Simulation of LEU and MOX fuels in Russian VVER-1000 reactor with the OpenMC code and recent data libraries

TAOUFIQ BOUASSA [1], ABDELOUAHED CHETAINE [1], ABDELHAMID JALIL [1], OUADIE KABACH [1], HAMID AMSIL [2]
[1] Mohammed V University of Rabat (Rabat, Morocco)
[2] Nuclear Center of Energy Science and Nuclear Technics, Rabat, Morocco
taoufiqbouassa@gmail.com

Abstract

This article analyses the OpenMC Monte Carlo code's ability to predict eigenvalue values for low-enriched uranium (LEU) and weapons-grade (MOX) fuel assemblies of the Russian VVER-1000 reactor. Besides, the differences in performance of the five most recent data libraries, i.e. ENDF/B-VII.0, ENDF/B-VII.1, ENDF/B-VIII.0, JEFF-3.2, and JEFF-3.3 have been evaluated by comparing the resulting reactivities of three calculation states, namely soluble boron effect, Fuel temperature (Doppler) effect, and total temperature effect.

Keywords: OpenMC code, Monte Carlo, eigenvalue calculation, nuclear data libraries, VVER-1000 assembly.

1. Introduction

Experts Groups have proposed and carried out several numerical benchmark exercises that involve comparing different code results for reference calculations as a form of code verification and as a means of evaluating code performance concerning other codes and data used by industry and research [[1],[2]]. However, extensive and systematic comparisons of calculated values and experimental data are required to validate the simulation tools' performances. As a result, the primary goal of this work is to analyze the VVER-1000 LEU and MOX assembly computational benchmark [3] using Monte Carlo simulations by OpenMC code [4] and recent data libraries, namely ENDF/B-VII.0, ENDF/B-VII.1, ENDF/B-VIII.0, and JEFF-3.2 [[5],[6],[7],[8],[9]], and to compare the results with the references. The OECD/NEA Expert Group proposed the VVER-1000 LEU and MOX assembly computational benchmark as a theoretical benchmark for investigating the physics of a whole VVER-1000 reactor core using two-thirds (LEU) and one-third (MOX) fuel [[10],[11]]. The OpenMC Monte Carlo version 0.13 was used in this study. For calculations, continuous energy cross-section data were taken from the HDF5 format, which can be generated from the ENDF format or the ACE file using the script integrated with the code for data library utilizations. The results of the above-mentioned libraries are intercomparisoned, and the reasons for the differences in the results are discussed.

2. Assembly description

VVER-1000 LEU and MOX assembly computational benchmark are proposed by Experts Group established at OECD/NEA to study the neutronics properties of VVER-1000 core with 30% MOX-fuel loading. The geometry and material composition specifications described in the benchmark report were used in the current study [3]. The following is a brief description.

The benchmark models used in this study include two different assemblies that are typical of the VVER-1000's advanced designs (i.e. UGD and MOXGD). Each assembly is hexagonal and is made up of one central tube, 312 fuel pin locations (12 of which are U/Gd rods), and 18 guide tubes.

In the UGD assembly (Figure 1), the enrichment of the fuel rods is 3.7 wt.% in U-235, the 12 U/Gd pins have a Gd_2O_3 content of 4.0 wt.% and the U-235 enrichment is set to 3.6 wt.%. The MOXGD assembly contains three different zones of fuel rods. The central zone contains MOX pins containing 4.2 wt.% fissile plutonium, the inner ring of fuel rods containing 3.0 wt.% fissile plutonium, and the outer ring of fuel rods containing 2.0 wt.% fissile plutonium. The positions of the U/Gd rods in the MOXGD assembly are identical to those in the UGD assembly (Figure 2). For, the clad and structural material in both studied assemblies are Zr-Nb alloys.

