APPLICATION OF THE TUD-W BENCHMARK FOR NUCLEAR DATA AND CODE ASSESSMENT

CAMPOS FORNÉS, MARTA
ATG Science & Engineering S.L.
Barcelona, Spain
Email: marta.campos@ext.f4e.europa.eu

FABBRI, MARCO
Fusion for Energy (F4E)
Barcelona, Spain
Email: marco.fabbri@f4e.europa.eu

PETRIZZI, LUIGINO
Retiree, former employée EU Commission
Rome, Italy
Email: luiginopetrizzi2@gmail.com

KOLSEK, ALJAZ
Fusion for Energy (F4E)
Barcelona, Spain
Email: aljaz.kolsek@f4e.europa.eu

LAGHI, DAVIDE
Fusion for Energy (F4E)
Barcelona, Spain
Email: davide.laghi@f4e.europa.eu

Abstract

The paper provides an assessment of tungsten nuclear data using the TUD-W SINBAD benchmark across two different Monte Carlo transport codes. Simulations have been conducted by means of both MCNP6.2 and OpenMCv0.15.0 to compute neutron and photon flux spectra at four depths (5, 15, 25, and 35 cm) within a thick tungsten alloy (DENSIMET-176/180) block irradiated by 14 MeV neutron source. Experimental data, measured with an NE 213 scintillation spectrometer, served as a reference for the assessment. Starting from the original MCNP benchmark model, its conversion to OpenMC is briefly discussed in the paper and the equivalence of the resulting models is demonstrated. Comparisons of simulation results using various nuclear data libraries were performed and, while general agreement was observed, significant discrepancies have been found for photon spectra above 6 MeV. The origin of these deviations was investigated using MCNP's PKMT card and identified as originating from (n,γ) reactions in ^{183}W and ^{58}Ni. Differences between FENDL 2.1, ENDF/B-VII.0 and other libraries were detected and, following further investigation, attributed to variations in the tungsten isotopes nuclear data.

1. INTRODUCTION

Tungsten (W) is a key material in fusion reactor designs, particularly for plasma-facing components. Accurate nuclear data for tungsten is essential for reliable neutronic simulations, impacting reactor safety, shielding, and operational performance. Additionally, the replacement of beryllium (Be) in ITER's First Wall (FW) with tungsten (W) during the 2023 ITER rebaselining exercise has further increased the interest in this material and the accuracy of computed responses.

This work is an assessment of tungsten nuclear data employing the TUD-W SINBAD benchmark [1], ranked as the highest-quality benchmark for this purpose. This benchmark consists of a thick tungsten alloy block (DENSIMET-176/180) irradiated by a 14 MeV neutron source (Fig. 1). Spectral neutron

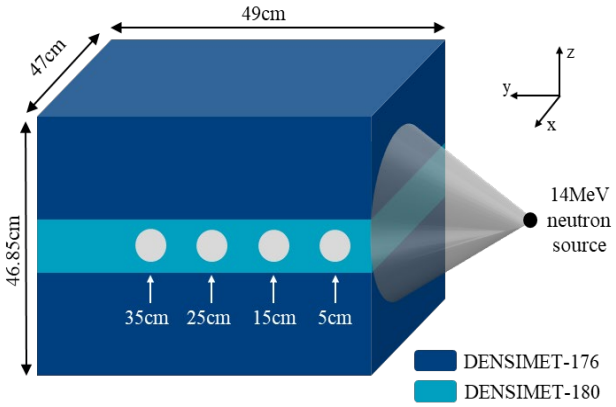

FIG 1. Diagram of the TUD-W SINBAD benchmark.

and photon flux were measured experimentally and computationally at four different positions in depth throughout the block: 5 cm (position 1), 15 cm (position 2), 25 cm (position 3) and 35 cm (position 4).

Two nuclear transport codes were used for the computational simulations: MCNP 6.2 and OpenMC v0.15.0. The experimental results, obtained using an NE 213 scintillation spectrometer, served as a reference for the nuclear data assessment.

Nuclear spectra in the different positions were recorded independently, both experimentally and computationally. When results were tallied for a specific position in depth, the cavities corresponding to the rest of positions were filled with a DENSIMET cylinder. Computationally, this involved performing a different simulation for each position, with the model geometry adjusted accordingly between runs.

Statistical optimization techniques were applied, including weight window generators and customized Python-based scripts to refine various cell parameters. Weight windows were iteratively computed both in OpenMC and MCNP as a global variance reduction technique to improve statistical accuracy in deeper regions (positions 2, 3, and 4). Moreover, a geometry error caused by a small undefined volume was corrected, and the corresponding patch was communicated to the NEA Data Bank.

This contribution is structured in two sections. The first one contains a brief description of the methodology used to convert the already-existent SINBAD MCNP TUD-W computational benchmark model to OpenMC, as well as a successful comparison between the nuclear spectra results obtained with both transport codes employing the FENDL 3.2c nuclear data library. The second one explores the main objective of this paper: the assessment of tungsten nuclear data across multiple nuclear data libraries, with a focus on discrepancies between experimental and computational results, as well as among libraries.

