Calculation of VVER MOX pin-cell benchmark with OpenMC code

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Abstract. This article presents the results of the 'Weapons-Grade MOX VVER-1000 Neutronics Benchmarks' calculated with the OpenMC code. The purpose of this work was to master the OpenMC code and adapt it for VVER calculations in order to use it in the research work conducted at the department. Previously the benchmark was calculated with the SAS2H, HELIOS and MCU codes. Cases calculated with the OpenMC code consist of eight fuel variants with a specific sets of reactor conditions which represent normal and off-normal situations. The obtained infinite neutron multiplication factors are consistent with the presented in the benchmark at the level of 0.02% to 4.71%. The best consistency is observed with the HELIOS code, deviations are less than 1.6% . Despite the rather large deviations for some variants, it can be argued that the OpenMC code allows getting close to other codes results and can be used for similar calculations of VVER-1000.

1. Introduction

One of the most accurate methods for modeling nuclear reactors is the Monte Carlo method. Today, there are dozens of programs based on this method in the world, but most of them are distributed for money. The OpenMC code [1] is free of charge and open to everyone, so it can be easily used for scientific research. It is a popular code, and there are many publications mentioning it, for example [2, 3]. However, there are no publications related to the calculation of a VVER-type reactor.

The purpose of this work was to master the OpenMC code and document its installation and usage, calculate infinite neutron multiplication factors for different benchmark cases, and compare the results with the presented in the benchmark. We showed how the results obtained in modeling of a VVER-type reactor are consistent with the results obtained with other codes. The OpenMC is planned to be used at the Department of Nuclear Physics for VVER-1200 calculations of the Belarusian NPP.

Benchmark calculation [4, 5] is necessary to confirm the codes (SAS2H, HELIOS, MCU) and nuclear data libraries, which could be used to model VVER-type reactors with different types of fuel. The results of the benchmark calculation with the MCU code are not presented for all the states and variants, so it is not possible to make a full comparison with the MCU code. The OpenMC has not been used for calculating VVER-type reactor before, that is why the analysis of the results gives good prospects for using the code in further calculations.

2. Geometry representation

In real fuel assemblies of the VVER-1000 reactor, the fuel pins have a central hole, and they are located in a hexagonal (triangular) lattice. The benchmark proposes to calculate an infinite lattice of fuel rods

with a pitch of 1.275 cm. The diameter of the cylindrical fuel area is 0.772 cm. For simplicity of modeling, the central hole in the fuel is not taken into account. The outer diameter of the shell is 0.9164 cm, with a cladding thickness of 0.0772 cm (figure 1).

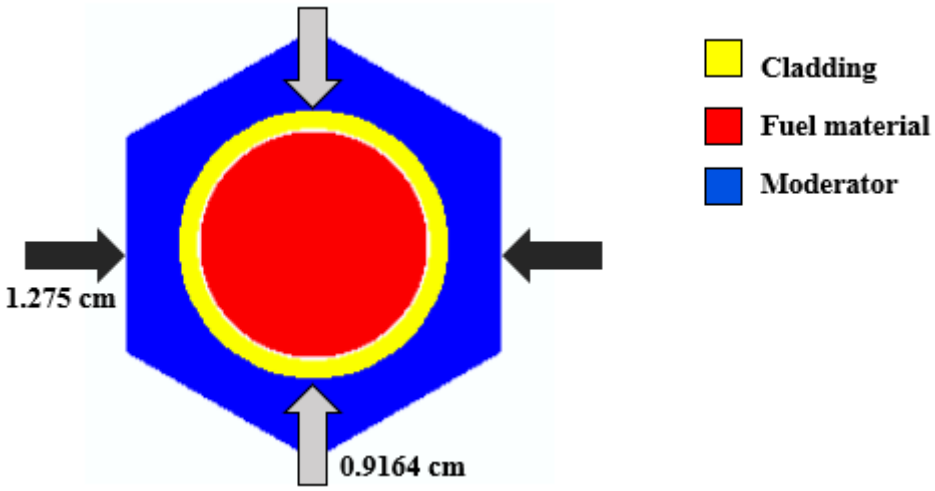

Figure 1. VVER-1000 neutronics benchmark pin-cell model.

