Nuclear Science
NEA/NSC/R(2020)5
March 2021
www.oecd-nea.org

Benchmark Specifications for the Fluoride-salt High-temperature Reactor (FHR) Reactor Physics Calculations

Phase I-A and I-B: Fuel Element 2D Benchmark

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18 March 2021

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JT03473032

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Phase I-A and I-B: Fuel Element 2D Benchmark

B. Petrovic, K. Ramey, I. Hill

March 2021

Nuclear Energy Agency

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Foreword

Under the auspices of the NEA Nuclear Science Committee (NSC), the Working Party on Scientific Issues of Reactor Systems (WPRS) has been established to study reactor physics, fuel performance, radiation transport and shielding, reactor core thermal-hydraulics, and the uncertainties associated with modelling of these phenomena in present and future nuclear power systems. The WPRS has different expert groups to cover a wide range of scientific issues in these fields.

The Expert Group on Reactor Physics and Advanced Nuclear Systems (EGRPANS) was created in 2011 to perform specific tasks associated with reactor physics aspects of present and future nuclear power systems. The EGRPANS provides expert advice to the WPRS and the nuclear community on the development needs (data and methods, validation experiments, scenario studies) for different reactor systems and also provides specific technical information regarding core reactivity characteristics, including fuel depletion effects; core power/flux distributions; core dynamics and reactivity control.

Starting in early 2000s, and expanding over the last decade, there has been significant interest in several member countries to investigate advanced reactors systems, the so-called Fluoride-salt High-temperature Reactors (FHR), cooled with liquid (molten) salt, fuelled with TRISO-based fuel. Such reactor designs share certain similarity (heat removal by molten salt) with the historic Molten Salt Reactor Experiment (MSRE), but also present a fundamental difference in having solid fuel – either in form of circulating pebbles or in hexagonal fuel elements. Either fuel form, due to its double heterogeneity, leads to complex reactor physics and present significant modelling challenges. This is further exacerbated in the case of hexagonal fuel elements, with fuel TRISO particles embedded in plates ("planks"), due to the complex fuel geometry, which could be considered a form of "triple heterogeneity". At the same time, there are no experimentally obtained results that would allow validation. This makes cross-verification using different reactor physics codes and methods on carefully defined benchmarks the most viable approach to improve confidence in results obtained by numeric simulations.

This benchmark focuses on FHR reactors with plate fuel. Several phases are planned, starting with single fuel element simulation without burn-up, and gradually extending to full core depletion.

Phase I – Fuel assembly (2D/3D with depletion):

- Phase I-A – "2D" (pseudo-2D) model, steady state (no depletion);
- Phase I-B – 2D model depletion;
- Phase I-C – 3D model depletion.

Phase II – 3D full core with depletion:

- Phase II-A – Steady state (no depletion);
- Phase II-B – Depletion.

Phase III – 3D full core with feedback and multicycle analysis:

- Phase III-A – Full core depletion with feedback;
- Phase III-B – Multicycle analysis.

This document describes Phase I-A and I-B. Phase I-C and Phase II specifications are planned to be prepared and released within about one year of releasing these specifications. Phase III is envisioned in principle, but its timing will depend on the progress of the first two phases.

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List of abbreviations

AHTR	Advanced High-Temperature Reactor
BP	Burnable poison
CR	Control rod
EGRPANS	Expert Group on Reactor Physics and Advanced Nuclear Systems (NEA)
FHR	Fluoride-salt High-temperature Reactor
HFP	Hot full power
HZP	Hot zero power
IPyC	Inner Pyrolytic Carbon
MSRE	Molten Salt Reactor Experiment
NEA	Nuclear Energy Agency
NSC	Nuclear Science Committee (NEA)
OD	Outer diameter
OPyC	Outer Pyrolytic Carbon
ORNL	Oak Ridge National Laboratory (United States)
TRISO	Tristructural-isotropic
WPRS	Working Party on Scientific Issues of Reactor Systems (NEA)

1. Background and introduction

Starting in early 2000s, and over the last decade, there has been significant interest in several OECD Nuclear Energy Agency (NEA) member countries to investigate advanced reactors systems; Fluoride-salt High-temperature Reactors (FHR) cooled with liquid (molten) salt and fuelled with tristructural-isotropic (TRISO)-based fuel. Such reactor designs share certain similarity (heat removal by molten salt) with the historic Molten Salt Reactor Experiment (MSRE), but also present a fundamental difference in having solid fuel, either in form of circulating pebbles or in hexagonal fuel elements. Either fuel form, due to its double heterogeneity, leads to complex reactor physics and present significant modelling challenges. This is further exacerbated in the case of hexagonal fuel elements, with fuel TRISO particles embedded in plates ("planks"), because of the complex fuel geometry, which could be considered a form of "triple heterogeneity". At the same time, there are no experimentally obtained results that would allow validation. This makes cross-verification using different reactor physics codes and methods on carefully defined benchmarks the most viable approach to improve confidence in results obtained by numeric simulations.

This benchmark focuses on FHR reactors with plate fuel. Several phases are planned, starting with single fuel element simulation without burn-up, and gradually extending to full core depletion:

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- Phase I-B – 2D model depletion;
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Phase II – 3D full core with depletion:

- Phase II-A – Steady state (no depletion);
- Phase II-B – Depletion.

Phase III – 3D full core with feedback and multicycle analysis:

- Phase III-A – Full core depletion with feedback;
- Phase III-B – Multicycle analysis.

This document provides benchmark specification for Phase I-A and Phase I-B (see Chapter 2), describes quantities to be calculated and reported (see Chapter 3), and provides some illustrative results (see Chapter 4).

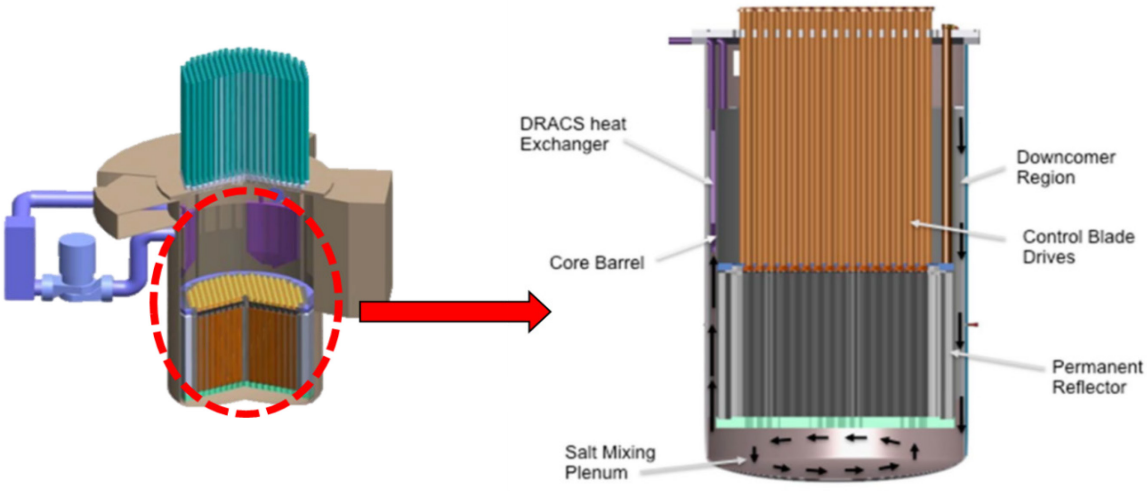
2. Benchmark specifications

2.1. Framework – Reference reactor design

There are several Fluoride-salt High-temperature Reactor (FHR) designs being developed worldwide. This benchmark has been developed relying primarily on the ORNL pre-conceptual design of the Advanced High-Temperature Reactor (AHTR), documented in [1]. The main characteristics of ORNL AHTR are presented in this section; the purpose is solely to provide the framework and not to define the benchmark. Consistent and complete benchmark specifications describing fuel element, to be used for this benchmark, are provided in subsequent sections of this chapter. Note that some specification differ from the ORNL AHTR design specifications, which should not be used in this benchmark. For example, ORNL AHTR thermal power is 3 400 MW. However, for the purpose of this benchmark, the power is set to 3 636 MW in order to round the specific power to 200.0 W/gU which simplifies conversion between the full power depletion (days) and burn-up (MWd/tU).

ORNL AHTR reactor schematic and reactor vessel vertical cut are shown in Figure 2.1 (left and right, respectively).

