UDC 621.039.51

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USING SOFTWARE BASED ON THE MONTE CARLO METHOD FOR RECEIVING THE FEW-GROUP HOMOGENIZED MACROSCOPIC INTERACTION CROSS-SECTIONS

В.В. Гальченко, А.М. Абдулаев, І.І. Шлапак. **Використання програмного продукту на базі методу Монте-Карло для отримання малогрупових гомогенізованих макроскопічних перерізів взаємодії**. При проведенні малогрупових розрахунків різних станів реакторної установки важливе значення мають питання підготовки малогрупових констант. Від того, як це було зроблено, залежить точність і якість подальших розрахунків кінетики реактора. Для підготовки малогрупових характеристик зазвичай використовуються транспортні програмні продукти (детерміністичні коди), які на основі теорії переносу нейтронів розраховують потоки нейтронів в залежності від енергії і положення в чарунці. Наведено опис розрахункової схеми ТВЗ, для цілей підготовки малогрупових характеристик, для програмного продукту Serpent, який використовує метод Монте-Карло та безперервну за енергією бібліотеку мікроскопічних констант і який розроблено для розрахунку характеристик ТВЗ, включно з розрахунком вигоряння і підготовкою малогрупових гомогенізованих макроскопічних перерізів взаємодії, для розрахунку активної зони. Наведено розрахункову схему для програмного продукту Serpent для ТВЗА та результати порівняльних розрахунків основних нейтронно-фізичних характеристик з кодами PHOENIX-H і WIMSD5B.
Ключові слова: Serpent, PHOENIX-H, WIMS, комп'ютерні коди, ВВЕР-1000, метод Монте-Карло, перерізи взаємодії, коефіцієнт розмноження

V.V. Galchenko, A.M. Abdulaev, I.I. Shlapak. **Using software based on the Monte-Carlo method for receiving the few-group homogenized macroscopic interaction cross-section.** The constant preparation issues are important for performing the few-group analysis for different states of the reactor core. Besides, the constant preparation method influences the further calculations accuracy and quality. The transport software products (deterministic codes) are usually used for the few-group characteristics preparation. On the basis of the neutron transport theory these codes calculate neutron fluxes depending on the energy and on the location in the cell. In present paper the description of fuel assembly calculation scheme for preparing the few-group characteristics is given for the Serpent code. This code uses the Monte-Carlo method and energy continuous microscopic data library. Serpent code was developed for calculating the fuel assembly characteristics including burnup calculations and preparation of the few-group homogenized macroscopic interaction cross-sections for the core calculating. The calculation scheme for the Serpent code for FAA and the results of the basic neutron-physical characteristics comparative calculations with PHOENIX-H and WIMSD5B codes are presented.
Keywords: Serpent, PHOENIX-H, WIMS, computer codes, VVER-1000, Monte-Carlo method, cross-sections, multiplication factor

Introduction. Typically, the neutron-physical processes modeling is based on two main types of methods: deterministic methods and stochastic methods (for example, the Monte Carlo method). The neutron transport equations numerical solution lies in the basis of the deterministic methods (for example, the discrete ordinates method or the characteristic method). The Monte Carlo methods are based on analyzing the probabilities of many events by simulating millions of elementary particles for the given material characteristics and geometry. The Monte Carlo methods are the most suitable for modeling the critical systems with complex geometry, where the deterministic methods cannot be applied. The most famous computer code using the Monte Carlo method for calculating the reactor systems is the MCNP code, developed by the Los Alamos National Laboratory (LANL, USA) [11].

Recently other reactor codes based on the Monte Carlo method have actively been developing. Among them the Serpent code is distinguished [2]. This code has been developing since 2004 at the VTT Technical Research Center (Finland). It quickly ingratiated with many scholars all over the world

due to its convenience, accuracy of calculations and wide range of tasks that it is capable to solve. At present, the Serpent code is actively used for studying reactors both on "fast" and on "thermal" neutrons [3, 4].

Today Monte Carlo calculations are considered to be the most precise. Criticality calculations of different systems with fuel, as well as various radiation characteristics calculations are carried out using such codes. Another possibility to use software based on the Monte Carlo method is calculating the whole core characteristics.

