Applicability of Legacy and New Calculation Tools for 2D Fuel Assembly Depletion as defined by VERA Benchmark

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ABSTRACT

Consortium for Advanced Simulation of LWRs (CASL) published in 2015 "Specification for the VERA Depletion Benchmark Suite". The benchmark contains specification for 16 fuel assembly configurations and 10 pin cells configurations covering almost all features of modern LWR fuel. It is of interest to investigate how the so called legacy 2D spectral codes perform against more modern deterministic and probabilistic codes. In calculations, we used 3 deterministic codes: FA2D collision probability code developed at the University of Zagreb Faculty of Electrical Engineering and Computing, TRITON and Polaris from SCALE 6.2.4 package, and one probabilistic code Serpent 2.1.32. The comparison between the codes is performed in terms of multiplication factors and pin power factors. We were interested in differences in calculated effective multiplication factors and pin power factors as well as in overall performance of the codes from point of view of required CPU time and memory allocation.

Keywords: *2D spectral codes, VERA benchmark, group constants, pin powers*

1 INTRODUCTION

The Consortium for Advanced Simulation of LWRs (CASL) published "Specification for the VERA Depletion Benchmark Suite" in 2015. It contains a set of benchmark problems involving 10 single pin and 16 fuel assembly problems. They differ in fuel temperature, U-235 enrichment, control rods, and burnable poisons. The problems describing fuel pins are denoted 1A – 1J and fuel assemblies 2A – 2P. The purpose of that document was to prepare basis for code-to-code comparison using selected benchmark problems [1].

The aim of this paper is to investigate how the so called legacy 2D spectral codes perform against more modern deterministic and probabilistic codes. Three deterministic codes, FA2D collision probability code developed at the University of Zagreb Faculty of Electrical Engineering and Computing, TRITON and Polaris from SCALE 6.2.4 package, and one probabilistic code Serpent 2.1.32 were used in the calculations. Three VERA benchmark cases were considered, namely 2C, 2M and 2G. These were of interest due to similarities with the NPP Krško fuel assembly configuration (fuel temperature, boron concentration and the number of integral fuel burnable absorber – IFBA). It was of interest to study the differences among the codes in calculated multiplication factors and pin power factors. We were interested in obtaining information on overall performance of the codes too (including if they are user friendly, what are required CPU time and memory allocation).

2 VERA BENCHMARK PROBLEMS

The "Specification for the VERA Depletion Benchmark Suite" is a publicly available document and the data are based on actual fuel from the initial core loading of Watts Bar Nuclear 1 Plant, a Westinghouse PWR reactor with 17×17 fuel assembly type. The fuel pin is composed of 120 inches axially uniform UO_2, cladding made of Zircaloy-4, upper gas plenum, plenum spring, and upper and lower plugs. As shown in Figure 1, each 17×17 fuel assembly contains 264 fuel pins, 24 guide tubes for rod cluster control assembly (RCCA) or discrete burnable poison rods, and one instrument tube in the centre for an incore neutron flux detector. The 17×17 lattice specification is provided in Table 1. The rest of the data can be found in [1].

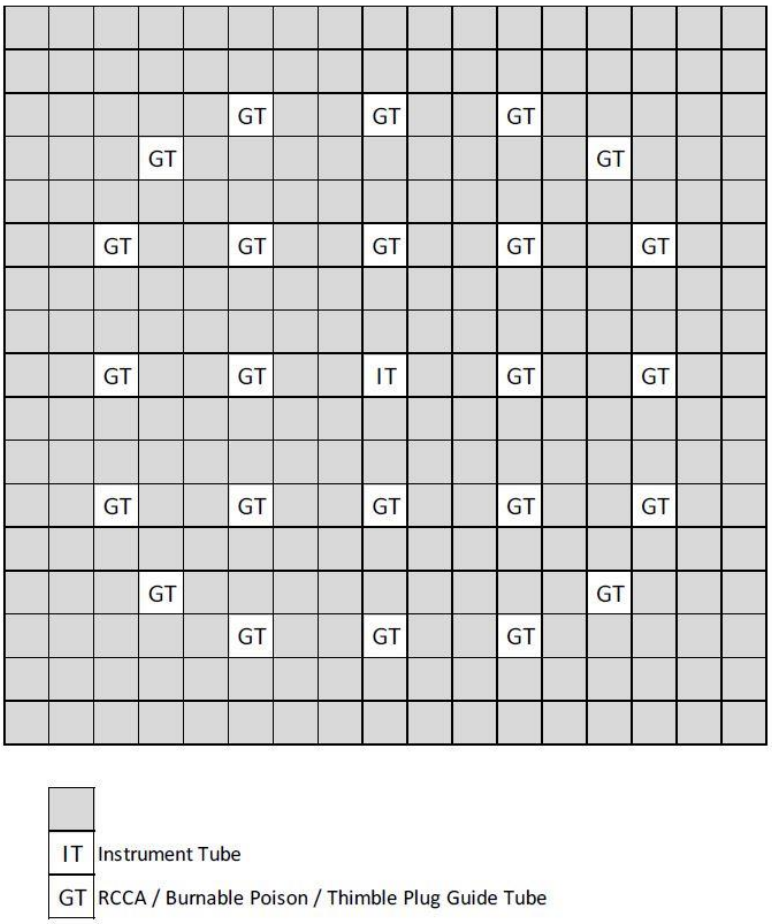


Figure 1: 17×17 Lattice fuel rod and guide tube layout

Table 1: 17×17 lattice specification

Input	**Value**
Inner Guide Tube Radius	0.561 cm
Outer Guide Tube Radius	0.602 cm
Inner Instrument Tube Radius	0.559 cm
Outer Instrument Tube Radius	0.605 cm
Tube Materials	Zircaloy-4
Rod Pitch	1.26 cm
Assembly Pitch	21.50 cm
Inter-Assembly Half Width Gap	0.04 cm

3 COMPUTER CODES

3.1 FA2D

The FA2D is a 2D transport collision probability code developed at the University of Zagreb Faculty of Electrical Engineering and Computing. It is used for calculation of cross section data at the fuel assembly level. The main objective of its development was the capability to generate cross section data to be used for fuel management and safety analyses of PWR reactors. The code uses 97-energy group structure based on ENDF/B-VI.5 evaluations.