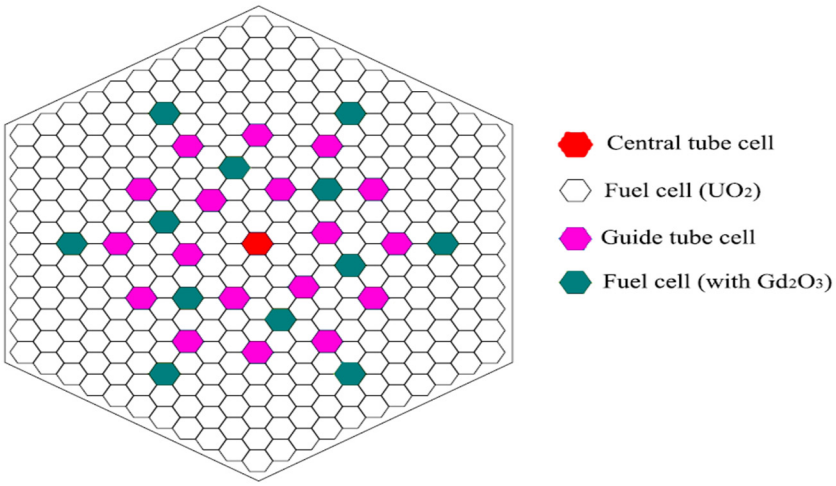

Figure 1. VVER-1000 assembly with LEU fuel

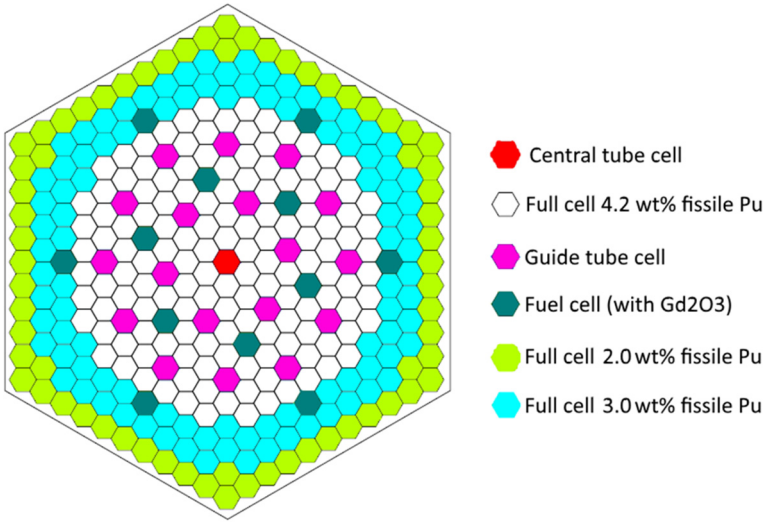

Figure 2. VVER-1000 assembly with MOX fuel

3. Calculation method

OpenMC [4] is a three-dimensional continuous-energy Monte Carlo particle transport code designed for a variety of applications such as reactor physics calculations, fuel cell and assembly calculations, spatial homogenization, few energy-group cross-section generations, full core criticality calculations, and fuel cycle studies. The geometry construction in the OpenMC code is based on constructive solid geometry with second-order surfaces. The cross-sections of interaction for continuous energy were based on a native HDF5 format that can be generated from the ENDF format or the ACE file using the script integrated with the code for data library utilizations.

The calculations in the OpenMC code for the determination of eigenvalues (i.e. K-inf) were done using 1000 neutron cycles with 100 non-active cycles and 106 histories per generation. For each proposed library, four calculations were performed, one for each of the operation states S2 - S5 described in Table 1. The fuel temperature used in this simulation is 1200 K rather than 1027 K. The resulting reactivities, as described below, have been calculated and compared to the benchmark K-inf mean.

1) Reactivity of the effect of the soluble boron 600 ppm, which has been calculated based on the K-inf values corresponding to reactor states S3 and S4;
2) Reactivity due to fuel temperature change from 575 K to 1027 K (Doppler), which has been calculated based on the K-inf values corresponding to the reactor states S2 and S3;
3) The reactivity resulted from the change of the temperature of the assembly from 300 K to 575 K, which has been calculated based on K-inf values corresponding to the reactor states S4 and S5.