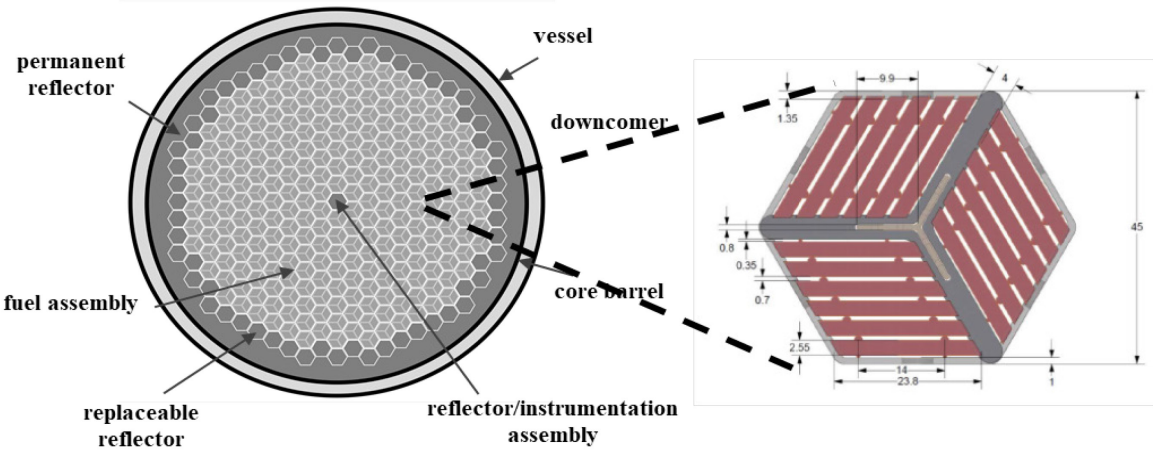
Figure 2.1. Reactor schematic (left) and vessel (right)



Source: ORNL, 2020.

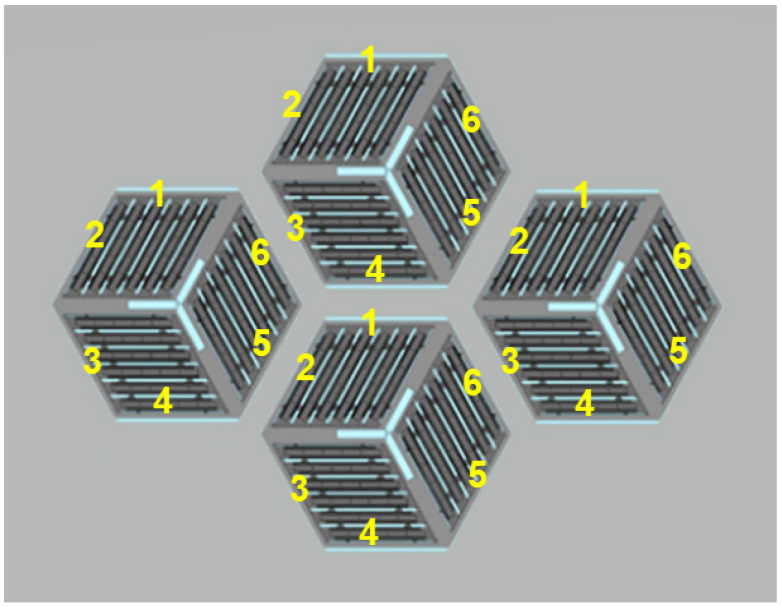
Vessel outer diameter (OD) is about 10 m. Reactor core, having equivalent radius of about 8 m, is composed of 252 hexagonal fuel elements. Each fuel element is 6 m high; the active core (section that includes fuel i.e. TRISO particles) corresponds to its middle section of 5.5 m, with 0.25 m top and bottom non-fuelled reflector regions. The core configuration is shown in Figure 2.2. Also shown is fuel element, measuring 45 cm across. Full core specifications for the benchmark will be defined in Phase II and III of this benchmark.

Figure 2.2. Core configuration and fuel element



Each fuel element has three diamond-shaped sections, each containing six fuel plates ("planks"). These sections correspond to each other with 120-deg rotational symmetry. Note that this is not the usual 60-deg mirror symmetry found in most designs with hexagonal fuel elements. Looking at a group of four neighbouring fuel elements in the core (shown in Figure 2.3, spread apart for clarity), it is clear that the internal 120-deg rotational symmetry may be represented by periodic boundary conditions when modelling a single fuel element. In other words, opposite surfaces, 1-4, 2-5 and 3-6 are periodic surfaces for boundary conditions.

Figure 2.3. Visualisation of periodic boundary conditions (for single assembly model)



Source: B. Petrovic and K. Ramey

2.2. Fuel element 2D ("pseudo-2D") model (for Phase I Benchmark)

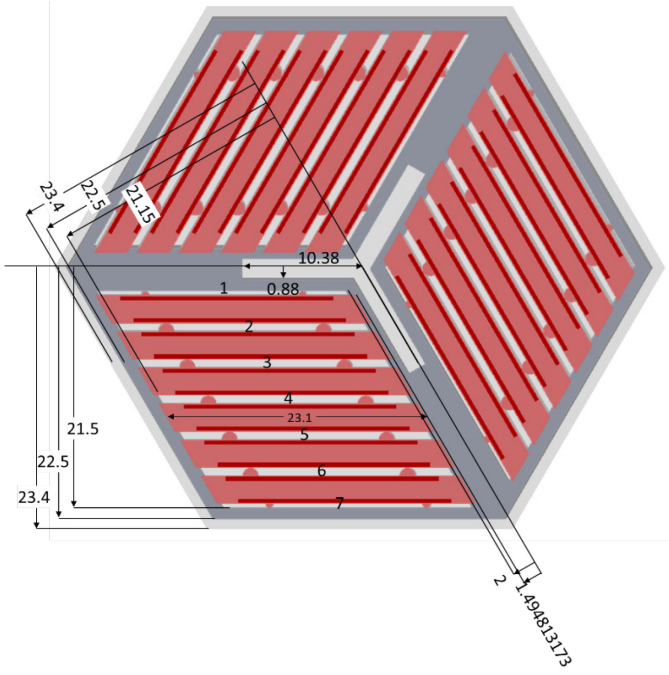
2.2.1. Fuel element geometry and dimensions

The pseudo-2D model consists of a finite slice of the active portion of fuel element, containing an integer number of TRISO particles, i.e. divisible with the assumed fuel lattice axial pitch value, with reflective top and bottom boundary conditions. It should be noted that, in contrast to extruded geometries such as the PWR fuel, the spherical shape of TRISO particles implies that the geometry is not uniform in the axial direction, hence there is no true 2D equivalent, and instead this "pseudo-2D" model is used. Periodic boundary conditions are assumed radially, as discussed in the previous section.

Main parameters characterising the FHR fuel element geometry are extracted from [1], [2] and [3]. The dimensions specified in these documents are "cold" (room temperature) dimensions. However, in Phase I and Phase II of this benchmark they will be used as-is and kept fixed for all cases and all temperatures. Phase III (with feedback) will address dimensional changes. Additional details are specified in this document to ensure that all geometrical characteristics are unambiguously defined.

Figure 2.4 shows the fuel element layout. Except for the fuel TRISO particles, all other fuel element structures are made of carbonaceous materials including graphite, carbon-carbon composite (C-C composite), or some compound of graphite and carbon (depending on the manufacturing process).

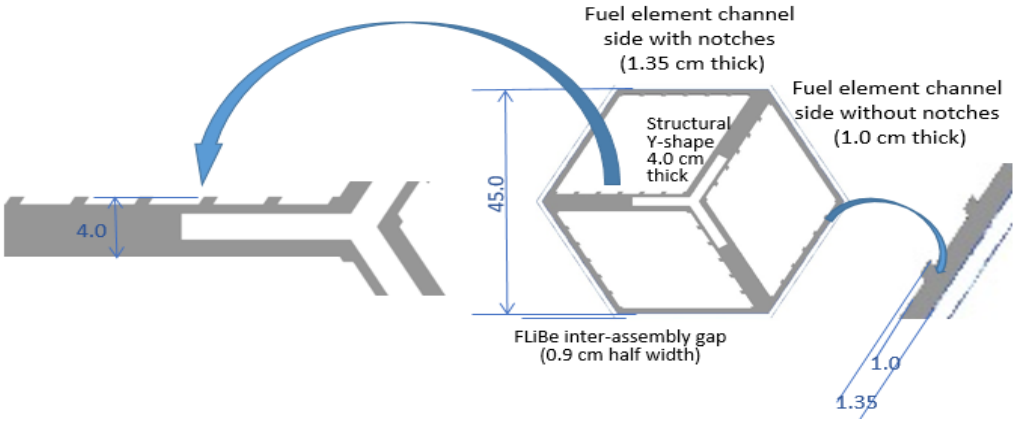
Figure 2.4. FHR fuel element geometry



Source: B. Petrovic and K. Ramey

The outer wrapper (channel) and structural Y-shape, shown in Figure 2.5, are made of C-C composite. Both have notches for fuel plates to slide in. The wrapper is 1.0 cm thick at its thinnest (i.e. the notches sides are extra and those sides that have notches are 1.35 cm thick), while the Y-shape is 4.0 cm thick at its thickest, i.e. notches are notched into that thickness. The apothem of the fuel hexagon is 22.5 cm, thus the outer dimension side-to-side is 45.0 cm. The gap between fuel elements, filled with bypass FLiBE, is 1.8 cm, i.e. the corresponding half-gap is 0.9 cm around each fuel assembly. The triangular core lattice pitch (centre-to-centre fuel element) is therefore 46.8 cm. There is a Y-shaped slot for control rod (CR) in the Y-shape structure in each fuel element. Its dimensions are marked in Figure 2.4. Control rods have the same Y-shape, with 0.38 cm clearance on each side, i.e. each wing is 10.0 cm long and 1.0 cm thick.

