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Verification of Monte Carlo Code OpenMC using VVER-1000 MOX Fuel Assembly against Criticality Benchmark Data

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ABSTRACT

In this study open source Monte Carlo code OpenMC is verified by evaluating criticality results with established benchmark data. OpenMC code has been chosen for this study as it uses three-dimensional and continuous-energy simulation which reduces all errors due to cross-section processing and geometry modeling approximations. The correctness of nuclear data used plays an important role in nuclear reactor and assembly configuration calculation and modeling also. The primary objective of this study is achieved by comparing the obtained values of effective multiplication factor using OpenMC code on designed model with the benchmark VVER-1000 mixed oxide (MOX) fuel assembly values provided by OECD Nuclear Energy Agency. Construction of fuel assembly geometry was performed using python programming language implementing the OpenMC application program interface for python. Updated standard continuous energy cross section data ENDF format of ENDF/B-VIII library and JEFF3.2 library in various temperatures were used to ensure the independence of nuclear data. The comparison of simulation results with benchmark data are analyzed and discussed in this paper including performance of the Monte Carlo OpenMC code.

Key words: OpenMC, Simulation, Neutronics, Benchmark, VVER

1. Introduction

Development of modern computers enabled high-fidelity modeling of nuclear assemblies and to utilize the power of latest parallel computing the open source Monte Carlo [1] reactor physics code OpenMC [2] have been developed. Other and more widely used Monte Carlo programs include codes such as MCNP [3] and SERPENT [4]. Any simulation code must be verified by modeling and simulating existing nuclear assembly specifications and comparing the results of simulation with the experimentally obtained data.

This ensures accuracy of simulations computed with this particular code is within acceptance. In this study, the calculated K_{eff} values obtained from the OpenMC simulation using the standard nuclear data library have been compared with the benchmark values. The benchmark chosen for this study is the VVER-1000 mixed oxide (MOX) fuel assembly [5] values provided by OECD Nuclear Energy Agency and it has been evaluated by multiple deterministic and

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probabilistic codes and also experimentally determined. The calculation simulation contains of 400 iterations with 100,000 particles per cycle. Large number of cycle and particles ensure lower value of statistical error (less than 0.1%). Modeling of fuel assembly with OpenMC and simulation using the standard ENDF/B-VIII [6] (Evaluated Nuclear Data Files, US based) nuclear data library has been performed successfully in the present study. JEFF-3.2 [7] (The Joint Evaluated Fission and Fusion Nuclear Data Library, EU based) library was also used to ensure the results are independent of nuclear data source and stable. Percent error was assessed from the OpenMC results, and values calculated were less than 5%. Thus the results presented in this study could be considered an approximate solution for the considered benchmark problem. It can be used as a reference for comparing performance of solutions based on Monte Carlo method.

2. OpenMC analysis of assembly

2.1 Geometry and Material specification

The VVER-1000 assembly like the other VVER designs is arranged in hexagonal formation. This particular assembly consists of 312 locations for fuel pins of which 12 positions are for the control rods. And an additional 18 locations are provided for guide tubes. There is also a central tube for the assembly. The composition of clad and structural material is Zr-Nb alloy. The Mixed oxide assembly in Figure 1 is made of three different loadings of plutonium. The regions are –

i. The central region pins of MOX fuel with fissile plutonium of 4.2 wt. % which consists of 93 wt. % ^{239}Pu

ii. Two middle rings of pins with fissile plutonium of 3.0 wt. %

iii. One outer ring of pins with fissile plutonium of 2.0 wt. %

The MOX assembly configuration specified in the benchmark specifications is presented in figure 1 -

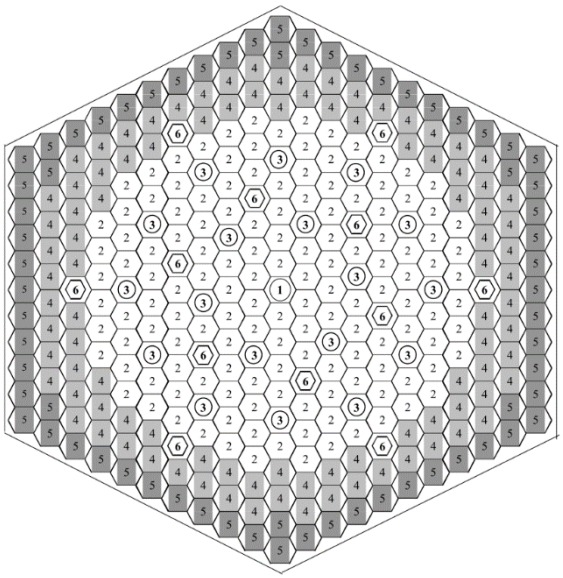

Fig. 1: MOX assembly configuration

Cells are divided into 6 types in the VVER-1000 MOX assembly –

Two types of tube cell (central and guide tube), three types of MOX cell (containing 4.2, 3.0 and 2.0 wt. % of Pu) and a fuel cell containing gadolinium (3.6 wt. %Uranium and 4.0 wt. % Gd_2O_3)

