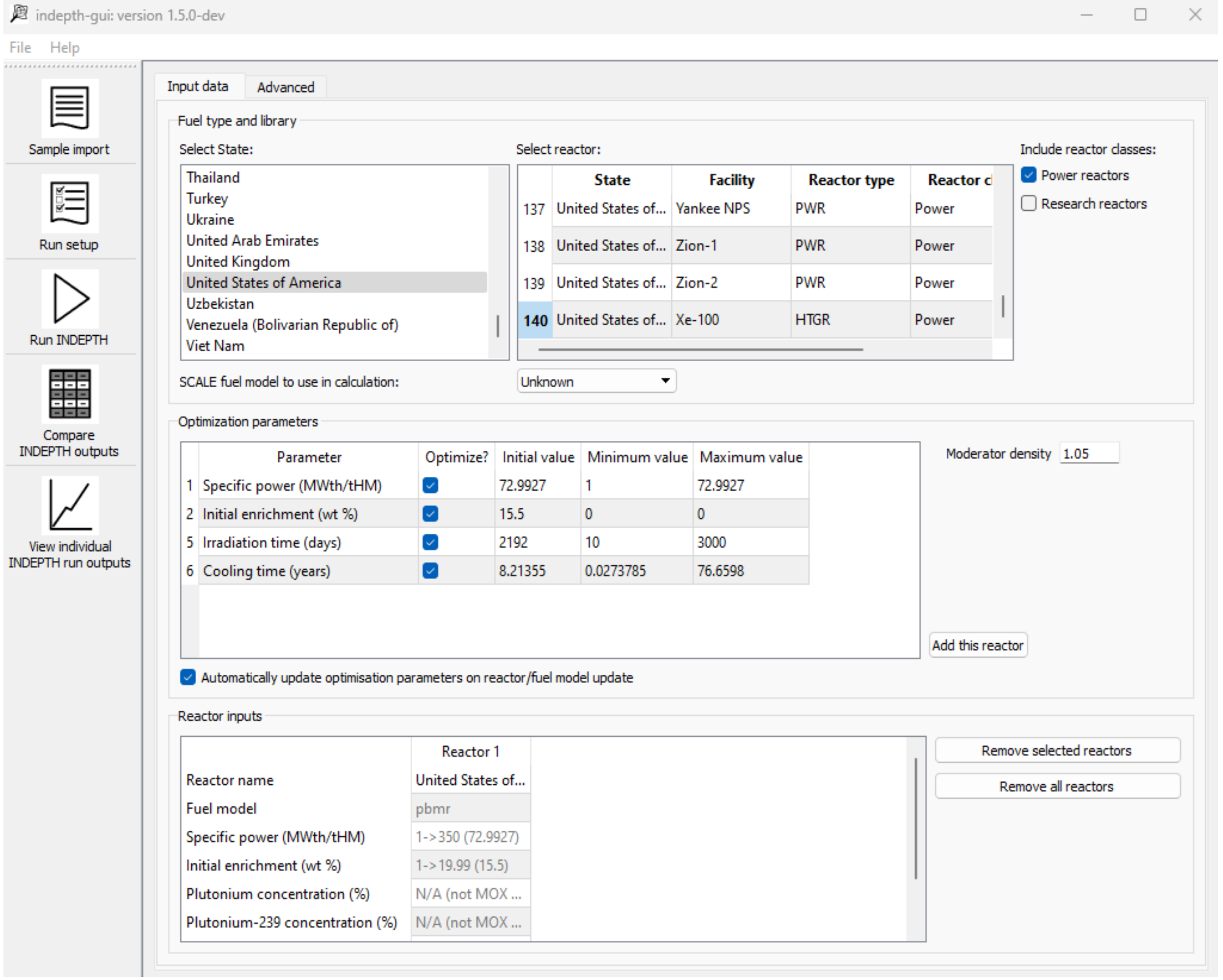
INDEPTH Analyses

INDEPTH


File Help
Sample import
Run setup
Run INDEPTH
Compare INDEPTH outputs
View individual INDEPTH run outputs
Isotope inventory input
Isotope ID
Ratio isotope ID
Mass ratio
Uncertainty
1 u-235 u-235 1 -1
Add row
Remove row
Import CSV
Ratio
Add this sample
Isotope inventory input
Sample 1
Sample 2
Sample 3
cm-244: 384.38...
cs-134: 689.476 ...
cs-137: 5790.26 ...
eu-152: 0.03434...
eu-154: 87.3044...
kr-85: 830 (8.3)
Remove selected samples
Remove all samples


indepth-gui: version 1.5.0-dev
File Help
Sample import
Run setup
Run INDEPTH
Compare INDEPTH outputs
View individual INDEPTH run outputs
Input data
Advanced
Fuel type and library
Select State:
Thailand
Turkey
Ukraine
United Arab Emirates
United Kingdom
United States of America
Uzbekistan
Venezuela (Bolivarian Republic of)
Viet Nam
Select reactor:
State Facility Reactor type Reactor c
137 United States of... Yankee NPS PWR Power
138 United States of... Zion-1 PWR Power
139 United States of... Zion-2 PWR Power
140 United States of... Xe-100 HTGR Power
Include reactor classes:
Power reactors
Research reactors
SCALE fuel model to use in calculation:
Unknown
Optimization parameters
Parameter Optimize? Initial value Minimum value Maximum value
1 Specific power (MWth/tHM) 72.9927 1 72.9927