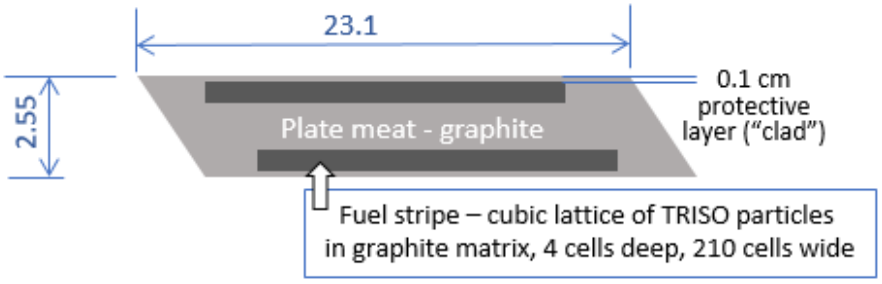
Figure 2.5. FHR fuel element – structural components (all dimensions in cm)



Source: B. Petrovic and K. Ramey

Fuel planks are made of isostatically pressed carbon, assumed to have graphite-like structure, and are 23.1 cm wide. The fuel stripes, one on each outer side of the plank close to coolant (see Figure 2.6). Fuel stripes are prismatic regions composed of graphite matrix filled with a cubic lattice of TRISO particles that is 210 TRISO particles wide in the x-direction, 4 particles deep in the y-direction, and 5 936 particles tall in the z-direction. The pitch of the TRISO lattice is 0.09266 cm. The fuel stripes are moved 0.1 cm inward, leaving a 0.1 cm thick protective layer ("clad" or "sleeve") between fuel and coolant. Fuel stripes are centred lengthwise, with respect to the coolant channel width. Specifically, geometric centre of each fuel stripe is located on the symmetry line between the left and right channel bounding planes.

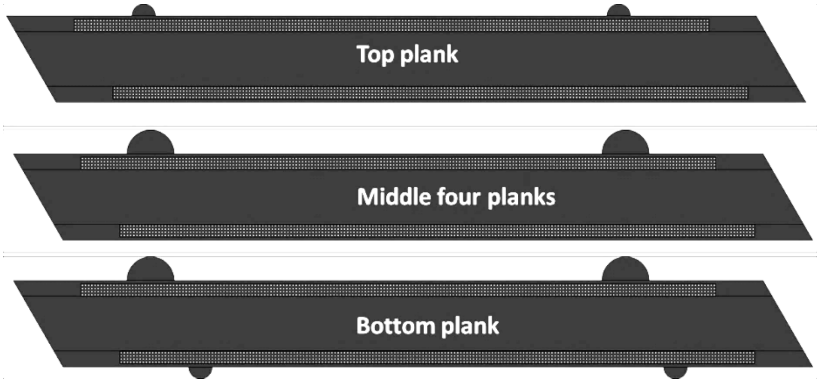
Figure 2.6. Fuel plank schematic (not to scale, all dimensions in cm)



Source: B. Petrovic and K. Ramey

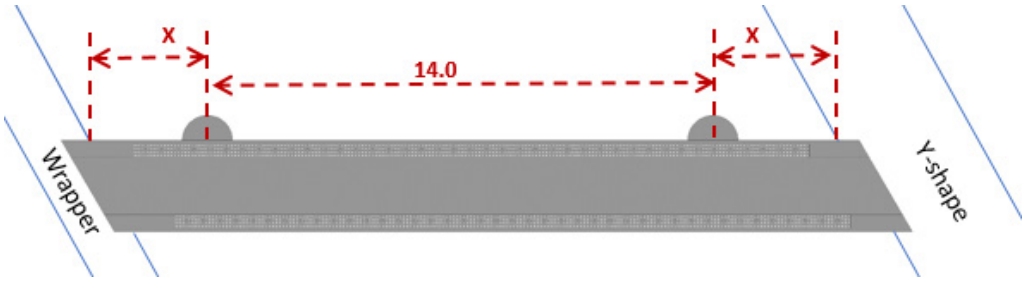
Fuel planks have semi-cylindrical spacers attached, their radius being equal to the coolant channel thickness, i.e. 0.35 cm for the narrow first and last channel (1 and 7 in Figure 2.4), and 0.70 cm for other channels (2 through 6). Specific shapes of fuel planks, with spacers, depending on their position (with reference to lower left diamond third in Figure 2.4) is shown in Figure 2.7. The two spacers on each plank are positioned in such a way that the distance between the centres of their defining cylinders is 14.0 cm, and they are located symmetrically with respect to the channel length (rather than with respect to the plank length; this makes a small difference of about 0.08 cm lengthwise), as illustrated in Figure 2.8. Note that the value of x should be derived from other given dimensions. (Channel width $2x+14 \approx 22.69587$ cm; hence, $x \approx 4.347935$ cm).

Figure 2.7. Fuel plank shapes depending on the position within a fuel element (to scale)



Source: B. Petrovic and K. Ramey

Figure 2.8. Position of the spacers (all dimensions in cm)



Source: B. Petrovic and K. Ramey

Schematic and dimensions of fuel TRISO particles are given in Figure 2.9 and Table 2.1. Note that the TRISO outer radius (OPyC radius) and TRISO lattice pitch result in a packing fraction of 40%. Also provided are material specifications and densities. Note that simplifications have been made in this benchmark definition as compared to the ORNL AHTR design report that aimed to estimate most likely manufactured densities. In the ORNL report, IPyC, OPyC, fuel stripe matrix (outside TRISO particles), fuel plate meat (with spacers), and structural C-C composite all have different densities ranging from 1.75 to 1.95 g/cm^3. In the benchmark, for simplicity, they are all prescribed to have a density of 1.8 g/cm^3. Moreover, they are all to be modelled as graphite, i.e. with the corresponding scattering matrix S(α,β), for pure graphite as the reference (additionally, for a sensitivity study, if available, also with 90% graphitisation), while in reality these would be somewhat different carbonaceous materials. Only the porous carbon is modelled as carbon, and at a different, low density of 1.0 g/cm^3.

Figure 2.9. TRISO particle schematic [1]

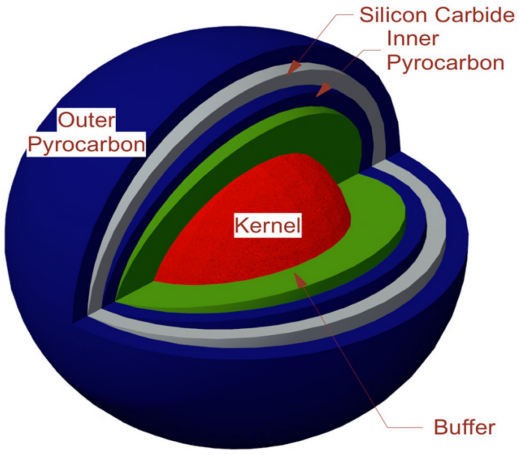


Table 2.1. TRISO fuel dimensions

Parameter	Size [cm]	Material model as	Density [g/cc]
Fuel Kernel (Oxycarbide) Radius	0.02135	UCO, 9% enriched	11.0
Buffer (Porous Carbon) Radius	0.03135	Carbon	1.0
Inner Pyrolytic Carbon (IPyC) Radius	0.03485	Graphite	1.8
Silicon Carbide (SiC) Layer Radius	0.03835	Silicon Carbide	3.2
Outer Pyrolytic Carbon (OPyC) Radius	0.04235	Graphite	1.8
Fuel Stripe Cubic Lattice Pitch	0.09266	Lattice matrix graphite	1.8

Source: B. Petrovic and K. Ramey

Fuel plank dimensions, including dimensions of all components, are given in Table 2.2. Most of these dimensions have already been provided and discussed, but they are summarised here for convenience.

Table 2.2. Fuel plate ("plank") and assembly dimensions

Parameter	Size [cm]
Fuel Plank Length	23.1
Large Spacer Radius	0.7
Small Spacer Radius	0.35
Spacers pitch (centre-to-centre)	14.0
Control Blade Slot Width	1.76
Control Blade Slot Length	10.38
Control Blade Arm Width	1.0
Control Blade Arm Length	10.0
Wrapper Minimum Thickness	1.0
Structural Y-shape Maximum Thickness Wrapper	4.0
Hex Wrapper Outer Apothem	22.5
FLiBe Inter Assembly Gap	1.8
Assembly Pitch	46.8

Source: B. Petrovic and K. Ramey

2.2.2. Materials and material compositions

Material compositions are given in Table 2.3 and Table 2.4. Note that both the total atom density (at/b-cm^3) and physical density (g/cm^3) are given. This is redundant and should be equivalent. It is preferred to use the total number density. However, physical density has been provided as a sanity check, as well as for use in codes that require physical density.