3. Benchmark specifications

The benchmark presents eight fuel variants V1-V4 and V7-V10 (table 1), with specific sets of reactor conditions (states S1-S6) which represent normal and off-normal situations (table 2). The simulated cases are pin-cell calculations with different fuel materials ranging from LEU UO_2 to MOX fuel with reactor-grade plutonium and with weapons-grade plutonium. The states include specified values for fuel temperatures, moderator temperature and density, fission products poison concentrations, boron concentrations.

Table 1 (a). Specifications for fuel and other materials.

Benchmark variant	Material	Comment	Nuclide	Content (a/b-cm)	Nuclide	Content (a/b-cm)	"Length" of fuel pin to contain 1 kg of heavy elements (cm)
V1	FU1	Fresh uranium fuel	^{235}U	8.7370×10^{-4}	^{16}O	3.9235×10^{-2}	275.643
			^{238}U	1.8744×10^{-2}			
V2	FU2	Fresh MOX fuel (WG Pu)	^{235}U	3.8393×10^{-5}	^{239}Pu	6.5875×10^{-4}	274.826
			^{238}U	1.8917×10^{-2}	^{240}Pu	4.2323×10^{-5}	
			^{16}O	4.1707×10^{-2}	^{41}Pu	7.0246×10^{-6}	
V3	FU3	Spent uranium fuel without FPs	^{235}U	3.7843×10^{-4}	^{241}Pu	2.1701×10^{-5}	284.204
			^{236}U	8.6365×10^{-5}	^{242}Pu	4.7576×10^{-6}	
			^{238}U	1.8327×10^{-2}	^{241}Am	4.9491×10^{-7}	
			^{16}O	3.9235×10^{-2}	^{242}Am	7.9194×10^{-9}	
			^{237}Np	2.4823×10^{-5}	^{243}Am	6.6925×10^{-7}	
			^{239}Np	1.8332×10^{-6}	^{242}Cm	1.2582×10^{-7}	
			^{238}Pu	6.7254×10^{-6}	^{243}Cm	2.0629×10^{-9}	
			^{239}Pu	1.3111×10^{-4}	^{244}Cm	1.2387×10^{-7}	
			^{240}Pu	3.6233×10^{-5}			

Table 1 (b).

V4	FU4	Spent uranium fuel with FPs	^{235}U	3.7843×10^{-4}	^{244}Cm	1.2387×10^{-7}	284.204
			^{236}U	8.6365×10^{-5}	^{103}Rh	1.8890×10^{-5}	
			^{238}U	1.8327×10^{-2}	^{131}Xe	1.4255×10^{-5}	
			^{16}O	3.9235×10^{-2}	^{143}Nd	2.6692×10^{-5}	
			^{237}Np	2.4823×10^{-5}	^{147}Pm	6.1574×10^{-6}	
			^{239}Np	1.8332×10^{-6}	^{133}Cs	3.5974×10^{-5}	
			^{238}Pu	6.7254×10^{-6}	^{99}Tc	3.3320×10^{-5}	
			^{239}Pu	1.3111×10^{-4}	^{152}Sm	2.6842×10^{-6}	
			^{240}Pu	3.6233×10^{-5}	^{151}Sm	3.0757×10^{-7}	
			^{241}Pu	2.1701×10^{-5}	^{145}Nd	1.9975×10^{-5}	
			^{242}Pu	4.7576×10^{-6}	^{153}Eu	2.4801×10^{-6}	
			^{241}Am	4.9491×10^{-7}	^{109}Ag	2.2037×10^{-6}	
			^{242}Am	7.9194×10^{-9}	^{155}Eu	9.6857×10^{-8}	
			^{243}Am	6.6925×10^{-7}	^{95}Mo	3.3720×10^{-5}	
			^{242}Cm	1.2582×10^{-7}	^{154}Eu	5.1189×10^{-7}	
			^{243}Cm	2.0629×10^{-9}	^{101}Ru	3.1134×10^{-5}	
V7	FU7	MOX fuel with ^{239}Pu only	^{235}U	3.8393×10^{-5}	^{239}Pu	6.5875×10^{-4}	275.505
			^{238}U	1.8917×10^{-2}	^{16}O	4.1707×10^{-4}	
V8	FU8	MOX fuel with ^{240}Pu only	^{235}U	6.9714×10^{-4}	^{240}Pu	4.2323×10^{-5}	275.063
			^{238}U	1.8917×10^{-2}	^{16}O	4.1707×10^{-2}	
V9	FU9	MOX fuel with ^{241}Pu only	^{235}U	3.8393×10^{-5}	^{241}Pu	6.6577×10^{-4}	275.330
			^{238}U	1.8917×10^{-2}	^{16}O	4.1707×10^{-2}	
V10	FU10	Fresh MOX fuel (RG Pu)	^{235}U	5.0000×10^{-5}	^{240}Pu	4.9000×10^{-4}	223.667
			^{238}U	2.2100×10^{-2}	^{241}Pu	1.9000×10^{-4}	
			^{16}O	4.6300×10^{-2}	^{242}Pu	1.0500×10^{-4}	
			^{238}Pu	3.0000×10^{-5}	^{241}Am	2.5000×10^{-5}	
			^{239}Pu	1.1600×10^{-3}			
	CL1	Cladding	Zr	4.2300×10^{-2}	-	-	-
	MOD1	Hot moderator with boron acid	H	4.7830×10^{-2}	^{10}B	4.7344×10^{-6}	-
			^{16}O	2.3910×10^{-2}	^{11}B	1.9177×10^{-5}	
	MOD2	Hot moderator without boron acid	H	4.7830×10^{-2}	^{16}O	2.3910×10^{-2}	-
	MOD3	Cold moderator with boron acid	H	6.6940×10^{-2}	^{10}B	6.6262×10^{-6}	-
			^{16}O	3.3470×10^{-2}	^{11}B	2.6839×10^{-5}	