The geometry of a single cell according to benchmark specifications is presented in figure 2 -

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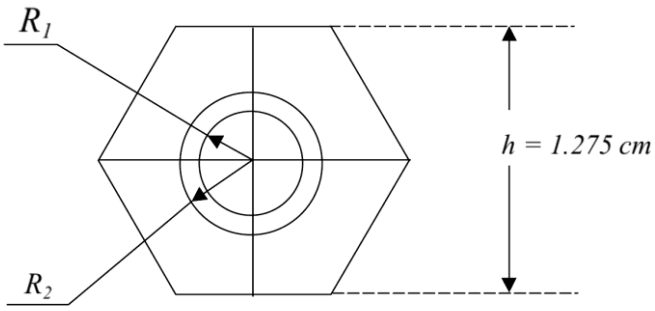

Fig. 2: Cell geometry

Table 1: Description of cell types geometry [5]

Cell Name	Zone Radius (cm)
Fuel cell	R1 = 0.386 R2 = 0.4582
Central tube cell	R1 = 0.48 R2 = 0.5626
Guide tube cell	R1 = 0.545 R2 = 0.6323

Table 2: Material description [5]

Material Name	Isotopic Content	
	Isotopes	Atoms / barn cm^3
U1 (LEU)	^{235}U ^{238}U ^{16}O	8.6264E-4 2.2169E-2 4.6063E-2
PU1 (MOX)	^{235}U ^{238}U ^{16}O ^{239}Pu ^{240}Pu ^{241}Pu	4.2672E-5 2.1025E-2 4.3047E-2 4.2414E-4 2.7250E-5 4.5228E-6
	^{235}U ^{238}U	4.2209E-5 2.0797E-2

ISSN: 2411-9997

PU2 (MOX)	^{16}O ^{239}Pu ^{240}Pu ^{241}Pu	4.3045E-2 6.3621E-4 4.0875E-5 6.7842E-6
PU3 (MOX)	^{235}U ^{238}U ^{16}O ^{239}Pu ^{240}Pu ^{241}Pu	4.1652E-5 2.0522E-2 4.3043E-2 8.9071E-4 5.7225E-5 9.4980E-6
GD1 (LEU & Gadolinium)	^{235}U ^{238}U ^{16}O ^{152}Gd ^{154}Gd ^{155}Gd ^{156}Gd ^{157}Gd ^{158}Gd ^{160}Gd	7.2875E-4 1.9268E-2 4.1854E-2 2.5159E-6 2.7303E-5 1.8541E-4 2.5602E-4 1.9480E-4 3.0715E-4 2.6706E-4

ISSN: 2411-9997

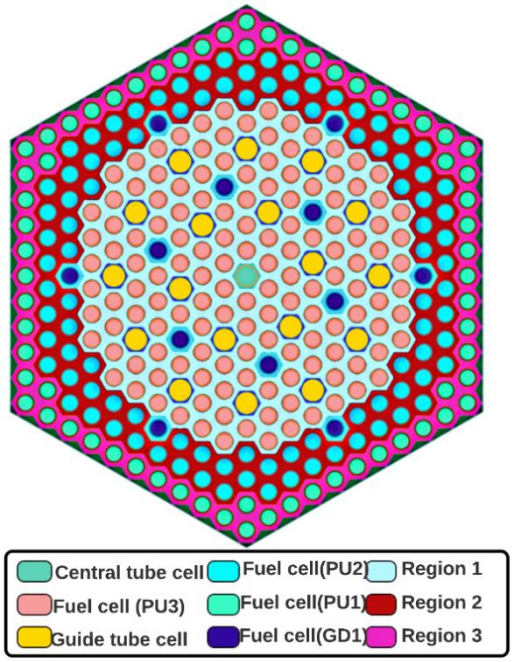

Fig. 3: OpenMC generated profiled MOX Fuel Assembly 2D section visualized using Matplotlib