3.2 TRITON

TRITON is a multipurpose SCALE control module for transport, depletion, sensitivity and uncertainty analysis for reactor physics applications. TRITON provides the capability to perform deterministic transport analyses for 2D geometries using NEWT. Neutron transport equation is solved using the discrete ordinate methods. In tandem with the ORIGEN depletion module, TRITON can predict isotopic concentration, source terms, and decay heats [3].

3.3 Polaris

As a part of SCALE 6.2.4 control module, Polaris provides 2D lattice physics analysis capability for light water reactor (LWR) fuel designs. Polaris uses multigroup self-shielding solver called the Embedded Self Shielding Method (ESSM) and transport solver based on the Method of Characteristics (MoC). Polaris is integrated with ORIGEN for depletion calculations. Both TRITON and Polaris can use either a fine 252-group or a broad 56-group neutron energy structure [3].

3.4 Serpent 2.1.32

Serpent 2.1.32 is a continuous energy neutron and photon Monte Carlo transport code. The code is used for many applications in reactor physics, but spatial homogenization based on the Monte Carlo method was the original intention of its development [4].

4 CALCULATION MODEL AND ASSPUMPTIONS

In this paper, three VERA benchmark problems were considered, namely 2C, 2G, and 2M. These were of interest because of the similarities in the configuration with the fuel assembly type used in the NPP Krško. The characteristics of the considered cases are summarized in Table 2. Cases 2C, 2G, and 2M have the same characteristics (fuel temperature 900 K, guide tube, cladding and moderator temperature 600 K, 1300 ppm boron concentration, moderator density of 0.700 g/cm^3 and 3.1 % uranium enrichment) except that 2G has inserted control rods made of Ag-In-Cd, and 2M has burnable material IFBA in 10 microns thin layer on selected number of fuel pins.

Table 2: Characteristics of the VERA benchmark problems 2A, 2C, 2G, and 2M

Case	**2C**	**2G**	**2M**
T_F (K)	900	900	900
T_G=T_C=T_M (K)	600	600	600
Boron concentration (ppm)	1300	1300	1300
Moderator density (g/cm^3)	0.700	0.700	0.700
Enrichment (%)	3.1	3.1	3.1
Control rod material	-	AgInCd	-
Burnable material	-	-	IFBA

This research was performed with the aim to compare our own developed FA2D code with the codes available for similar purposes. However, the results obtained with Serpent 2.1.32 are considered the representative ones and the comparison of other codes is made relative to the Serpent results. Serpent code is capable for detailed analysis of complex assembly geometries using continuous energy cross section data. It is first Monte Carlo code developed for calculation of fuel assembly depletion and it is able to generate collapsed and homogenized neutron cross section group data as an input to reactor physics nodal codes. That is original application for any 2D spectral physics code.

All two-dimensional depletion calculations were performed with reflective boundary conditions and the critical spectra in all calculations were determined by B1 method.

In FA2D code, the 17×17 fuel assemblies were modelled in full symmetry and the calculations were made with the 97-energy group structure based on ENDF/B-VI.5 evaluations.

For the TRITON calculations, the settings $S_N = 8$, and $P_N = 1$ (except for moderator where PN = 3) were selected. The fuel assemblies were modelled in a quadratic symmetry. Although it is possible to perform calculations with 252 energy groups, a broad 56-group structure based on ENDF/B-VII.1 Evaluated Nuclear Data Library was chosen to save computer time. In TRITON module, the control rod was modelled using a "multi-region" unit cell specification that contains the control rod in the centre, surrounded by a homogenized mixture of fuel, clad, gap and moderator (Figure 2). The resulting self-shielded mixtures were used in the construction of the 2D model. The calculations were also performed using ENDF/B-VII.1 library.

In Polaris, the fuel assemblies were modelled in an octant symmetry. For the case 2M, due to the thin IFBA layer, the spacing between MoC rays was set to 0.01 cm as a compromise between recommended value and default values of 0.003 cm and 0.04 cm, respectively. The Polaris model of the case 2G with a control rod inserted is shown in Figure 3 for lower right quadrant.

In Serpent 2.1.32, the fuel assemblies were modelled in an octant symmetry. Full symmetry Serpent model of fuel assembly is shown in Figure 4. The number of neutrons per generation was 10000, the number of active generations 560, and the number of inactive generations 60. ENDF/B-VII.0 library was used in the calculations.