Table 2.3. Material specifications for benchmark

Material	Region	Material details	Density [g/cc]
Oxycarbide	TRISO fuel kernel	9 and 19.75 wt% enriched U $(UO_2)_{0.714}(UC_{1.86})_{0.123}(UC)_{0.164}$	11.0
Porous Carbon	TRISO buffer layer	Model as carbon	1.0
Silicon Carbide	TRISO confinement layer	SiC	3.2
Graphite	TRISO IPyC and OPyC Fuel stripe matrix, fuel plank, spacer, wrapper, Y-shape	Model as graphite	1.8
FLiBe	Coolant channels, control rod slot, inter-assembly gap	$2LiF–BeF_2$ 99.995 wt% ^7Li/Li	1.95
Molybdenum–hafnium carbide alloy (MHC)	Control rods	Mo with 1.2 wt% Hf, 0.1% C	10.28
Europium	Burnable poison	Eu_2O_3; discrete and homogenised option	5.0

Source: B. Petrovic and K. Ramey

Table 2.4. Material compositions

Material	Material composition [at/b-cm^3]		Density [g/cc]
Uranium Oxycarbide	**9 wt%**	**19.75 wt%**	11.0
	92235 2.27325E-3	4.98781E-3	
	92238 2.269476E-2	2.001094E-2	
	8016 3.561871E-2	3.566255E-2	
	6012 9.79714E-3	9.80920E-3	
	TOTAL: 7.038386E-2	7.047050E-2	
Porous Carbon	6012 5.013980E-2		1.0
Silicon Carbide	14028 4.431240E-2		3.2
	14029 2.25887E-3		
	14030 1.48990E-3		
	6012 4.806117E-2		
	TOTAL: 9.612234E-2		
Graphite	6012 9.025164E-2		1.8
FLiBe	3006 1.383014E-6		1.95
	3007 2.37132E-2		
	4009 1.18573E-2		
	9019 4.74291E-2		
	TOTAL: 8.30097E-2		
Molybdenum–hafnium carbide alloy (MHC)	42092 9.328884E-3		10.28
	42094 5.850533E-3		
	42095 1.010836E-2		
	42096 1.061782E-2		
	42097 6.102080E-3		
	42098 1.546981E-2		
	42100 6.205246E-3		
	72174 6.659530E-7		
	72176 2.189321E-5		
	72177 7.741704E-5		
	72178 1.135450E-4		
	72179 5.668925E-5		
	72180 1.460102E-4		
	6012 5.154371E-4		
	TOTAL: 6.461439E-2		
Europia (europium oxide, Eu_2O_3)	63151 8.179510E-3		5.00 (discrete spheres)
	63153 8.932435E-3		
	8016 2.566792E-2		
	TOTAL: 4.277986E-2		
	63151 1.533453E-6		0.0521 wt% in fuel plate graphite at 1.8 g/cm^3
	63153 1.674607E-6		
	8016 4.812090E-6		
	TOTAL: 8.020151E-6		

Source: B. Petrovic and K. Ramey

The dimensions and densities specified in this section refer to room temperature conditions, except for FLiBe (liquid density near operating conditions). If available, use FLiBe S(α,β), and possibly also test the impact of using it, or not. In any case, specify whether and which S(α,β) was used for FLiBE. It is recognised that this S(α,β) is missing in most libraries. Specific temperatures and densities to be used in various benchmarks are specified later.

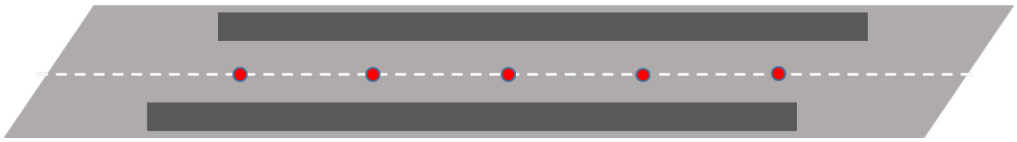
2.2.3. Burnable poison

Europium in the form of europium oxide, Eu_2O_3, is used as burnable poison. Two options are defined: discrete burnable poison option and integral (dispersed) burnable poison option.

Discrete option:

In the discrete option, small spherical particles of europium oxide, Eu_2O_3, are stacked axially, at 5 locations in each fuel plate. The 5 locations are equidistantly placed every 4 cm along the plank centreline, and centred lengthwise (see Figure 2.10) with respect to the coolant channel length (analogous to Figure 2.8). The axial pitch (sphere-to-sphere centre distance) is the same as for TRISO particles, 0.09266 cm. Sphere radius is 0.035 cm.

Figure 2.10. Schematic (not to scale) placement of axial stacks of burnable poison spheres



Source: B. Petrovic and K. Ramey

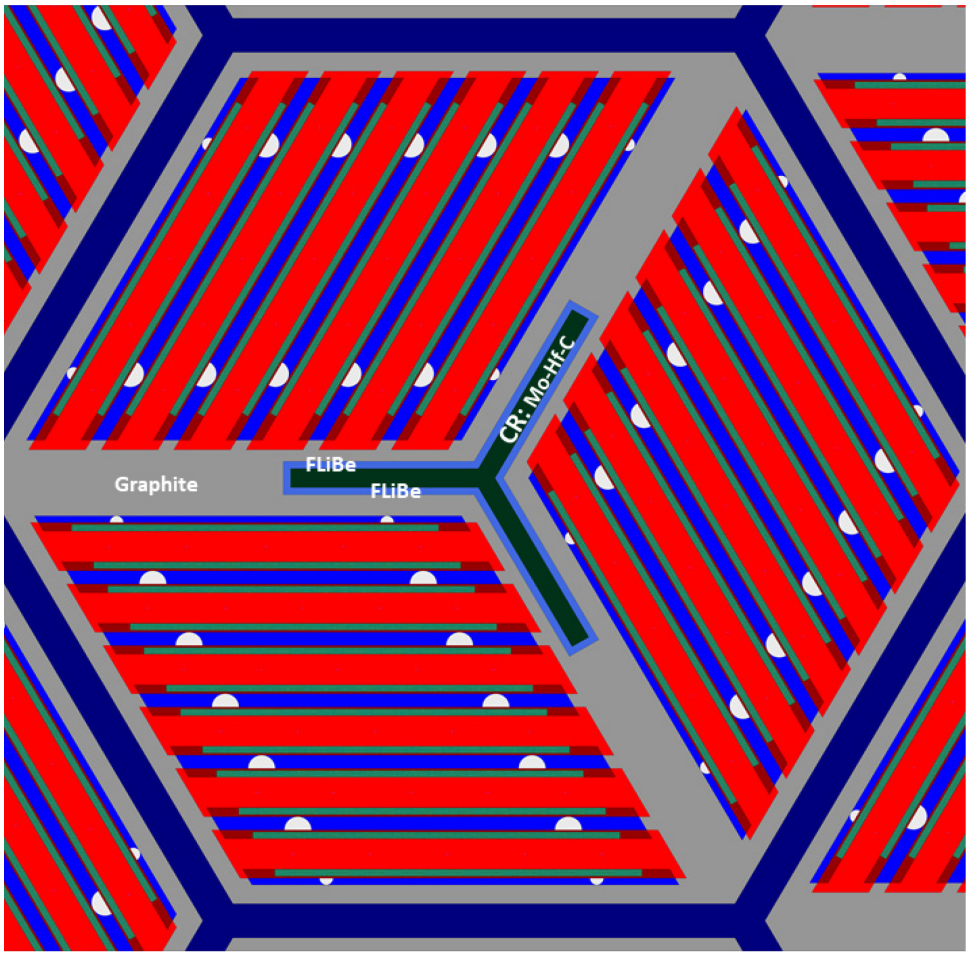
Integral (dispersed) option:

In the integral burnable poison option, europium oxide, Eu_2O_3, is homogeneously mixed with the plank graphite matrix (including the graphite in fuel stripes matrix, and the graphite in the plank ends indented to structural sides, but excluding the graphite in spacers and graphite in TRISO particles). Weight fraction of europium oxide in graphite is expected to be below 0.1% (most likely around 0.05%). Therefore, europium oxide atom densities are added to the graphite atom density, and the total atom density is increased by that same amount.

2.2.4. Control rods

Reactivity is also controlled by control rods. The dimensions of the Y-shaped slot and control rod are provided in Table 2.2. Fuel element with a control rod inserted is shown in Figure 2.11. It is assumed that control rod is uniformly composed of MHC with no cladding (shown in black) surrounded by a thin layer of FLiBe (shown in light blue).

Figure 2.11. Y-shaped control rod inserted



Source: B. Petrovic and K. Ramey

3. Analyses to be performed in Phase I-A and I-B

3.1.1. Quantities of interest

Quantities to be obtained by analyses in Phase I include:

- effective multiplication factor, and its change with depletion;
- reactivity coefficients, at selected depletion steps. (β-effective; fuel Doppler coefficient; FLiBe temperature coefficient; graphite temperature coefficient);
- tabulated fission source distribution, at several levels of granularity (by fuel plate, by fuel stripe, by 1/5-th fuel stripe), and its change with depletion, at selected burn-ups (details are specified in Section 3.1.4), optional: visualised fission density distribution;
- neutron flux, averaged over the whole model, tabulated in 3 coarse energy groups (upper energy boundaries 3 eV for thermal group and 0.1 MeV for intermediate group), and its change with depletion, at selected burn-ups (details are specified in Section 3.1.4.);
- visualised distribution of the neutron flux distribution, in 3 coarse energy groups, and its change with depletion, at selected burn-ups (details are specified in Section 3.1.4.);
- neutron spectrum, fuel assembly average; optional: by region;
- fuel (and burnable poison, when applicable) isotopic change with depletion (details, i.e. which isotopes at what burn-up are specified in Section 3.1.4.); note that FLiBe will be assumed non-depleting (constant isotopics) even in depletion calculations; the reason is that the FLiBe depletion cannot anyhow be correctly modelled without knowing the volume ratio of FLiBe in and out of the core; a separate Case to benchmark FLiBe isotopic change with depletion may be added at a later time.