2.2 Monte Carlo method

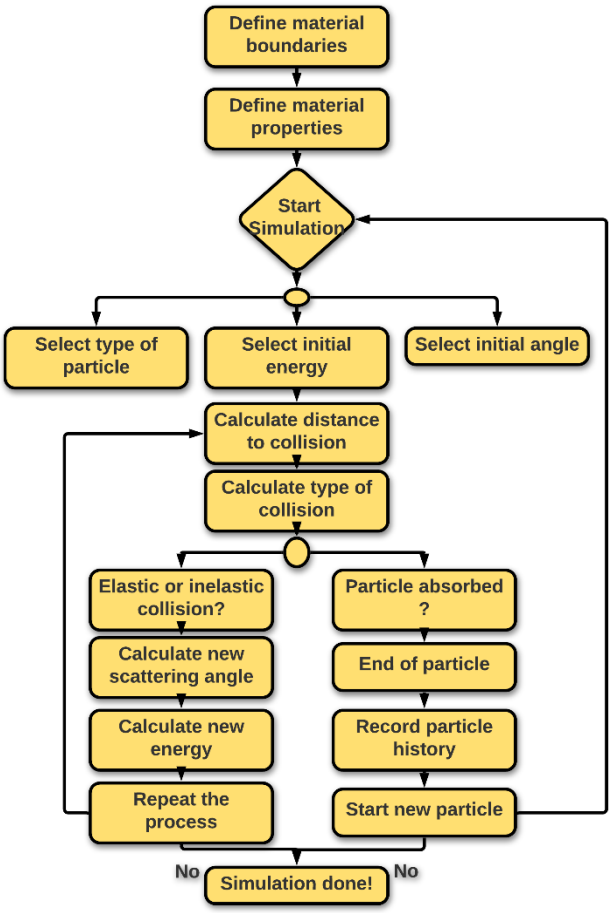

Fig. 4: Flow diagram of Monte Carlo method

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The Monte Carlo method used in this study is shown in figure 4 diagram. It represents the simplified steps involved in the simulation process. In this study the code version used was OpenMC – 0.10.0. This is a random walk process. Where particles interact with other particles or atoms with various chance of reaction. The chances of reaction are described by cross sections of those reactions. These continuous cross section data are contained in the various standard nuclear data libraries. By implementing the Monte Carlo method using the data libraries on specifically designed models and materials various neutronic parameter can be evaluated.

3. Results

Table 3: K_{eff} values of benchmark calculated using reference codes compared with OpenMC calculation

SL	Codes	K_{inf}	Mean	Deviation (from mean)
1	MCU	1.1551	1.1566	-0.002
2	TVS-M	1.1585		0.002
3	WIMS8A	1.1494		-0.007
4	HELIOS	1.1595		0.003
5	MULTICELL	1.1606		0.004
6	**OpenMC(JEFF – 3.2)**	**1.1984**		-0.0418
7	**OpenMC(ENDF-B/VIII)**	**1.2008**		-0.0442
8	VISWAM(JEFF -3.1)	1.1899		-0.0333

From the values presented above the deviation percentage can be calculated for OpenMC using JEFF-3.2 as **3.6%** and for ENDF-B/VIII it is **3.8%.** Also it should be noted that apart from OpenMC the VISWAM code is the latest of all and the results from OpenMC matches most with the VISWAM results **(only 0.7% deviation** using JEFF library).

4. Conclusion

Neutronics simulation is an important step in the design and verification of reactor cores. The simulated assembly in this work showed good agreement with the other standard codes results showing less than 4% deviation in average, which clearly indicates the validity of the OpenMC code. Due to limited resources the study was conducted in a narrow scope. With more rigorously detailed models and material specification coupled with higher computational power the achievement of lower levels of error could be a possibility. With wider available configurations of mixed oxide fuels a more in-depth study can be conducted. Assembly simulations done in this study can be further extended to perform a full core analysis of VVER-1200 in future.

References

ISSN: 2411-9997

[1] Nicholas Metropolis & S. Ulam (1949) The Monte Carlo Method, Journal of the American Statistical Association, 44:247, 335-341, DOI: 10.1080/01621459.1949.10483310

[2] 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

[3] X-5 Monte Carlo Team, "MCNP- A General MC N-Particle Transport Code, Version 5," vol. 836, 2008.

[4] J. Leppänen, "Serpent – a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code, VTT Technical Research Centre of Finland, March 6," 2013.

[5] A VVER-1000 LEU and MOX Assembly Computational Benchmark. Nuclear Energy Agency, Organisation for Economic Co-operation and Development, NEA/NSC/DOC 10, 2002.

[6] D.A. Brown, Chadwick, et al. ENDF/B-VIII.0: The 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data Nucl. Data Sheets, 148 (2018), pp. 1-142, 10.1016/j.nds.2018.02.001

[7] OECD/NEA Data Bank, JEFF-3.2 Evaluated Data Library - Neutron data (2014), http://www.oecd-nea.org/dbforms/data/eva/evatapes/jeff_32/

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