2 Initial enrichment (wt %) 15.5 0 0
5 Irradiation time (days) 2192 10 3000
6 Cooling time (years) 8.21355 0.0273785 76.6598
Moderator density 1.05
Add this reactor
Automatically update optimisation parameters on reactor/fuel model update
Reactor inputs
Reactor 1
Reactor name United States of...
Fuel model pbmr
Specific power (MWth/tHM) 1->350 (72.9927)
Initial enrichment (wt %) 1->19.99 (15.5)
Plutonium concentration (%) N/A (not MOX ...
Plutonium-239 concentration (%) N/A (not MOX ...
Remove selected reactors
Remove all reactors

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Isotope inventory input

Sample 1	Sample 2	Sample 3
cm-244: 384.38...	cs-134: 689.476 ...	cs-134: 689.476 ...
cs-134: 689.476 ...	cs-137: 5790.26 ...	cs-137: 5790.26 ...
cs-137: 5790.26 ...	eu-152: 0.03434...	eu-152: 0.03434...
eu-152: 0.03434...	eu-154: 87.3044...	eu-154: 87.3044...
eu-154: 87.3044...		kr-85: 830 (8.3)
kr-85: 830 (8.3)		

Burnup Condition	Value
Irradiation time (Days)	1304
Cooling time (Days)	30
Enrichment (%)	15.5

(Max Enrichment set to 19.99%)

Result	Sample 1	Sample 2	Sample 3
Irradiation Time (Days)	1987	1366	1976
Cooling time (Days)	9.99	9.99	9.99
Enrichment (%)	15.85	18.47	17.50

- Input data from heterogeneous MCNP single pebble model
- INDEPTH model uses homogeneous SCALE single pebble model