However, calculating the core using codes based on the Monte Carlo method is still of a single nature. Mainly it is used for research purposes since it requires significant machine resources and system's modeling volumes.

Currently the core characteristics calculations are carried out using software that solves the reactor kinetic equations in a two-group approximation. The accuracy of this calculation depends greatly on the constant software preparation quality.

The Serpent computer code gives a possibility to prepare the few-group homogeneous macroscopic characteristics. In order to do this it is necessary to carry out the verification calculations of the developed calculation scheme for the corresponding fuel assembly (FA) beforehand.

1. The VVER-1000 calculation scheme and the calculation methodology

1.1 VVER-1000 FA calculation scheme. The fuel assembly main type, currently operated at the NPP with VVER-1000 in Ukraine, is TVSA. Project fuel loading, formed mainly from fuel assembly of several types, is 439MT and 398MO. The configurations of these FA are shown in Fig. 1
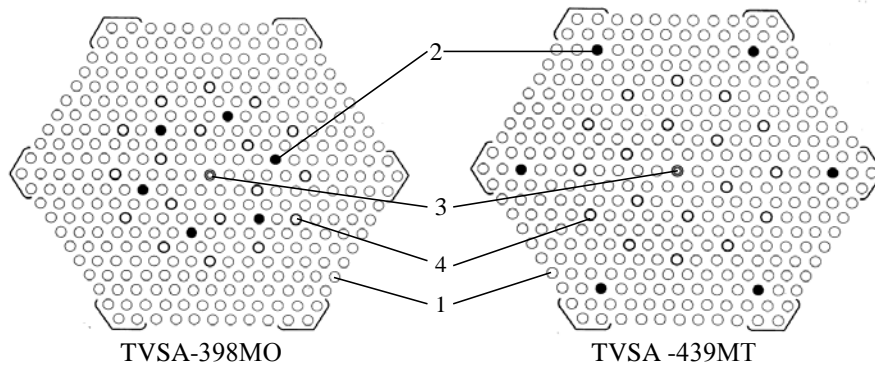

Fig. 1. Configuration of 398MO and 439MT fuel assemblies: fuel elements with 4,0% enrichment on 235U (1); fuel elements with 3,3% enrichment on 235U and 5% Gd2O3 (2); central tube (3); instrumental tubes (4)

Table 1

Material and geometric characteristics of VVER-1000 FA

Parameter	Value
Fuel rods step in FA, cm	1.275
Fuel	UO_2
Fuel pill diameter, fuel rod internal / external, cm	0.14 / 0.757
Diameter of fuel shell, internal / external, cm	0.772 / 0.91
Material of fuel shell	Zr + 1 % Nb
Diameter of guide channels, internal / external, cm	1.09/1.26
Diameter of the central tube, internal / external, cm	1.1 / 1.3
Coolant temperature, K	578
Coolant density, g/cm^3	0.723
Fuel temperature, K	890
Fuel rods fuel density, g/cm^3	10.45
Boron concentration in the coolant, ppm	200

The TVSA geometric and material characteristics, which were used in modeling and further calculations, are presented in Table 1.

The Serpent code geometry is based on the structures similar to MCNP [2]. These structures are based on the Universe-based combinatorial solid geometry (CSG) model. The FA calculation schemes, which were developed for the Serpent code, are shown in Fig. 2 and Fig. 3. The drawings are built directly by the Serpent code from the input file.
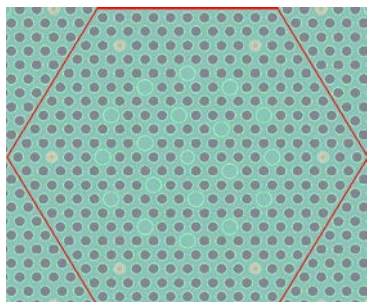
Fig. 2. 439MT FA calculation scheme
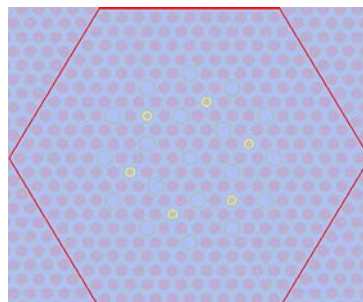*for Serpent code*

Fig. 3. 398MO FA calculation scheme
for Serpent code

The VVER-1000 FA calculation schemes for the WIMSD5B [5] and PHOENIX-H [6] computer codes, as well as some verification calculations for them are presented in [6–9].

