ЭКСПЛУАТАЦИЯ ОБЪЕКТОВ АТОМНОЙ ОТРАСЛИ

УДК : 621.039.517 : 621.039.519

ПРОВЕРКА ФИЗИЧЕСКИХ ПАРАМЕТРОВ КОДА МОНТЕ-КАРЛО OPENMC С ПОМОЩЬЮ КОДА UNK ДЛЯ РАЗЛИЧНЫХ ТВС ВВЭР-1200

© 2021 Х.А. Танаш, Д.А. Соловьёв, В.Г. Зимин, А.А. Семенов, Н.В. Щукин, А.З. Альхмуд, Б. Джарум, А. И. Аль-Шамайлех

Национальный Исследовательский Ядерный Университет «МИФИ», Москва, Россия

Новый код Монте-Карло под названием OpenMC был разработан Массачусетским технологическим институтом. В данной работе рассматривается проверка детерминированного транспортного кода решетки реактора OpenMC для различных типов тепловыделяющих сборок ВВЭР 1200. Трехмерная полная модель с обогащением по 3 урана 4,95%, 4,0% и 1,3% построена с использованием кода Монте-Карло для переноса частиц OpenMC. Значения эффективного коэффициента умножения () для свежего топлива с двумя конфигурациями топлива и конца жизненного цикла (EOL) выполнены для трех типов ТВС с разным обогащением и выполнены для каждого из девяти случаев; результаты показывают согласование с двумя другими кодами (Serpent и UNK). Значения интегральных параметров, рассчитанные OpenMC, сравнивались с кодом UNK, результат коэффициента диффузии показывает большое относительное отличие от UNK, поскольку метод кумулятивной миграции не реализован в коде OpenMC.

Ключевые слова: код Монте-Карло для переноса частиц OpenMC, ВВЭР-1200, эффективный коэффициент умножения, интегральные параметры.

Поступила в редакцию 13.07.2021
После доработки 03.09.2021
Принята к печати 07.09.2021

Introduction

The commissioning of WWER-1200 was one of the most important events in the nuclear power industry of Russia and the whole world [1]. The WWER technology [2] undoubtedly played a decisive role in the key stages of the formation and development of nuclear power in the Soviet Union and Russia. Different fuel assemblies of a WWER-1200 reactor indicated the calculation of this problem in order to compare the consistency of the reactor physics constant. Recently, many studies discussed this characteristic of reactor to validate reactor physics and neutronics by use several simulation code with different nuclear data libraries [3]. In this work, we use OpenMC Monte Carlo simulation platform, which was developed in 2011 by the Computational Reactor Physics Group members at the Massachusetts Institute of Technology (MIT) [4].

The initial work on OpenMC has focused on criticality calculations as applied to the simulation of nuclear reactors. The platform has its powerful from the huge numbers of tallies efficiently (reaction rate, fission, flux, etc.) that available to the user with progressing plotting to track geometry and post-processing the data. This continuous development makes OpenMC capable to design arbitrar ily complex geometric objects with advance plotting/post-processing. In the last decade, many studies for calculation of reactor physics and simulation of particle transport in reactor were performed using OpenMC Monte Carlo, because of its high performance and simply extensible for research purposes, In addition to its accuracy for neutron calculation and the ability of simulating 3D models using a constructive solid geometry representation. OpenMC uses data of particle interaction on HDF5 format, which

can be generated from the ACE or ENDF/B format as in the MCNP [5] and Serpent Monte Carlo platform.

