OECD/NEA COUPLED NEUTRONIC/THERMAL-FLUIDS BENCHMARK OF THE MHTGR-350 MW CORE DESIGN

VOLUME III: LATTICE PHYSICS EXERCISES

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III-1 LATTICE PHYSICS DEPLETION BENCHMARK EXERCISE

The depletion benchmark is intended to examine the variation in lattice calculation results between benchmark participants. The calculation will be performed on a super-cell arrangement with dimensions given in Table III-1 and the geometric representation shown in Figure III-1. There are 3 major regions defined: 1) central fresh fuel region (depleting region), 2) homogenized burned fuel region at the bottom (non-depleting region), and 3) reflector region at the top (non-depleting region). Note the presence of 6 FBP, one in each corner of the central block. The super-cell is a geometric representation of block 18 in Figure 14 with its orientation rotated 60^{O} counter-clockwise.

Table III-1: Dimensions for Super-Cell Calculations

		Dimension	Units
TRISO Fuel Particle	Kernel Radius	2.125E−02	cm
	Porous Carbon Buffer OR	3.125E−02	cm
	IPyC OR	3.475E−02	cm
	SiC OR	3.825E−02	cm
	OpyC OR	4.225E−02	cm
	TRISO Packing Fraction	0.35	
	Compact Radius	0.6225	cm
	Gap Radius	0.635	cm
Burnable Poison Particle	Kernel Radius	1.00E−02	cm
	Kernel Density	2.4696	g/cm^3
	Porous Carbon Buffer OR	1.18E−02	cm
	PyC OR	1.41E−02	cm
	BP Particle Packing Fraction	0.109	
	BP Compact Radius	0.5715	cm
	Gap Radius	0.635	cm
Large Coolant Channel Radius		0.794	cm
Small Coolant Channel Radius		0.635	cm
Pin pitch		1.88	cm
Block Flat-to-Flat Width		36.0	cm
Super-cell Flat-to-Flat Width		108.0	cm

The calculation will be repeated twice, once without burnable poisons and once with a burnable absorber in each of the six locations in the block. Both cases should be first run at zero burnup at 293.6 K in all regions (Exercises 1a and 1b). The data should be reported for this temperature. In the case without burnable poisons, block graphite should be placed in each of the six locations. The objectives of this benchmark are essentially an extension of the Benchmark Specification for HTGR Fuel Element Depletion [10]. Then, for the depletion of each model, a fixed temperature of 1200K will be used in all regions (Exercises 2a and 2b). The purpose of this simplification is to avoid differences in the interpolation of temperatures. Depletion is to be performed at a constant power assuming continuous burnup with no downtime as indicated in Table III-2. Note that only the central fresh fuel block needs to be depleted.