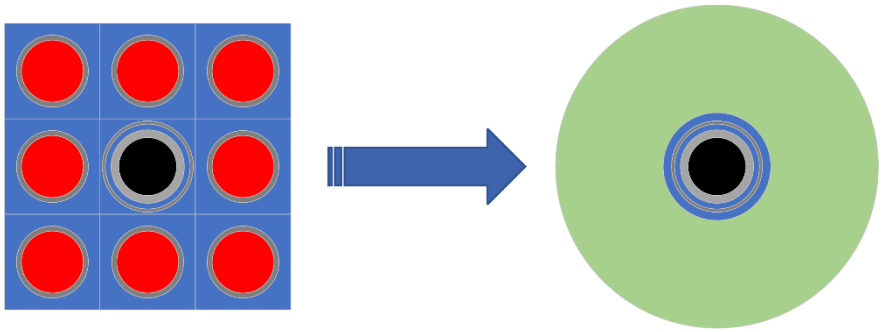


Figure 2: Control rod model in TRITON

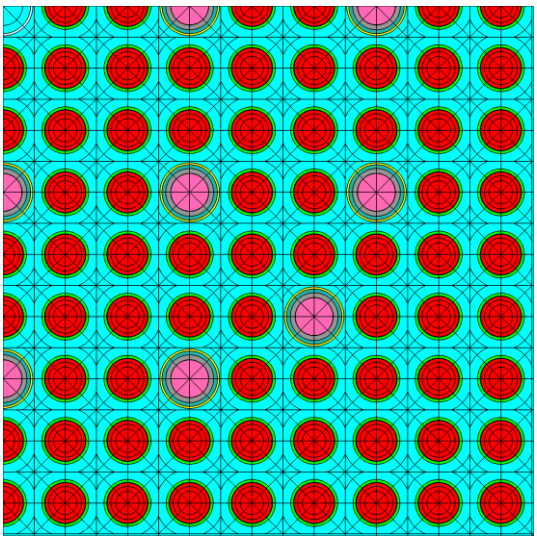


Figure 3: Polaris interpretation of fuel assembly lower right quadrant for case 2G (control rods inserted)

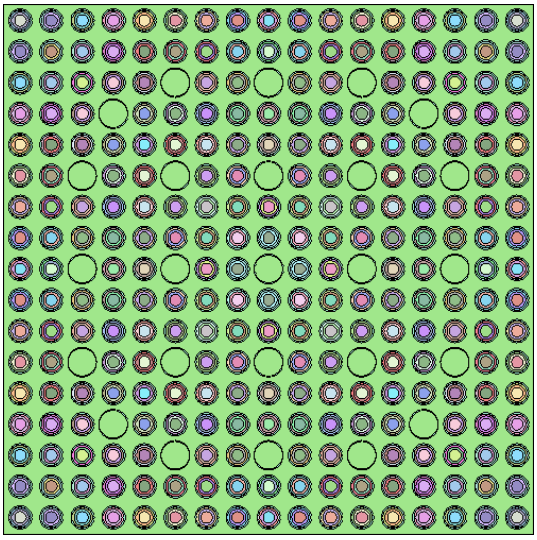
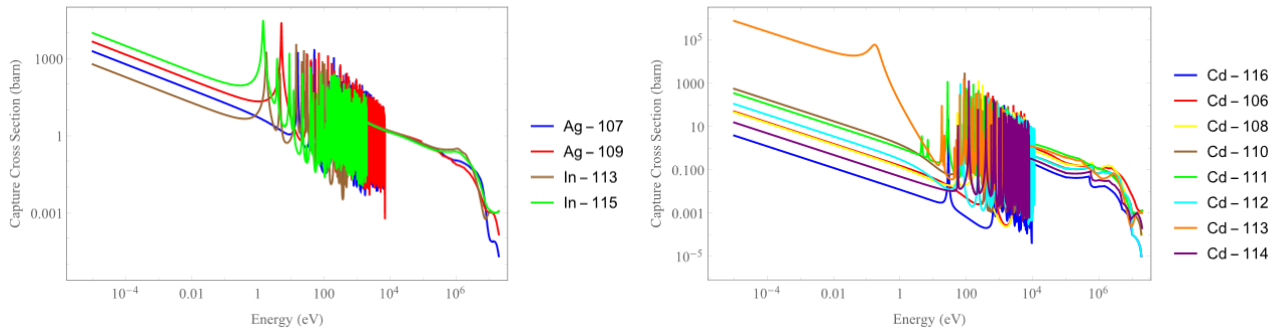


Figure 4: Fuel assembly modelled in Serpent

Figure 5 shows neutron capture cross sections for In and Ag (a), and Cd (b). Sharp resonance peaks are observed for the epithermal energies. These may cause some difficulties in the calculations for the case 2G.



a) b)

Figure 5: Capture cross section (barn) for a) In and Ag, and b) Cd isotopes

5 RESULTS

In this section, the comparisons of multiplication factor (k_{inf}) and pin power factors obtained with FA2D (w17x17), TRITON, Polaris, and Serpent 2.1.32 (s2) are provided. Multiplication factor k_{inf} as a function of burnup for cases 2C, 2G, and 2M is shown in Figure 6, Figure 7, and Figure 8, respectively. Note that for case 2G, due to problem with the resonance cross sections for In-Ag-Cd, the results were obtained only with TRITON, Polaris, and Serpent 2.1.32.