2 WWER-1200 Reactor

WWER reactors are undoubtedly one of the most important pressurized water reactors, which played a decisive role in key stages of the formation and development of nuclear power in the Soviet Union and Russia. All of its kind power units based on WWER technology [1]. The core of a WWER-1200 reactor assembled from 163 hexagonal fuel assemblies, close by design for fuel assemblies of a WWER-1000 reactor. The power frame of the fuel assembly is formed by 18 guide channels and 13 spacer grids welded to them. Each fuel assembly contains 312 fuel rod elements, located with spacers at the corners of a uniform triangular mesh, as shown in Fig. 1. The fuel is enriched uranium dioxide isotope uranium-235. Uranium enrichment is constant along the fuel rod height. Average enrichment fuel FA does not exceed 4.95%. With such fuel enrichment, one fuel assembly subcritical in cold water without boron taking into accounts the calculation error. In fuel loads presented in the work use fuel elements with fuel enrichment U-235 equal to 1.3%, 4.0% and 4.95%. Where the basic characteristics of the core WWER-1200 shown in Table 1.

3 Material and methods

In this work, WWER-1200 fuel assemblies have been used to analyse and the simulation was generated. Three-dimensional fuel assembly model was built using the design specifications data of the WWER-1200. Reactor analysis was performed at three enrichments 1.3%, 4%, and 4.95%. In addition, two states of the fuel life configuration: fresh and end of lifecycle were also taken into account for different enrichment.

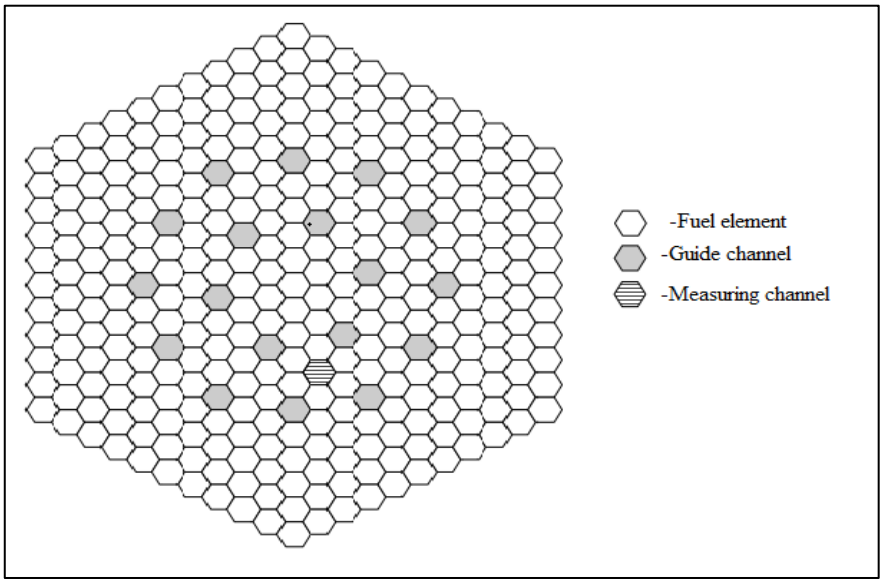

Figure 1– Cartogram fuel assemblies Z13, Z40, and Z49 of the reactor WWER-1200

In this study, we used OpenMC Monte Carlo simulation platform, the simulation platform is supported by the Python programming language, which make it conforming to perform and having the contemporaneous standard rather than a complex language like FORTRAN. This Monte Carlo simulation code focused criticality on neutron calculations and particle transport calculation. The simulation platform OpenMC uses 3D models that depend on constructive solid geometry representation with second-order surfaces. OpenMC can represent any closed volume as the union, intersection, and/or difference of multiple half-spaces. This allows to design all available geometry surfaces of nuclear reactor. All input user files in OpenMC platform uses Extensible Markup Language (XML), which make it very easy to examine the input file and get the determined data from output file.