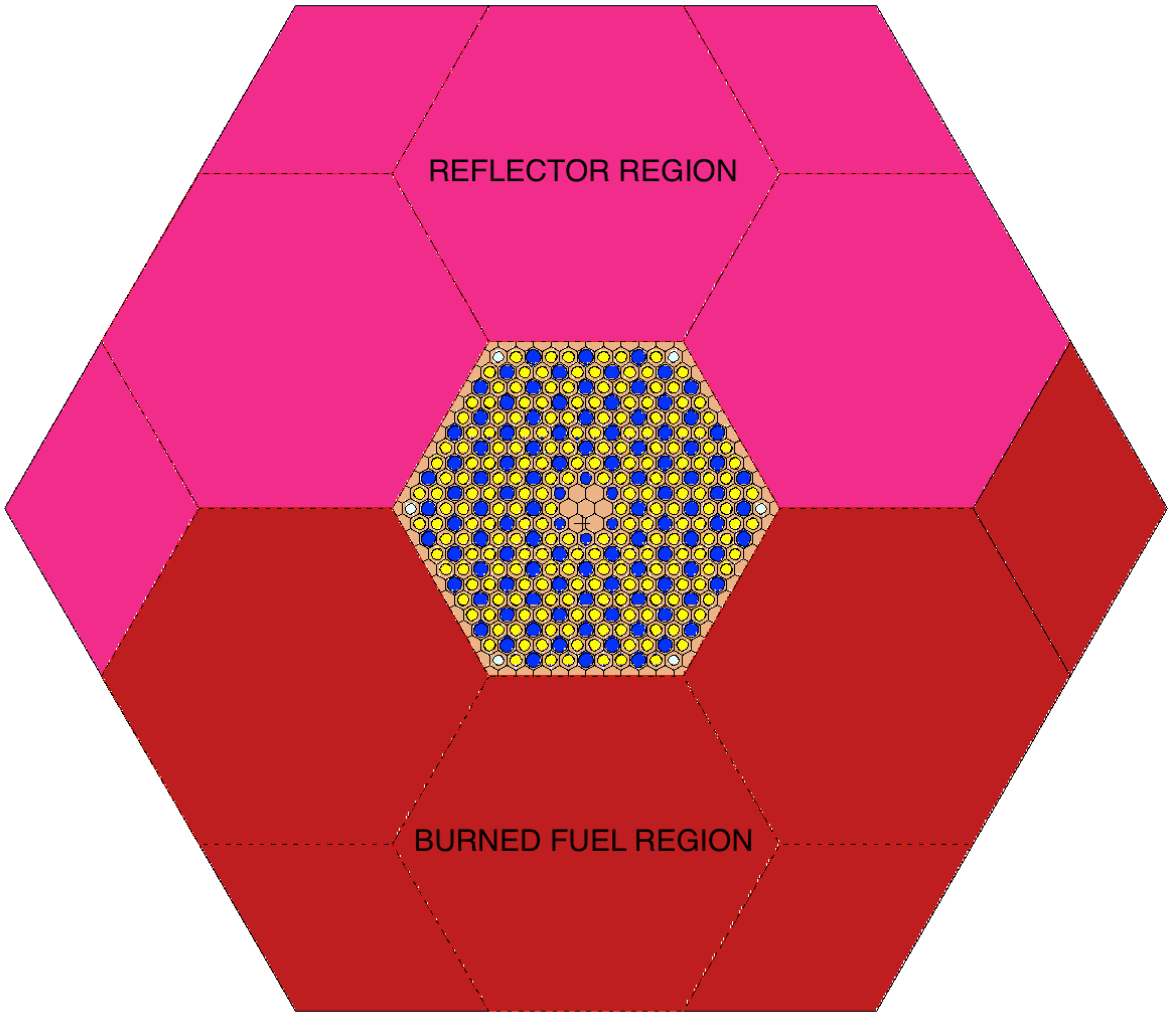


Figure III-1: Graphical Representation of the Super-Cell

The initial number densities for the fresh fuel block are provided in Table III-3. The material C-nat refers to natural carbon (with abundance 98.9% C-12 and 1.1% C-13). The material C-graph refers to natural carbon corrected for thermal binding and crystal lattice effects. The number densities for the burned fuel and reflector regions are provided in Table III-4.

To be able to include calculations from as many different methods as possible, depletion calculations are to be performed without a critical spectrum correction. Reflective/mirror boundary conditions should be used where available; white boundary conditions may be used where reflection is not an option. The participants are strongly encouraged to submit results from neutron libraries based on **ENDF/B-VII.r0** in order to better ascertain the differences in the models. Other libraries will be accepted for comparisons.