2. CONVERSION OF THE TUD-W BENCHMARK COMPUTATIONAL MODEL TO OPENMC

The TUD-W benchmark model for OpenMC was constructed through the conversion of the MCNP model provided by SINBAD. While the geometry and materials translations were automatized using the csg2csg repository [2], converting the source proved to be significantly more challenging.

The latter conversion required a thorough understanding of source definition for both transport codes and a detailed manual translation process. The source examples presented in the openmc_fusion_benchmarks repository [3] were used as a reference, but the necessary deeper understanding of source definition equivalence between MCNP and OpenMC was obtained from the documentation of each transport code [4][5].

Another point that had to be considered was the definition of code-specific weight windows. Since the cell-based approach was adopted for MCNP, the model implementation in OpenMC entailed computing weight windows from scratch, as cell-based weight windows are not supported in OpenMC v0.15.0 and, therefore, the direct translation was not a possibility.

Results from a series of ITER-relevant simulations have suggested the underperformance of OpenMC weight windows once compared to MCNP [6], both in terms of computation time and quality of standard deviation outputs. This conclusion resulted in the need to perform an OpenMC weight windows scoping study specific to the TUD-W benchmark in order to optimize the efficiency of this global variance reduction technique for positions 2, 3 and 4. In this investigation, several OpenMC parameters were considered, among which the number of batches chosen, the deactivation of survival biasing and the use of softening proved to be critical. Moreover, additional feedback was communicated to the code developers to further enhance this essential variance reduction technique.

2.1. Comparison of MCNP and OpenMC

Neutron and photon spectra results along four different positions in the TUD-W benchmark were compared between MCNP 6.2 and OpenMC v0.15.0. To reduce the sources of potential discrepancies between the two sets of results, the same nuclear data library was employed for all simulations: FENDL 3.2c [7].

The comparison between the two transport code results is presented in Fig.2 in the form of C/E step plots. A very good agreement can be observed for both neutron and photon computational spectra in all positions, with the mean of the discrepancy between OpenMC and MCNP being 3.43% for neutrons and 4.23% for photons. This result

compatibility led to the validation of the developed OpenMC model and the confirmation of the proper operation of OpenMC as a transport code in the context of the TUD-W benchmark.

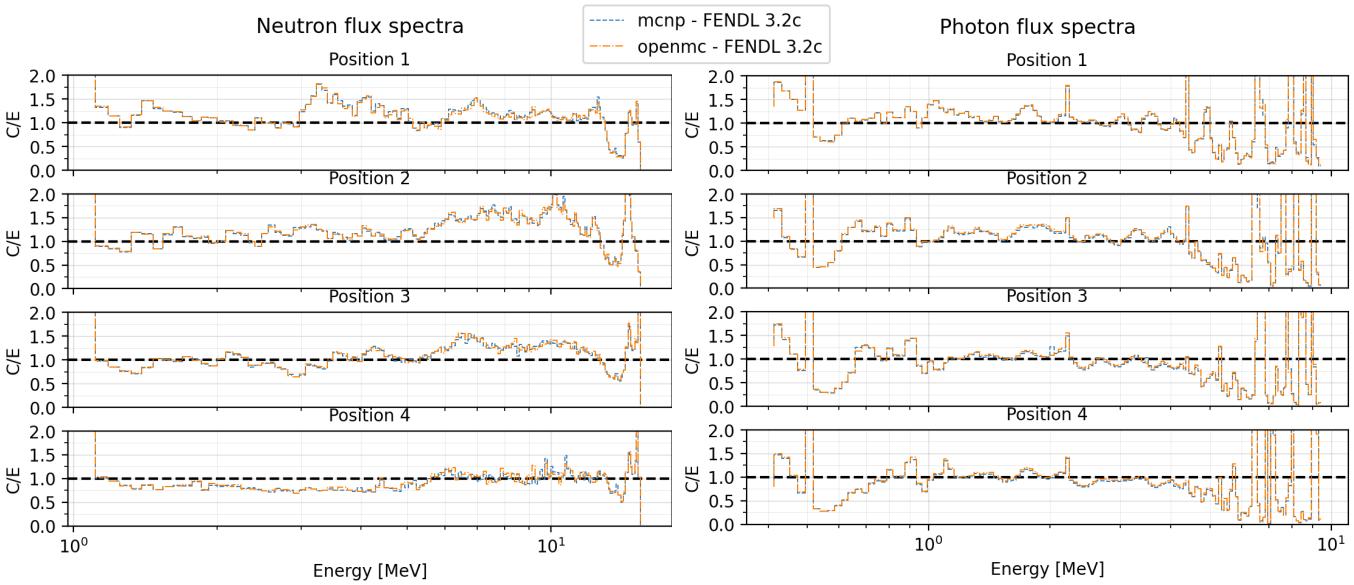

FIG 2. Ratio representation of the OpenMC (orange) and MCNP (blue) neutron (left) and photon (right) flux spectra results for the TUD-W benchmark compared to the measured experimental values. A different plot is presented for each position (5 cm, 15 cm, 25 cm and 35 cm in depth, respectively). The first energy group results were excluded, both for neutron and photon spectra, following the benchmark's documentation indications [1]. JADE [8] was employed to produce these plots.

