COMPUTATIONAL BENCHMARK FOR FUEL ASSEMBLY OF VVER-1000 USING THE MONTE CARLO SERPENT CODE

by

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The use of a new Monte Carlo Serpent code for the calculation of water-cooled reactors is presented and a calculation scheme of the fuel assembly for VVER-1000 reactors developed. The calculation of neutron-physical characteristics for the fuel assembly of VVER-1000 is carried out for different states and the results obtained by the Serpent model compared with the results of other reactor codes. The analyses of these results are presented in the paper submitted here. Based on this article, the Monte Carlo Serpent code could be used for neutron-physical calculations of VVER-1000 reactors.

Key words: VVER-1000, Monte Carlo method, reactor calculation, Serpent code

INTRODUCTION

A sustained development of nuclear energy needs application of new types of software for neutron-physical analysis of nuclear reactors [1-3], as well as the investigation of advanced nuclear reactors [4-7], is currently in operation.

Generally, neutron-physical modelling is based on two types of methods: deterministic methods and stochastic methods (for example, the Monte Carlo method) [8]. The base of deterministic methods is a numerical solution of the neutron transport equation (for example, discrete ordinate method [9] or characteristic method [10]). Stochastic methods, such as the Monte Carlo method, are based on the analysis of the probabilities of many events by simulating millions of elementary particles for given material characteristics and geometry [11]. Monte Carlo methods are most convenient for modeling reactor systems with complicated geometries where deterministic methods cannot be applied. The most well-known software product using the Monte Carlo method for calculating reactor systems is the MCNP code that was developed at the Los Alamos National Laboratory (LANL, USA) [12, 13].

Other reactor codes based on the Monte Carlo method such as the Serpent Monte Carlo code [14] are being actively developed as well. The development of the Serpent code started in 2004 at the VTT Technical Research Center (Finland) and has since gained the commitment of many scientists around the world due to convenience, accuracy of calculations and a wide range of tasks that it can solve [15].

Currently, the Serpent code is being actively used for investigating both fast reactors and thermal reactors [16, 17]. In the paper presented here, the authors investigate the possibility of using the Serpent code for the calculation of fuel assemblies (FA) characteristics for VVER-1000 reactors and a verification tool for deterministic codes that calculate the entire core of the VVER-1000 reactor (for example, VOYAGE/KRUIZ [18] and HELIOS [19]). This is especially urgent from the viewpoint of the need to develop a genuine Ukrainian deterministic code for the calculation of VVER reactor cores with Westinghouse fuel [20].

CALCULATION MODEL AND METHOD

Research aims

The verification of a reactor software which performs calculations of the physical characteristics for nuclear fuel is always a complex task since there is either not enough necessary experimental data or (in case of homogenous macroscopic interaction characteristics), the data is absent. Therefore, the cross-verification procedure is often used. Cross-verification is the implementation of same set of comparison calculations with other similar software products that have already been verified [21].

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In study [22], the calculations for FA VVER-1000 are done with the use of the well-verified codes for VVER fuel: TVS-M code [23], MCU code [24], WIMS8A code [25], HELIOS 1.4 code [19], MCNP4B code [26], and MULTICELL code [27].

The aim of this work is to repeat the calculations presented in report [22] by utilizing the Serpent code for the verification of software for calculations of VVER-1000 fuel.

Model description and input data

Within the scope of the present work, calculations were made for U/Gd FA of a VVER-1000 reactor [28]. The configuration of such U/Gd FA is shown in fig. 1. This FA consists of the fuel element (FE) of the main fuel and the mixed uranium-gadolinium fuel with oxide Gd_2O_3 (U/Gd FE). Fuel assemblies of the presented configuration are in use in all current Ukrainian nuclear power plants.

The FA in fig. 1 consists of: 300 FE, 12 U/Gd FE [29], 18 instrumental tubes and 1 central tube. The radius of fuel for FE and U/Gd FE: $R_1 = 0.386$ cm, the outer radius of cladding for FE and U/Gd FE: $R_2 = 0.4582$ cm (see fig. 2).