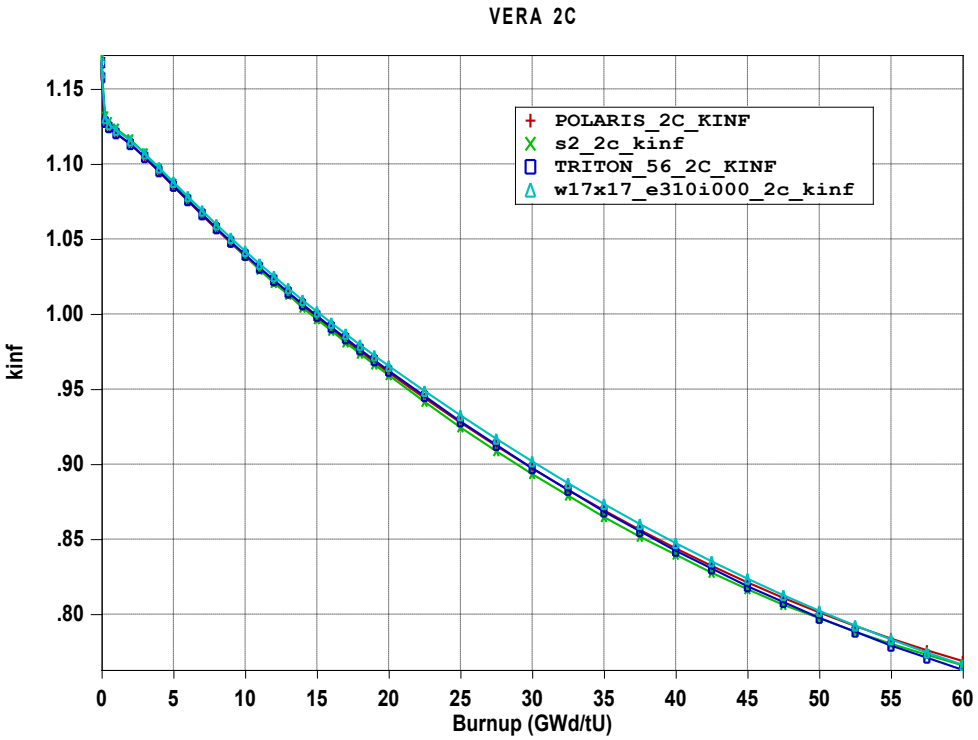


Figure 6: Multiplication factor k_{inf} as a function of burnup for case 2C

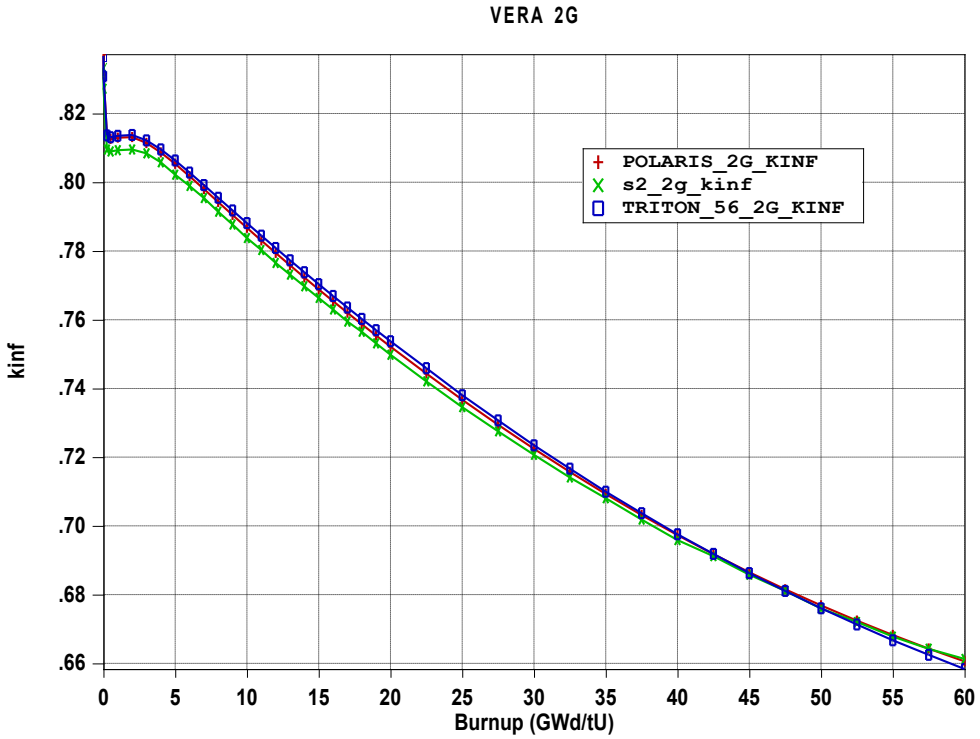


Figure 7: Multiplication factor k_{inf} as a function of burnup for case 2G (control rod inserted)

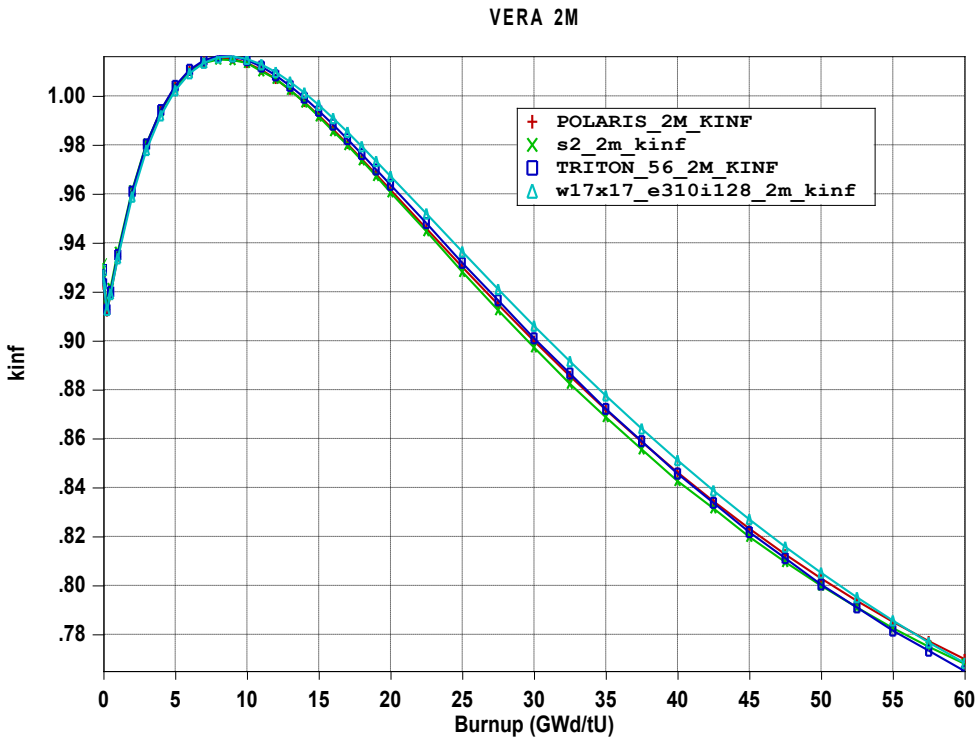


Figure 8: Multiplication factor k_{inf} as a function of burnup for case 2M (IFBA case)

Taking Serpent results as the reference, in Figure 9, Figure 10, and Figure 11 we provided relative errors of the k_{inf} results obtained by Polaris, TRITON, and FA2D for cases 2C, 2G, and 2M, respectively. From these figures it can be seen that the multiplication factors are typically within 1 % compared to Serpent results. Some problems were encountered (error was above 2 %) in case 2G in FA2D calculation due to difference in control rod material resonance cross sections in used library.