3. ASSESSMENT OF TUNGSTEN NUCLEAR DATA

The assessment of tungsten nuclear data was approached through the comparison of TUD-W experimental results with those resulting from computational simulations. Similarly to the validation of the OpenMC v0.15.0 model, neutron and photon spectra were analysed separately for each position in depth within the DENSIMET block.

In computational simulations, neutron and photon spectra were recorded using specific energy groups provided by the detector supplier. In accordance with the benchmark's documentation [1], since neutron flux was experimentally measured in an energy range starting from 1 MeV, the first energy group used in simulations to record neutron flux ([0,1.1) MeV) was excluded from the comparison.

In the following subsections, two different types of plots are presented with the objective of illustrating the agreements and discrepancies between experimental and computational TUD-W data. Both types of graphs consist of a C/E ratio representation of results, but differ in format: while the first is a step plot of the nuclear spectra data (neutron and photon, respectively) produced with JADE [8], the second is a point graph showing flux integrated over broader energy intervals.

Numerous versions of reference nuclear data libraries were tested in this assessment, as outlined below:

- Fusion Evaluated Nuclear Data Library [7]: FENDL 2.1, FENDL 3.1d, FENDL 3.2c;
- Evaluated Nuclear data File [9]: ENDF/B VII.0, ENDF/B VIII.0, ENDF/B VIII.1;
- Joint Evaluated Fission and Fusion Nuclear Data Library [10]: JEFF-4.0, JEFF-4T5.

As a result of the demonstrated equivalence between the OpenMC v0.15.0 and MCNP 6.2 TUD-W models, results from both transport codes were treated as completely equivalent and interchangeable. Consequently, each nuclear data library was evaluated using only one of the codes, avoiding redundant simulations.

3.2. Comparison across all tested nuclear data libraries

3.2.1. Neutron spectra

Neutron spectra results for all the tested libraries are presented in Fig. 3. Additionally, the neutron flux for five different energy intervals is plotted in Fig 4 where, as a reference, three times the experimental relative error is included.

The low-energy neutron responses ([1,6) MeV) showed consistency across all nuclear data libraries, as well as a general agreement with experimental results. The only observable discrepancy in this range was for position 1 within the [3,6) MeV energy interval, where none of the nuclear data libraries accurately reproduced the experimental neutron spectra to the same extent as for the other positions in the TUD-W benchmark (Fig. 3).

Computational results in positions 2 and 3 showed a larger divergence from experimental measurements for energies above 6 MeV (Fig. 3). The [6,12) MeV energy range also presented pronounced differences among the tested libraries (Fig. 4). In the [9,12) MeV energy interval, the responses separated into two distinguishable library groups: while FENDL 2.1 and ENDF/B-VII.0 produced similar results, the remaining libraries formed a differentiated set. In the [6,9) MeV range, although distinctions across libraries were still apparent, results didn't present such a grouping.

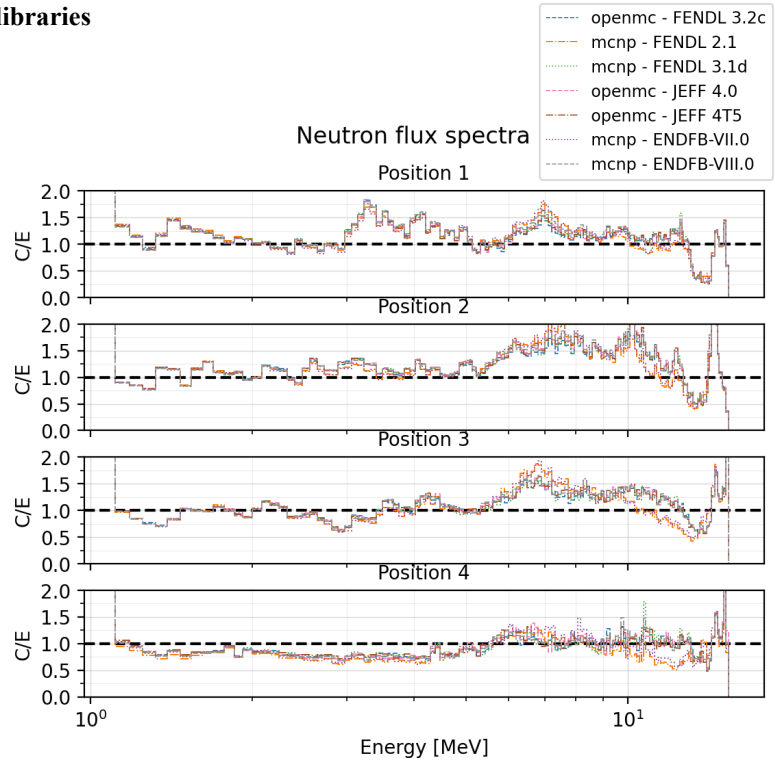

FIG 3. Ratio representation of the neutron flux spectra results for all the tested nuclear data libraries compared to the measured experimental values (orange). A different plot is presented for each position (5 cm, 15 cm, 25 cm and 35 cm in depth, respectively). JADE [8] was employed to produce these plots.