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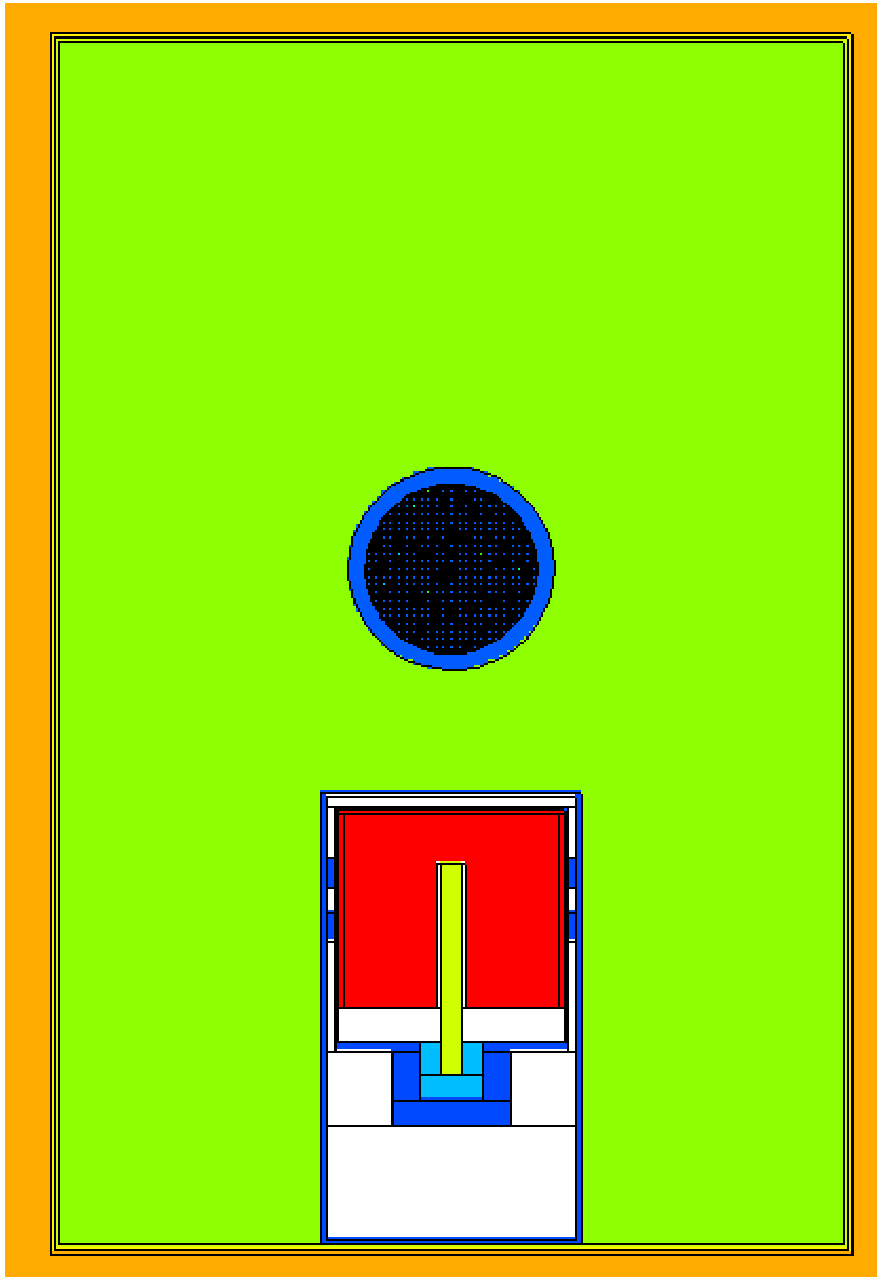
Gamma Ray Signature

Gamma Ray Sampling

- MCNP6.2
- Gamma rays are generated in the fuel region of the pebble
  - Each gamma emitting nuclide in used fuel is modeled independently
- HPGe detector is used to measure the gammas
  - Energy range from 0 MeV to 8192 MeV with 16384 bins at 0.5 keV per bin



