FHR Benchmark Equations

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1 Phase 1a Required Results

(a) Effective multiplication factor

(b) Reactivity coefficients (β_{eff}, fuel Doppler coefficient, FLiBe temperature coefficient, graphite temperature coefficient)

(c) Tabulated fission source distribution, at several levels of granularity (by fuel plate, by fuel stripe, by 1/5-th fuel stripe). Optional: visualized fission density distribution.

(d) Visualized distribution of the neutron flux distribution, in 3 coarse energy groups

(e) Neutron spectrum, fuel assembly average. Optional: by region.

1.1 Reactivity coefficients (b)

We assume 1 energy group and 6 delayed neutron groups for β_{eff}.

$$\beta_{eff} = \sum_k \beta_k$$

Doppler reactivity coefficient (fuel):

$$\frac{\Delta\rho}{\Delta T_f} = \frac{\rho_{1150K} - \rho_{1100K}}{1150 - 1100}[\frac{pcm}{K}]$$

$$\delta\frac{\Delta\rho}{\Delta T_f} = \frac{\sqrt{\delta(\rho_{1150K})^2 + (\delta\rho_{1100K})^2}}{1150 - 1100}[\frac{pcm}{K}]$$

Coolant reactivity coefficient (FLiBe):

$$\frac{\Delta\rho}{\Delta T_c} = \frac{\rho_{1150K} - \rho_{1100K}}{1150 - 1100}[\frac{pcm}{K}]$$

$$\delta\frac{\Delta\rho}{\Delta T_c} = \frac{\sqrt{\delta(\rho_{1150K})^2 + (\delta\rho_{1100K})^2}}{1150 - 1100}[\frac{pcm}{K}]$$

Graphite reactivity coefficient (graphite):

$$\frac{\Delta\rho}{\Delta T_g} = \frac{\rho_{1150K} - \rho_{1100K}}{1150 - 1100} [\frac{pcm}{K}]$$

$$\delta\frac{\Delta\rho}{\Delta T_g} = \frac{\sqrt{\delta(\rho_{1150K})^2 + (\delta\rho_{1100K})^2}}{1150 - 1100} [\frac{pcm}{K}]$$

1.2 Fission source distribution (c)

Fission density (FD) is calculated by using openmc's 'fission' score (f) divided by the average of all 'fission' scores:

$$FD_i = \frac{f_i}{f_{ave}}$$

Fission density standard deviation calculation:

$$\delta FD = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(FD_i - f_{ave})^2}$$

1.3 Neutron Flux (d, e, f)

Openmc's 'flux' score is given in units of $[\frac{n*cm}{src}]$. For the benchmark, we need to convert it to units of $[\frac{n}{cm^2s}]$. The conversion:

$$\Phi_c = \frac{N * \Phi_o}{V}$$

$$N = \frac{P * \nu}{Q * k}$$

where:

$$\Phi_c = \text{Converted Flux } [\frac{neutrons}{cm^2 s}]$$

$$\Phi_o = \text{Original Flux } [\frac{neutrons*cm}{src}]$$

$$N = \text{Normalization factor } [\frac{src}{s}]$$

$$V = \text{Volume of fuel assembly } [cm^3]$$

$$P = \text{Power } [\frac{J}{s}]$$

$$\nu = \frac{\nu_f}{f} [\frac{neutrons}{fission}]$$

$$Q = \text{Energy produced per fission } [\frac{J}{fission}]$$

$$= 3.2044 * 10^{-11} \text{ J per } U_{235} \text{ fission}$$

$$k = k_{eff} [\frac{neutrons}{src}]$$

Flux standard deviation:

$$\delta\Phi_c = \Phi_c * \sqrt{(\frac{\delta\Phi_o}{\Phi_o})^2 + (\frac{\delta\nu_f}{\nu_f})^2 + (\frac{\delta k}{k})^2 + (\frac{\delta f}{f})^2}$$

Reactor power is calculated based on the given reference specific power (P_{sp}) of 200 $\frac{W}{gU}$.

$$P = P_{sp} * V_F * \rho_F * \frac{wt\%_U}{100}$$

where:

$$P = \text{Reactor power [W]}$$
$$V_F = \text{Volume of fuel } [cm^3]$$
$$= \frac{4}{3}\pi r_1^3 * 101 * 210 * 4 * 2 * 6 * 3$$
$$\rho_F = \text{density of fuel } [g/cc]$$
$$wt\%_U = \frac{at\%_{U235} * AM_{U235} + at\%_{U238} * AM_{U238}}{\sum(at\%_i * AM_i)} * 100$$
$$AM = \text{atomic mass}$$

2   Phase 1b

2.1   Depletion steps

Openmc requires the user to input the time instances to conduct depletion till as opposed to the burnup value to conduct depletion till. In the benchmark, the burnup value is specified, therefore, we need a method to determine how long the assembly must be depleted to reach the desired burnup.

$$T = \frac{tU * BU}{P}$$

where:

$$T = \text{depletion time [day]}$$
$$tU = \text{mass of enriched Uranium [metric tonnes]}$$
$$BU = \text{Burnup [MWd/t]}$$
$$P = \text{thermal power [MW]}$$

2.2 Choosing depletion step size

Openmc states:

> A general rule of thumb is to use depletion step sizes around 2 MWd/kgHM, where kgHM is really the initial heavy metal mass in kg. These are typically valid for the predictor scheme, as the point of recent schemes is to extend this step size. A good convergence study, where the step size is decreased until some convergence metric is satisfied, is a beneficial exercise.

The 'maximum' depletion step:

$$\Delta t_{max} = \frac{2 MWd/khHM * hm_{op}}{P}$$

where:

$$\Delta t_{max} = \text{Maximum depletion step [days]}$$
$$hm_{op} = \text{mass of initial heavy metal [g]}$$
$$P = \text{Power [W]}$$

2.3 Unit conversion

After running depletion, openmc returns the total number of atoms for each nuclide. The benchmark requests results returned in relative density units [g/tHMi]. Unit Conversion:

$$\rho_{rel} = \frac{A_{Ti} * amu}{NA * hm_{op}}$$

where:

$$\rho_{rel} = \text{Relative density [g/tHMi]}$$
$$A_{Ti} = \text{total no. of atoms per nuclide [atoms]}$$
$$amu = \text{atomic mass unit [g/mol]}$$
$$NA = \text{Avogadro constant [atoms/mol]}$$
$$hm_{op} = \text{mass of initial heavy metal [tHM]}$$