Further specifics are provided in Sections 3.1.3 and 3.1.4 and 4.

3.1.2. Analysis specifications

All relevant details of the performed analysis should be reported, including but not limited to:

- all codes (with their version) used in analysis;
- computational resources used and run-times for all cases;
- nuclear data libraries and temperature treatment of cross-sections and scattering matrices (interpolation or use of the closest temperature);
- all relevant calculation/simulation parameters;
- convergence, i.e. calculation parameters and estimated residual error for deterministic codes and statistical uncertainty for stochastic codes;

- any modelling deviations from the prescribed benchmark (e.g. as necessitated by the relatively complex fuel element geometry.)

3.1.3. Analyses matrix

Phase I-A

The following cases (Phase IA) will be analysed for fresh fuel, without depletion analysis:

- CASE 1A: Reference case. Hot full power (HFP), with prescribed temperatures for coolant (948 K) and fuel kernel (1 110 K). In all cases in Phase I-A all other materials (including TRISO particle layers other than fuel kernel) are to be modelled at the coolant temperature. Nominal (cold) dimensions, 9wt% enrichment, no burnable poison (BP), control rods (CR) out.
- CASE 2AH: Hot zero power (HZP) with uniform temperature of 948 K in all regions, otherwise same as CASE 1A. Comparison with CASE 1A provides HZP-to-HFP power defect.
- CASE 2AC: "Cold" Zero Power (CZP), i.e. cooled down while still keeping FLiBe liquid. Same as CASE 2AH, but with uniform temperature of 773 K. Comparison with CASE 2AH provides isothermal temperature coefficient.
- CASE 3A: CR inserted, otherwise same as CASE 1A.
- CASE 4A: Discrete europia BP, otherwise same as CASE 1A.
- CASE 4AR: Discrete europia BP, and CR inserted, otherwise same as CASE 1A.
- CASE 5A: Integral (dispersed) europia BP, otherwise same as CASE 1A.
- CASE 6A: Increased HM loading (4 to 8 layers of TRISO), hence decreased C/HM (from about 400 to about 200) and decreased specific power to 100 W/gU, otherwise same as CASE 1A.
- CASE 7A: Fuel enrichment 19.75wt%, otherwise same as CASE 1A.

Table 3.1 summarises the cases to be analysed, associated conditions and the results to be reported.

Table 3.1. Cases to be analysed in Phase I-A

CASE	Enr.[wt%]	FLiBe Temp[K]	CR	BP	Sp.Pow. [W/gU]	Comment	Results to be reported (see 3.1.1)
1A	9.0	948	Out	No BP	200.0	Reference HFP	a, b, c, d, e, f
2AH	9.0	948	Out	No BP	0.0	HZP	a, b, c, d, e
2AC	9.0	773	Out	No BP	0.0	CZP	a, b, c, d, e
3A	9.0	948	In	No BP	200.0	CR in	a, b, c, d, e
4A	9.0	948	Out	Eu-discrete	200.0	BP/discrete	a, b, c, d, e
5A	9.0	948	Out	Eu-integral	200.0	BP/integral	a, b, c, d, e
6A	9.0	948	Out	No BP	100.0	Increase HM	a, b, c, d, e
7A	19.75	948	Out	No BP	200.0	19.75% enr	a, b, c, d, e

Source: B. Petrovic and K. Ramey

Note: For consistency check, the participants should specify the model axial height and the resulting loading (gU) and power (W) corresponding to their pseudo-2D model.

Phase I-B

In Phase I-B, depletion analysis will be performed for CASE 1B, CASE 4B and CASE 7B. These are the same as cases 1A, 4A and 7A, but with depletion steps added. Preferably, depletion will be performed under critical spectrum assumption. Only fuel, and BP when present, should be depleted (in reality, neutronically significant transmutations would occur in FLiBe, but the magnitude depends, among others, on the ratio of FLiBe mass in and out of core, therefore, it is prescribed to keep the composition constant; a separate case may be defined later to study this issue).

Depletion model and assumptions should be clearly reported, including the depletion spectrum. Depletion should be performed to obtain and report results at specified burn-ups. Additional intermediate burn-up steps should be used to obtain converged results (this will partly depend on the code, e.g. use of corrector-predictor or not; also, the case with BP may require initially additional steps). Some results should be reported at all steps, some only on a subset, as specified in Table 3.2. Note that results for Phase IA are essentially identical to the zero-burn-up

Table 3.2. Burn-up steps at which results should be reported

Burn-up [GWd/tU]	k-eff (a)	Fission source distribution (c)	3-group flux (d)	3-group flux distrib. (e)	Neutron spectrum (f)	Isotopics (g)
0	All	All	All	All	All	All
0.1	All		All			All
0.5	All		All			All
1	All	All	All	All	All	All
2	All		All			All
4	All		All			All
6	All		All			All
8	All		All			All
10	All		All			All
14	All		All			All
18	All		All			All
22	All		All			All
26	All		All			All
30	All	All	All	All	All	All
40	All		All			All
50	All		All			All
60	All		All			All
70	All	All	All	All	All	All
Only CASE 7B for burn-ups beyond 70 GWd/tU						
80	CASE 7B		CASE 7B			CASE 7B
90	CASE 7B		CASE 7B			CASE 7B
100	CASE 7B		CASE 7B			CASE 7B
120	CASE 7B		CASE 7B			CASE 7B
140	CASE 7B		CASE 7B			CASE 7B
160	CASE 7B	CASE 7B	CASE 7B	CASE 7B	CASE 7B	CASE 7B

Source: B. Petrovic and K. Ramey

Isotopic evolution with depletion, averaged over the model, is requested. Isotopics should be reported in grams per tonne of initial heavy metal (uranium), g/tHMi; alternatively, in atom densities at/b-cm3. Key nuclides (shown in bold) are required; extended table including all nuclides listed below is optional. (See Section 4.1.8).

Actinides:

- ^{232}U, ^{233}U, ^{234}U, **^{235}U**, ^{236}U, **^{238}U**;
- ^{236}Np, ^{237}Np;
- ^{236}Pu, ^{238}Pu, **^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu**, ^{243}Pu, ^{244}Pu;
- **^{241}Am**, ^{242m}Am, ^{243}Am;
- ^{242}Cm, ^{243}Cm, **^{244}Cm, ^{245}Cm**, ^{246}Cm, ^{247}Cm, ^{248}Cm;
- ^{226}Ra, ^{228}Ra;
- ^{227}Ac;
- ^{229}Th, ^{230}Th, ^{232}Th;
- ^{252}Cf.

Additionally:

- For CASE 4B with BP, also report all relevant Eu isotopes;
- Treat FLiBe as non-depletable, i.e. keep its isotopics fixed.

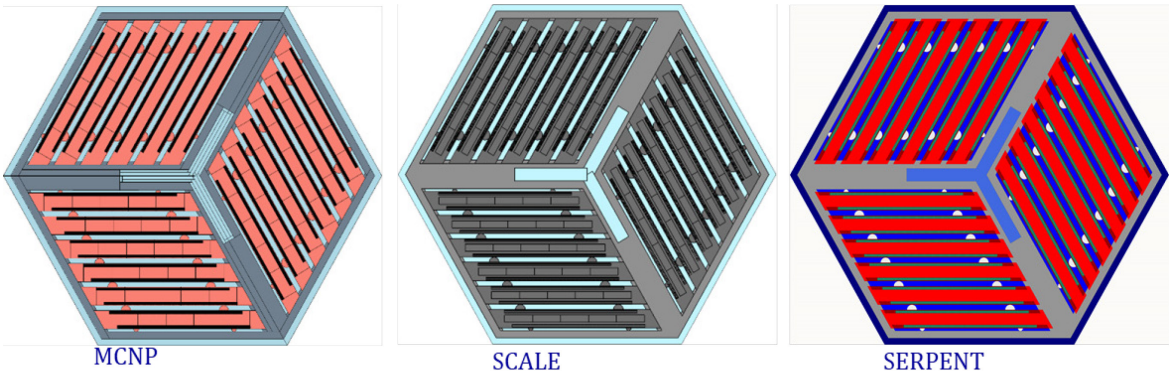
3.1.4. Output examples

Analyses for a very similar problem were performed and reported in [2] and [4].

The fuel element model used in these analyses is nearly identical, except for a number of small modifications that have been made to simplify the benchmark model. Reference [2] examined sensitivity to modelling assumptions (which is not addressed in this benchmark). Reference [4] compared basic results obtained using SERPENT [5], SCALE [6], and MCNP [7]. The corresponding models are shown in Figure 3.1. However, no depletion was performed.