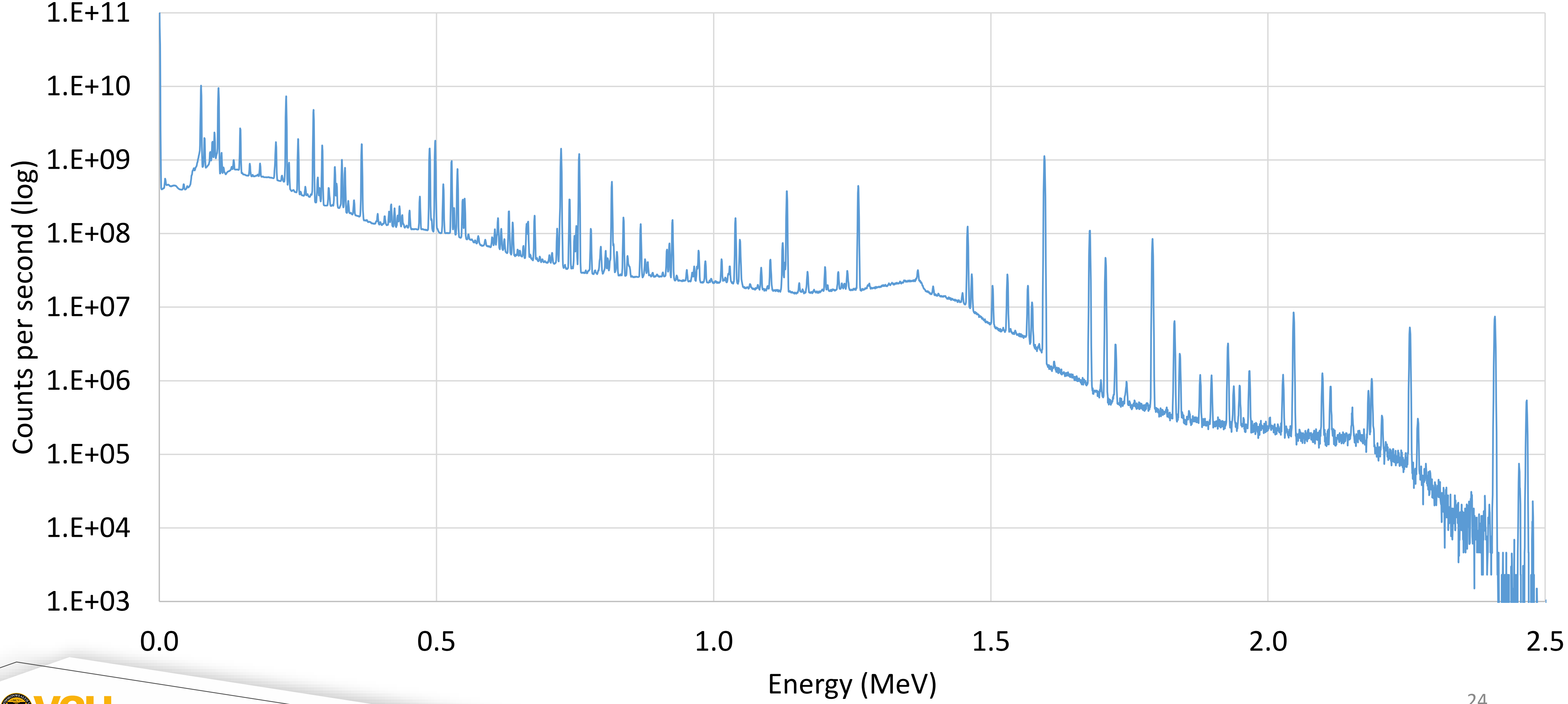
Spreadsheet has 2 inputs

- Scales pre-tabulated results based on ZAID and mass

ZAID	Name	Mass
92234	U234	2.53E-10
92235	U235	3.71E-05
92236	U236	4.30E-06
92237	U237	7.31E-09
92238	U238	3.19E-04
92239	U239	5.27E-10
93237	Np237	1.50E-07
93238	Np238	4.32E-10
93239	Np239	7.59E-08