Table 2. Reactor operating conditions.

State	Temperature of the fuel material (K)	Temperature of the non-fuel components (K)	Moderator	^{135}Xe and ^{149}Sm concentration
S1	1027	579	(Hot) light water, dissolved B, 579K	^{135}Xe: 9.4581×10^{-9} ^{149}Sm: 7.3667×10^{-8}
S3	1027	579	(Hot) light water, no dissolved B, 579K	^{135}Xe: 9.4581×10^{-9} ^{149}Sm: 7.3667×10^{-8}
S4	1027	579	(Hot) light water, dissolved B, 579K	-
S5	579	579	(Hot) light water, dissolved B, 579K	-
S6	300	300	(Cold) light water, dissolved B, 579K	-

4. Analysis of the obtained results

We used the method of interpolation [6] of the temperature dependence of the cross-sections to obtain the results. The interaction cross sections are not actually interpolated between each other in the usual sense. Each time a neutron collides with a nucleus, the code randomly selects data at a temperature above or below the actual temperature of the material in proportion to how close the material temperature is to the temperature for which the interaction cross section is known.

You can notice a good consistency of the results (see figures below). The calculation time for a single state was 2 hours and 30 minutes on a laptop using a single core 1.10 GHz processor and 4 GB of RAM. The standard deviation in the value of infinite neutron multiplication factor (k-inf) was about 0.00023.

In the V1 variant (figure 2), the S3 state calculated with the MCU is knocked out of the general trend, this state differs from other states by the absence of boron in the moderator. It is similar for the V2 (figure 3), but the difference is smaller. You can see that the smallest values are obtained with the SAS2H for the variants V1 and V2 in all states.

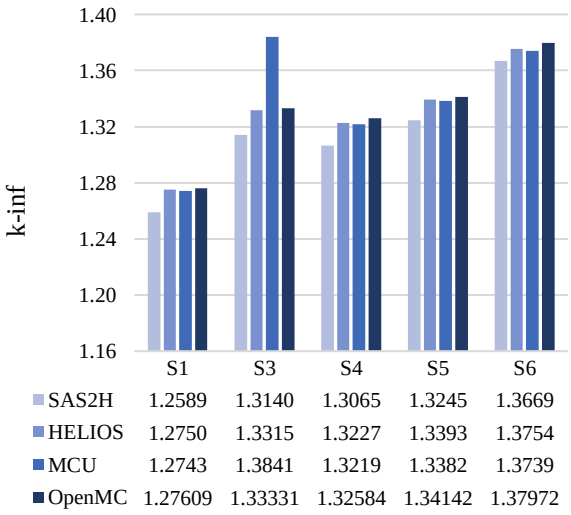

Figure 2. Variant 1.