Table 1. Assembly state descriptions [10].

State	Description	Fuel temp. (K)	Non-fuel temp. (K)	Soluble Boron [ppm]
S2	Operating non-poisoned state	1027	575	600
S3	Hot state	575	575	600
S4	Hot state without boron acid	575	575	0
S5	Cold state	300	300	0

4. Result and discussion

The results of the simulations of the UGD assembly and the benchmark mean are presented in table 2. The (C/E-1) (i.e. calculated to expected value) values in pcm are shown in Figure 1, based on the results. For the states S2, S3, and S4, for all the libraries the values of K-inf are lower than the mean. The results based on JEFF-3.2 have a higher difference compared to other libraries which have a good agreement with each other according to (C/E-1) value. On the other hand, for the S5 state have a positive (C/E-1) value.

Table 2. UGD results of K-inf using OpenMC.

State	B.mean*	ENDFVII.0	ENDFVII.1	ENDFVIII.0	JEFF-3.2	JEFF-3.3
S2	1.1754	1.1704+/-0.0003	1.1711+/-0.0003	1.1699+/-0.0003	1.1660+/-0.0003	1.1707+/-0.0003
S3	1.1891	1.1876+/-0.0003	1.1877+/-0.0003	1.1865+/-0.0003	1.1836+/-0.0003	1.1880+/-0.0003
S4	1.2489	1.2476+/-0.0003	1.2472+/-0.0003	1.24582+/-0.0003	1.2427+/-0.0003	1.2466+/-0.0003
S5	1.3175	1.3230+/-0.0003	1.3227+/-0.0003	1.31929+/-0.0003	1.3215+/-0.0003	1.3223+/-0.0003
* benchmark mean						

