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Usage of Monte Carlo Code Serpent2 for Calculation of FHR Fuel Assembly

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ABSTRACT

In this paper our initial results are presented for Fluoride-salt High-temperature Reactor (FHR) reactor physics benchmark calculations, Phase I-C. Phase I-C extends to 3D previous OECD benchmark Phase I-A and I-B, which defined pseudo-2D calculation of a single FHR fuel assembly with TRISO fuel, moderated with graphite and cooled with FLiBe coolant. Pseudo-2D fuel element geometry is extruded in axial direction with addition of axial top and bottom reflectors (FLiBe and graphite). Radially, periodic boundary conditions (BC) were applied, and axially, vacuum BCs were used. The characteristics of the benchmark, complicated 2D geometry of a plate type assembly with TRISO fuel, double heterogeneity spectral calculation and use of 'exotic' materials (FLiBe coolant, Eu as burnable poison, molybdenum-hafnium-carbide (MHC) control rods), mean that the most suitable calculation tool should be Monte Carlo computer code. We used Serpent2 code (versions 2.1.32 and 2.2.1, compiled for Cygwin environment) with three versions of ENDF/B library (ENDF/B-VI.8, ENDF/B-VII.0 and ENDF/B-VII.1). In addition, CSAS6 module from SCALE 6.2.4 and SCALE 6.3.1 package was used to check the obtained k_{eff} values. This paper covers the results (k_{eff}, fission density spatial distribution, group fluxes, and selected isotopes number densities) of the first 4 Phase I-C benchmark exercises. The first two exercises assume axially symmetric core, with uniform temperature distribution, without depletion. The third exercise analyses control rod insertion and the fourth is the same as the first one, but with depletion up to 70 GWd/tU. Our goal was to check the differences when using the two most recent Serpent2 versions (almost the same results and small change in CPU time) and what are differences in results and calculation time when three versions of ENDF/B library were used. The decision was to use faster (and less memory demanding) ENDF/B-VI.8 library for scoping calculation and ENDF/B-VII.1 library for production calculation.

1 INTRODUCTION

Fluoride-salt-cooled High-temperature Reactor (FHR) is an advanced reactor system cooled with liquid (molten) salt and fuelled with tristructural-isotropic (TRISO)-based fuel. The fuel is dispersed in a graphite matrix and the coolant is fluoride salt $2LiF\text{-}BeF_2$ (FLiBe). The main difference between this reactor and historical Molten Salt Reactor Experiment is that the fuel is solid in form of circulating pebbles or in hexagonal fuel elements. The latter design type has TRISO particles contained within the fuel stripes of the fuel planks, which introduces

double heterogeneity in the already complex geometry. This is why benchmark was needed to evaluate the applicability of the methodologies and methods to simulate FHR core physics [1]

OECD (Organisation for Economic Co-operation and Development) FHR benchmark proposal was accepted in 2019 at the Expert Group on Reactor Physics and Advanced Nuclear Systems meeting. The benchmark exercises are divided in three phases. Phase I covers a model of a single fuel assembly. A 3D full core model with depletion is considered in Phase II and Phase III deals with a 3D full core model with feedback and multicycle analysis. Phase I has three subphases: I-A and I-B which cover the pseudo 2D model without and with depletion, respectively [2], and a 3D model of a single fuel assembly is analysed in I-C [3]. The results of simulations of the pseudo 2D fuel assembly (Phase I-A and Phase I-B) performed by different FHR benchmark participants are published in [4].

In this paper, our initial results for FHR reactor physics benchmark calculations, Phase I-C are presented. Phase I-C extends to 3D previous OECD benchmark Phase I-A and I-B, which defined pseudo-2D calculation of a single FHR fuel assembly with TRISO fuel, moderated with graphite and cooled with FLiBe coolant. Pseudo-2D fuel element geometry is extruded in axial direction with addition of axial top and bottom reflectors (FLiBe and graphite). Radially, periodic boundary conditions (BC) were applied, and axially, vacuum BCs were used. The characteristics of the benchmark, complicated 2D geometry of plate type assembly with TRISO fuel, double heterogeneity spectral calculation and use of 'exotic' materials (FLiBe coolant, Eu as burnable poison, molybdenum-hafnium-carbide (MHC) control rods), mean that the most suitable calculation tool should be Monte Carlo computer code. We used Serpent2 code [5] (versions 2.1.32 and 2.2.1, compiled for Cygwin environment) with three versions of ENDF/B library (VI.8, VII.0, and VII.1). The goal of this work is to check the differences when using the two most recent Serpent2 versions and what are differences in results and calculation time when three versions of ENDF/B library are used. In addition, CSAS6 module from SCALE 6.2.4 [6] and SCALE 6.3.1 [7] package was used to check the obtained k_{eff} values.

2 METHODOLOGY

2.1 Computer codes

The main calculation tool is Serpent 2.1.32 and 2.2.1 (libraries ENDF/B-VI.8, ENDF/B-VII.0 and ENDF/B-VII.1). The check of results for non-depletion cases is performed with SCALE 6.2.4 and SCALE 6.3.1 (libraries (ENDF/B-VII.1 and ENDF/B-VIII.0). Short description of the used codes follows.