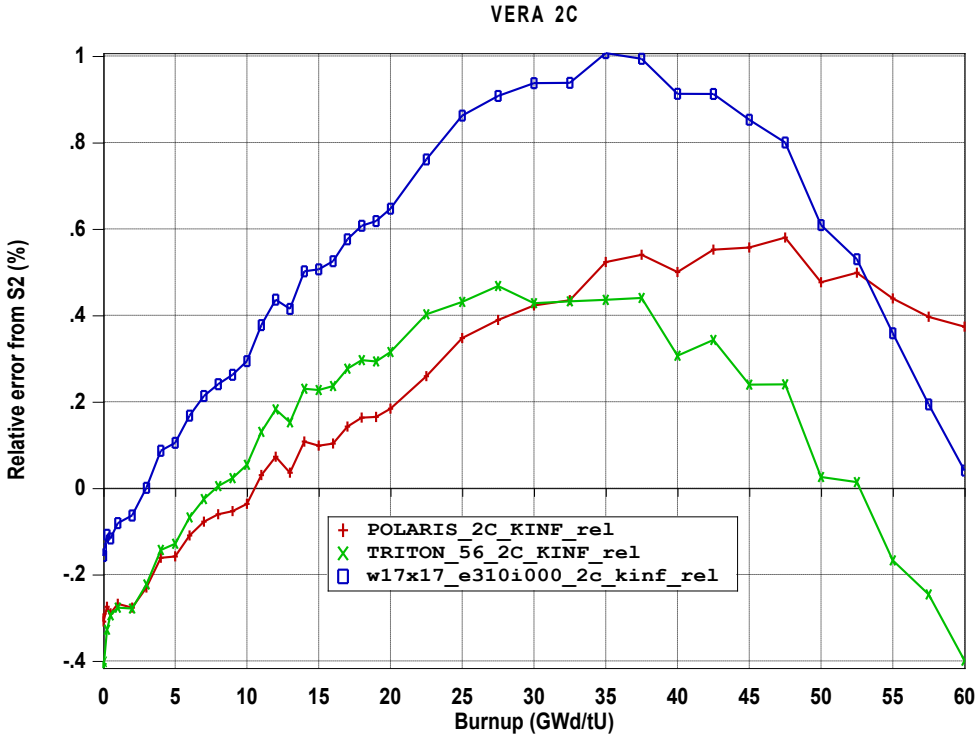


Figure 9: Relative errors of multiplication factor k_{inf} as a function of burnup for case 2C

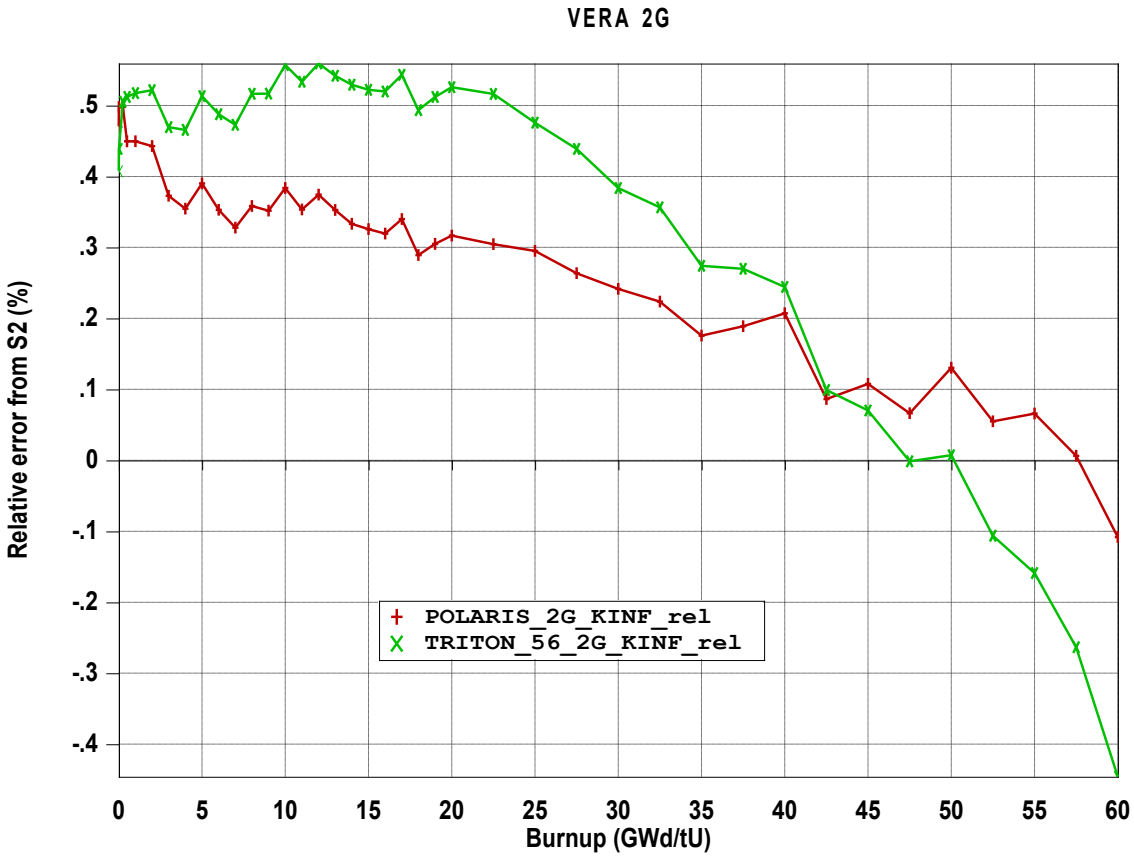


Figure 10: Relative errors of multiplication factor k_{inf} as a function of burnup for case 2G