The codes presented in *Research aims* section are used for the preparation of small-group macroscopic interaction characteristics. In the preparation of such characteristics, campaign values of the fuel temperature averaged by the reactor, the cooling temperature and the concentration of boric acid are commonly used for the calculation of the change in isotopic composition with burn-up, as well as the base states and derived states [30, 31].

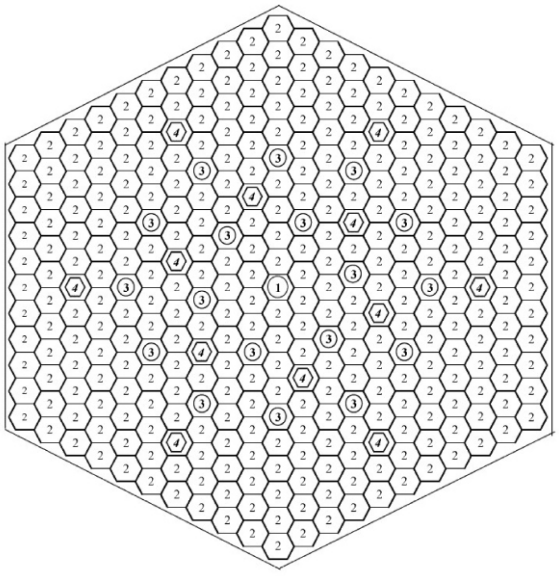

Figure 1. The configuration of considered U/Gd FA; *1 – central tube, 2 – FE with 3.7 % enrichment in U-235, 3 – instrumental tubes, 4 – U/Gd FE (UO_2 with 3.6 % enrichment in U-235 + 4.0 % Gd_2O_3)*

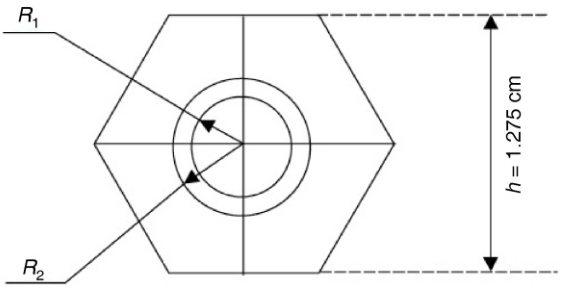

Figure 2. The configuration of the elementary fuel cell, where *h* is the key size

Table 1. Calculated states [22]

State	Description	Fuel temperature [K]	Non-fuel temperature [K]	Xe-135, Sm-149
S1	Operating poisoned state	1027	575	Eq.*
S2	Operating non-poisoned state	1027	575	0.0
S3	Hot state	575	575	0.0
S4	Hot state without boron acid	575	575	0.0
S5	Cold state	300	300	0.0

*Eq. Indicates equilibrium Xe-135 and Sm-149 concentrations

The analysis of characteristics of FA (fig. 1) was carried out for the five states shown in tab. 1.

The states indicated in tab. 1 correspond to the base and derived states for reactors VVER-1000. State S1 is the operating poisoned state where the burn-up calculation is carried out with the concentration of natural boron in the coolant of 0.6 gkg^{-1}.

Serpent code as an instrument for reactor calculations and calculation model

The Serpent code has been developed at the VTT Technical Research Centre of Finland since 2004. Serpent is a Monte Carlo code which uses a continuous energy library of neutron-physical constants, an approach similar to that used in the MCNP code for the determination of the neutron multiplication factor. The difference between the Serpent code and the MCNP code lies in the use of the Woodcock Delta-Tracking Method for neutron transport simulation, unlike the traditional Surface-to-surface ray-tracing method of the MCNP code. The main advantage of the Woodcock Delta-Tracking Method is that it greatly simplifies geometry processing during the calculation which leads to a reduction in modeling time, especially for complex geometries [32]. In the present paper, calculations were done with the help of the Serpent Monte Carlo transport code version 1.1.7 which employs the ENDF/B-VI.8 nuclear data library [33].