Serpent is a 3D continuous energy neutron and photon transport code that has been developed at the VTT Technical Research Centre of Finland since 2004. It may be used for a wide range of particle transport applications such as reactor modelling, group constants generation, radiation transport, fusion, etc. The physics model covers neutron, photon and coupled neutron-photon simulations. Cross sections are read from ACE format data libraries. The continuous-energy interaction data is obtained from evaluated nuclear data files without major approximations. Standard tallies in Serpent enable calculating flux, power and reaction rate distributions in geometry cells and materials, as well as regular structures, such as lattices and super-imposed meshes [5].

The Criticality Safety Analysis Sequence with KENO-VI (CSAS6) is a control module of the SCALE code system. It is used for performing k_{eff} calculations in a reliable and efficient way. There is a multigroup and continuous energy calculation mode. In the multigroup mode, CSAS6 uses XSProc to process the cross sections for temperature corrections and problem-dependent resonance self-shielding and calculates the k_{eff} of three-dimensional (3-D) system models. In continuous energy mode there is no need for resonance processing and the continuous energy cross sections are used directly in KENO-VI, with temperature corrections

provided as the cross sections are loaded. The module can analyse complex 3-D systems since it features geometric modelling capabilities and the automated cross section processing [6].

2.2 Serpent model of FHR

As already mentioned, in Phase I-C a single 3D model of the fuel element is analysed. The FHR fuel element has hexagonal form containing three diamond sections (120-deg rotational symmetry), each containing six fuel planks as shown in Figure 1 (plot SCALE – Fulcrum). The apothem of the fuel hexagon is 22.5 cm, thus the outer dimension side-to-side is 45.0 cm. Each fuel plank is composed of two fuel stripes and burnable poisons at 5 equidistant locations. Fuel stripes are prismatic regions composed of graphite matrix filled with a cubic lattice of TRISO particles shown in Figure 2. Burnable poison is in the form of small spherical particles made of europium oxide. The TRISO particle contains 5 layers from the inside out: fuel kernel, buffer, inner pyrolytic carbon, silicon carbide layer, and outer pyrolytic carbon. The TRISO lattice pitch is 0.09266 cm. Axial distribution of TRISO particles is shown in Figure 3. The control rod is a Y-shape structure made of MHC (Molybdenum-hafnium carbide alloy) with no cladding, surrounded by a thin layer of FLiBe. Each wing is 10 cm long and 1 cm thick.

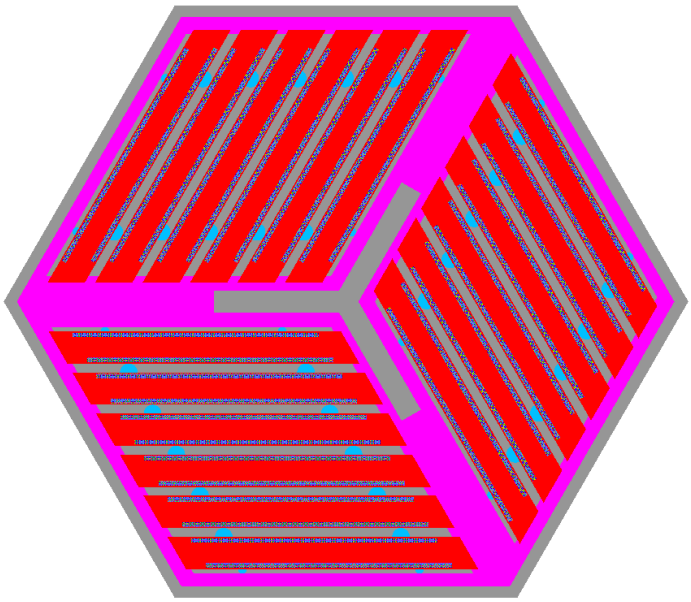

Figure 1: FHR fuel assembly XY cross section in active fuel part, SCALE model

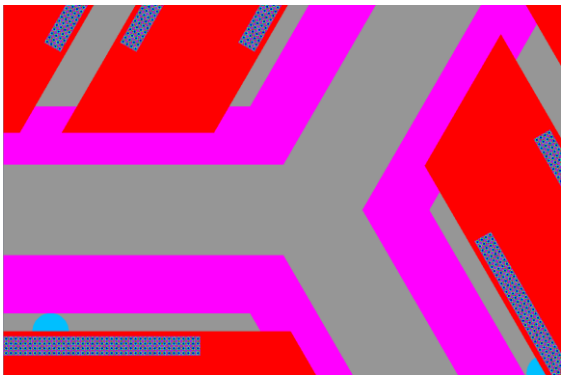

Figure 2: FHR fuel assembly XY cross section in active fuel part zoomed to view TRISO spheres

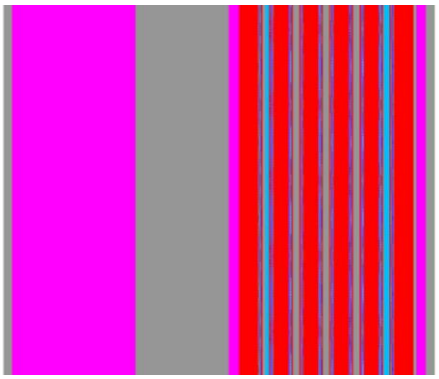

Figure 3: Axial distribution of TRISO spheres

The 3D model of the FHR fuel element was extruded from the pseudo-2D fuel element geometry in axial direction with addition of axial top and bottom reflectors (FLiBe and graphite). Radially, periodic boundary conditions (BC) were applied, and axially vacuum BCs were used (Figure 4).