1.2 The Monte Carlo method in Serpent code. Serpent code uses an energy-continuum library of neutron-physical constants. In this research the library of neutron-physical constants, based on the evaluated nuclear data ENDF/B6.8 file, was used. Although, Serpent allows to use libraries based on other evaluated nuclear data files (e.g. JEF2.2 [10]). The implemented in Serpent, Monte Carlo method defines the neutron multiplication factor for the system as the ratio of the one generation's neutrons number to the previous generations' neutrons number. Thus, the neutrons flow interaction with the matter nuclei is "played out" directly in the program.

The difference between Serpent and MCNP is in the use of the "Woodcock delta-tracking" method for the neutron transfer modeling, unlike the traditional for the Monte Carlo codes "Surface-to-surface ray-tracing" method. The "Woodcock delta-tracking" method's main advantage is that it greatly simplifies the geometry processing during the calculation. It leads to a decrease in the modeling time, especially for complex geometry [11].

2. Calculations results. The calculation was made for the system parameters given in Table 1 with the burnup step of 1.5 MW·day/t(U) to 60 MW·day/t(U). In Fig. 4 and Fig. 5 the neutron multiplication factor dependence on the burnup, received by various codes, is presented.

The figures show that at the initial burnup stage the results between Serpent PHOENIX-H have rather high coincidence level. This is an integrated into Gd fuel burnup stage. Then the results for different codes are aligned. But the neutron multiplication factor obtained by Serpent is slightly lower than WIMSD5B and PHOENIX-H. Eventually at the end of the burnup they reach the same values. But the deviation between the neutron multiplication factor values concerning these three softwares does not exceed the value of 1.5 %.
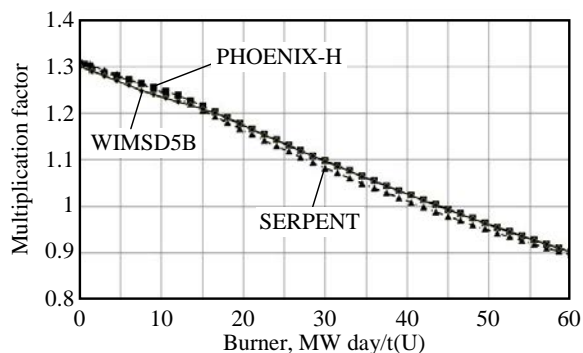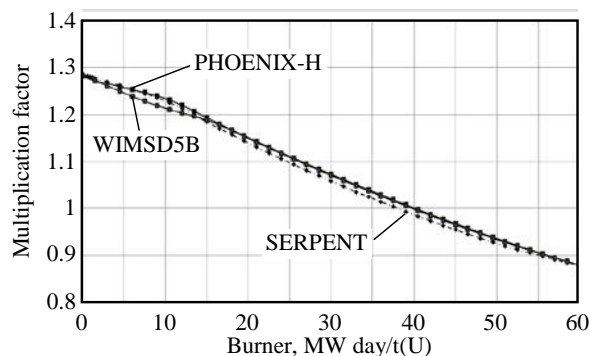

Fig. 4. Dependence of the neutron multiplication
factor on the burnup for 439MT FA

Рис. 5. Dependence of the neutron multiplication
factor on the burn up for 398MO FA

The main goal to use WIMSD5B and PHOENIX-H computer codes is few-group homogeneous macroscopic cross-section preparation. Tables 2–4 show the main interaction of cross-sections comparison in two energy groups.