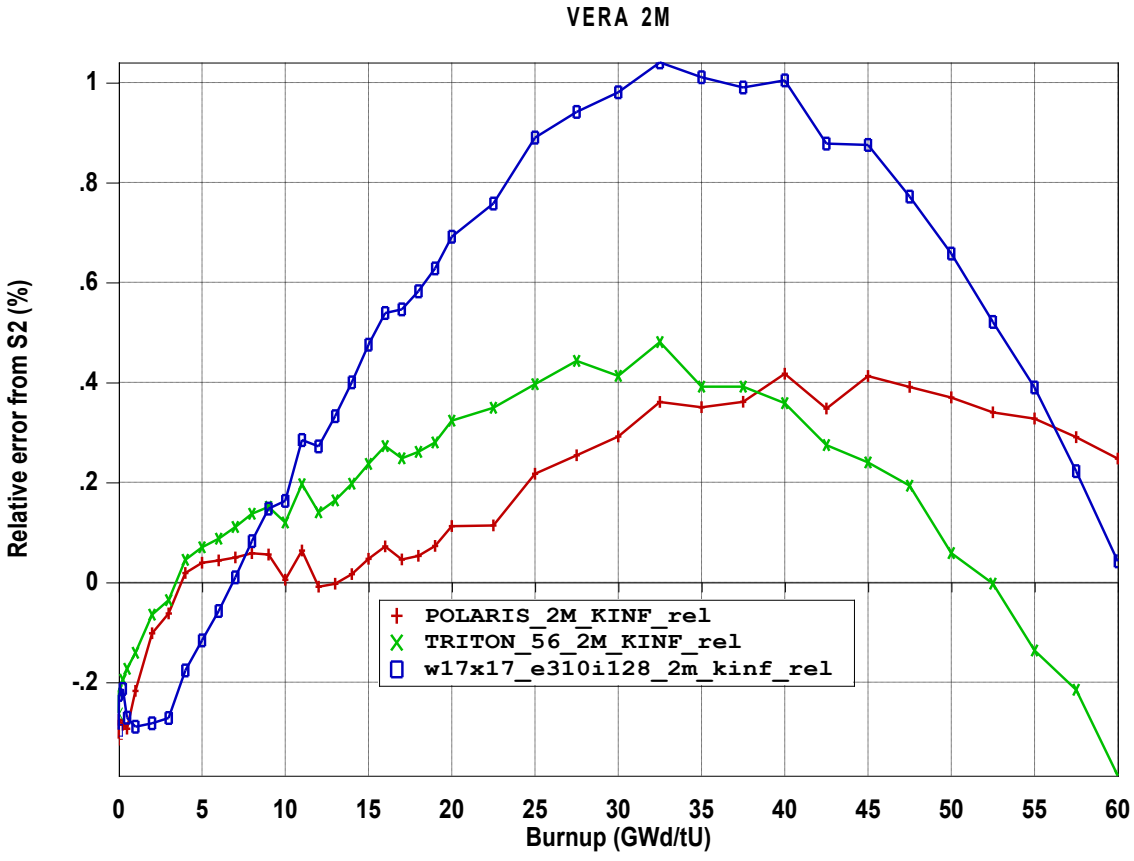
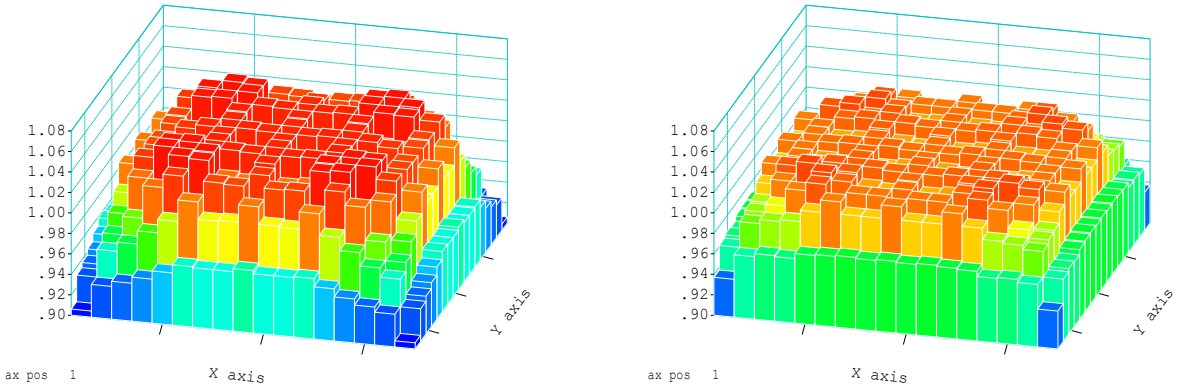