Table III-2: Burnup Specifications

Variable	Value
Specific power	100 W/g HM
Burnup	0, 0.5, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, and 120 GWd/tonne

Table III-3: Number Densities for the Fresh Fuel Region

NUMBER DENSITIES		Nuclide	N (at/b-cm)
TRISO Fuel Particle	Kernel	U-235	3.70E−03
		U-238	1.99E−02
		O-16	3.55E−02
		C-nat	1.18E−02
	Porous Carbon	C-graph	5.02E−02
	IpyC	C-graph	9.53E−02
	SiC	Si-28	4.43E−02
		Si-29	2.25E−03
		Si-30	1.49E−03
		C-nat	4.81E−02
	OpyC	C-graph	9.53E−02
Burnable Poison Particle	Kernel	B-10	2.14E−02
		B-11	8.63E−02
		C-nat	2.69E−02
	Buffer	C-graph	5.02E−02
	PyC	C-graph	9.38E−02
BP Compact Matrix		C-graph	6.87E−02
Fuel Compact Matrix		C-graph	8.27E−02
Block Graphite		C-graph	9.28E−02
Coolant Channels		He-4	2.46E−05

Table III-4: Number Densities for the Burned Fuel and Reflector Regions

Number Densities	Nuclide	N (at/b-cm)	Nuclide	N (at/b-cm)
Homogenized Burned Fuel Block	U-234	4.92E−10	Rh-103	4.34E−07
	U-235	1.83E−05	Rh-105	9.75E−10
	U-236	3.30E−06	Pd-107	1.26E−07
	U-238	1.78E−04	Xe-131	3.68E−07
	Np-237	2.49E−07	Xe-135	3.03E−10
	Np-239	5.33E−08	Cs-133	9.56E−07
	Pu-238	4.97E−08	Cs-134	9.75E−08
	Pu-239	3.51E−06	Nd-143	7.65E−07
	Pu-240	5.96E−07	Nd-145	5.52E−07
	Pu-241	6.42E−07	Pm-147	1.58E−07
	Pu-242	9.34E−08	Sm-149	3.77E−09
	Am-241	1.83E−08	Sm-151	1.63E−08
	Am-243	1.31E−08	Sm-152	6.93E−8
	Cm-242	3.21E−09	Eu-153	6.97E−08
	Cm-243	5.01E−11	Eu-154	1.47E−08
	Cm-244	2.53E−09	Eu-155	3.82E−09
	Cm-245	1.38E−10	O-16	3.06E−04
	Cm-246	4.12E−12	C-graph	6.90E−02
	Kr-83	3.36E−08	Si-28	5.07E−04
	Sr-90	7.82E−07	Si-29	2.57E−05
	Mo-95	8.02E−07	Si-30	1.70E−05
	Tc-99	8.82E−07		
Reflector Block	C-graph	8.63E−02		
	B-10	2.76E−08		

III-1.1 Convergence Criteria

General convergence criteria guidelines are provided in Table III-5. Each participant should ensure that a well-converged result is obtained by performing a sensitivity study on the code- specific input parameters, mesh sizes, and acceleration parameters.

Table III-5: Suggested Convergence Criteria

Parameter	Unit	Convergence Criteria
k-eff		1.0E−5
Local Fluxes		5.0E−5

III-2 Requested Output

All output data files should use the XML format delineated in this section. The files should adhere to the UTF-8 (UCS Transformation Format) encoding standard. Any files submitted will be verified for the appropriate format before being accepted for analysis. Sample files as well as a computer code to generate the XML will be provided. The results submitted should be included with the folder structure shown in Figure III-2. The structure will be checked to make sure that it meets the desired organization.

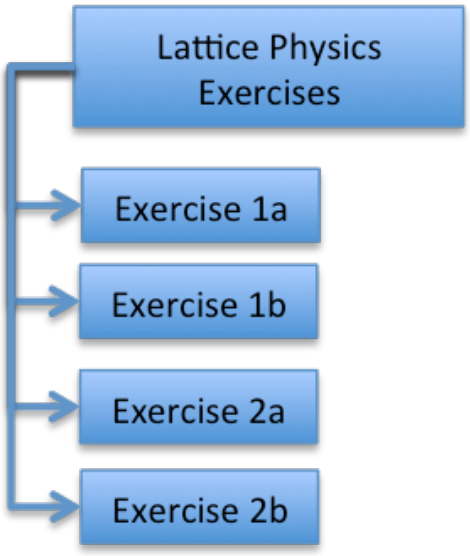


Figure III-2: Schematic of the Benchmark Results Folder

NOTE: *Any data point for which data is unavailable should be reported as −999.*

III-2.1.1 Reporting Mesh/Geometry

For these exercises the asymmetry in the super-cell is not considered important enough to warrant full datasets on all of the pins in the domain. Therefore, full datasets will only be required in a few representative pins. Only the relative compact powers will be reported for all the fuel compacts (210 locations) in the fresh fuel region for all burnup points specified in Table III-2.