Table 2

Main macroscopic interaction characteristics, counted using difference codes for 439MT FA,
burnup 30 MW·day/t(U)

Parameter	PHOENIX-H	WIMS	Serpent
Diffusion coefficient for the 1st group D_1, cm	1.3968	1.4831	1.3024
Diffusion coefficient for the 2nd group D_2, cm	0.3911	0.3839	0.3768
Absorption cross-section for the 1st group Σ_a^1, cm^{-1}	0.0097	0.0098	0.0103
Absorption cross-section for the 2nd group Σ_a^2, cm^{-1}	0.1014	0.1039	0.1043
Multiplication capability for the 1st group $\upsilon\Sigma_f^1$, cm^{-1}	0.0075	0.0077	0.0081
Multiplication capability for the 2nd group $\upsilon\Sigma_f^2$, cm^{-1}	0.1681	0.1711	0.1731
For the 1st group $\chi\Sigma_f$	0.6124	0.6129	0.6469
For the 2nd group $\chi\Sigma_f$	14.1244	14.2209	14.3650
Multiplication factor	1.3047	1.2983	1.3118

As it can be seen from the tables the interaction cross-sections values in the "thermal" energy group have a rather high level of coincidence. A noticeable deviation occurs for the diffusion coefficient in the "fast" energy group. Although transport approximation was used for all three computer codes, Serpent has the lowest diffusion coefficient value in the "fast" energy group. It should be noted that this coefficient's magnitude does not affect further calculations significantly.

However, it must be noted that the calculation time (with all burnup points) for WIMSD5B/PHOENIX-H was about 2 minutes, while SERPENT spent an hour.

Conclusions. The relatively new Monte Carlo Serpent code, which can be used for the nuclear reactors neutron analysis, is presented. The main Serpent calculating capabilities are shown; VVER-1000 FA is used as an example.

The further direction in the Serpent verification will be aimed at studying the calculating of homogeneous interaction cross-sections for VVER-1000 fuel methods and analyzing the microscopic constants libraries effects, since Serpent code makes it possible to use the microscopic constants library based on the evaluated nuclear data JEFF file.

Table 3

Main macroscopic interaction characteristics, counted using difference codes for 439MT FA,
burnup 30 MW·day/t(U)

Parameter	PHOENIX-H	WIMS	Serpent
Diffusion coefficient for the 1st group D_1, cm	1.4285	1.4777	1.3133
Diffusion coefficient for the 2nd group D_2, cm	0.3777	0.3734	0.3696
Absorption cross-section for the 1st group Σ_a^1, cm^{-1}	0.0108	0.0109	0.0113
Absorption cross-section for the 2nd group Σ_a^2, cm^{-1}	0.1020	0.1026	0.1085
Multiplication capability for the 1st group $\upsilon\Sigma_f^1$, cm^{-1}	0.0056	0.0058	0.0059
Multiplication capability for the 2nd group $\upsilon\Sigma_f^2$, cm^{-1}	0.1565	0.1568	0.1660
For the 1st group $\chi\Sigma_f$	0.4388	0.4469	0.4583
For the 2nd group $\chi\Sigma_f$	12.2950	12.1771	12.8255
Multiplication factor	1.0985	1.0972	1.0832

Table 4

*Main macroscopic interaction characteristics, counted using difference codes for 398MO FA,
burnup 0 MW·day/t(U)*

Parameter	PHOENIX-H	WIMS	Serpent
Diffusion coefficient for the 1st group D_1, cm	1.39721	1.481411	1.29387
Diffusion coefficient for the 2nd group D_2, cm	0.39001	0.384645	0.37702
Absorption cross-section for the 1st group Σ_a^1, cm^{-1}	0.00946	0.009635	0.01001
Absorption cross-section for the 2nd group Σ_a^1, cm^{-1}	0.09602	0.097977	0.09901
Multiplication capability for the 1st group $\upsilon\Sigma_f^2$, cm^{-1}	0.00709	0.007269	0.00759
Multiplication capability for the 2nd group $\upsilon\Sigma_f^2$, cm^{-1}	0.15601	0.158997	0.16063
For the 1st group $\chi\Sigma_f$	0.5759	0.5776	0.6068
For the 2nd group $\chi\Sigma_f$	13.0987	13.2151	13.3340
Multiplication factor	1.2818	1.2803	1.2853

It is important to note that in order to use code for preparing a few-group constants software, a great number of verification calculations must be executed for multilateral investigation of all factors that influence the calculations result, since the further core calculations quality and accuracy depends on the constant software preparation.

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