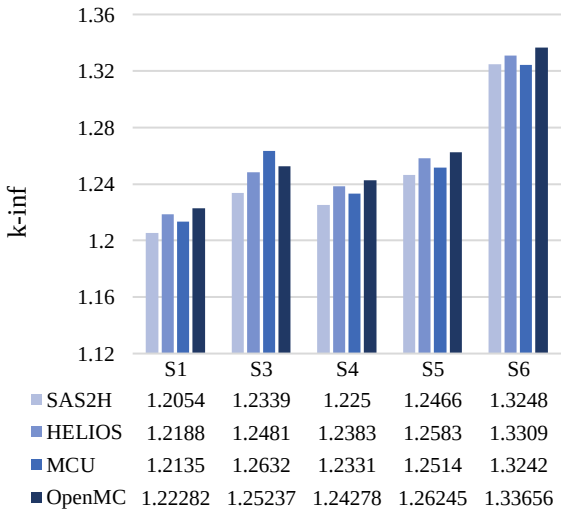

Figure 3. Variant 2.

In the V3 variant (figure 4), the result for the MCU code is presented only for the S6 state, it is noticeably larger compared to the other codes. In the V4 variant (figure 5), there is a difference in the S3 state calculated with the MCU, it differs from other states by the absence of boron in the moderator.

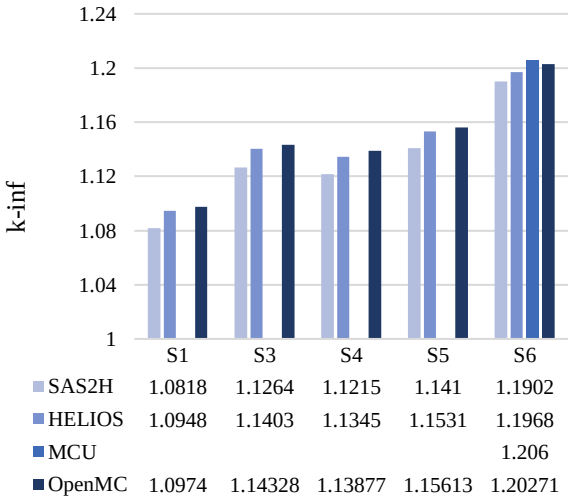

Figure 4. Variant 3.

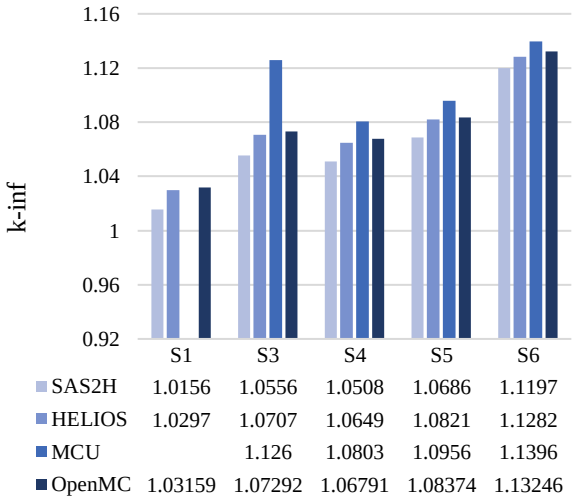

Figure 5. Variant 4.

In the V7 variant (figure 6), the k-inf value calculated using OpenMC is the largest. In this variant, there is only one plutonium isotope in fuel – ^{239}Pu. In the V8 variant (figure 7), the SAS2H values are less than the values from other codes.

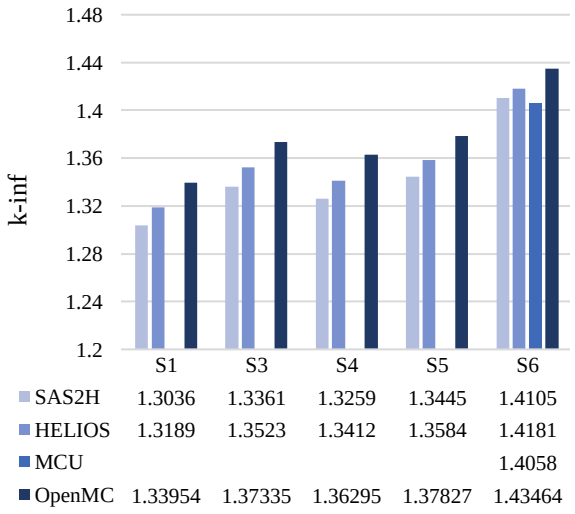

Figure 6. Variant 7.