The numbering of the compacts/pins starts at the upper left-hand corner (near the reflector region) and proceeds from left to right. Note that the numbering includes the BP pins. **Note:** Pin number 1 is the representative FBP that is closest to the reflector region and 216 is the representative FPB near the burned fuel region. There are 16 fuel and 3 burnable poison reporting locations in the central block that will include additional information, shown in Figure III-3. These 16 fuel regions will include relative powers, spectral indices, actinides, fission products, and spectrum data. The FBP locations will include the B-10 concentration and the spectrum.

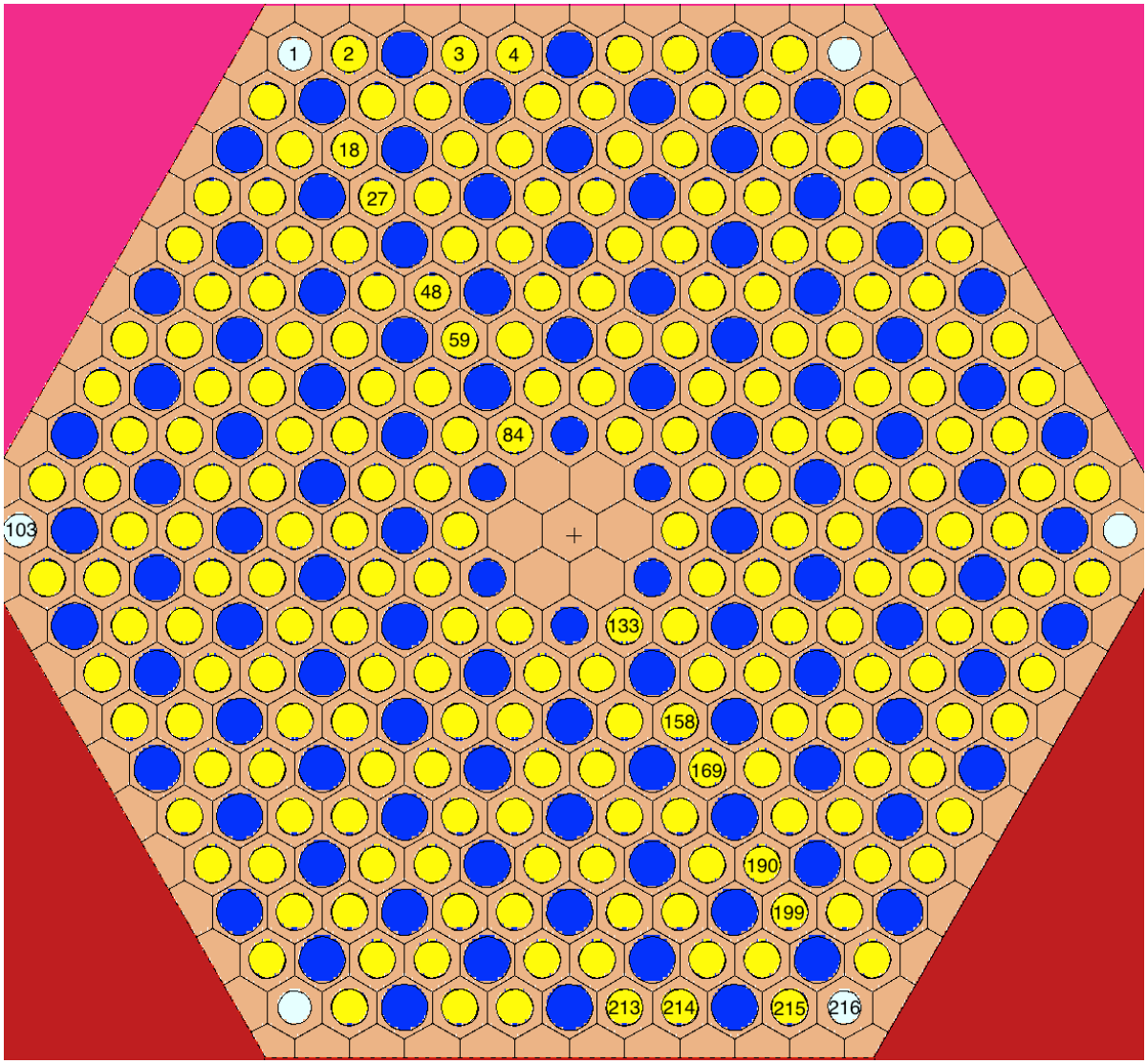


Figure III-3: Reporting Locations for the Depletion Calculation

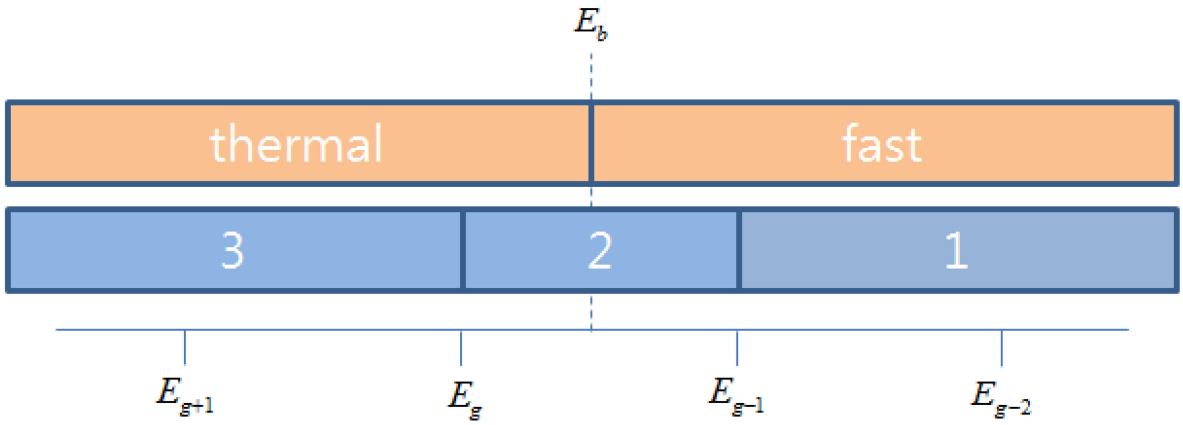
III-2.1.2 Reporting File Structure for Lattice Physics Exercises

The files submitted by each participant will meet certain requirements for processing. All files should contain a “Header” and a “Data-body” element sections. The header section includes the metadata shown in Table III-6. This dataset describes the origination of the file and provides some key values to read the spectrum. Note: The XML tags are not case sensitive, since the data reader converts all of the XML tags to lower case when loading the data.

Table III-6: Header Metadata for Lattice Physics Exercises

Sub element name	Data Type	Definition
PHASE	integer	*3*
Exercise	string	*(1a, 1b, 2a, 2b)*
Contact	string	
Institution	string	
Country	string	
Time-stamp *Attributes: Date, Time*	Date and time	*Date and time when the calculation was completed* *Date* YYYY-MM-DD *Time* hh:mm:ss
Computer-code	string	
Computer-code-description	string	Please provide a description of the code system: library processing, number of energy groups, transport solution, DH treatment, self-shielding method, geometry modeling, etc.
Library-source	string	(ENDF/B-VII.r0, JENDL-4.0, JEFF-3.1.1, etc.)
Number-spectrum-points	integer	Number of data points in neutron spectrum reported
Spectrum-energy	array of floats	Average energy in each bin of the reported neutron spectrum in eV $\tilde{E}_i = 10^{\left(\frac{log_{10}(E_{i+1})+log_{10}(E_i)}{2}\right)}$
Kconvg	float	Kinf convergence
Fconvg	float	Flux convergence