The cross section treatments in OpenMC support in tow energy modes (continuous-energy and multi-group), for continuous energy particle interaction data, native HDF5 format is utilized by OpenMC that can be created from ACE and ENDF/B files like the MCNP and Serpent Monte Carlo codes. As most Monte Carlo codes OpenMC can create the HDF5 files data with the NJOY. In this study was used ENDF/B-VII.1 version for nuclear material cross-sectional data by The National Nuclear Data Centre (NNDC). The version of OpenMC used in this study was 0.12.0. A three-dimensional geometric model of the fuel assembly (FA) of WWER-1200 reactor was designed to do our neutronic calculations. Using Python package gives the user more flexibility to generate plots and in data post-processing and enables us to simply manipulate of the HDF5 data. In our work the reading of criticality calculation was taken for 50000 particles with 100 batches and 50 inactive batches, all the reactions rates are obtained with relative statistical errors in the average of 0.005%. The source space was treated as a box with dimensions 37 cm -37 cm in X- axis, 35 cm -35 cm in Y-axis and 187 to -187 in Z-axis direction.

Table 1 – Main characteristics of the WWER-1200 core

Parameter name	Value
Reactor thermal power (nominal), MW.	3200
Number of fuel assemblies in the core.	163
Number of fuel rods in fuel assembly.	312
Pitch between fuel elements, mm.	12.75
Fuel height, nominal, mm.	3730
Outer diameter of the fuel element cladding, mm.	9.10
Inner diameter of the fuel element cladding, mm.	7.73
Clad material.	Alloy E110
Fuel material.	UO2
fuel mass (UO2) in a fuel element (nominal), kg.	1.71
Outer diameter of the fuel element , mm.	7.6
Number of guide channel.	18
Outer diameter of guide channel, mm.	12.9
Inner diameter of guide channel, mm.	11.0

Serpent is three-dimensional continuous-energy Monte Carlo particle transport code, developed by the VTT Technical Research Center of Finland. Serpent uses ACE cross-sectional libraries based on the converted JEFF-2.2, JEFF-3.1, JEFF-3.1.1, ENDF/B-VI.8 and ENDF/B-VII evaluated nuclear data files. ACE is a special format for presenting data from various libraries of cross sections for the interaction of neutrons with nuclei in the epithermal energy range. Data are available for 432 nuclides at 6 temperatures from 300 to 1800 K. While the UNK program is intended for calculating the neutronic characteristics of cells and fuel assemblies of various types of nuclear reactors. The nuclear data library of the program includes about 300 isotopes and was calculated using the NJOY program from the evaluated data files ENDF / B-VI, JEFF-2.2 and JENDL-3.2. The main energy grid includes 89 groups: 24 groups in the region of deceleration to 2.15 eV and 65 thermal groups. The integral equation of neutron transport in the transport approximation is solved by the method of the probability of the first collisions (ITF). Matrices of the IPM method are calculated analytically in the case of one-dimensional geometry, for complex geometry matrices are determined by numerical integration using the method of characteristics.

4 Discussion of results

In this study three-dimensional FA model was built by OpenMC to perform the calculations reactor physics parameters. The simulation calculation runs in the OpenMC was taken for 50000 particles with 100 batches and 50 inactive batches. The values of multiplication factor K_{eff} was calculated for FA with three different enrichments at three

different cods (OpenMC, Serpent, UNK), after that we analyzed the value of Integral parameters, that getting in OpenMC with other code UNK.

4.1 Validation OpenMC code

The values of multiplication factor K_{eff} was calculated at three different enrichment shown in Table 2, the calculation was performed under a hot state condition (Tf=1027 K, Tc=575 K, without boric acid, density of water=0.7235 g/cm^3), the results of OpenMC are compared with two differences codes Serpent [6] and UNK [7]. The results show good agreements with each other as shown in Table 3, while the slightly difference refer to the different in the nuclear data libraries which used and to the computational method of each codes. In this study, we used ENDF/B-VII.1 nuclear cross-sectional data for OpenMC and Serpent.

At the same hot state condition, the values of the K_{eff} versus burnup for Z40, TVS obtained by three codes are presented in Figure 2.