Given the previously proven agreement between the MCNP and OpenMC models, the discrepancies appearing above 6 MeV were most likely attributable to the nuclear data rather than to the Monte Carlo codes. The neutron flux integrated over the whole energy spectrum (Fig. 4) demonstrated a strong agreement across all nuclear data libraries, with deviations from experimental measurements not exceeding 15%.

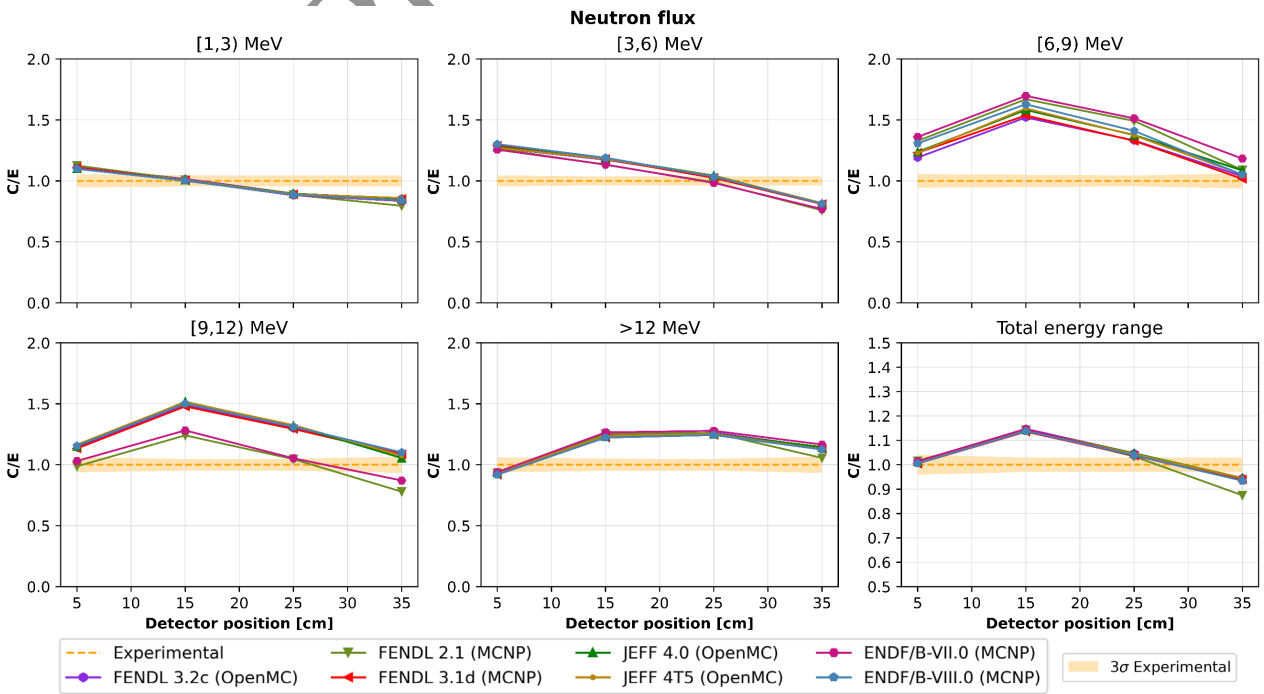

FIG 4. C/E plot of neutron flux for all the tested nuclear data libraries at different energy ranges. Every plot presents 4 data points, each corresponding to a different position in depth within the DENSIMET block. The last graph shows the neutron flux integrated across the full energy spectrum. The orange shadow represents three times the experimental relative error.

3.2.2. *Photon spectra*

The photon spectra and flux results across all tested nuclear data libraries are displayed in Fig. 5 and Fig. 6, respectively.

As illustrated in both figures, low-energy photon responses ([0,3) MeV) showed a general agreement between nuclear data libraries and a satisfactory compatibility with experimental results. While computational data for intermediate-energy photons ([3,6) MeV) was consistent with experimental results, Fig. 6 shows that FENDL 2.1 and ENDF/B-VII.0 slightly underperformed compared to the other nuclear data libraries. The divergence of these two libraries from the rest was accentuated in high-energy photon responses ([6,10) MeV). Nonetheless, in this case FENDL 2.1 and ENDF/B-VII.0 performed more accurately than the other libraries in reproducing the experimental data (Fig. 6). In this energy range, significant deviations were observed for all nuclear data libraries in several peaks over 6 MeV when compared to experimental data (Fig. 5).