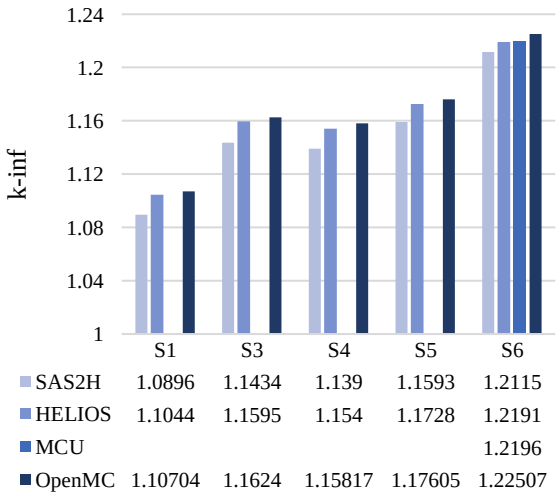

Figure 7. Variant 8.

In the V9 variant (figure 8), the HELIOS value is noticeably higher. In the V10 variant (figure 9), the OpenMC results are in very good agreement with the HELIOS. In all variants, the values calculated by the SAS2H are the smallest.

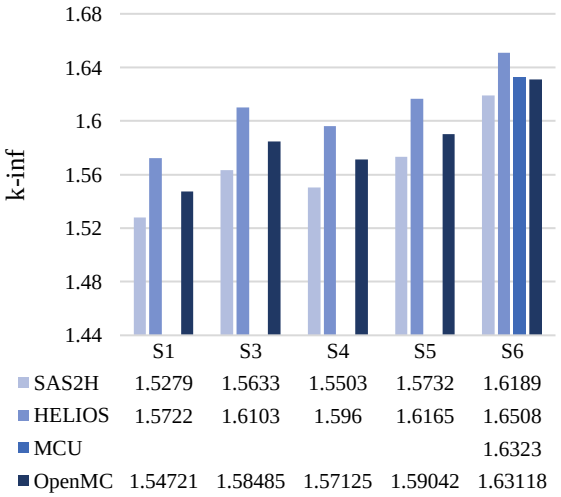

Figure 8. Variant 9.

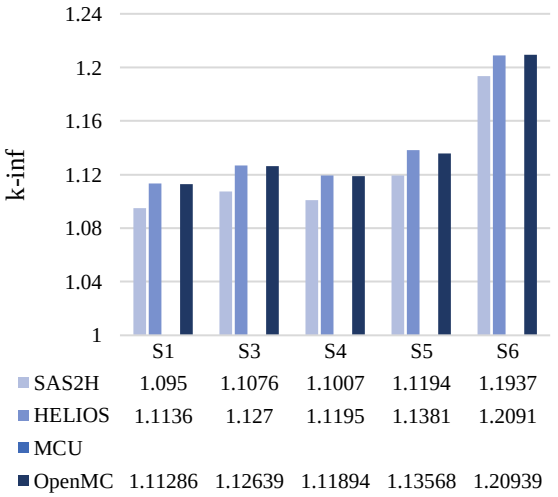

Figure 9. Variant 10.

Deviation tables were also compiled. The results of the OpenMC were compared with the average values (table 3, (OpenMC-average)/average), which were obtained by averaging the results for the SAS2H, MCU, and HELIOS codes taken from the benchmark. We can see that the largest deviations are in the V7 variant of the S1-S4 states – about 2.2 %, also the S5 and S6 states have the deviation close to 2%. The V7 fuel composition differs from other variants by the presence of ^{239}Pu in the fuel in addition to uranium. Although the same ^{239}Pu content is present in the V2 variant, there are also other plutonium isotopes that probably have a positive effect on the similarity of the results, since there are smaller deviations of less than 1%.

If we compare the results obtained with the SAS2H and HELIOS codes (table 4, (SAS2H- HELIOS)/ HELIOS), the largest deviations are in the V9 of the states S1-S5, about 3%, and the smallest deviations are in the V1-V8 of the states S6 and V2(S5), no more than 1%. It can be argued that the OpenMC deviations vary in the same range as deviations between SAS2H and HELIOS codes, that is why the OpenMC allows getting similar results and can be used for similar calculations of VVER-1000.

Analysing the sum of the deviations absolute values, we can say that the smallest deviation was obtained for the S6 variant, which is not surprising, since the temperature of all materials there is 300K. In other variants, the cross-sections were adjusted to the desired temperatures by the methods implemented in the codes.