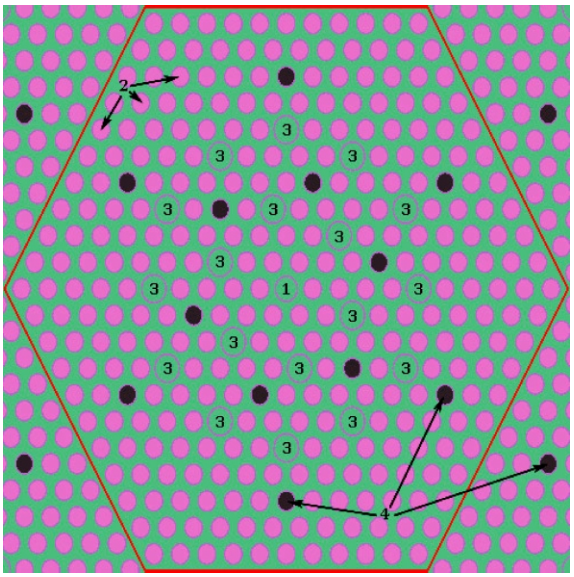

Figure 3. Calculation scheme of FA VVER-1000 from the Serpent code;
1 – central tube, 2 – FE with 3.7 % enrichment in U-235, 3 – instrumental tubes, 4 – U/Gd FE (UO_2 with 3.6 % enrichment in U-235 + 4.0 % Gd_2O_3)

The geometry in the Serpent code is based on structures very similar to the MCNP code [15]. These structures are based on the universe-based combinatorial solid geometry (CSG) model. The visualization of the FA VVER-1000 cross-section from the Serpent code is shown in fig. 3.

In the calculation scheme presented in fig. 3, the material composition and geometric characteristics of the cell are fully consistent with those given in [15].

The ENDF/B-VI.8 nuclear data library was used for all calculations in the present paper. It contains data for a number of temperatures – 300, 600, 900, 1200, 1500, and 1800 K for all the isotopes. The temperature range for light water for the thermal scattering library has the form: 296, 350, 400, 450, 500, and 600 K [34].

For Monte Carlo simulations, 320 cycles per 10000 neutrons were used in one neutron generation while disregarding the first 20 cycles to provide a value of the mean-square deviation of less than 0.0003 [35].

RESULTS AND DISCUSSION

Neutron multiplication factor calculations

The neutron multiplication factor is an integral characteristic of any nuclear fuel system and is one of the main informative indicators of the nuclear system's state. The correctness of the calculated value of the neutron multiplication factor will show the correctness of the used mathematical models, the correctness of the developed design scheme and ensure the correct values of interaction cross-sections. In the present paper, we have investigated the neutron multiplication factor, the concentrations of the main isotopes and pin-by-pin power distributions. The simulation results of S1 state with different calculation codes are given in tab. 2.

The BIPR code [36] is usually used for analyzing fuel loading of VVER reactors and the group con-