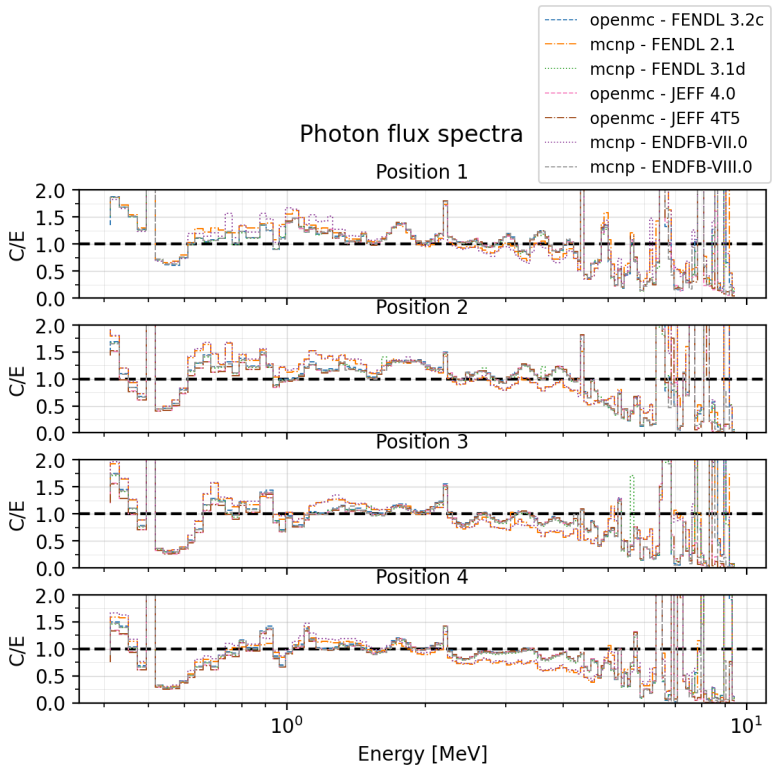

FIG 5. Ratio representation of the photon flux spectra results for all the tested nuclear data libraries compared to the measured experimental values (orange). A different plot is presented for each position (5 cm, 15 cm, 25 cm and 35 cm in depth, respectively). JADE [8] was employed to produce these plots.

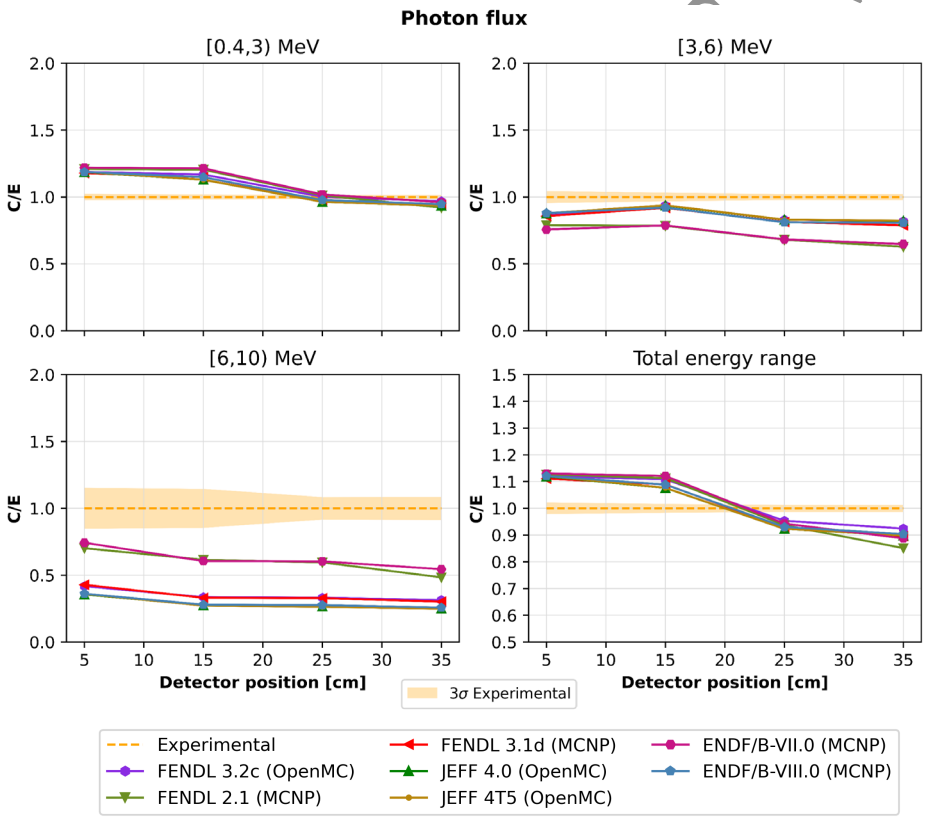

FIG 6. C/E plot of photon flux for all the tested nuclear data libraries at different energy ranges. Every plot presents 4 data points, each corresponding to a different position in depth within the DENSIMET block. The last graph represents the neutron flux integrated across the full energy spectrum. The orange shadow represents three times the experimental relative error.