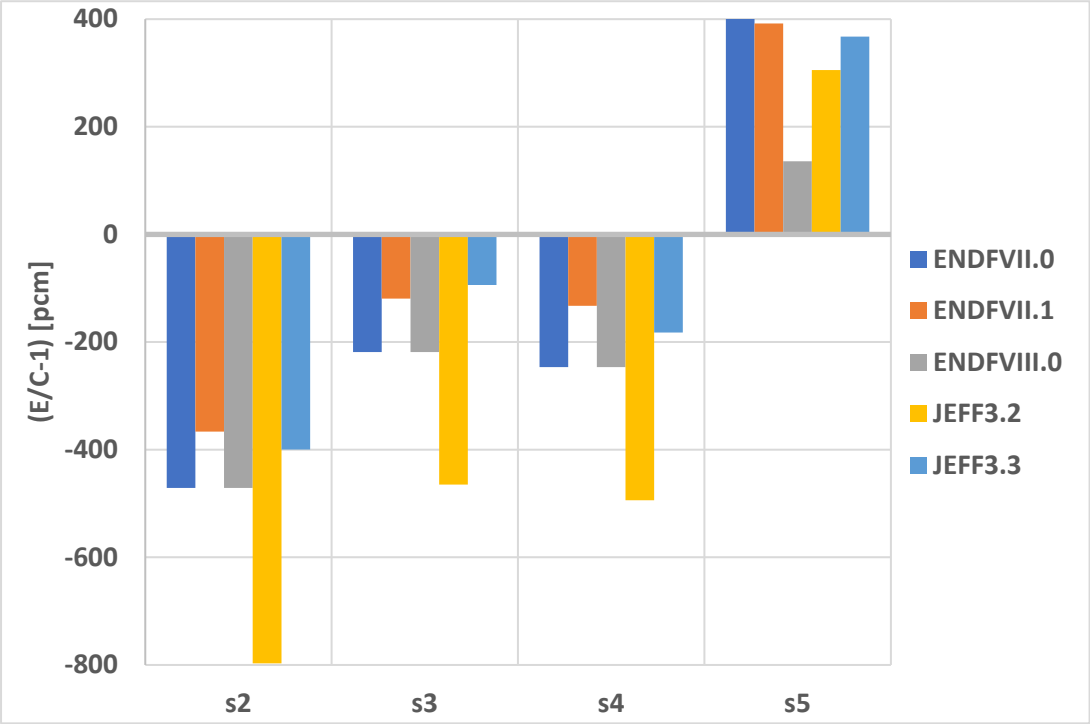

Figure 3. Values of (C/E-1) in pcm per state, UGD assembly

For MOXGD assembly the results are shown in Table 3. The values of (C/E-1) for the S2 are in very code agreements except for the library ENDFVII.1 that has the negative higher value of -325 pcm. The values of the (C/E-1) are around 300-400 pcm; however for the library ENDFVII.1 they have the lower values -23, -97 for S3 and S4 respectively. Finally, for S5 the values of the (C/E-1) are around 500 pcm.

Table 3. MOXGD results of K-inf using OpenMC.

State	B.mean	ENDFVII.0	ENDFVII.1	ENDFVIII.0	JEFF-3.2	JEFF-3.3
S2	1.1899	1.1899+/-0.0003	1.1860+/-0.0003	1.1908+/-0.0003	1.1914+/-0.0003	1.1914+/-0.0003
S3	1.2073	1.2113+/-0.0003	1.2070+/-0.0003	1.2117+/-0.0003	1.2124+/-0.0003	1.2124+/-0.0003
S4	1.2422	1.2456+/-0.0003	1.2409+/-0.0003	1.2459+/-0.0003	1.2469+/-0.0003	1.2469+/-0.0003
S5	1.3209	1.3289+/-0.0003	1.3267+/-0.0003	1.3285+/-0.0003	1.3280+/-0.0003	1.3280+/-0.0003