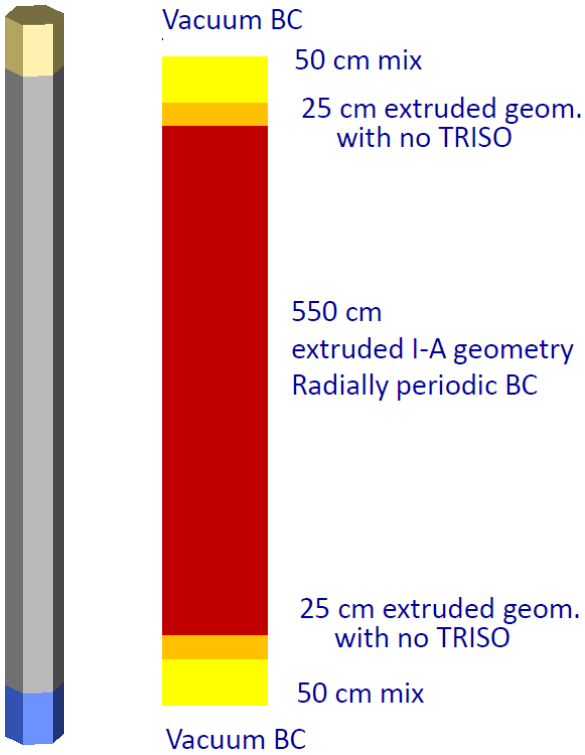

Figure 4: FHR fuel assembly axial division and boundary conditions [3]

2.3 Benchmark exercises

This paper covers the results (k_{eff}, fission density spatial distribution, group fluxes, and selected isotopes number densities) of the first 4 benchmark exercises. The first two exercises assume axially symmetric core, with uniform temperature distribution (fuel kernel 1110 K, everything else 948 K), without depletion. The third exercise analyses control rod insertion and the fourth uses the same configuration as the first one, but with depletion up to 70 GWd/tU.

3 RESULTS

3.1 Exercise 1

The fission density rate is shown in Figure 5. The comparison is made between the two version of the Serpent code using available ENDF/B libraries. Axially, active length of the fuel assembly is divided into sixteen zones of equal height, marked 1-16. The lowest number corresponds to the lowest zone. As expected, there are no significant discrepancies in the results for the two versions of Serpent2 code and libraries used.

Figure 6 shows the normalized neutron spectrum over 252-group energy structure used in SCALE package. Again, just small differences can be noticed (energy range between 0.01 and 1 MeV) when three versions of library were used.

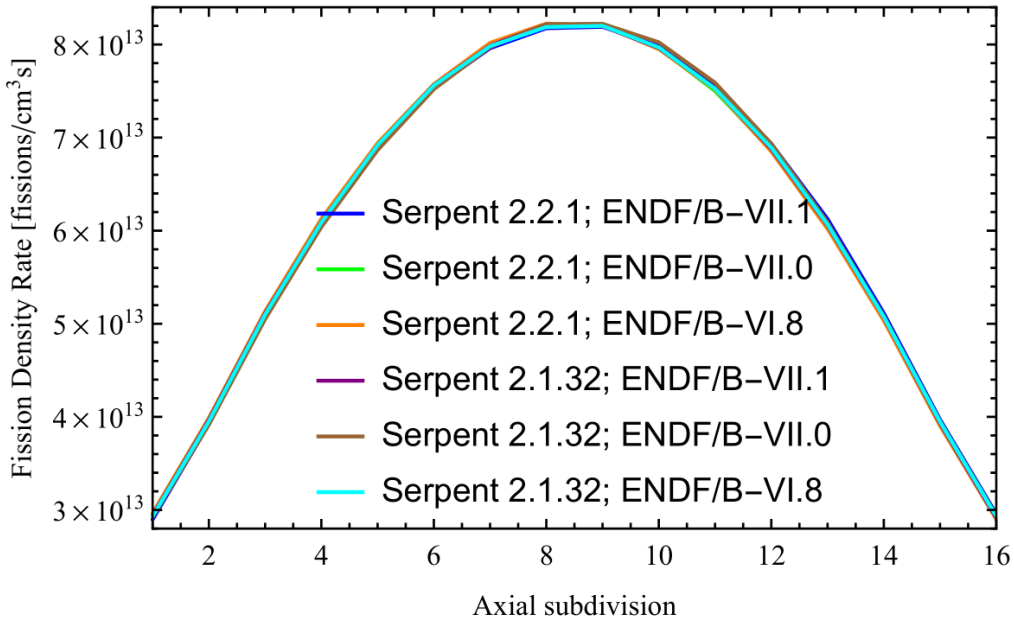

Figure 5: Fission density rate for two Serpent versions and three libraries (16 axial subdivisions)