With the caveat that the models are not identical, both references provide useful examples of presenting results, and may help to speed up the process of generating the models and performing analyses. Examples from [4] that follow illustrate the tentative format for presentation of output b (optional), d and e. Templates with exact specifications of the format are provided in Section 4.

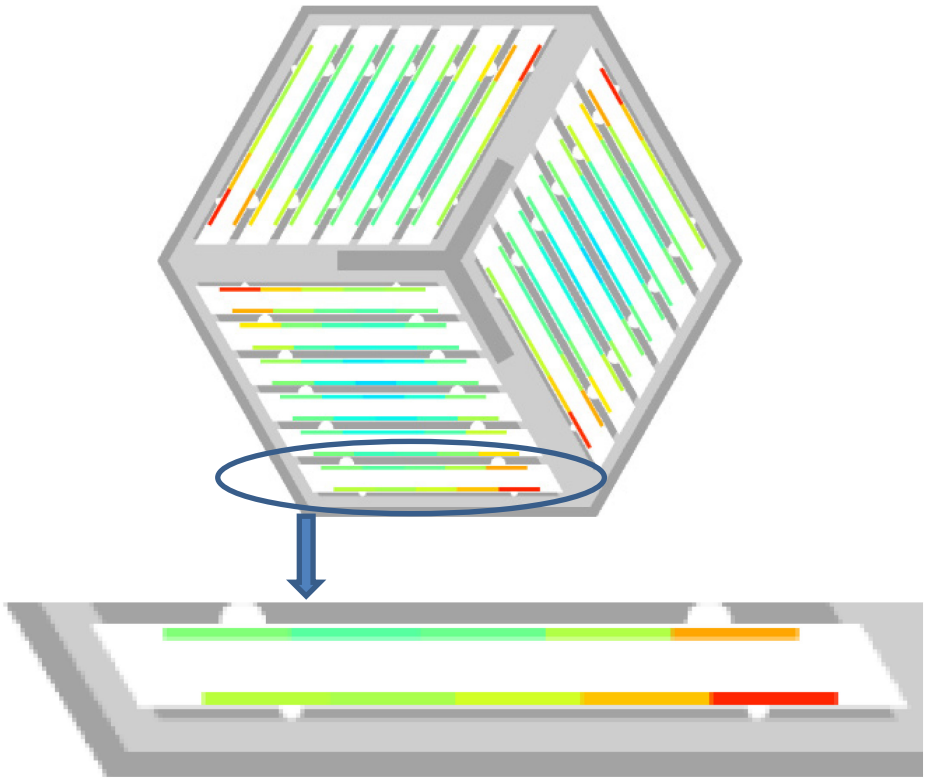
Figure 3.1. MCNP, SCALE and SERPENT model



Source: B. Petrovic and K. Ramey

Example (b, optional result): Visualisation of fission source distribution by stripe, or by 1/5-th stripe, see Figure 3.2.

Figure 3.2. Fission density (colour-coded, 1/5-stripe granularity)

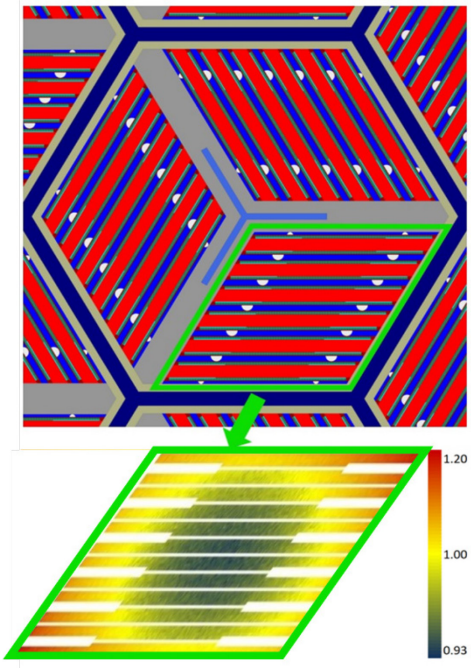


Source: B. Petrovic and K. Ramey

Insert shows that each fuel stripe (two stripes per fuel plate) is split into five equal-length regions with TRISO particles, and fission density for each is shown colour-coded.

Example (b, optional result): Visualisation of fission source by TRISO particle, see Figure 3.3.

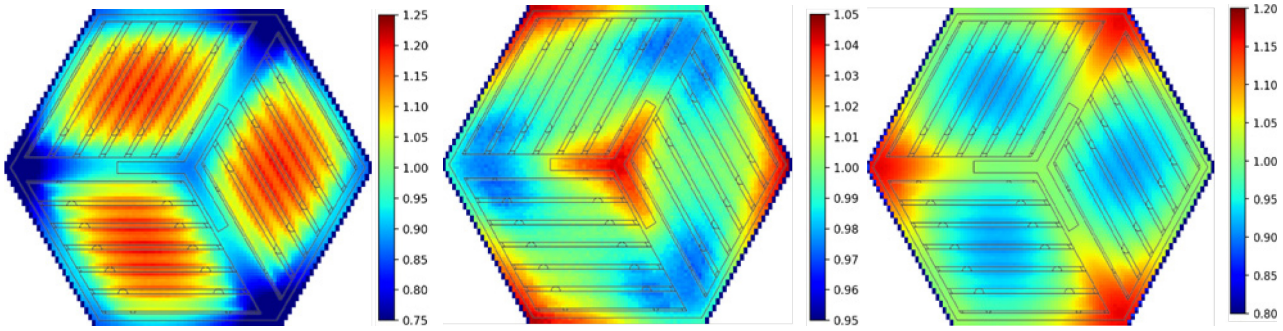
Figure 3.3. Fission density by individual TRISO particle (colour-coded)



Source: B. Petrovic and K. Ramey

Example (output d): Visualisation of 3-group flux distribution, see Figure 3.4.

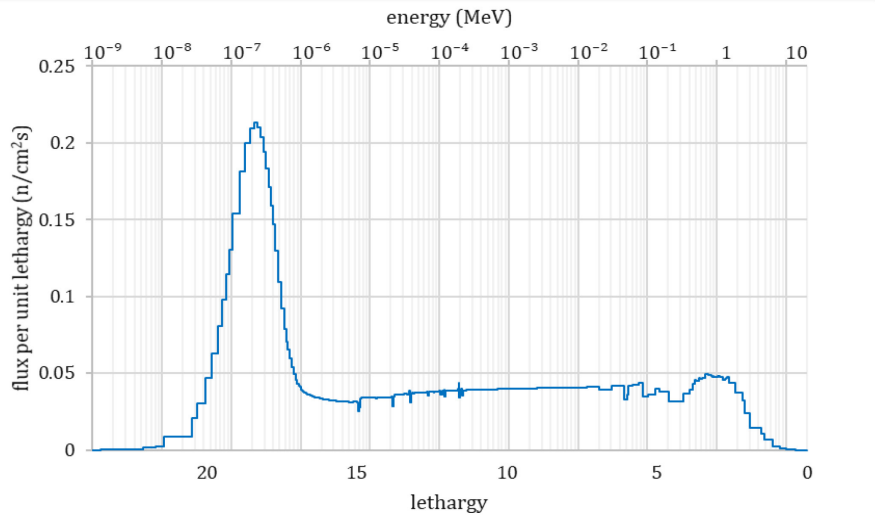
Figure 3.4. Three-group flux distribution (on 100x100 spatial mesh)



Source: B. Petrovic and K. Ramey

Example (output e): Visualisation of the average neutron spectrum (also to be provided as raw data), see Figure 3.5.