Table 2 – Critically calculation of $\mathbf{K_{eff}}$ for VVER-1200 FA, with three different enrichment, for fresh fuel and end life of cycle

%		OpenMC	Serpent	UNK
1.30%	Fresh fuel	1.08370+/-0.00060	1.08416 +/- 0.00033	1.07752
	EOL	1.00128+/-0.00062	1.00720 +/- 0.00035	1.00526
	CR(B_4C)	0.74788 +/- 0.0005	0.74807 +/- 0.00045	0.72773
4.00%	Fresh fuel	1.37029+/-0.00104	1.37124 +/- 0.00030	1.37711
	EOL	1.014981+/-0,00064	0.99951 +/- 0.00045	1.00270
	CR(B_4C)	1.05514 +/- 0.00066	1.05647 +/- 0.00054	1.05667
4.95%	Fresh fuel	1.40444 +/- 0.00114	1.40622 +/- 0.0004	1.41594
	EOL	1.014981+/-0.00064	0.98261 +/- 0.00050	1.00589
	CR(B_4C)	1.10314 +/- 0.00062	1.10396 +/- 0.00055	1.10685

Table 3 – Mean deviation between OpenMC-UNK and OpenMC-Serpent for three cases

%		Fresh fuel	CR(B_4C)	End of life
Mean deviation %	OpenMC-UNK	0.628	1.058	1.110
	OpenMC-Serpent	0.0795	0.075	0.172
Maximum deviation %	OpenMC-UNK	0.819	2.694	1.226
	OpenMC-Serpent	0.126	0.126	0.364
Standard deviation	OpenMC-UNK	0.168	1.419	0.186
	OpenMC-Serpent	0.043	0.050	0.174