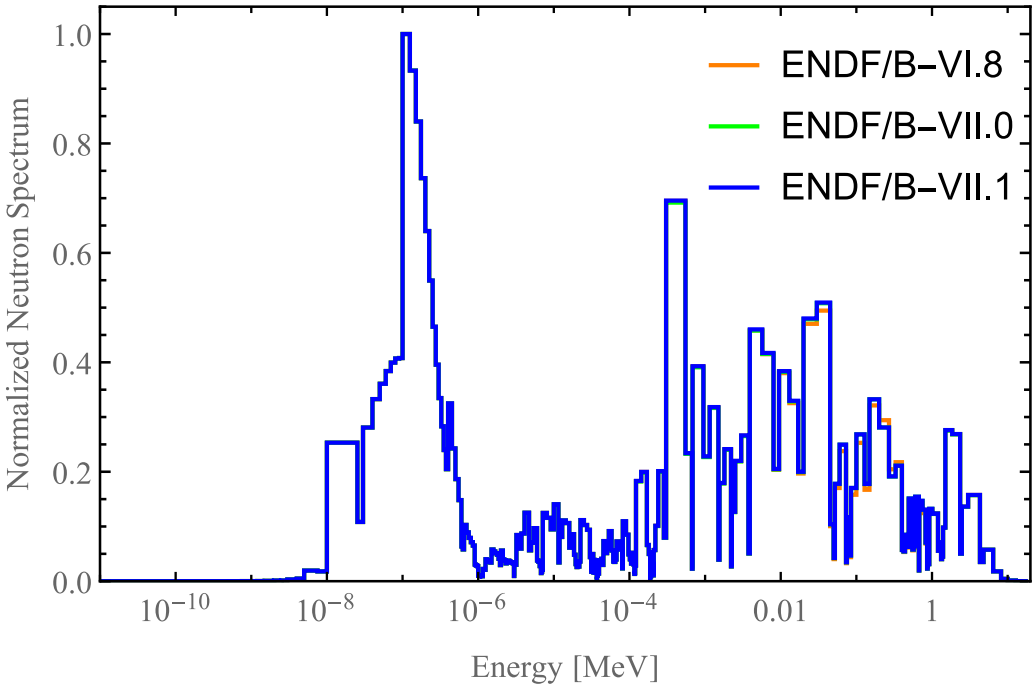

Figure 6: Normalized neutron spectrum – fuel (Serpent 2.2.1), 252 groups SCALE energy structure

3.2 Exercise 2

The axial offset (AO) and associated uncertainties for two versions of Serpent as well as for SCALE 6.3.1, and different libraries are shown in Table 1. The results in terms of multiplication factor obtained with different programs and libraries are shown in Table 2. The axial offset was small, as expected for symmetric core configuration. When using the same library, Serpent 2.2.1 and SCALE 6.3.1 gave almost the same AO and k_{eff}. The influence of changing library for the same version of the code can be seen, but it is small. Similar AO differences exist between different Serpent2 versions for the same library. For k_{eff} values the influence of Serpent2 code version is negligible. The uncertainty was limited to 0.00019 for Serpent2 calculations.

Table 1: Axial offset

Program	Library	Axial Offset	Uncertainty
Serpent 2.2.1	ENDF/B-VII.1	0.00343	0.00019
Serpent 2.2.1	ENDF/B-VII.0	-0.00232	0.00019
Serpent 2.2.1	ENDF/B-VI.8	-0.00608	0.00019
Serpent 2.1.32	ENDF/B-VII.1	-0.00254	0.00019
Serpent 2.1.32	ENDF/B-VII.0	0.00318	0.00019
Serpent 2.1.32	ENDF/B-VI.8	-0.00125	0.00019
SCALE 6.3.1	ENDF/B-VIII.0	0.00524	
SCALE 6.3.1	ENDF/B-VII.1	-0.00331	

Table 2 k_{eff} results

	Serpent 2.2.1 ENDF-B/VII.1	Serpent 2.2.1 ENDF-B/VII.0	Serpent 2.2.1 ENDF-B/VI.8	Serpent 2.1.32 ENDF-B/VII.1	SCALE 6.3.1 ENDF/B-VIII.0	SCALE 6.2.4/6.3.1 ENDF/B-VII.1
k_{eff}	1.37908	1.38305	1.38056	1.37904	1.37898	1.37934
σ	0.00005	0.00005	0.00006	0.00006	0.00019	0.00019

3.3 Exercise 3

The dependence of k_{eff} values on the control rod insertion for Serpent 2.1.32 (ENDF/B-VII.1), SCALE 6.2.4 (ENDF/B-VII.1) and SCALE 6.3.1(ENDF/B-VIII.0) is shown in Figure 7. The differences are generally small except close to fully inserted position (between 15 and 16), where one spatial midpoint is added in 16-steps equidistant subdivision.

Figure 8 shows grouped neutron flux for the control rod insertion 12-04. The results are presented for two axial slices (axial slice 20 and 30) and three neutron flux groups (group 1, 2, and 3). The different influence of neutron production and absorption can be seen in the selected group structure. Spatial subdivision was 100x100x112.