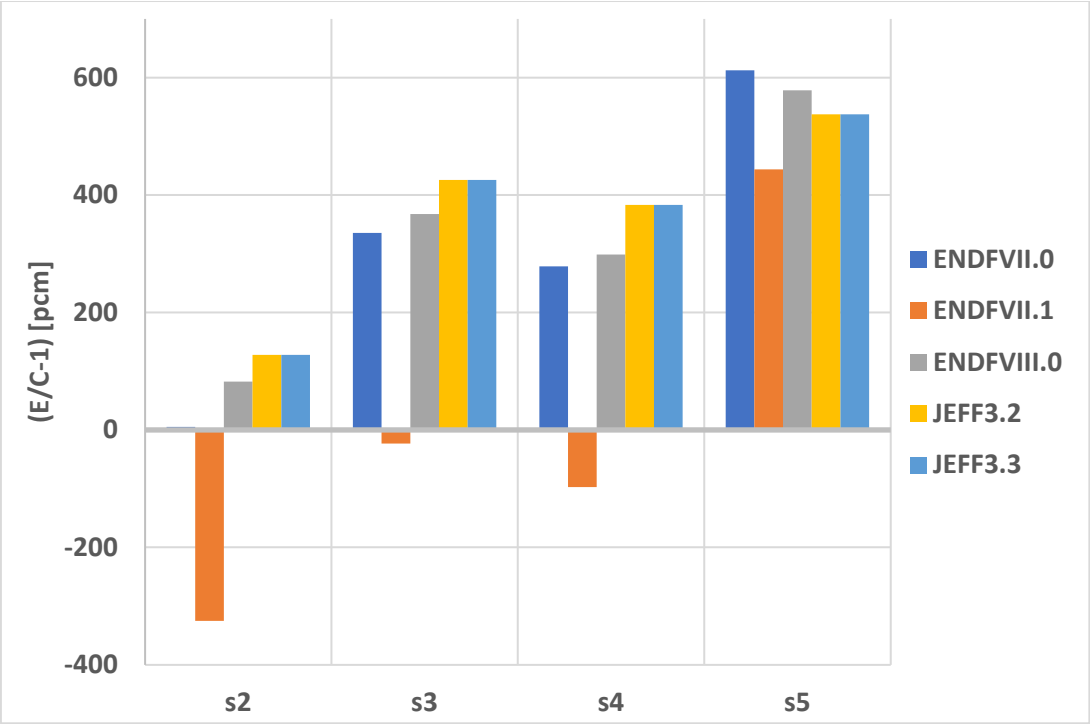

Figure 4. Values of (C/E-1) in pcm per state, MOXGD assembly

From Tables 4 and 5, the values of the reactivity effect of fuel temperature and total temperature effect are higher than the benchmark means. On other hand, the reactivity of the soluble boron effect values is in good agreement with the benchmark provided data.

Table 4. Variant. Reactivity effects for UGD. (K_{Si} means K-inf at the state Si)

	B.mean	ENDFVII.0	ENDFVII.1	ENDFVIII.0	JEFF-3.2	JEFF-3.3
Fuel temperature (Doppler) effect, [(K_{S2}-K_{S3}) *100]	-1,37	-1,72	-1,66	-1,66	-1,75	-1,73
Soluble boron effect, [(K_{S3}-K_{S4}) *100]	-5,98	-6,00	-5,96	-5,93	-5,92	-5,86
Total temperature effect, [(K_{S4}-K_{S5}) *100]	-6,86	-7,53	-7,54	-7,35	-7,88	-7,57

Table 5. Variant. Reactivity effects for MOXGD.

	B.mean	ENDFVII.0	ENDFVII.1	ENDFVIII.0	JEFF-3.2	JEFF-3.3
Fuel temperature (Doppler) effect, [(K_{S2}-K_{S3}) *100]	-1,74	-2,13	-2,09	-2,08	-2,10	-2,10
Soluble boron effect, [(KS3-K_{S4}) *100]	-3,49	-3,43	-3,39	-3,41	-3,45	-3,45
Total temperature effect, [(K_{S4}-K_{S5}) *100]	-7,87	-8,33	-8,57	-8,26	-8,10	-8,10

Generally, the reactivity of the total temperature effect for MOXGD assembly is lower than UGD assembly. Where this difference varies between the libraries, 12 %, 7 %, 4 %,2 %, and 1 % respectively for library JEFF-3.2, JEFF-3.3, ENDFVII.0, ENDFVIII.0 and, ENDFVII.1.