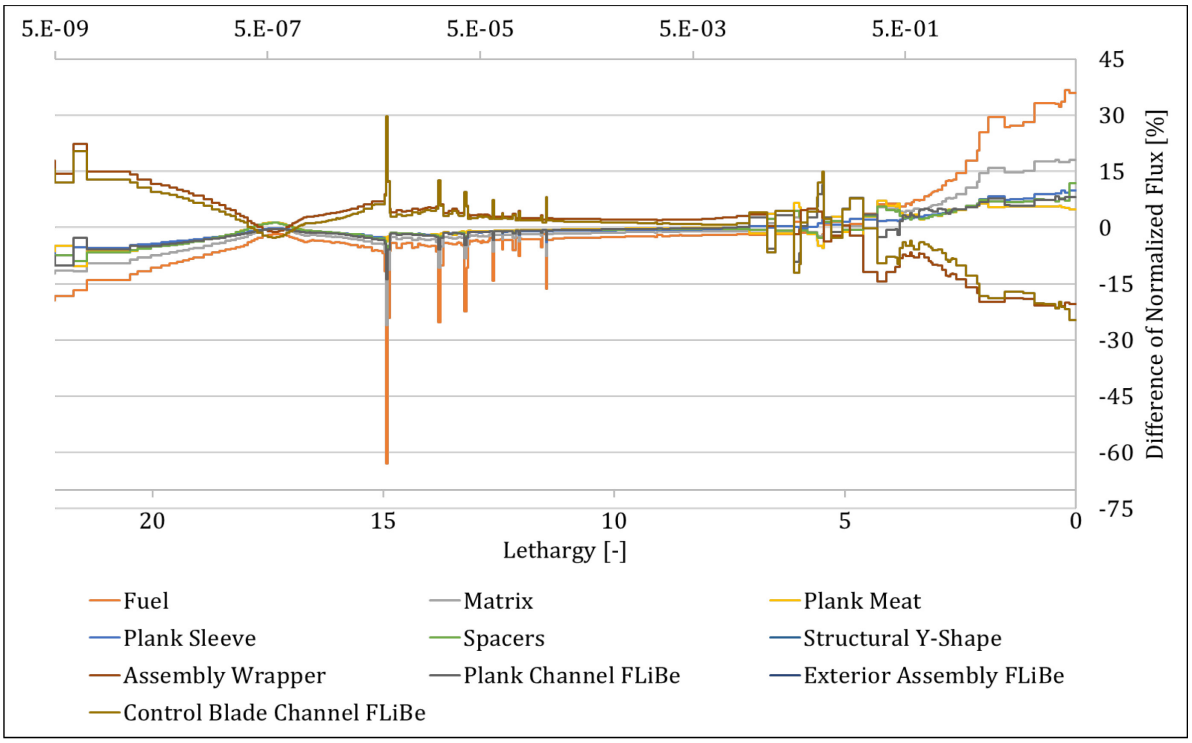
Figure 3.5. Average neutron spectrum (over the whole problem)



Source: B. Petrovic and K. Ramey

Example (output e, optional): Visualisation of region-wise neutron spectra, see Figure 3.6. Present spectra in all regions and/or difference to the average spectrum over the whole problem.

Figure 3.6. Fission density (1/5-stripe granularity)



Source: B. Petrovic and K. Ramey

4. Output specifications and templates

4.1. Phase I-A and Phase I-B results

Results required in Phase I include Phase I-A results (no depletion) and Phase I-B results (selected I-A cases with depletion):

(a) Effective multiplication factor, and its change with depletion.

(b) Reactivity coefficients, at selected depletion steps (β-effective; 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), and its change with depletion, at selected burn-ups (details are specified in Section 3.1.4). Optional: visualised fission density distribution.

(d) Neutron flux, averaged over the whole model, tabulated in three coarse energy groups (upper energy boundaries 3 eV for thermal group and 0.1 MeV for intermediate group), and its change with depletion, at selected burn-ups (details are specified in Section 3.1.4).

(e) Visualised distribution of the neutron flux distribution, in three coarse energy groups, and its change with depletion, at selected burn-ups (details are specified in Section 3.1.4).

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

(g) Fuel (and burnable poison, when applicable) isotopic change with depletion. Only in Phase I-B (details, i.e. which isotopes at what burn-up are specified in Section 3.1.4).

Specifications for output format of results requested in Phase I follow. Please follow the format specifications exactly.

Note that in most cases the format is the same for Phase I-A and Phase I-B, except that multiple results will be provided in Phase I-B (in the same format) for multiple burn-ups, rather than a single result. This is different in cases (a) and (g), where the results will be tabulated in a single file for all specified burn-ups.

4.1.1. Effective multiplication factor (a), Phase I-A

Provide both k-eff and 1σ(k-eff) (or equivalent estimated uncertainty) to 5 decimal places.

Specify 1σ(k-eff) as absolute value (not relative).

Table 4.1. Requested format of effective multiplication factor Phase I-A

	k-eff	1σ(k-eff)
CASE 1A		
CASE 2AH		
CASE 2AC		
CASE 3A		
CASE 4A		
CASE 5A		
CASE 6A		
CASE 7A		

Source: B. Petrovic and K. Ramey

4.1.2. Effective multiplication factor (a), with depletion, Phase I-B

Provide both k-eff and 1σ(k-eff) (or equivalent estimated uncertainty) to 5 decimal places.

Specify 1σ(k-eff) as absolute value (not relative).

Table 4.2. Requested format of effective multiplication factor with depletion Phase I-B

	CASE 1B		CASE 4B		CASE 7B	
Burn-up [GWd/tU]	k-eff (a)	1σ(k-eff)	k-eff (a)	1σ(k-eff)	k-eff (a)	1σ(k-eff)
0						
0.1						
0.5						
1						
2						
4						
6						
8						
10						
14						
18						
22						
26						
30						
40						
50						
60						
70						
Only CASE 7B for burn-ups beyond 70 GWd/tU						
80						
90						
100						
120						
140						
160						

Source: B. Petrovic and K. Ramey

4.1.3. Delayed neutron parameters and reactivity coefficients (b)

Provide βeff and 1σ(βeff) (or equivalent estimated uncertainty) to 5 decimal places. Specify 1σ(βeff) as absolute value (not relative).

Provide reactivity coefficients defined as:

$$\left(\frac{\partial \rho}{\partial T}\right)_i \approx \frac{\Delta \rho}{\Delta T_i} \left[\frac{pcm}{K}\right]$$

where index i denotes:

f = Fuel for Doppler reactivity coefficient

c= FLiBe for coolant reactivity coefficient

g= graphite for graphite reactivity coefficient

It is suggested to use ΔT=±50K when calculating temperature coefficients. In any case, specify the temperatures used.

Specify the coefficients and the associated (absolute) uncertainty to two decimal places.

Table 4.3. Requested format of effective multiplication factor Phase I-B

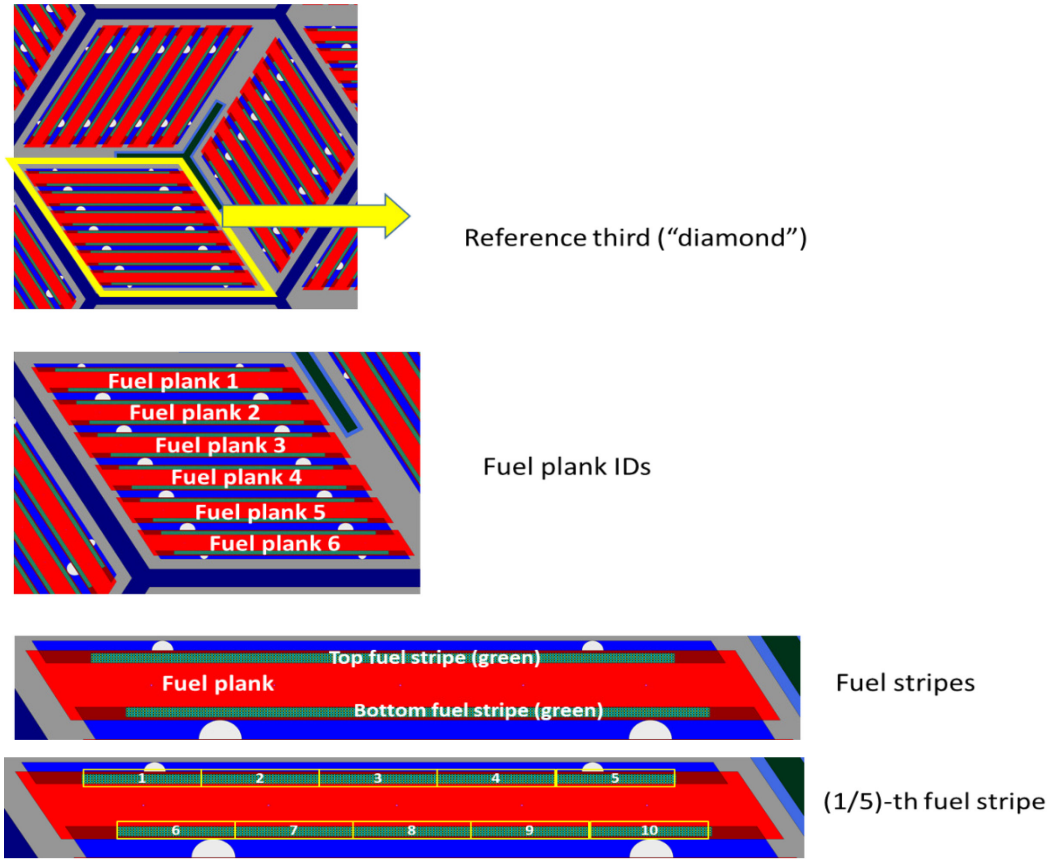
	βeff	1σ(βeff)	Fuel (Δρ/ΔT) [pcm/K]	1σ [pcm/K]	FLiBe (Δρ/ΔT) [pcm/K]	1σ [pcm/K]	Graphite (Δρ/ΔT) [pcm/K]	1σ [pcm/K]
CASE 1A								
CASE 2AH								
CASE 2AC								
CASE 3A								
CASE 4A								
CASE 5A								
CASE 6A								
CASE 7A								

Source: B. Petrovic and K. Ramey

4.1.4. Fission source distribution (c)

For each case analysed, provide results for the bottom left third of the fuel assembly. Provide normalised fission source to three decimal places with the corresponding uncertainty. Use the following figures and table to relate region ID to its position within the assembly.