Table 3. Comparison of OpenMC and average values.

	S1	S3	S4	S5	S6
V1	0.53%	–0.74%	0.67%	0.56%	0.56%
V2	0.85%	0.32%	0.86%	0.83%	0.75%
V3	0.84%	0.48%	0.95%	0.79%	0.42%
V4	0.87%	–1.03%	0.24%	0.15%	0.29%
V7	2.16%	2.17%	2.20%	1.98%	1.64%
V8	0.92%	0.95%	1.02%	0.86%	0.69%
V9	–0.18%	–0.13%	–0.12%	–0.28%	–0.17%
V10	0.78%	0.81%	0.79%	0.61%	0.67%
Sum of abs	7.1%	6.6%	6.9%	6.1%	5.2%

Table 4. Comparison of SAS2H and HELIOS.

	S1	S3	S4	S5	S6
V1	–1.26%	–1.31%	–1.22%	–1.11%	–0.62%
V2	–1.10%	–1.14%	–1.07%	–0.93%	–0.46%
V3	–1.19%	–1.22%	–1.15%	–1.05%	–0.55%
V4	–1.37%	–1.41%	–1.32%	–1.25%	–0.75%
V7	–1.16%	–1.20%	–1.14%	–1.02%	–0.54%
V8	–1.34%	–1.39%	–1.30%	–1.15%	–0.62%
V9	–2.82%	–2.92%	–2.86%	–2.68%	–1.93%
V10	–1.67%	–1.72%	–1.68%	–1.64%	–1.27%
Sum of abs	11.9%	12.3%	11.8%	10.8%	6.7%

Table 5. Comparison of OpenMC and SAS2H.

	S1	S3	S4	S5	S6
V1	1.37%	1.47%	1.48%	1.28%	0.94%
V2	1.45%	1.5%	1.45%	1.27%	0.89%
V3	1.44%	1.5%	1.54%	1.33%	1.05%
V4	1.57%	1.64%	1.63%	1.42%	1.14%
V7	2.76%	2.79%	2.79%	2.51%	1.71%
V8	1.60%	1.66%	1.68%	1.45%	1.12%
V9	1.26%	1.38%	1.35%	1.09%	0.76%
V10	1.63%	1.7%	1.66%	1.45%	1.31%
Sum of abs	13.1%	13.5%	13.6%	11.8%	8.9%

Table 6. Comparison of OpenMC and HELIOS.

	S1	S3	S4	S5	S6
V1	0.09%	0.14%	0.24%	0.16%	0.31%
V2	0.33%	0.34%	0.36%	0.33%	0.43%
V3	0.24%	0.26%	0.38%	0.27%	0.49%
V4	0.18%	0.21%	0.28%	0.15%	0.38%
V7	1.56%	1.56%	1.62%	1.46%	1.17%
V8	0.24%	0.25%	0.36%	0.28%	0.49%
V9	–1.59%	–1.58%	–1.55%	–1.61%	–1.19%
V10	–0.07%	–0.05%	–0.05%	–0.21%	0.02%
Sum of abs	4.3%	4.4%	4.8%	4.5%	4.5%

Table 7. Comparison of OpenMC and MCU.

	S1	S3	S4	S5	S6
V1	0.14%	–3.67%	0.3%	0.24%	0.42%
V2	0.77%	–0.86%	0.79%	0.88%	0.93%
V3	–	–	–	–	–0.27%
V4	–	-4.71%	-1.15%	-1.08%	–0.63%
V7	–	–	–	–	2.05%
V8	–	–	–	–	0.45%
V9	–	–	–	–	–0.07%

Comparing the results of the OpenMC with the SAS2H (table 5), the smallest deviations are in V1-V2, V9 of the S6 state – about 1%, and the largest deviations are in the V7 variant of the S1-S5 states – about 2.8 %.

Comparison of the results with the MCU (table 6) cannot be performed completely, because there was not enough data obtained with this code. The largest deviation is in the V4 variant of the S3 state – 4.7%. Also in the V7 variant of the S6 state is a large deviation around 2%.

The best agreement of the OpenMC is observed with the HELIOS (table 7). The smallest deviations are in the V1-V4, V8, V10 variants, no more than 0.5%, and the largest deviations are in the V7 and V9 variants, about 1.6%.

