EPJ Web of Conferences **302**, 07006 (2024) https://doi.org/10.1051/epjconf/202430207006
SNA + MC 2024

Discrepancy across various OpenMC versions due to thermal neutron scattering law

Tianxiang Wang[1], *Shengli* Chen[1*], *Shuqi* Xu[2], *Zhuo* Li[1]

[1]Sino-French Institute of Nuclear Engineering and Technology, Sun Yat-sen University, Zhuhai, 519082, Guangdong, China
[2]European Spallation Source ERIC, Box 176, Lund, SE-221 00, Sweden

Abstract. The performance of neutron transport calculations is heavily reliant on the fidelity of nuclear data. The Free Gas Model (FGM) is no longer applicable at low neutron energy range due to nucleus binding effects, necessitating the implementation of the Thermal Scattering Law (TSL). The present study systematically reports the unexpected discrepancies in k_{eff} calculations with TSL across different versions of OpenMC, an open-source Monte Carlo code developed by MIT. Based on four representative benchmark series (HMT-026, HMT-027, BEAVRS, and TRIGA fuel rod), the analysis reveals that updates in OpenMC v0.13.0 significantly contribute to these discrepancies, sometimes up to ~1000 pcm. After further review, a modification in the source code for coherent elastic scattering (suggestion #1949) may affect the sampling of the cosine of the coherent scattering angle. Additionally, recompilation of OpenMC v13.2 using the older segment code aligns reactivity calculations closely with version 0.12.2 and thus confirms the above conclusion. Nevertheless, both the developers and we are still uncertain whether this update is correct until now. A systematic examination of the source code is necessary in the near future. Another direct conclusion from the present study is the importance of including diverse benchmarks for code verification and validation.

1 Introduction

The performance of reactor simulations relies on the fidelity of nuclear data used in neutron transport calculations. In most cases, the target nuclei are treated as free gas that does not interact with other nuclei during neutron moderation. This approach is referred to as the Free Gas Model (FGM). However, when fission neutrons are moderated to a low energy range (often below a few eV) in thermal reactors, the aforementioned FGM is no longer applicable because the binding of the scattering nucleus in a solid, liquid, or gas moderator material significantly influences the neutron cross section as well as the energy and angular distributions of secondary neutrons [1, 2], which in turn affect the reactor physics calculations. Thus, a more accurate description of this scattering process, known as Thermal Scattering Law (TSL), contributes to improving the accuracy of numerical simulations.

* Corresponding author: chenshli23@mail.sysu.edu.cn

Monte Carlo simulation is a key tool for numerically studying intractable problems and widely used to solve particle transport equations. OpenMC, originally initiated by the Massachusetts Institute of Technology (MIT) since 2011 and under development, is an open-source Monte Carlo particle transport code that supports solid constructive geometry and continuous-energy cross sections [3]. Its simulation accuracy in some typical reactors has been validated and verified through comparisons with other codes and experiments, such as light water reactors [4], fast reactors [5], and others. Currently, it has been updated to the 0.15.0 stable version.

However, some discrepancies in k_{eff} calculations among different versions of the OpenMC code are discovered when employing TSL. Until now, these issues have not yet been publicly reported. In the present study, the differences are systematically compared across various OpenMC versions based on four representational benchmark series, which are described in Section 2. Additionally, the source code of the relevant version is checked and compared to identify the potential main issues inducing the discrepancy. Section 3 discusses the deviations across different versions and pinpoints the potential sources. Section 4 summarizes the principal conclusions of the present study.

2 Benchmark modelling

2.1 Graphite benchmarks

The simplified geometric configuration of the HMT-026 series is illustrated in **Fig. 1**. The reactor core is a 4×6 fuel elements lattice with a 13-cm pitch. The core is fully surrounded by graphite reflector blocks. The fuel element is designed in a tubular form and consists of metal U-Al with 37% uranium with 80% ^{235}U enrichment. The lateral layer of the fuel assembly consists of rectangular beryllium blocks for moderation. More details of these benchmarks are given in Refs [6, 7]. The reference k_{eff} values for all 27 experiments are consistently 0.9998±0.0041. The present study employs a total of 2.5×10^7 active histories for simulations, which result in statistical uncertainties of around 20 pcm. Additionally, the TSL for Be metal and graphite is used in simulations.