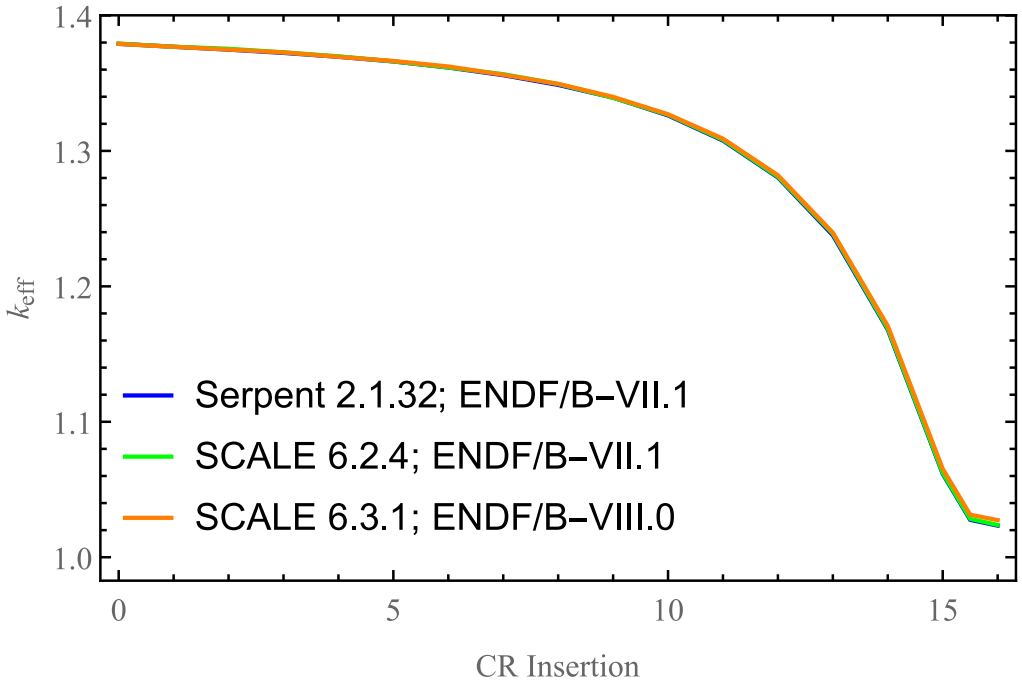

Figure 7: k_{eff} vs control rod insertion

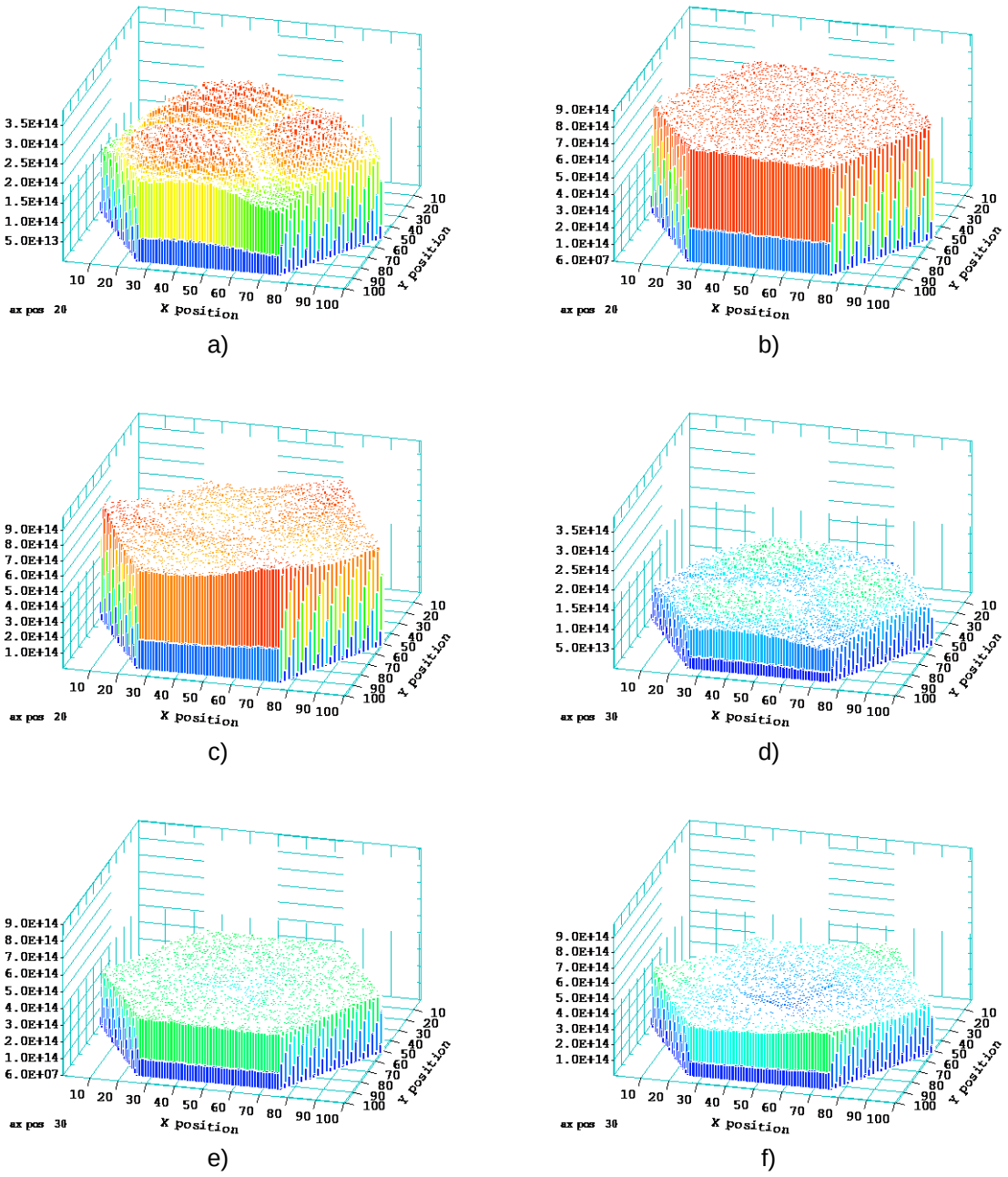

Figure 8: Serpent 2.2.1 ENDF/B-VII.1 control rod insertion 12-04: a) axial slice 20, neutron flux group 1; b) axial slice 20, neutron flux group 2; c) axial slice 20, neutron flux group 3; d) axial slice 30, neutron flux group 1; e) axial slice 30, neutron flux group 2; f) axial slice 30, neutron flux group 3

In Figure 9 the differences in k_{eff} values (Δk_{eff}) are shown, during control rod insertion, obtained with SCALE 6.2.4 and Serpent 2.1.32, when using the same library (ENDF/B-VII.1), as well as with SCALE 6.3.1 (ENDF/B-VIII.0) and Serpent 2.1.32 (ENDF/B-VII.1) when using different libraries. It can be seen that the Serpent and SCALE results agree well when using the same cross section library (ENDF/B-VII.1) and in the worst case the difference is 110 pcm. However, when using newer library, the results agree well up to and including 5 steps of the control rod insertion. The differences are below 100 pcm up to and including 10 steps of the control rod insertion. It may be expected that for initial insertion (e.g., 5 steps) the impact of

cross section library is small, since the impact of control rod is small. After that, a constant increase in the Δk_{eff} is noticed and in case of the full control rod insertion (16 steps) the difference is 407 pcm. It would be interesting to find out which nuclide in the control rod leads to the difference, but that will be analysed in next step.

The 3-group distribution of neutron flux for four and eight steps of control rod insertion obtained over the 100x100x148 square mesh in SCALE 6.2.4 is shown in Figure 10. The boundaries between the groups are 3 eV and 0.1 MeV. Expectedly, deeper insertion („0808“) resulted in the skewed fluxes towards the lower parts of the fuel assembly. The Source Vectors (SV) for selected control rod insertion depths, obtained using SCALE 6.2.4 and SCALE 6.3.1 and different libraries, generally show small differences.