As you can see for the V7, there is a significant discrepancy between the OpenMC and all other codes.

The deviation of the obtained results may be due to a difference in the cross-section libraries used for calculating the benchmark. The ENDF/B-V library was used in the SAS2H calculations, ENDF/B-VI – MCU and HELIOS, ENDF/B-VII – OpenMC. It is also likely that the method of cross-section adjustment for a given temperature have a significant impact. However, even if there are large deviations for some variants, it can be argued that OpenMC allows getting similar to other codes results.

Using the results obtained for all codes, namely SAS2H, HELIOS, MCU and OpenMC, a table of neutron multiplication factors for all variants and in all states was made (table 8).

Table 8. K-inf by variant, state and computer code.

		S1	S3	S4	S5	S6
V1	SAS2H	1.2589	1.314	1.3065	1.3245	1.3669
	HELIOS	1.275	1.3315	1.3227	1.3393	1.3754
	MCU	1.2743	1.3841	1.3219	1.3382	1.3739
	OpenMC	1.27609	1.33331	1.32584	1.34142	1.37972
V2	SAS2H	1.2054	1.2339	1.225	1.2466	1.3248
	HELIOS	1.2188	1.2481	1.2383	1.2583	1.3309
	MCU	1.2135	1.2632	1.2331	1.2514	1.3242
	OpenMC	1.22282	1.25237	1.24278	1.26245	1.33656
V3	SAS2H	1.0818	1.1264	1.1215	1.141	1.1902
	HELIOS	1.0948	1.1403	1.1345	1.1531	1.1968
	MCU	–	–	–	–	1.206
	OpenMC	1.0974	1.14328	1.13877	1.15613	1.20271
V4	SAS2H	1.0156	1.0556	1.0508	1.0686	1.1197
	HELIOS	1.0297	1.0707	1.0649	1.0821	1.1282
	MCU		1.126	1.0803	1.0956	1.1396
	OpenMC	1.03159	1.07292	1.06791	1.08374	1.13246
V7	SAS2H	1.3036	1.3361	1.3259	1.3445	1.4105
	HELIOS	1.3189	1.3523	1.3412	1.3584	1.4181
	MCU	–	–	–	–	1.4058
	OpenMC	1.33954	1.37335	1.36295	1.37827	1.43464
V8	SAS2H	1.0896	1.1434	1.139	1.1593	1.2115
	HELIOS	1.1044	1.1595	1.154	1.1728	1.2191
	MCU	–	–	–	–	1.2196
	OpenMC	1.10704	1.1624	1.15817	1.17605	1.22507
V9	SAS2H	1.5279	1.5633	1.5503	1.5732	1.6189
	HELIOS	1.5722	1.6103	1.596	1.6165	1.6508
	MCU	–	–	–	–	1.6323
	OpenMC	1.54721	1.58485	1.57125	1.59042	1.63118
V10	SAS2H	1.095	1.1076	1.1007	1.1194	1.1937
	HELIOS	1.1136	1.127	1.1195	1.1381	1.2091
	MCU	–	–	–	–	–
	OpenMC	1.11286	1.12639	1.11894	1.13568	1.20939

5. Conclusion

In this work the OpenMC code was mastered and different benchmark states were calculated in order to provide the evidence that the code could be used for VVER-type reactor calculations.

The following conclusions can be drawn from the work:

1. We studied the main features of the OpenMC code and documented its installation, indicating the specifics and ways of solving the problems.
2. Values of infinite neutron multiplication factors for different variants and states of the VVER MOX benchmark were obtained.
3. It is shown that:
    - The values of infinite neutron multiplication factors obtained with the OpenMC are usually higher than the values obtained with the SAS2H, HELIOS, MCU.
    - The OpenMC deviations from other codes vary in the same range as the deviations between the SAS2H and HELIOS. Therefore, OpenMC allows getting similar results and is not inferior to other codes in similar calculations of VVER-1000.
    - The best agreement of the OpenMC values are with the HELIOS code.

- For the V7 variant, there is a significant discrepancy between the results obtained by each code. In this variant, the ^{239}Pu is added into uranium fuel.

In the future, it is proposed to calculate changes in the isotopic composition and compare it with the results from the benchmark. The OpenMC code is planned to be used at the Department of Nuclear Physics of the Belarusian State University for the calculations of the VVER-1200 (Belarusian NPP).

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