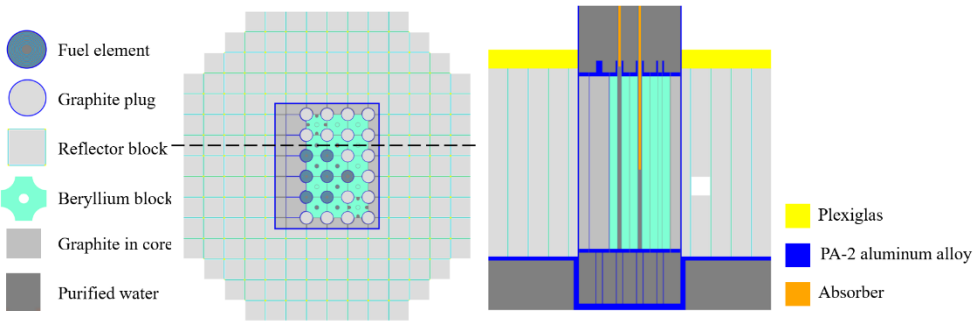

Fig. 1 Horizontal and vertical cross-sections (along the line) of the HMT-026 experiment [6].

2.2 BeO benchmarks

The HMT-027 series comprises a total of 15 experiments, characterized by relatively simple geometric configurations. In each experiment, one or more high-enriched uranium foils are stacked between BeO moderation blocks. These fuel foils are mostly in a square metal form, with dimensions of 5.25 inches by 5.25 inches and thicknesses of either 0.001 or 0.002 inches. For example, in experimental configuration 2, the specific parameters of this

assembly are 60.96×60.96 cm^2. Each column, 22 inches tall, is arranged in the pattern of a 4×4 design. The column is composed of a stack of BeO blocks, as shown in **Fig. 2**.

Since there are different stacking arrangements for each experiment, the BeO/^{235}U ratio varies from 247 to 7660. This not only highlights the significance of validating BeO data but also indicates the HMT-027 series as a suitable choice for validation of the related TSL. More details of these benchmarks can be found in Refs. [8, 9]. The present study employs a total of 10^7 histories for simulations, which results in statistical uncertainties of approximately 40 pcm.

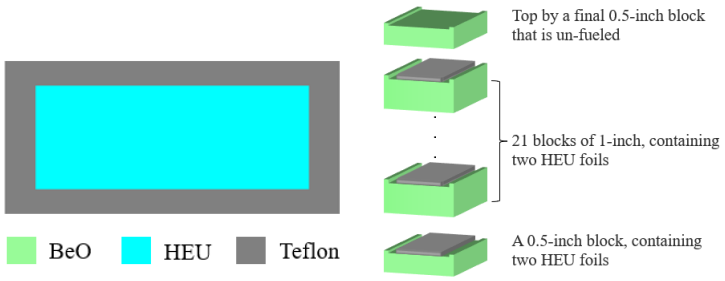

Fig. 2 Vertical cross-sections of HEU foil (left) and a 22-inch column (right) [6].

2.3 BEAVRS

BEAVRS is developed by the Massachusetts Institute of Technology (MIT) and now becomes one of the most important benchmarks in various directions of reactor physics study. This high-fidelity multi-physics benchmark enables researchers to test and validate the coupled neutron transport, thermal-hydraulics, and fuel isotopic depletion [10]. As shown in **Fig. 3**, the BEAVRS reactor is loaded with 193 varying fuel assemblies arranged in 17×17 and involved in five different enrichments: 1.6, 2.4, 3.1, 3.2, and 3.4 wt.% ^{235}U. The active fuel height measures 365.76 cm and includes components such as the Baffle, Core Barrel, and Neutron Shield Panel. The total heavy metal loading in BEAVRS amounts to 81.8 metric tons. Control rods are available in two types, constructed from Ag-In-Cd and B_4C, respectively. Simulations are performed employing a total of 2.5×10^9 histories, resulting in statistical uncertainties of approximately 2 pcm. Currently, only the TSL for H_2O is used in BEAVRS simulations.