The “Data-body” element contains all of the data in a structured format, as shown in Table III-7. The “Data-block” is the only sub-element of “Data-body” and is used to separate state points. The attributes for “Data-block” are the depletion step, the temperature state (cold/hot), and the infinite multiplication factor. Each “Data-block” includes a “Block_XS” and “Pin” sub-elements. The “Block_XS” sub-element, included in Table III-8, is used to report macroscopic cross sections and six factor formula factors for the central block. The cross sections will be provided in two groups with a thermal cutoff of E_b= 4.95 eV. If the participant’s energy boundaries do not match the value of E_b provided, then a three-group structure condensation must be utilized as shown in Figure III-4.



$$\Sigma_x^{fast} = \frac{\Sigma_{x,1}\phi_1 + \Sigma_{x,2}\phi_2\alpha}{\phi_1 + \phi_2\alpha}, \quad \Sigma_x^{thermal} = \frac{\Sigma_{x,2}\phi_2(1-\alpha) + \Sigma_{x,3}\phi_3}{\phi_2(1-\alpha) + \phi_3}$$

$$\alpha = \frac{E_{g-1} - E_b}{E_{g-1} - E_g}$$

Figure III-4: Three-group Condensation Example

Table III-7: "Data-body" Element Description

Sub-element name (all floats)	**Definition/units**
Data-block *Attributes: step, state, kinf, kinf-err*	step in GWd/MTU state = cold/hot kinf= inf. Multiplication factor kinf-err = relative error (if available)
Sub-element: Block_XS	
Sub-element: Pin *Attributes: ID, fuel*	ID = pin number Fuel = t/f

Table III-8: "Block_XS" Sub-element Description

Sub-element Name (all floats)	**Definition/Units**
Total	Macroscopic total cross section [cm^{-1}] (fast and thermal)
Absorption	Macroscopic absorption cross section [cm^{-1}] (fast and thermal)
Nufission	Macroscopic nufission cross section [cm^{-1}] (fast and thermal)
Fission	Macroscopic fission cross section [cm^{-1}] (fast and thermal)
Scattering	Macroscopic scattering cross section [cm^{-1}] (1➔1,2➔1,1➔2,2➔2)
Fast_fission_fact	$\varepsilon = \frac{\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2}{\nu\Sigma_{f2}\phi_2}$

Sub-element Name (all floats)	**Definition/Units**
Resonance_escape	$p = \frac{\Sigma_s \phi_1}{\Sigma_{a1}\phi_1 + \Sigma_s \phi_1}$
Thermal_utilization	$f = \frac{\Sigma_{a2}^F \phi_2}{\Sigma_{a2}\phi_2}$ where F stands for fuel (all fissionable isotopes*)
Eta	$\eta = \frac{\nu\Sigma_{f2}\phi_2}{\Sigma_{a2}^F \phi_2}$ where F stands for fuel (all fissionable isotopes*)
Fast_nonleak	$L_{fast} = \frac{k_{eff}\left(\Sigma_{a1}\phi_1 + \Sigma_s \phi_1\right)}{\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2}$
Thermal_nonleak	$L_{thermal} = \frac{\Sigma_{a2}\phi_2}{\Sigma_s \phi_1}$
* U234, U235, U236, U237, U238, U239, Np237, Np238, Np239, Pu238, Pu239, Pu240, Pu241, Pu242, Pu243, Pu244, Am241, Am242, Am243, Am244, Am242m, Cm242, Cm243, Cm244, Cm245, Cm246	

The “Pin” sub-element, included in Table III-9, is used to separate the various compacts within the geometry. The “Pin” sub-element has two attributes: 1) an id to determine the pin of interest and 2) the fuel logical flag, which identifies the region as fuel or BP.