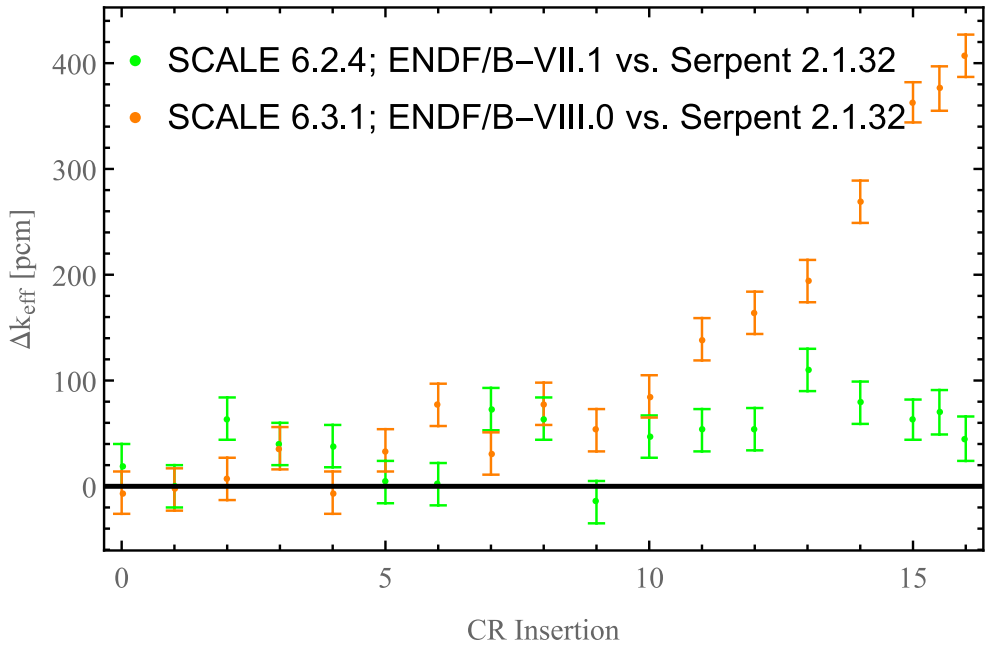

Figure 9: Δk_{eff} (SCALE vs. Serpent) during control rod insertion

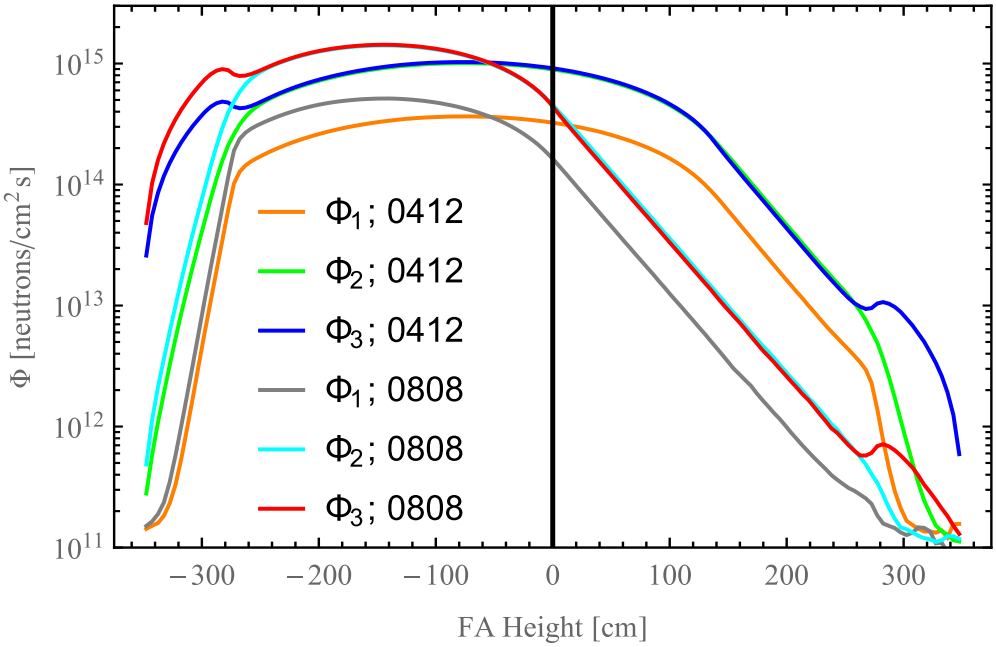

Figure 10: 3 group fluxes for 4/16 and 8/16 inserted control rod

3.4 Exercise 4

The depletion calculations were performed for the 18 predefined burnup steps. Three calculations were performed using Serpent 2.1.32 with ENDF/B-VII.1 and ENDF/B-VII.0 libraries, as well as using Serpent 2.2.1 with ENDF/B-VII.1 library. The results in terms of $k_{eff}(B)$ and $\Delta k_{eff}(B)$ are shown in Figure 11 and Figure 12. It can be seen that the version of the code has almost no influence on the k_{eff}(B). The maximum absolute difference of the multiplication factors is (78 ± 18) pcm. However, the variation of the used library has far greater influence on the obtained results. Using the older ENDF/B-VII.0 library gives higher values of $k_{eff}(B)$, whereas the maximum difference of (512 ± 18) pcm is achieved for B = 2.0 GWd/tU. The higher the burnup the lower the differences, but no lower than (270 ± 23) pcm. The change in isotopic concentration of the fuel during depletion is given in Figure 13. Again, while not shown in the figure, when using the same library, both Serpent2 versions are giving almost the same results. Similar results for this FHR problem and for VII.1 vs VII.0 difference (Figure 13) were reported in ANS summary [8].