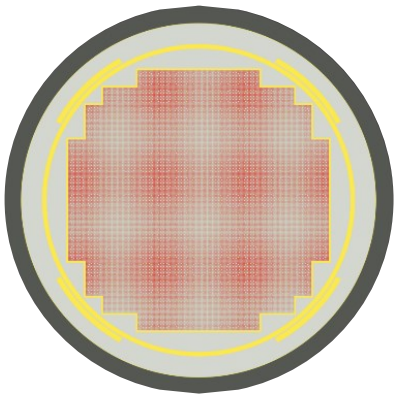

Fig. 3 Horizontal cross section of the BEAVRS benchmark.

2.4 TRIGA fuel rod

Given the significant enhancement in thermal conductivity, UO_2 doped with BeO has been proposed to increase the accident tolerance of the current nuclear fuel [11, 12]. The present study also evaluates the discrepancy in reactivity calculation across different versions of OpenMC for UO_2-BeO fuel. For simplicity and to reduce the computation burden, the present work includes the fuel rod of TRIGA, as the geometry shown **Fig. 4**. The studied fuel consists of a BeO volume fraction of 36.4% and a ^{235}U enrichment of 4.9% [13]. The simulation is performed with a total of 2.5×10^9 histories, leading to uncertainties around 2 pcm. Additionally, the TSL for H_2O or BeO is employed to facilitate direct comparison with the BEAVRS or HMT-027 benchmarks, which also utilize the same TSL.

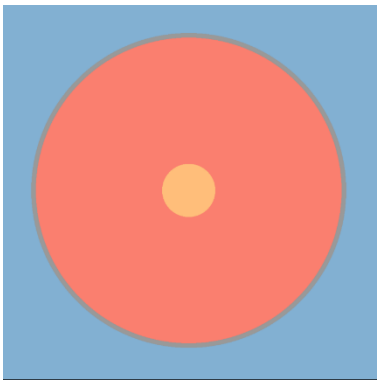

Fig. 4 Horizontal cross section of the TRIGA fuel rod benchmark. (From inside to outside: zirconium alloy, BeO-doped UO_2, stainless steel, and water.)

3 Results and discussion

3.1 Discrepancy across various versions

The reactivity differences between the 0.13.0-dev and 0.13.4-dev versions are shown in **Fig. 5**. The discrepancy remains within one standard deviation (1σ) when the TSL for any material is not considered. However, employing the TSL leads to an increase in deviation, even reaching nearly 1000 pcm (vs. ~40 pcm statistical uncertainty) for HMT-027-015. As the examples of HMT-027 benchmarks, this discrepancy becomes more pronounced with increasing content of materials related to the TSL.

To more precisely highlight discrepancies among each version, the reactivity calculations corresponding to these versions are presented in **Fig. 6**. Notably, the significant discrepancy is primarily observed between versions 0.12.2-stable (in fact, including 0.13.0-dev) and 0.13.0-stable, suggesting that the main sources inducing such large discrepancy is due to some updates in 0.13.0 release. However, according to the release notes of version 0.13.0-stable, the modification concerning the thermal scattering law is only limited to changes in the function to get the TSL name (suggestion #1945), which typically should not affect the computational process [14].