These discrepancies between computational and experimental results in high-energy photon responses appeared across both nuclear transport codes, MCNP and OpenMC (Fig. 2). Similarly to the case of neutron spectra, this confirmed that the deviations were likely driven by the nuclear data itself rather than the Monte Carlo codes.

The degree of divergence between computational responses and experimental results for high-energy photons across all nuclear data libraries prompted further investigation into their origin. As a result, a dedicated study, presented in section 3.3, was conducted to examine these discrepancies in more detail.

Considering the photon flux integrated across the full energy spectrum (Fig. 6), results from all nuclear data libraries show a general agreement and fall within a 15% deviation from the experimental measurements.

3.3. Discrepancies in high-energy photon responses

The discrepancy observed between computational and experimental results for high-energy photons was investigated using the PKMT card in MCNP. This card was employed to selectively disable the secondary gamma production for different isotopes.

The results obtained from this methodology are presented in Fig. 7. The high-energy photon spectra ([4,10] MeV) for position 4 was computed for 3 different cases:

- Secondary gamma production enabled for all nuclides in the geometry;
- Secondary gamma production disabled for all isotopes except ^{183}W;
- Secondary gamma production enabled only for ^{56}Fe and ^{58}Ni.

This analysis revealed that one of the first photon lines responsible for a substantial deviation, corresponding to an energy of 7 MeV, originated from ^{183}W(n,γ) reactions. Following the same approach, the higher-energy peaks that introduced discrepancies were found to originate predominantly from radiative capture, (n,γ), in ^{58}Ni [11], one of the main impurities present in DENSIMET.

This finding underscored the critical role of impurities, not only in activation studies, but also in prompt radiation transport. Consequently, it highlighted the necessity for thorough material characterization and certification to ensure accurate response predictions.

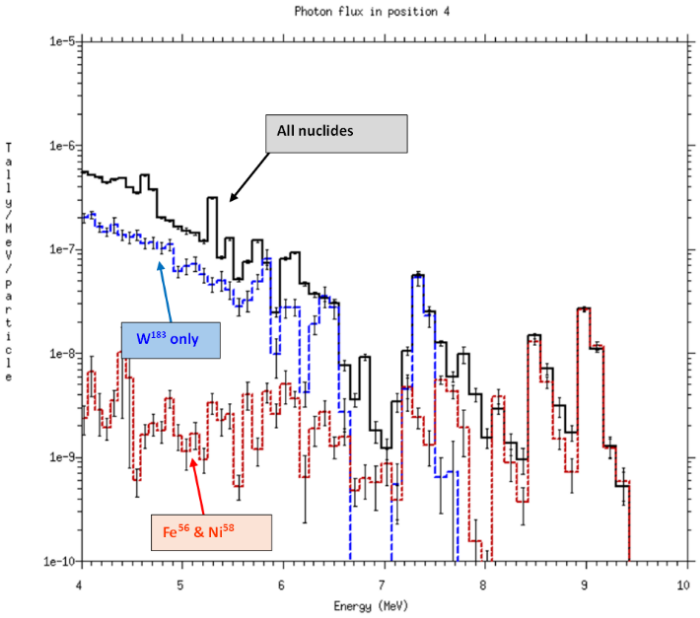

FIG 7. High-energy photon spectra results in position 4 for: secondary gamma production enabled for all isotopes (black), secondary gamma production disabled for all isotopes except ^{183}W (blue) and secondary gamma production enabled only for ^{56}Fe and ^{58}Ni (red).

3.4. FENDL 2.1

Following the observed discrepancies between FENDL 2.1 and the newer FENDL releases, a decision was made to further investigate their origin. Two potential sources of these differences were identified:

- Nuclear data of W isotopes;
- Nuclear data of the main impurities in DENSIMET, corresponding to the isotopes of Fe and Ni.

The objective of this assessment was to isolate the responsible elements for the significant variation in nuclear response. Accordingly, a plan was established to efficiently compare FENDL 2.1 results to those obtained using FENDL 3.2c.

Firstly, while using FENDL 3.2c as a base, the nuclear data for Fe and Ni (TUD-W main impurities) was exchanged for the FENDL 2.1 one. Simulations for all positions were run, and the results were compared to the original results of FENDL 3.2c and FENDL 2.1. This comparison is presented in Fig. 8, where the graphs which showed the biggest discrepancy between FENDL 2.1 and the newer FENDL releases in the previous subsection (Fig. 4 and Fig. 6) are plotted.

As shown in Fig. 8, the substitution of the Fe and Ni nuclear data from FENDL 3.2c with those from FENDL 2.1 did not lead to any significant deviation from the original FENDL 3.2c results. This allowed the impurities to be ruled out as the primary cause of the observed discrepancies.