Table 2. Obtained simulation results of the multiplication factor for S1 state

Burn-up* [MWdkg^{-1}]	MCU	TVS-M	WIMS8A	HELIOS	MULTICELL	Averaged**	Serpent	Deviation serpent from averaged [%]	Deviation serpent from TVS-M [%]	Deviation serpent from HELIOS [%]
0	1.1353	1.1353	1.1328	1.1355	1.1363	1.135	1.1341	0.08	0.10	0.12
1	1.1364	1.1345	1.1303	1.1361	1.137	1.1349	1.1326	0.20	0.17	0.31
2	1.1354	1.1355	1.1318	1.1377	1.1382	1.1357	1.1340	0.15	0.13	0.33
3	1.1388	1.1359	1.133	1.1387	1.1386	1.137	1.1345	0.22	0.13	0.37
4	1.1377	1.1365	1.1341	1.1395	1.1389	1.1373	1.1349	0.21	0.14	0.41
5	1.139	1.1375	1.1358	1.1407	1.1394	1.1385	1.1355	0.26	0.18	0.46
6	1.1408	1.139	1.138	1.1421	1.1404	1.1401	1.1366	0.31	0.21	0.48
7	1.1427	1.1403	1.1392	1.143	1.1414	1.1413	1.1379	0.30	0.21	0.45
8	1.1421	1.139	1.1371	1.1414	1.1404	1.14	1.1369	0.27	0.19	0.40
9	1.1344	1.1346	1.1318	1.1365	1.1363	1.1347	1.1329	0.16	0.15	0.32
10	1.1284	1.1273	1.124	1.1291	1.1295	1.1277	1.1259	0.16	0.12	0.28
11	1.1178	1.1185	1.115	1.1203	1.1209	1.1185	1.1177	0.07	0.07	0.23
12	1.1099	1.1092	1.1058	1.1112	1.1117	1.1096	1.1084	0.10	0.07	0.25
13	1.0996	1.1	1.0966	1.102	1.1025	1.1002	1.0997	0.05	0.03	0.21
14	1.0923	1.091	1.0877	1.0931	1.0935	1.0915	1.0912	0.02	–0.02	0.17
15	1.0827	1.0821	1.079	1.0843	1.0846	1.0825	1.0826	–0.01	–0.05	0.16
20	1.0403	1.0405	1.0383	1.0435	1.0427	1.0411	1.0416	–0.05	–0.11	0.18
25	1.0039	1.0022	1.0017	1.0061	1.0041	1.0036	1.0049	–0.13	–0.26	0.12
30	0.9703	0.9665	0.9681	0.9714	0.9681	0.9689	0.9715	–0.26	–0.51	–0.01
35	0.9415	0.9332	0.9372	0.9391	0.9343	0.9371	0.9401	–0.32	–0.74	–0.11
40	0.9091	0.9025	0.9088	0.9091	0.9029	0.9065	0.9110	–0.49	–0.93	–0.21

* Here and throughout this work the burn-up in units MWdkg^{-1} of heavy metal are used in all the paper's tables
** Averaged value of K_{eff} calculated by MCU, TVS-M, WIMS8A, HELIOS, MULTICELL codes in report [15]

Table 3. Obtained simulation results of the multiplication factor for different states

State\Burnup [MWdkg^{-1}]	S1	S2	S3	S4	S5
MCU					
0	1.1353	1.1779	1.1899	1.2499	1.3197
20	1.0403	1.0809	1.0950	1.1496	1.2192
40	0.9091	0.9432	0.9562	1.0063	1.0632
TVS					
0	1.1353	1.1768	1.1900	1.2504	1.3213
20	1.0405	1.0781	1.0928	1.1484	1.2138
40	0.9025	0.9325	0.9460	0.9954	1.0470
WIMS8A					
0	1.1328	1.1695	1.1845	1.2433	1.3122
20	1.0383	1.0781	1.0941	1.1477	1.2173
40	0.9088	0.9422	0.9566	1.0041	1.0604
HELIOS					
0	1.1355	1.1750	1.1894	1.2490	1.3181
20	1.0436	1.0828	1.0988	1.1535	1.2198
40	0.9092	0.9422	0.9572	1.0063	1.0577
MULTICELL					
0	1.1363	1.1776	1.1919	1.2518	1.3164
20	1.0427	1.0835	1.0989	1.1543	1.2192
40	0.9029	0.9368	0.9509	1.0005	1.0505
Serpent					
0	1.1368	1.1720	1.1805	1.2385	1.3137
20	1.0416	1.0825	1.0918	1.1444	1.2175
40	0.9110	0.9449	0.9543	1.0003	1.0594

stant is prepared using the TVS-M code for BIPR calculations. In addition, the software product HELIOS is widely used in Ukraine for the preparation of constant support [31]. Therefore, tab. 2 provides separate comparisons with TVS-M and HELIOS codes.

The analysis of the obtained results shows good agreement between the neutron multiplication factor calculated by the Serpent code compared with other codes. There is an increase in deviation in comparison with the TVS-M code, but a similar situation can be seen when comparing the TVS-M code with other codes as well. Serpent's results lie in the range of a 0.5 % deviation compared by HELIOS code results, which is most likely due to the possible uncertainty of the input data (the presence or absence of distant grids, the format of input of isotopic composition, *etc.*).