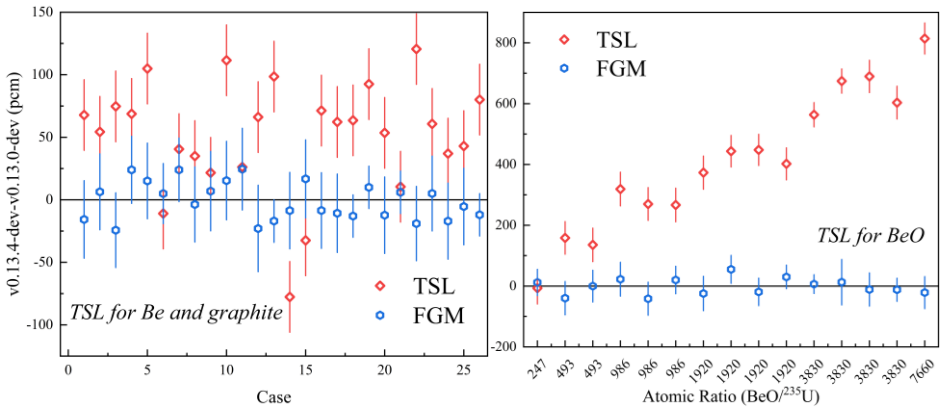

Fig. 5 Difference in k_{eff} between OpenMC 0.13.4-dev and 0.13.0-dev versions, with and without considering TSL(s). (Left: HMT-026; Right: HMT-027).

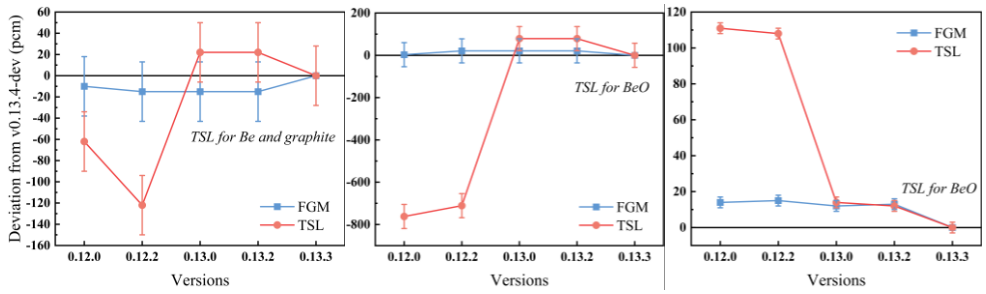

Fig. 6 Reactivity deviation from 0.13.4-dev across various stable versions of OpenMC. From left to right, they respectively correspond to HMT-026-01, HMT-027-15, and TRIGA fuel rod benchmarks.

3.2 Identifying the main source inducing discrepancy

Numerical studies show that the impact of TSL on various materials varies. As shown in **Fig. 7**, employing the TSL for H_2O does not result in similar discrepancies. Although there is a shift in the discrepancy for v0.13.3-stable for the TRIGA fuel rod benchmark, the variation is relatively small (~15 pcm vs. 3 pcm uncertainties) and both TSL and FGM exhibit this shift. Thus, it is reasonable to conclude that this change is a normal consequence of a routine update that slightly enhances the accuracy.

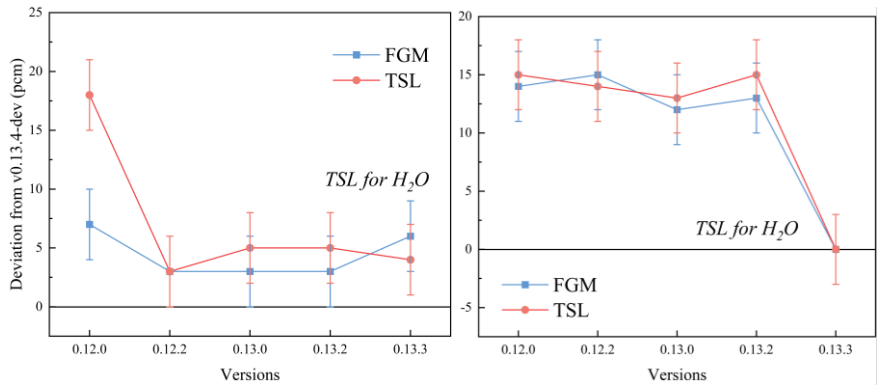

Fig. 7 Reactivity deviation from v0.13.4-dev across various stable versions of OpenMC, with and without considering the TSL for H_2O. (Left: BEAVRS, Right: TRIGA fuel rod).