As a result, a second test was performed focusing on the tungsten nuclear data. Using FENDL 3.2c as a base, the nuclear data for W, Fe and Ni was exchanged for the FENDL 2.1 one. In this case, as illustrated in Fig. 8, a larger

discrepancy with the original FENDL 3.2c results was observed, accompanied by a good alignment with the FENDL 2.1 data. The slight discrepancies with the FENDL 2.1 responses are suspected to result from the W isotopes that were not substituted in FENDL 3.2c by FENDL 2.1 nuclear data due to only being included in more recent FENDL releases.

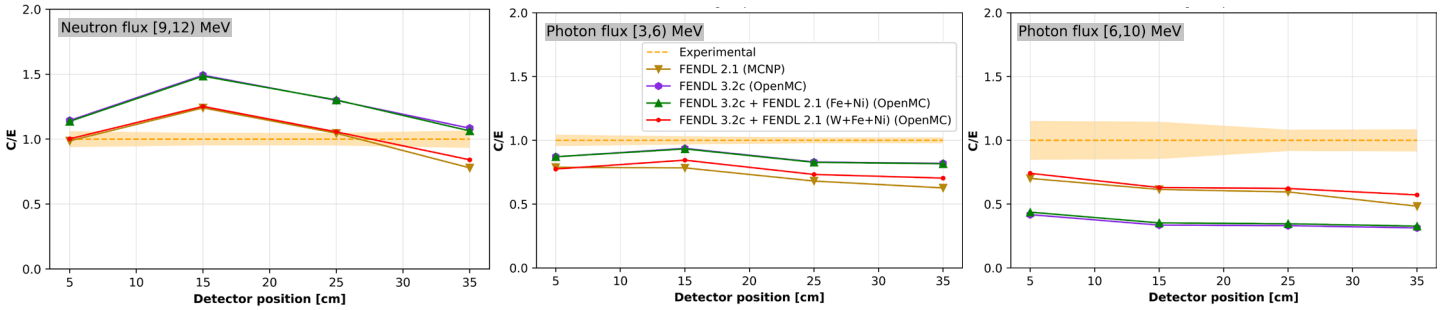

FIG 8. Neutron and photon flux plots at the energy ranges showing the biggest discrepancy between FENDL 2.1 and the rest of the tested nuclear data libraries.

3.5. ENDF/B-VII.0

An equivalent approach to FENDL 2.1 was taken for ENDF/B-VII.0 as a consequence of the observed deviations in the responses of this library in comparison to the majority of nuclear data libraries tested in this study (Fig. 4 and Fig. 6).

Since a similar behaviour was observed in the neutron and photon responses of FENDL 2.1 and ENDF/B-VII.0 across all positions, it was suspected that the discrepancies seen in ENDF/B-VII.0 had the same origin as those in FENDL 2.1. This was confirmed by the results in Fig. 9, where replacing the W nuclear data in FENDL 3.2c with that from ENDF/B-VII.0 successfully reproduced the original ENDF/B-VII.0 responses.

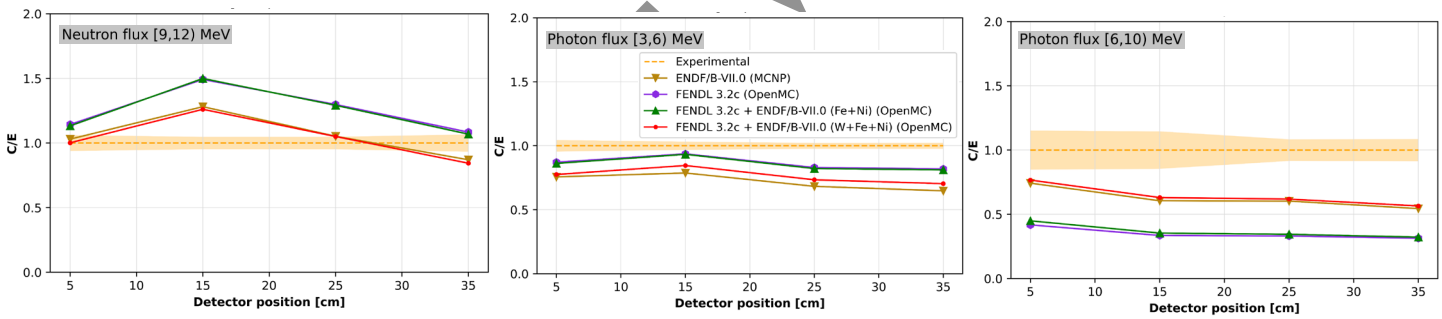

FIG 9. Neutron and photon flux plots at the energy ranges showing the biggest discrepancy between ENDF/B-VII.0 and the rest of nuclear data libraries.