Figure 4.1. Illustration depicting the fuel region to report fission source distribution



Source: B. Petrovic and K. Ramey

Table 4.4. Requested fuel regions to report fission source distribution

PLANK	Top	1	2	3	4	5
	Bottom	6	7	8	9	10
	ID					
1	Top	101	102	103	104	105
	Bottom	106	107	108	109	110
2	Top	201	202	203	204	205
	Bottom	206	207	208	209	210
3	Top	301	302	303	304	305
	Bottom	306	307	308	309	310
4	Top	401	402	403	404	405
	Bottom	406	407	408	409	410
5	Top	501	502	503	504	505
	Bottom	506	507	508	509	510
6	Top	601	602	603	604	605
	Bottom	606	607	608	609	610

Source: B. Petrovic and K. Ramey

Provide results in the following format:

Table 4.5. Requested format of the fission source distriution

PLANK	Stripe	Region	ID	Fission density	1σ (abs.)	Relative unc.
1	Top	1	101			
		2	102			
		3	103			
		4	104			
		5	105			
	Bottom	6	106			
		7	107			
		8	108			
		9	109			
		10	110			
…						
…						
6	Top	1	601			
		2	602			
		3	603			
		4	604			
		5	605			
	Bottom	6	606			
		7	607			
		8	608			
		9	609			
		10	610			

Source: B. Petrovic and K. Ramey

Optionally, provide visualised fission density distribution (see examples in Section 3.1.4).

4.1.5. Neutron flux (d)

Provide results for the neutron flux, averaged over the whole model, tabulated in three coarse energy groups (upper energy boundaries 3 eV for thermal group and 0.1 MeV for intermediate group).

Provide absolute values, for the reference specific power, 200 W/gU.

Table 4.6. Requested format of the neutron flux

Group	Energy range	Flux Φ[n/cm²s]	1σ (abs.)	Relative unc.
1	E>0.1MeV			
2	0.1MeV>E>3eV			
3	3eV>E			

Source: B. Petrovic and K. Ramey

4.1.6. Neutron flux distribution (e)

To facilitate consistent comparison, it is suggested to capture 3-group flux distribution on a rectangular 100x100 spatial mesh. The co-ordinate X-Y system should be positioned so that its origin is at the fuel assembly centre. Results should be provided in the EXCEL file in the following format:

- ---------- intro block ----------
- TITLE – 3 lines identifying the case
- NX (number of X intervals),
- X0,X1,X2,….XNX (NX+1 interval boundaries)
- NY (number of Y intervals)
- Y0,Y1,Y2, ,YNY (NY+1 interval boundaries)
- ---------- table with fluxes for group 1 (NY lines, NX columns) --------
- Φ1(1,1), Φ1(2,1), … , Φ1(NX,1)
- …..
- Φ1(1,NY), Φ1(2,NY), … , Φ1(NX,NY)
- ---------- table with fluxes for group 2 (NY lines) --------
- Φ2(1,1), Φ2(2,1) , Φ2(NX,1)
- …..
- Φ2(1,NY), Φ2(2,NY), … , Φ2(NX,NY)
- ---------- table with fluxes for group 3 (NY lines) --------
- Φ3(1,1), Φ3(2,1), … , Φ3(NX,1)
- …..
- Φ3(1,NY), Φ3(2,NY), … , Φ3(NX,NY)

For examples of visualised neutron flux distribution, see Section 3.1.4.

4.1.7. Neutron flux distribution (f)

See examples in Section 3.1.4.

Average spectrum for the whole problem is required. Additional spectra by region are optional.

The tabulated results should be provided in the EXCEL file as (absolute) multi-group fluxes with specified energy group boundaries. This will enable post-processing into spectrum per energy or per lethargy.

It is suggested to tabulate spectra in the SCALE 252-group energy structure.

Visualisation may be performed in a format equivalent to Figure 3.5.

The EXCEL file should include, for each spectrum, the following information:

- ---------- intro block ----------
- TITLE – 3 lines identifying the case
- NG – number of energy groups
- Header line for the columns that follow:
- ---------- table with fluxes by group, NG lines --------
- Each line should contain columns with:
- IG (group index, 1 to NG)
- Emax upper energy boundary (MeV)
- Emin lower energy boundary (MeV)
- Flux (n/cm2s) for nominal full power

4.1.8. Fuel and burnable poison isotopic vs. depletion (g): Only for Phase I-B

For each case (CASE 1B, 4B, 7B) provide change of atom densities with depletion for fuel isotopes, and when applicable for burnable poison (CASE 4B). Note that for zero burn-up these numbers are identical to the ones in Phase I-A. Provide numbers in scientific format with five decimal places, e.g. 1.23456E-02. Provide results for burn-ups specified in Table 3.2. One EXCEL sheet per case. If possible, also provide uncertainty estimate. Identical format, one sheet per case.

Isotopics is requested in relative density, g/tHMi. However, it is also acceptable to provide results in atom density units at/b-cm^3.

Results will be provided at two levels of detail:

(a) key nuclides, required;

(b) extended list of actinides, optional.

Results will be provided in the following format:

a) Key nuclides, required

Table 4.7. Requested format of nuclide concentration vs. burn-up for Phase I-B'

CASE ID	Burn-up [GWd/tU]					
Nuclide [g/tHMi]	0	0.1	0.5	1	…	Etc.
Actinides						
^{235}U						
^{238}U						
^{239}Pu						
^{240}Pu						
^{241}Pu						
^{242}Pu						
^{243}Pu						
^{244}Pu						
^{241}Am						
^{242m}Am						
^{243}Am						
^{242}Cm						
^{243}Cm						
^{244}Cm						
^{245}Cm						
Fission products						
^{85}Kr						
^{90}Sr						
^{110m}Ag						
^{137}Cs						
^{135}Xe						
^{149}Sm						
^{151}Sm						
CASE 4B only						
Eu isotopes						

Source: B. Petrovic and K. Ramey

b) Extended list of actinides, optional

Table 4.8. Requested format for optional nuclide concentrations vs. burn-up for Phase I-B

CASE ID	Burn-up [GWd/tU]					
Nuclide [g/tHMi]	0	0.1	0.5	1	…	Etc.
^{232}U						
^{233}U						
^{234}U						
^{235}U						
^{236}U						
^{238}U						
^{236}Np						
^{237}Np						
^{236}Pu						
^{238}Pu						
^{239}Pu						
^{240}Pu						
^{241}Pu						
^{242}Pu						
^{243}Pu						
^{244}Pu						

Table 4.8. Requested format for optional nuclide concentrations vs. burn-up for Phase I-B (Cont'd)

^{241}Am						
^{242m}Am						
^{243}Am						
^{242}Cm						
^{243}Cm						
^{244}Cm						
^{245}Cm						
^{246}Cm						
^{247}Cm						
^{248}Cm						
^{226}Ra						
^{228}Ra						
^{227}Ac						
^{229}Th						
^{230}Th						
^{232}Th						
^{252}Cf						

Source: B. Petrovic and K. Ramey

The results should be sent to **bojan.petrovic@gatech.edu** **and cc: wprs@oecd-nea.org.**

5. References

[1] Varma, V.K., D.E. Holcomb, F.J. Peretz, E.C. Bradley, D. Ilas, A.L. Qualls, N.M. Zaharia (2011), *AHTR Mechanical, Structural, and Neutronic Preconceptual Design*, ORNL/TM-2012/320, Oak Ridge National Laboratory. DOI: 10.2172/1054145.

[2] Ramey, K., B. Petrovic (2018), "Monte Carlo modeling and simulations of AHTR fuel assembly to support V&V of FHR core physics methods", *Annals of Nuclear Energy*, 118, 272-282. DOI: 10.1016/j.anucene.2018.04.003.

[3] Rahnema, F., B. Petrovic, P. Singh, P. Burke, H. Noorani, X. Sun, G. Yoder, P. Tsvetkov, J. Zhang, D. Zhang, D. Ilas (2017), "The Challenges in Modeling and Simulation of Fluoride-Salt-Cooled High-Temperature Reactors", White Paper CRMP-2017-9-001, Georgia Institute of Technology. http://hdl.handle.net/1853/58808.

[4] Petrovic, B., T. Flaspoehler, K. Ramey (2018), "Benchmarking FHR core physics simulations: 2D fuel assembly model", *Proc. 12th Intl. Conf. on Nuclear Option in Countries with Small and Medium Electricity Grid*s, Zadar, Croatia, 3-6 June 2018.

[5] Leppänen, J., M. Pusa, T. Viitanen, V. Valtavirta, T. Kaltiaisenaho (2015), "The SERPENT Monte Carlo code: status, development, and applications", *Annals of Nuclear Energy*, 82, 142-150. DOI: 10.1016/j.anucene.2014.08.024.

[6] ORNL (2016), *SCALE 6.2.1: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design; Includes ORIGEN and AMPX*, ORNL/TM-2005/39, Version 6.2.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee. DOI: 10.2172/1326509.

[7] LANL (2013), *MCNP: A General Monte Carlo N-Particle Transport Code*, Version 6.1, LA-CP-00634, Los Alamos National Laboratory, Los Alamos, N.M.