Actually, compared with other materials like graphite and BeO, the TSL for H_2O does not include the coherent elastic scattering (CES) part due to its liquid phase. It is thus reasonable to guess that the main cause of the discrepancies is due to the CES. Thus, to simplify the verification, the CES cross sections in the TSL files for BeO are set to zero, and the inelastic scattering cross sections are replaced with the MT2 data block of the FGM. The results are summarized in **Fig. 8**, which indicates that the new discrepancies among different versions generally remain within a 3σ statistical uncertainty range. Therefore, this suggests that the main issue is related to the treatment of the coherent elastic scattering.

After further review, it is discovered that the developer has addressed an invalid access issue in a class named 'CoherentElasticAE' (suggestion #1949) [15]. Although the relevant function is reworked and the results are changed, the developer states that he is still not sure if it is correct. Therefore, by replacing this segment of the source code and recompiling OpenMC v0.13.2, more consistent calculation results with 0.12.2 version are achieved. As the results shown in **Fig. 9**, the calculated reactivity of the recompiled version with the previous CES energy-angular function aligns more closely with that of v0.12.2 rather than the original v0.13.2, indicating that the above deviations across various versions are likely mainly due to changes in this segment of the source code. Nevertheless, until now, we are also uncertain, like the developer, if this modification is correct. Preliminary analysis suggests that the modifications primarily affect the sampling related to the cosine of the coherent scattering angle. Since all these versions have been widely used, a systematic examination of the source code is necessary to verify its accuracy in future work.

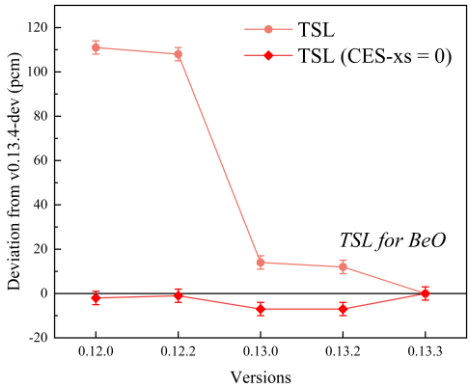

Fig. 8 Reactivity deviation from the 0.13.4-dev version across various stable versions of OpenMC removing the coherent elastic scattering cross section for TRIGA fuel rod benchmark.

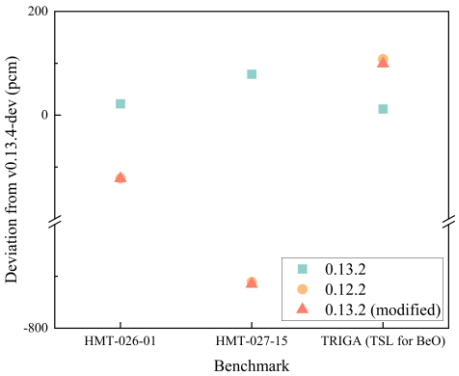

Fig. 9 Reactivity deviation from v0.13.4-dev following the modification of OpenMC v0.13.2.

According to the above findings, it is important to include diverse benchmarks (i.e., for more general representativity) for code verification and validation. If only typical LEU with H_2O moderator benchmarks is considered, the significant discrepancies between different OpenMC versions identified in the present work cannot be observed.

4 Conclusions

The present study reports the issue of discrepancies in k_{eff} calculations across different versions of the OpenMC when employing the TSL. Based on the four representative benchmark series (HMT-026, HMT-027, BEAVRS, and TRIGA fuel rod), these differences are systematically compared. The research indicates that updates in OpenMC v0.13.0 are primarily responsible for these discrepancies, which are quite significant, even reaching deviations up to ~1000 pcm for HMT-027-001. Additionally, the impact of TSL on various materials varies. Compared with other materials, the discrepancy introduced by the TSL for H_2O is nearly negligible.

Furthermore, after removing the coherent scattering cross section in the data blocks of the TSL for BeO, the discrepancies are almost eliminated. Thus, it can be determined that the main issue inducing the significant discrepancy across various versions is related to the treatment of the coherent elastic scattering. After further review, a minor modification (in the sense of coding) is found in a class named 'CoherentElasticAE', which may affect the sampling of the cosine of the coherent scattering angle. By replacing this segment of the source code with that of v0.12.2 and recompiling OpenMC v0.13.2, calculation results are more consistent with those of v0.12.2. This further confirms the above conclusion. Nevertheless, we, both the developers and us, are still uncertain whether this update in v0.13.0 is correct or better. A systematic examination of the source code is necessary in future work.