Table III-9: “Pin” Sub-element Description

Sub-element Name (all floats)	**Definition/units**
Spectral-indices	Unitless ρ238, δ235, δ238, c/f235
Actinides	Grams/MTU ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{244}Cm, and ^{245}Cm in order
Fission-products	Grams/MTU ^{85}Kr, ^{90}Sr, ^{110m}Ag, ^{135}Xe, ^{137}Cs, ^{149}Sm, and ^{151}Sm in order
Relative-power	Compact power relative to fresh fuel block average compact power
Spectrum-value	Magnitude of spectrum
B-10	Fraction of initial Average concentration of ^{10}B in BP
Spectral-indices-err	Relative error (if available)
Actinides-err	Relative error of Actinide concentration (if available)
Fission-products-err	Relative error of fission product concentration (if available)
Relative-power-err	Relative error of relative power (if available)
Spectrum-value-err	Relative error of spectrum (if available)
B-10-err	Relative error ^{10}B concentration (if available)

III-2.1.3 Cross Section Generation Output Parameters

Table III-10: Output Parameter Definition

Parameter	Description	Unit
kinf	Infinite medium multiplication factor for the super-cell	none
Spectral indices	The following spectral indices from averages over the fuel kernels in the 16 fuel reporting locations (assuming a fast/thermal boundary at 4.95 eV) $\rho_{238} = \frac{\int dV \int_{4.95}^{E_{max}} dE\ \sigma_\gamma^{238}(r,E)\phi(r,E)}{\int dV \int_{E_{min}}^{4.95} dE\ \sigma_\gamma^{238}(r,E)\phi(r,E)}$ $\delta_{235} = \frac{\int dV \int_{4.95}^{E_{max}} dE\ \sigma_f^{235}(r,E)\phi(r,E)}{\int dV \int_{E_{min}}^{4.95} dE\ \sigma_f^{235}(r,E)\phi(r,E)}$ $\delta_{238} = \frac{\int dV \int_{E_{min}}^{E_{max}} dE\ N_{238}(r)\sigma_f^{238}(r,E)\phi(r,E)}{\int dV \int_{E_{min}}^{E_{max}} dE\ N_{235}(r)\sigma_f^{235}(r,E)\phi(r,E)}$ $c/f_{235} = \frac{\int dV \int_{E_{min}}^{E_{max}} dE\ N_{238}(r)\sigma_\gamma^{238}(r,E)\phi(r,E)}{\int dV \int_{E_{min}}^{E_{max}} dE\ N_{235}(r)\sigma_f^{235}(r,E)\phi(r,E)}$	
Actinide concentrations	Volume averaged over the fuel kernels for the 16 fuel reporting locations for ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{244}Cm, and ^{245}Cm	grams/MTU
Fission product concentrations	Volume averaged over the fuel kernels for the 16 fuel reporting locations for ^{85}Kr, ^{90}Sr, ^{110m}Ag, ^{137}Cs, ^{135}Xe, ^{149}Sm, and ^{151}Sm	grams/MTU
Flux per unit "lethargy"	Volume averaged energy-dependent flux for fuel kernels in the 16 fuel reporting locations scaled by the energy-integrated flux and divided by the "lethargy" interval (using participant's own group structure) $\tilde{\phi}(E_i) = \frac{1}{\sum_{i=1}^{G} \phi(E_i)} \ \frac{\phi(E_i)}{log_{10}(E_{i+1}) - log_{10}(E_i)}$ where, $\phi(E_i)$ = Volume averaged energy-dependent flux for fuel kernels in one reporting location G = total number of groups E_{i+1} = upper energy boundary in the energy bin E_i = lower energy boundary in the energy bin This normalization enables comparison of several spectra through the entire energy domain. All the spectra have an integral equal to 1 on a logarithmic scale. Note that for this reason the traditional natural logarithm has been replaced with a base 10 logarithm in the definition of "lethargy."	

B-10 concentration	^{10}B nuclide concentrations from averages over the BP kernels in the 3 BP reporting locations (fraction of initial ^{10}B BP loading)	