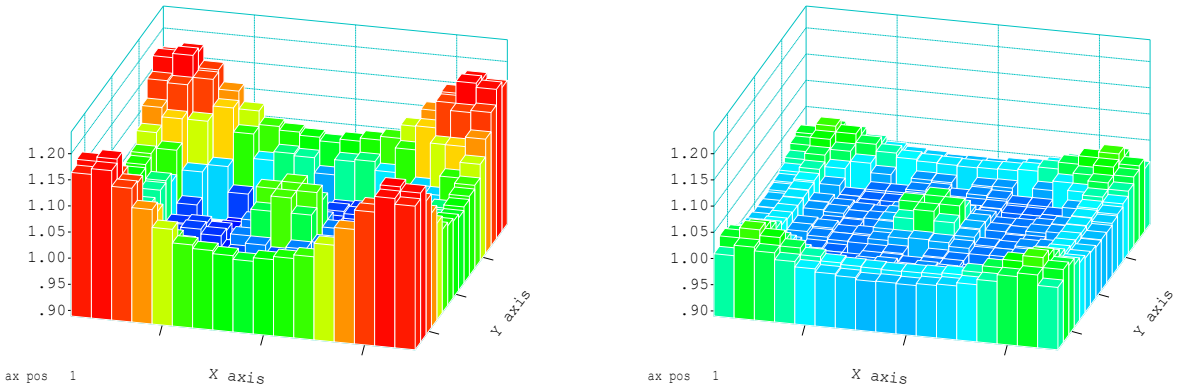
Figure 11: Relative errors of multiplication factor k_{inf} as a function of burnup for case 2M

Figure 12, Figure 13, and Figure 14 show pin power factors calculated using FA2D code at a burnup of 0 and 60 GWd/tU for the cases 2C (regular fuel assembly), 2G (assembly with inserted control rods) and 2M (fuel assembly with IFBAs).



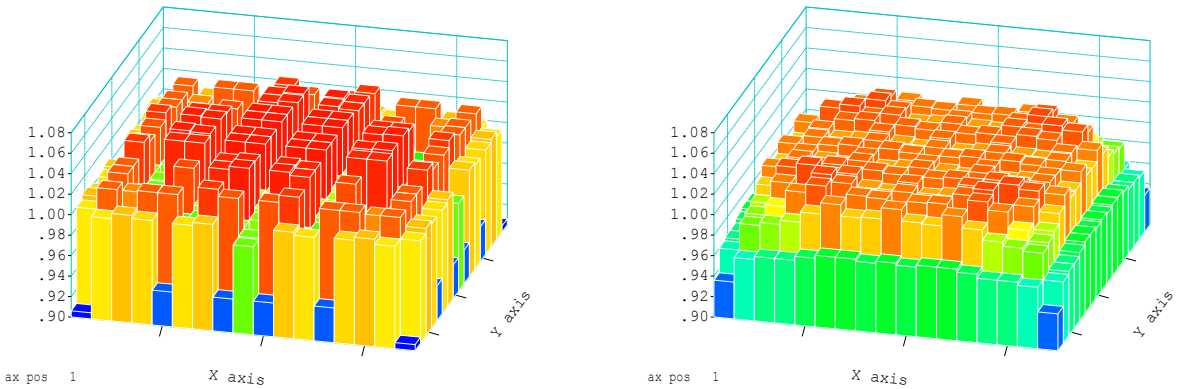
a) b)

Figure 12: Pin powers for case 2C at a) 0 GWd/tU, and b) 60 GWd/tU



a) b)

Figure 13: Pin powers for case 2G at a) 0 GWd/tU, and b) 60 GWd/tU



a) b)

Figure 14: Pin powers for case 2M at a) 0 GWd/tU, and b) 60 GWd/tU

The comparison between the codes is provided in terms of Root Mean Square Error (RMSE), expressed as:

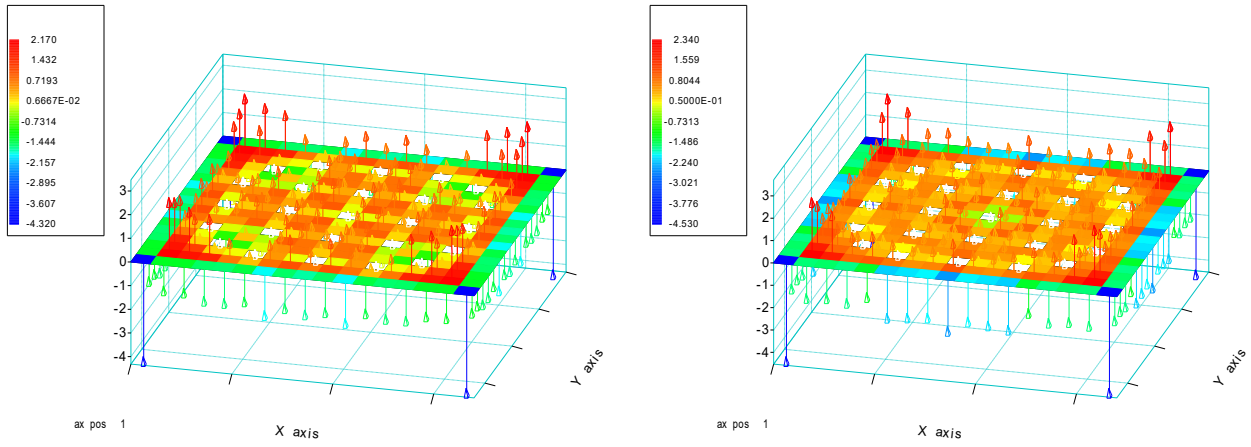
$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{N}(y-z)^2}{N}} \tag{1}$$

where y is the pin power calculated by FA2D, Polaris or TRITON, z is the pin power calculated by Serpent, and N is the sample size. The results are shown in Table 3. RMSE for FA2D is typically around 1% except for 2G where it is around 4 %. For Polaris and TRITON, RMSE is around 2 ‰ to 4 ‰. In case of 2C, RMSE increases with burnup, slightly for FA2D and POLARIS and almost two times for TRITON. For case 2M, RMSE decreases with burnup except for TRITON. For case 2G RMSE also decreases with burnup, except for Polaris.