Finally, the research underscores the importance of including diverse benchmarks for code verification and validation. For example, if only the typical LEU benchmarks with H_2O moderators are considered, the significant discrepancies between different OpenMC versions identified cannot be observed.

References

[1] G. L. Squires, *Introduction to the Theory of Thermal Neutron Scattering*, 3rd ed. Cambridge University Press, 2012.

[2] H. Schober, 'An introduction to the theory of nuclear neutron scattering in condensed matter', *J. Neutron Res.*, **17**(3–4), 109–357, 2014.

[3] P. K. Romano, N. E. Horelik, B. R. Herman, A. G. Nelson, B. Forget, K. Smith, 'OpenMC: A state-of-the-art Monte Carlo code for research and development', *Ann. Nucl. Energy*, **82**, 90–97, 2015.

[4] H. El Yaakoubi, H. Boukhal, T. El Bardouni, L. Erradi, E. Chakir, K. Benaalilou, M. Lahdour, S. El Ouahdani, *et al.*, 'Validation study of the reactor physics lattice transport code DRAGON5 & the Monte Carlo code OpenMC by critical experiments of light water reactors', *J. King Saud Univ. - Sci.*, **31**(4), 1271–1275, 2019.

[5] H. Guo, X. Huo, K. Feng, H. Gu, 'Verification of OpenMC for fast reactor physics analysis with China experimental fast reactor start-up tests', *Nucl. Eng. Technol.*, **54**(10), 3897–3908, 2022.

[6] T. Wang, S. Chen, S. Xu, Z. Li, S. Chen, X. Wu, 'OpenMC interpretation and analysis of two series highly-enriched-uranium thermal-spectrum benchmarks for nuclear data validation', *Ann. Nucl. Energy*, **192**, 110017, 2023.

[7] D. Heinrichs, B. Lloyd, J. Scorby, 'Highly Enriched Uranium Metal Moderated by Beryllium Oxide', NEA/NSC/DOC/(95)03/II.
[8] 'Nuclear Energy Agency (NEA) - International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook'. https://www.oecd-nea.org/jcms/pl_20291/international-criticality-safety-benchmark-evaluation-project-icsbep-handbook (accessed Jan. 12, 2023).
[9] R. M. Buck, D. E. Cullen, D. P. Heinrichs, E. M. Lent, K. E. Sale, 'COG - Publicly Available Now to Criticality Safety Practitioners', Lawrence Livermore National Lab. (LLNL), Livermore, CA (United States), UCRL-CONF-224715, 2006.
[10] N. Horelik, B. Herman, B. Forget, K. Smith, 'Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS)', in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering*, Sun Valley, Idaho, 2013.
[11] D. E. Johnson, R. Mills, 'Irradiation Behavior of BeO-UO2 Fuel as a Function of Fuel-Particle Size', General Atomic Division of United States Atomic Energy Commission, 1963.
[12] S.-L. Chen, X.-J. He, C.-X. Yuan, 'Recent studies on potential accident-tolerant fuel-cladding systems in light water reactors', *Nucl. Sci. Tech.*, **31**(3), 32, 2020.
[13] S. Chen, C. Yuan, 'Neutronic study of UO_2-BeO fuel with various claddings', *Nucl. Mater. Energy*, **22**, 100728, 2020.
[14] OpenMC Development Team, 'S(a,b) name suggestions · Issue #1945 · openmc-dev/openmc — github.com'. [Online]. Available: https://github.com/openmc-dev/openmc/issues/1945. [Accessed: 15-Jul-2024].
[15] OpenMC Development Team, 'Fixes for various bugs · Pull Request #1949 · openmc-dev/openmc — github.com'. [Online]. Available: https://github.com/openmc-dev/openmc/pull/1949. [Accessed: 15-Jul-2024].