Name	Zr95	Zr93	Y91	Y90	Xe135	Xe134	Xe133	U239	U238	U237	U236
Specific Activity	7.9513E+14	93055000	9.08E+14	2.01E+16	9.4E+16	0	6.93E+15	1.24E+18	12435.7	3.02E+15	239279
Yield	0.9892	4.3E-06	0.0026	1.4E-08	1.745797	2.7	0.475749	0.595744	0.000742	0.64102	0.00097
	Norm	Norm	Norm	Norm	Norm	Norm	Norm	Norm	Norm	Norm	Norm
Norm	7.8654E+14	400.1365	2.36E+12	2.82E+08	1.64E+17	0	3.3E+15	7.39E+17	9.227289	1.94E+15	2322.4
	Tallies	Tallies	Tallies	Tallies	Tallies	Tallies	Tallies	Tallies	Tallies	Tallies	Tallies
	6.56E-03	3.00E-09	8.10E-03	9.97E-03	4.27E-03	5.96E-03	0.000763	2.85E-04	1.12E-04	1.00E-03	1.55E-0
	3.65E-03	2.00E-09	4.51E-03	5.55E-03	2.38E-03	3.32E-03	0.000426	1.58E-04	6.23E-05	5.62E-04	8.63E-0
	2.09E-03	0.00E+00	2.58E-03	3.17E-03	1.37E-03	1.90E-03	0.000246	9.14E-05	3.60E-05	3.25E-04	5.02E-0
	6.90E-04	1.00E-09	8.47E-04	1.04E-03	4.59E-04	6.30E-04	8.44E-05	3.07E-05	1.24E-05	1.11E-04	1.74E-0
	1.39E-04	0.00E+00	1.64E-04	1.96E-04	1.01E-04	1.29E-04	2.06E-05	6.85E-06	3.34E-06	2.73E-05	4.56E-0
	2.68E-05	0.00E+00	2.58E-05	2.57E-05	2.88E-05	2.69E-05	7.92E-06	1.93E-06	1.50E-06	1.03E-05	2.07E-0
	1.44E-05	0.00E+00	1.01E-05	6.89E-06	2.09E-05	1.54E-05	6.31E-06	1.46E-06	1.19E-06	8.57E-06	1.67E-0
	1.36E-05	1.00E-09	8.91E-06	5.85E-06	2.06E-05	1.47E-05	6.15E-06	1.48E-06	1.20E-06	8.56E-06	1.53E-0
	1.35E-05	1.00E-09	8.54E-06	5.76E-06	2.06E-05	1.47E-05	6.25E-06	1.45E-06	1.25E-06	8.55E-06	1.68E-0
	1.34E-05	0.00E+00	8.87E-06	5.77E-06	2.05E-05	1.45E-05	6.12E-06	1.41E-06	1.27E-06	8.60E-06	1.66E-0
	1.38E-05	0.00E+00	9.01E-06	6.05E-06	2.06E-05	1.47E-05	6.3E-06	1.56E-06	1.26E-06	8.63E-06	1.67E-0
	1.38E-05	0.00E+00	9.12E-06	5.92E-06	2.06E-05	1.48E-05	6.41E-06	1.71E-06	1.29E-06	8.71E-06	1.72E-0

Gamma Estimation



Neutron Signature

SOURCES-4C

- MCNP6.2
- Neutrons are generated in the fuel region of the pebble
  - Each neutron emitting nuclide in used fuel is modeled independently
    - Includes both spontaneous fission and (α,n) reactions
- Output will be energy dependent neutron flux at the surface of the pebble

Acknowledgements

- This work is performed with the support of U.S. Department of Energy's Nuclear Energy University Program (NEUP) with the Award No. DE-NE0009304

Spoiler Alert

New NEUP MC&A Grant Awarded

- Development of a Benchmark Model for the Near Real-Time Radionuclide Composition Measurement System using Microcalorimetry for Advanced Reactors
  - Braden Goddard (VCU), Kyle C. Hartig (UF), Zeyun Wu (VCU), Mark Croce (LANL), and Shayan Shahbazi (ANL)
  - Aug. 2024 – Sept. 2027
  - $1,000k + $100k





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