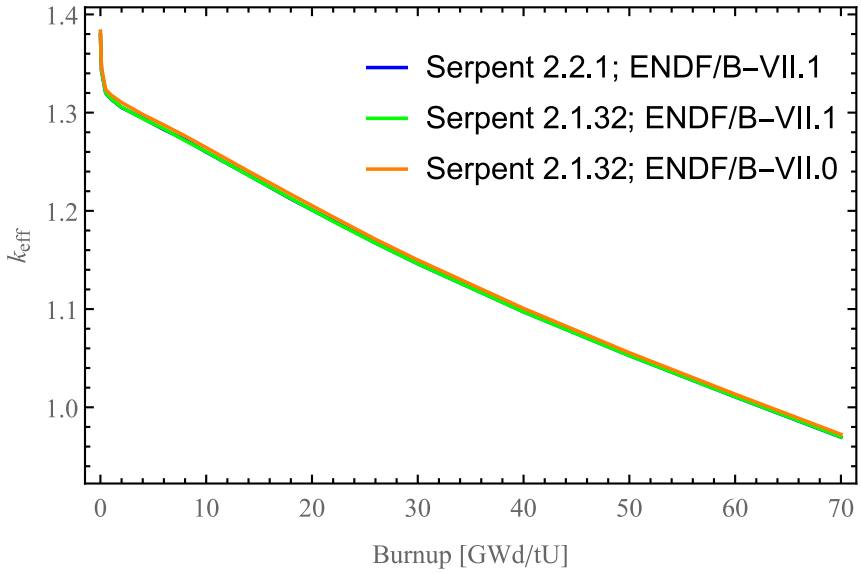

Figure 11: k_{eff}(B) obtained with different Serpent programs

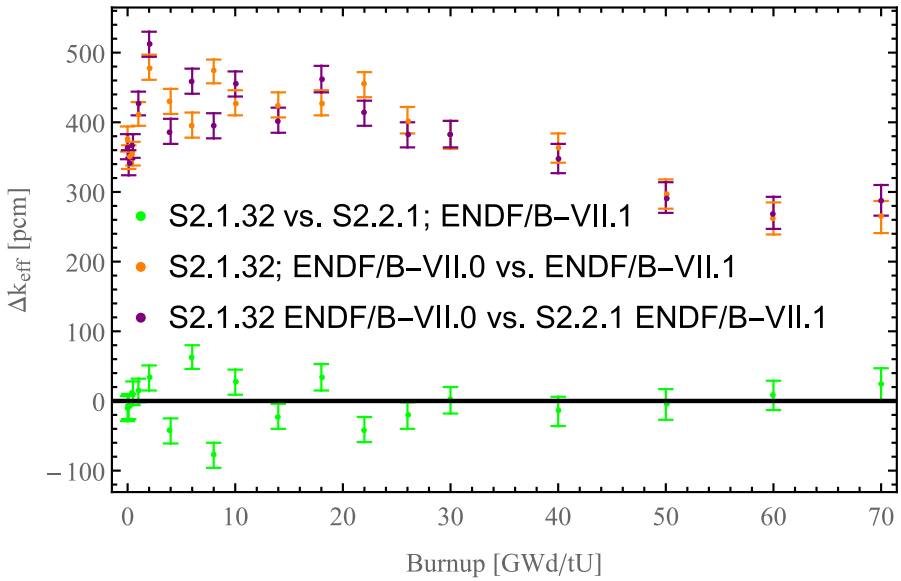

Figure 12: Comparison of Δk_{eff}(B) between the codes and libraries

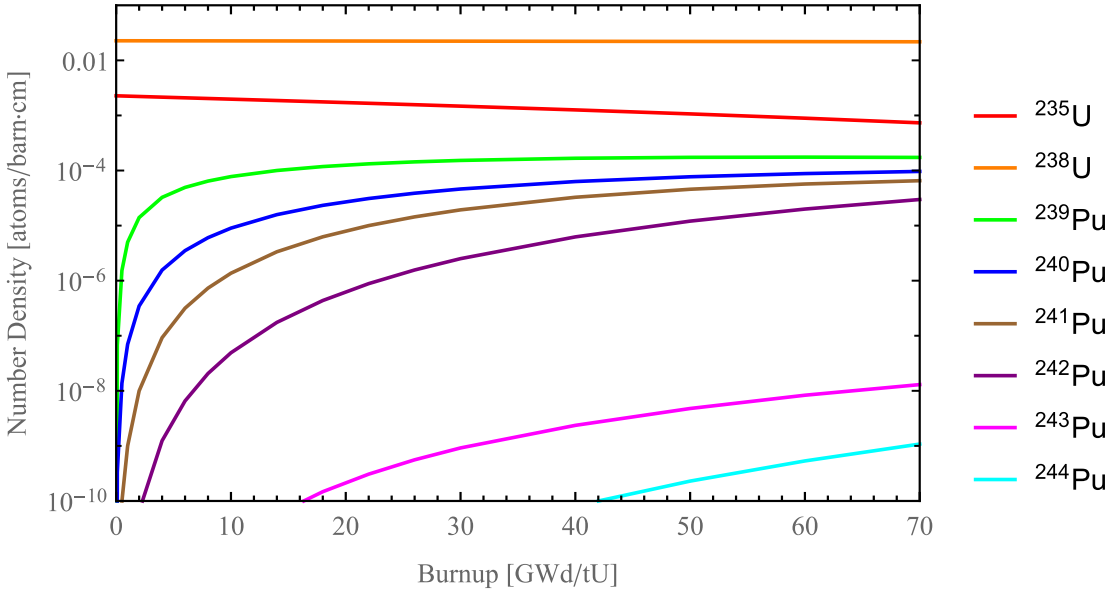

Figure 13: Concentration of U and Pu isotopes, Serpent 2.1.32 with ENDF/B-VII.1

4 CONCLUSIONS

The goal of the paper was to check the prediction capabilities when using two most recent Serpent2/SCALE versions in modelling challenging advanced reactor fuel assembly configuration. The differences between different versions of the same program (Serpent) and between different programs (Sperpent, SCALE) were small and the same is true for required CPU time. When different versions of ENDF/B library were used, the differences in results and in calculation time were larger. In Serpent case we decided to use faster (and less memory demanding) ENDF/B-VI.8 library for scoping calculation and ENDF/B-VII.1 library for production depletion calculation. In SCALE 6.2.4/6.3.1 case the natural library choice was ENDF/B-VII.1/VIII.0 combination. Both codes (Serpent 2 and SCALE) were able to provide reliable results for FHR fuel assembly, but Serpent2, being faster due to parallelization, was used for depletion calculation.

ACKNOWLEDGMENTS

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