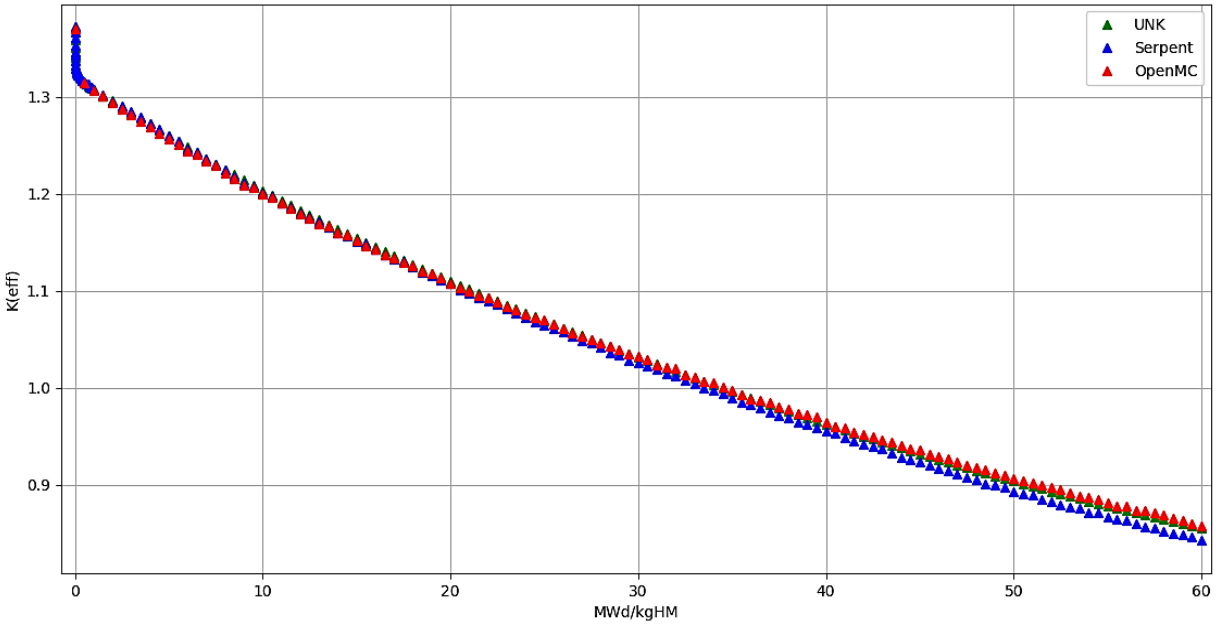

Figure 2 – $\mathbf{K_{eff}}$ versus burnup for Z40 TVS

4.2 Integral parameters calculations

The values of the reactor parameters were computed by OpenMC code, diffusion coefficient D, absorption Σ_a, fission Σ_f and nu-fission Σ_{nf} macro cross-sections, at hot state condition (Tf=1027 K, Tc=575 K, without boric acid, density of water=0.7235 g/cm^3) and without control rods for 2-group energy, after that these value were compared by the values which getting in UNK code as shown in table 4. The thermal cutoff energy in our calculations is set to 2.15 eV. For both codes neutron cross sections are processed based on the ENDF/B-VII.1 evaluated data file.

Table 4 – Integral parameters calculated by UNK and OpenMC for VVER-1200 TVS

TVS	Code	Integral parameter							
		D_1(cm)	D_2(cm)	$\Sigma_{a1}(cm^{-1})$	$\Sigma_{a2}(cm^{-1})$	$\Sigma_{nf1}(cm^{-1})$	$\Sigma_{nf2}(cm^{-1})$	$\Sigma_{f1}(cm^{-1})$	$\Sigma_{f2}(cm^{-1})$
Z13	OpenMC	1.0681E+00	3.9318E-01	9.1617E-03	4.7799E-02	4.3758E-03	6.6159E-02	1.6628E-03	2.7151E-02
	UNK	0.6694E+00	2.6856E+00	7.8367E-03	4.1058E-02	3.7085E-03	5.4766E-02	1.4047E-03	2.2486E-02
Z40	OpenMC	1.0729E+00	4.0859E-01	1.1035E-02	9.0612E-02	7.8921E-03	1.6008E-01	3.0969E-03	6.5697E-02
	UNK	0.6813E+00	2.6028E+00	0.9555E-02	7.8606E-02	6.7714E-03	1.3690E-01	2.6524E-03	5.6274E-02
Z49	OpenMC	1.0705E+00	4.1147E-01	1.1575E-02	1.0280E-01	9.0033E-03	1.8646E-01	3.5514E-03	7.6524E-02
	UNK	0.6814E+00	2.5877E+00	1.0037E-02	0.8860E-01	7.7316E-03	1.5878E-01	3.0454E-03	3.04544E-03

In the comparison of the values of Integral parameters, which calculated by OpenMC to UNK code for fuel assembly Z40, it is showing good agreement except for the values of the diffusion coefficient. The maximum relative difference from UNK was 0.843 % for the fast group diffusion coefficient these large values of relative difference because the cumulative migration method is not implemented into OpenMC code until now, while the relative difference for other parameters was not more than 2%. OpenMC and other Monte Carlo codes used B_1 equations to tally micro-group cross sections, these equations are solved for a critical spectrum, which is used to recondense the cross sections into leakage-corrected few-group constants. While generating micro-group cross sections need more tallying and computation work, so diffusion coefficients cannot be tallied directly into the desired group structure. This is one of the main challenges in the implementation of Monte Carlo codes; an accurate theory for computing diffusion coefficients and transport cross sections is yet to be implemented, more details you can see in this paper [8].

Table 5 – The relative difference from UNK = [(OpenMC- UNK)/UNK] ×100 in %, for Z40

D_1	D_2	Σ_{a1}	Σ_{a2}	Σ_{nf1}	Σ_{nf2}	Σ_{f1}	Σ_{f2}
0.575	0.843	0.155	0.153	0.166	0.1.69	0.168	0.167

4 Conclusions

The importance of this work lies in studying. The WWER-1200 benchmark problems were chosen for this work, based on requirements technical specifications and requirements of regulatory documents in Russian Federation, and experience in the design and operation of WWER reactors in Russia. In our calculation, we used OpenMC Monte Carlo simulation platform, which is a powerful simulation platform for analyzing integral parameters of nuclear reactors using continuous energy cross-section data provided by the NNDC.