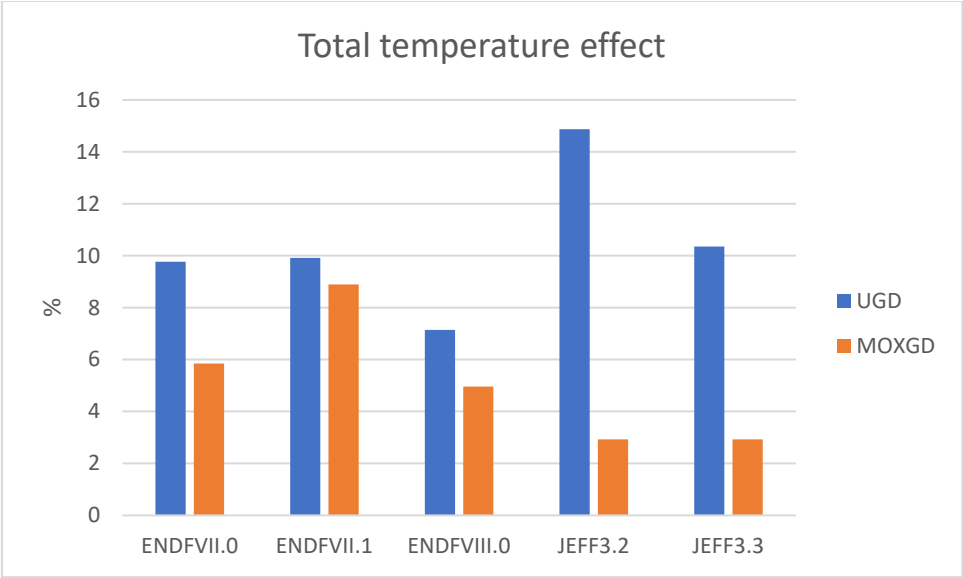

Figure 5. Values of reactivity total temperature effect in % per library

On the another hand, the reactivity of the soluble boron effect has the lowest deviation compared with other reactivities effects. Furthermore, these values are higher using libraries ENDF's for assembly MOXGD compared to JEFF-3.3. Where in case using JEFF--3.2 there is an equality in value of the reactivity about -1%.