The calculated isotopic compositions at state S1 are exported to other states (S2-S5) and the calculation of the neutron multiplication factor is carried out in the final stage. The calculation results for some burn-up points are shown in tab. 3.

The obtained difference of isotopic composition calculation for state S1 similarly affects calculations results for other states in which the isotope composition was exported (tab. 3).

The difference of the neutron multiplication factor for different states indicates a change in reactivity with a change of parameters. Table 4 shows the coefficients of reactivity at these burning points.

In tab. 4 we can note lower values of coefficients of reactivity for fuel temperature in the Serpent code

Table 4. Coefficients of reactivity

	Burn-up [MWdkg^{-1}]	MCU	TVS-M	WIMS8A	HELIOS	MULTICELL	Serpent
S1-S2 (Xe, Sm effects)	0	–4.26	–4.15	–3.67	–3.95	–4.13	–3.53
	20	–4.06	–3.76	–3.98	–3.92	–4.08	–4.08
	40	–3.41	–3.00	–3.33	–3.30	–3.39	–3.39
S3-S4 (boron effect)	0	–6.00	–6.04	–5.88	–5.96	–5.99	–5.79
	20	–5.46	–5.56	–5.36	–5.48	–5.54	–5.26
	40	–5.01	–4.94	–4.75	–4.91	–4.96	–4.59
S3-S2 (fuel temperature, Cb > 0)	0	1.20	1.32	1.50	1.44	1.43	0.85
	20	1.41	1.47	1.60	1.60	1.54	0.94
	40	1.30	1.35	1.44	1.50	1.41	0.95
S4-S5 (change of fuel temperature and cooling temperature)	0	–6.98	–7.09	–6.89	–6.91	–6.46	–7.52
	20	–6.96	–6.54	–6.95	–6.63	–6.49	–7.31
	40	–5.69	–5.16	–5.63	–5.15	–5.00	–5.92

than in other codes between states S3 and S2. This is because the used nuclear data library for Serpent calculations does not contain data for the temperature of 1027 K. In that case, the cross-sections with a temperature of 900 K were used. According to [37], in the second version of Serpent code, there is an option that allows adjusting the microscopic cross-sections to the required temperature values for fuel and other materials. Table 4 also shows that Serpent code gives a good match compared to the MCU, WIMS8A, and HELIOS codes. The deviation from the results of the TVS-M code was discussed before.

The pin-by-pin power distribution

The pin-by-pin power distribution makes it possible to analyze the distribution of energy in the FA and, as a result, the distribution of neutron flux in the FA. Information about pin-by-pin power distribution is important when analyzing the characteristics of a fuel inventory of a nuclear reactor since it provides an opportunity to control the values of the energy output in fuel and thus prevent excess of heat fluxes passport values. This, in turn, ensures the safe operation of nuclear fuel.

Figure 4 shows the numbers of FE in FA for the 60-degree sector.

Table 5 shows the values of pin-factors for different states at several burn-up points for considered neutron-physical codes. Pin numbers in tab. 5 are taken according to [15].

Analysis of data obtained in tab. 5 shows that the results of the Serpent calculation for the pin-by-pin power distribution provide acceptable values in comparison with other codes. It can also be noted that Monte Carlo codes Serpent and MCU are in very good agreement with each other. In addition to data presented in tab. 5, the changes of isotope composition with burn-up for: transuranium elements, Xe, Sm, and other isotopes are analyzed within the scope of the present investigation. The deviation in the isotopic composition for the main isotopes given in [15] agrees with the deviations obtained by the Serpent code.

CONCLUSIONS

A relatively new Monte Carlo Serpent code which can be used for analysis of neutron-physical characteristics for nuclear fuel systems, burn-up calculations, preparation of homogenized macroscopic characteristics, and simulation of fuel loading characteristics is presented.