Table 3: RMS deviation of pin powers from Serpent 2.1.32 results

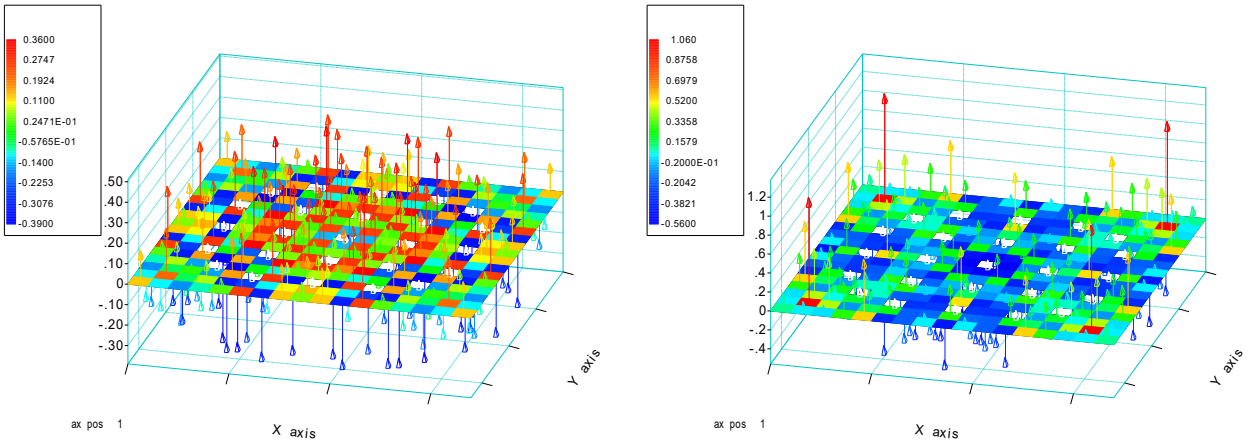
CASE	**FA2D**		**POLARIS**		**TRITON**	
	0 GWd/tU	**50 GWd/tU**	**0 GWd/tU**	**50 GWd/tU**	**0 GWd/tU**	**50 GWd/tU**
VERA 2C	1.10754E-02	1.22258E-02	2.00029E-3	2.83442E-3	2.13451E-3	4.08840E-3
VERA 2M	1.45852E-02	1.16219E-02	4.20448E-3	3.85997E-3	2.61383E-3	3.98179E-3
VERA 2G	3.15402E-02	1.90376E-02	2.78999E-3	4.84882E-3	3.63126E-3	2.99402E-3

Finally, a graphical representation of pin power relative errors for case 2C is shown in Figure 15 for FA2D, in Figure 16 for Polaris, and in Figure 17 for TRITON. For any pin location relative error is within 5 % for FA2D (most likely due to older ENDF/B library used in calculation) and within 1 % for other deterministic codes.



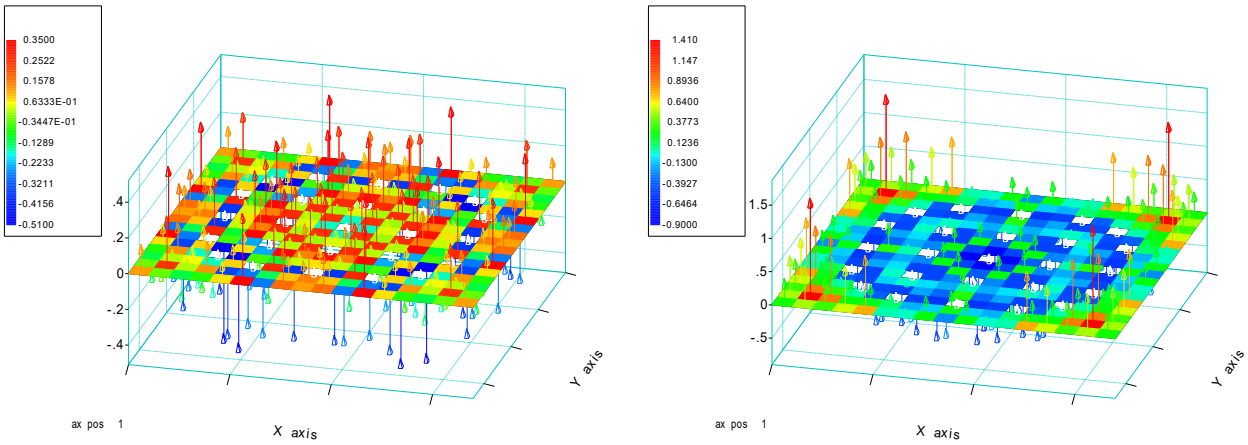
a) b)

Figure 15: Pin power relative error of FA2D compared to Serpent results for VERA 2C at 0 GWd/tU (a) and 50 GWd/tU (b)



a) b)

Figure 16: Relative error of POLARIS compared to SERPENT results for VERA 2C at 0 GWd/tU (a) and 50 GWd/tU (b)



a) b)

Figure 17: Relative error of TRITON compared to SERPENT results for VERA 2C at 0 GWd/tU (a) and 50 GWd/tU (b)

6 CONCLUSION

VERA Depletion Benchmark Suite was used to assess applicability of different transport codes in depletion calculation of PWR fuel assemblies. The regular fuel assembly without and with inserted control rods and IFBA fuel assembly were analysed. The first check was intended to be limited to multiplication factor and pin power comparisons. In next step calculated collapsed and homogenized cross sections will be compared. The results obtained with Monte Carlo code Serpent were used as a reference. Generally speaking, all three deterministic transport codes provided similar results, with some deviation experienced in case of FA2D, mainly due to older used ENDF/B neutron cross section library. FA2D code was easier to use, with lower calculation time and less allocated memory. Deterministic transport codes were serial applications and Serpent was used as parallel OMP application. In order to reduce statistical uncertainties inherent to Monte Carlo codes (especially in pin power distributions) Serpent needed the same wall clock time with 6-cores CPU as FA2D as serial application on the same computer. For typical PWR fuel assemblies both legacy codes and state of the art codes give similar results when the same cross section libraries were used.

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