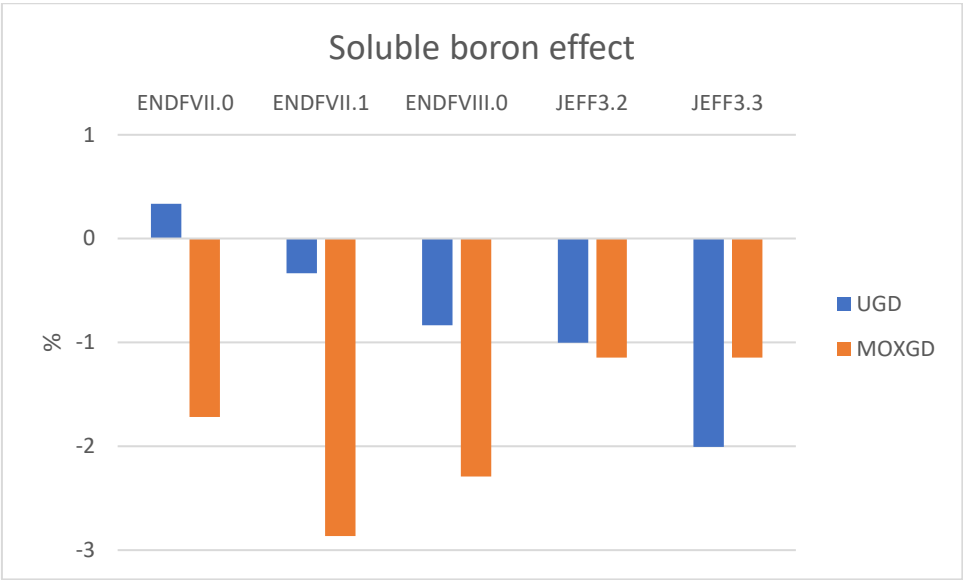

Figure 6. Values of reactivity soluble boron effect in % per library

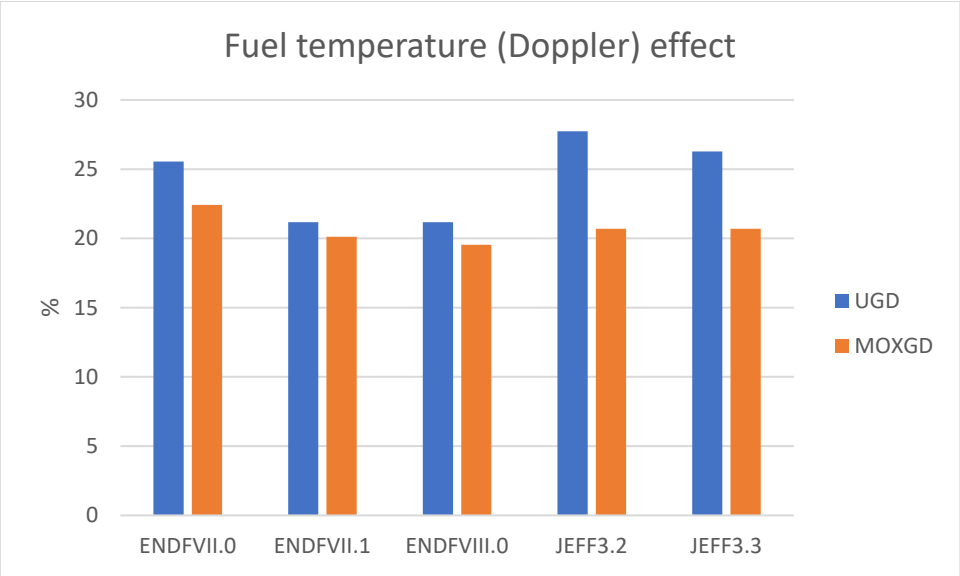

Figure 7. Values of reactivity fuel temperature (Doppler) effect in % per library

5. Conclusion

In this study, OpenMC was used to calculate the simulation of the VVER-1000 reactor core's UGD and MOXGD fuel assemblies using several cross-section libraries. When compared to the OECD/NEA group's benchmark mean results, the K-inf results show generally good agreement. Other findings revealed:

- Compared to other libraries, using JEFF-3.2 in UGD assembly results in a minor deviation for the states S2, S3, and S4.
- ENDFVII.0 has a lower deviation of 5 pcm for MOXGD, whereas ENDFVII.1 has a higher standard deviation of -325 pcm for the case state S2. ENDFVII.1 has the lowest deviation for S3 and S4.
- Rather than the cases mentioned above, most cases have minor deviations and the variations in the reactivity effect are virtually the same.

References

[1] L. Mercatali, N. Beydogan, and V. H. Sanchez-Espinoza, “Simulation of low-enriched uranium burnup in Russian VVER-1000 reactors with the Serpent Monte-Carlo code,” *Nucl. Eng. Technol.*, 2021.

[2] O. Kabach, A. Chetaine, A. Benchrif, and H. Amsil, “An inter-comparison between ENDF/B-VIII.0-NECP-Atlas and ENDF/B-VIII.0-NJOY results for criticality safety benchmarks and benchmarks on the reactivity temperature coefficient,” *Nucl. Eng. Technol.*, vol. 53, no. 8, pp. 2445–2453, Aug. 2021.

[3] NEA, *A VVER-1000 LEU and MOX Assembly Computational Benchmark Specification and Results*. 2002.

[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, Aug. 2015.

[5] M. B. Chadwick *et al.*, “ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology,” *Nucl. Data Sheets*, vol. 107, no. 12, pp.

2931–3060, 2006.

[6] M. B. Chadwick *et al.*, “ENDF/B-VII.1 nuclear data for science and technology: Cross sections, covariances, fission product yields and decay data,” *Nucl. Data Sheets*, vol. 112, no. 12, pp. 2887–2996, 2011.

[7] D. A. Brown *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*, vol. 148, pp. 1–142, 2018.

[8] O. Cabellos, “Processing of the new JEFF-3.2T4 Cross Section Library with the NJOY Code System into Various Formats for Testing Purposes,” no. February, 2014.

[9] O. Cabellos *et al.*, “Benchmarking and validation activities within JEFF project,” *EPJ Web Conf.*, vol. 146, p. 06004, 2017.

[10] L. Thilagam, V. Jagannathan, C. Sunil sunny, and K. V. Subbaiah, “VVER-1000 MOX Core Computational Benchmark analysis using indigenous codes EXCEL, TRIHEX-FA and HEXPIN,” *Ann. Nucl. Energy*, vol. 36, no. 10, pp. 1502–1515, 2009.

[11] L. Thilagam, R. Karthikeyan, V. Jagannathan, K. V. Subbaiah, and S. M. Lee, “Inter-comparison of JEF-2.2 and JEFF-3.1 evaluated nuclear data through Monte Carlo analysis of VVER-1000 MOX Core Computational Benchmark,” *Ann. Nucl. Energy*, vol. 37, no. 2, pp. 144–165, 2010.