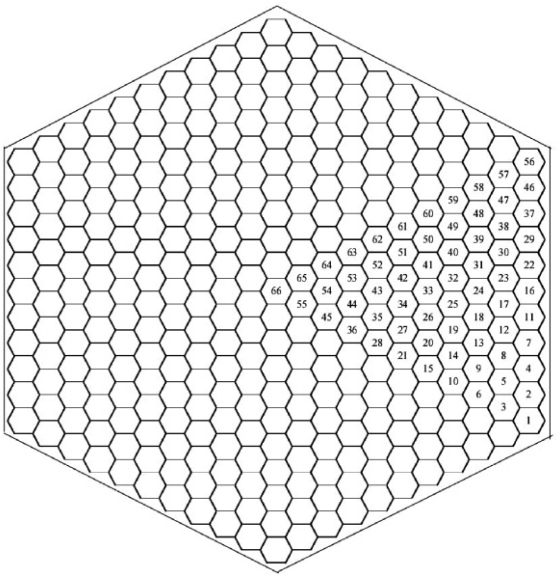

Figure 4. Numbering of cells in FA for calculation of pin-by-pin power distribution

A calculation scheme of the FA for the VVER-1000 reactor was developed with the use of the Serpent code. Performed calculations affirm the correctness of the developed calculation scheme for analyzing critical systems with VVER-1000 fuel. It can be noted that the results of Serpent calculations are in good agreement with the results of HELIOS calculations. The deviation of the results of Serpent calculations from the results of TVS-M calculations for increasing burn-ups is similar to the deviation of TVS-M results from MCU, WIMS8A, and HELIOS codes. This is very important since the variation in the calculation of the neutron multiplication factor equal to 1 % will give a deviation in the concentration of boric acid of 0.5 gkg^{-1} (depending on the method of constant preparation) for the calculation of the reactor campaign. This deviation of concentration is very significant since the error in the prediction campaign time can last up to 10 effective days. But, this deviation will not have a significant effect on the error in the determination of the energy-release distribution.

Table 5. Pin-factors

Code	Burn-up per cell [$MWdkg^{-1}$]														
	State – S1			State – S2			State – S3			State – S4			State – S5		
	0	20	40	0	20	40	0	20	40	0	20	40	0	20	40
	63	19	6	35	1	6	35	64	6	35	58	6	35	1	6
MCU	1.005	0.965	0.959	0.318	1.048	0.963	0.320	1.062	0.958	0.308	0.953	0.957	0.218	1.084	0.943
TVS-M	0.993	0.983	0.987	0.319	1.032	0.989	0.318	1.037	0.989	0.308	0.972	0.987	0.217	1.070	0.971
WIMS8A	0.998	0.987	0.990	0.336	1.028	0.992	0.333	1.032	0.992	0.323	0.978	0.991	0.229	1.050	0.985
HELIOS	0.981	0.975	0.979	0.329	1.047	0.981	0.327	1.038	0.981	0.317	0.966	0.979	0.222	1.078	0.967
MULTI CELL	0.957	0.979	0.985	0.317	1.045	0.986	0.316	1.037	0.986	0.306	0.967	0.984	0.215	1.056	0.986
Serpent	1.010	1.000	0.981	0.377	1.015	0.962	0.381	1.041	0.962	0.362	0.979	0.963	0.262	1.044	0.963

The papers [38, 39] show that the value of the diffusion coefficient in the „fast" energy region requires clarification. Therefore, considering the results presented in this article, it is logical to switch to the use of the second version of the Serpent code.

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РАЧУНАРСКО ТЕСТИРАЊЕ ГОРИВНОГ СКЛОПА VVER-1000 РЕАКТОРА ИЗВРШЕНО МОНТЕ КАРЛО СЕРПЕНТ КОДОМ

Применом новог Монте Карло Серпент кода извршен је прорачун реактора хлађених водом и развијена је прорачунска шема горивног склопа VVER-1000 реактора. Прорачун неутронско-физичких карактеристика горивног склопа VVER-1000 реактора урађен је за различита стања, а резултати добијени Серпент кодом упоређени су са резултатима других реакторских програмских пакета. Из анализе ових резултата закључује се да се Монте Карло Серпент код може користити за неутронско-физичке прорачуне VVER-1000 реактора.

Кључне речи: VVER-1000, Монте Карло метода, реакторски прорачун, Серпент код