The aspects of this study with different enrichments of the fuel assembly of WWER-1200 reactor were compared and verified the values of multiplication factor [9], which calculated in this OpenMC simulation with two codes (Serpent and UNK) and showed reasonable agreement with each other. The integral parameters show no significant differences between UNK and OpenMC except for the value of the diffusion coefficient. This reflects that the benchmark models developed by the OpenMC code was good in predicting the integral parameters of light water reactors, while the slight difference between the other

parameters are due to the different solution methods of each code with its associated nuclear data. Therefore, Monte Carlo code OpenMC is a reliable neutronic code to make calculation scheme and nuclear data for further neutronic analysis.

REFERENCES

[1] V. G. Asmolov, I. N. Gusev, V. R. Kazanskiy, V. P. Povarov, and D. B. Statsura, "New generation first-of-the kind unit – VVER-1200 design features," *Nucl. Energy Technol.*, vol. 3, no. 4, pp. 260–269, Dec. 2017.

[2] S. B. Ryzhov *et al.*, "VVER-Type Reactors of Russian Design," in *Handbook of Nuclear Engineering*, Springer US, 2010, pp. 2249–2320.

[3] S. Dawahra, K. Khattab, and G. Saba, "Study the effects of different reflector types on the neutronic parameters of the 10 MW MTR reactor using the MCNP4C code," *Ann. Nucl. Energy*, vol. 85, pp. 1115–1118, Apr. 2015.

[4] P. K. Romano, N. E. Horelik, B. R. Herman, A. G. Nelson, B. Forget, and K. Smith, "OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development," *Ann. Nucl. Energy*, vol. 82, pp. 90–97, 2015.

[5] E. Breismeister, J.F., "MCNP - A General Monte Carlo N-Particle Transport Code," Los Alamos, 1997.

[6] J.Leppänen., *Serpent – a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code*. VTT Technical Research Centre of Finland, 2015.

[7] В. Ф. Цибульский, В.Ф. Давиденко, "UNK программа детального расчета спектра в элементарной ячейке реактора," Нейтроника-97, 2008.

[8] J. O. Zhaoyuan Liu a, Kord Smith a, Benoit Forget a, "Cumulative migration method for computing rigorous diffusion coefficients and transport cross sections from Monte Carlo," *Ann. Nucl. Energy*, vol. 112, pp. 507–516, 2018.

[9] C. K. S. and M. S. M,"Burnup dependent Monte Carlo neutron physics calculations of IAEA MTR benchmark," *Prog.Nucl.Energy*, vol. 81, pp. 43–52, 2015.

Validation of the Physical Parameters of Monte Carlo Code Openmc by Unk Code for Different WWER 1200 Fuel Assemblies

H.A. Tanash[1], D.A.Solovyev[2], V.G.Zimin[3], A.A.Semenov[4], N.V. Schukin[5], B. Djaroum[6], A.I. Al-Shamayleh[7]

National Research Nuclear University «MEPhI», Kashirskoye shosse, 31, Moscow, Russia 115409

[1]ORCID iD: 0000-0002-7831-8516
e-mail: tanash_hamza@yahoo.com
[2]ORCID iD: 0000-0002-0507-0839
e-mail: vulture@inbox.ru
[3]ORCID iD: 0000-0002-0334-3741
e-mail: vgzimin@mail.ru
[4]ORCID iD: 0000-0002-5495-3662
e-mail: dozaand@mail.ru
[5]ORCID iD: 0000-0002-4228-7228
e-mail: pikenv@gmail.com
[6]ORCID iD: 0000-0002-1862-8838
e-mail: bel.djar111215@gmail.com
[7]ORCID iD: 0000-0002-7831-8516
e-mail: tanash_hamza@yahoo.com