3.6. ENDF/B-VIII.1

The procedure presented in sections 3.4 and 3.5 was also implemented for ENDF/B-VIII.1, using FENDL 3.2c as a base library. In this case, with no previous indications of a potential deviation from the other tested libraries, this decision was driven by the availability of nuclear data only for W, Fe and Ni isotopes in ENDF/B-VIII.1. This analysis was still considered relevant as a result of the significant influence of these elements on the measured nuclear spectra, as shown in prior simulations for this benchmark.

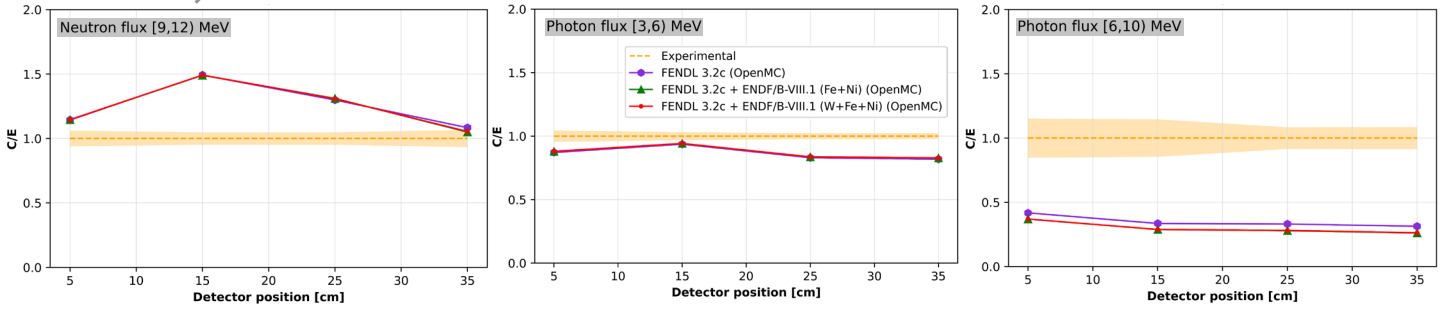

FIG 10. Neutron and photon flux plots at the energy ranges showing the biggest discrepancies between the tested nuclear data libraries in Fig. 4 and Fig. 6.

As shown in Fig. 10, no relevant discrepancies with FENDL 3.2c were detected for any of the tested nuclear data combinations including ENDF/B-VIII.1 W, Fe and Ni isotopes.

4. CONCLUSIONS

This study has provided a comprehensive assessment of tungsten nuclear data using the TUD-W SINBAD benchmark across multiple nuclear data libraries and the two different transport codes MCNP 6.2 and OpenMC v0.15.0.

The analysis provided new insights into the performance of the tested nuclear data libraries, highlighting the differences identified for FENDL 2.1 and ENDF/B-VII.0, which were traced back to the nuclear data of tungsten isotopes in both libraries.

A general underestimation of high-energy photon responses was observed across several libraries when compared to experimental data, particularly above 6 MeV. This discrepancy was most probably linked to Ni, one of the main impurities in DENSIMET, but it remained unclear whether the root cause lied in the inaccurate reporting of impurity concentrations or in the nuclear data associated with these elements, which was difficult to understand decades after the experiment.

Following the results of this study, the TUD-W SINBAD benchmark post-processing was added to JADE [8], both for MCNP and OpenMC, and suggestions for further development were provided to OpenMC developers.

ACKNOWLEDGEMENTS

The authors would like to thank Daniel López Aldama for his valuable suggestions and recommendations throughout the development of this work. His support in providing the ENDF/B-VIII.1 nuclear data was instrumental to the analysis efforts presented in this study.

REFERENCES

[1] NEGOITA, C., Measurement of Neutron Flux Spectra in a Tungsten Benchmark by Neutron Foil Activation Method, University of Dresden (2004)

[2] DAVIS, A., et al., csg2csg: A TOOL TO ASSIST VALIDATION & VERIFICATION, EPJ Web Conf. (2021), 247 04012, https://doi.org/10.1051/epjconf/202124704012

[3] PETERSON, E., et al., openmc_fusion_benchmarks GitHub repository, https://github.com/eepeterson/openmc_fusion_benchmarks

[4] WERNER, C., et al., Los Alamos National Laboratory, MCNP User's Manual Code Version 6.2 (2017), http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-17-29981

[5] ROMANO, P. et al., Massachusetts Institute of Technology and UChicago Argonne LLC, OpenMC v0.15.0 documentation, https://docs.openmc.org/en/v0.15.0/

[6] VALENTINE, A., et al., Investigation of OpenMC for fusion neutronics, UKAEA, 15th-ITER Neutronics meeting and Fusion Neutronics Workshop (2024)

[7] Fusion Evaluated Nuclear Data Library (FENDL), IAEA Nuclear Data Section, Vienna, Austria, https://www-nds.iaea.org/fendl/

[8] LAGHI, D., et al., "JADE, a new software tool for nuclear fusion data libraries verification & validation", Fusion Engineering and Design (2020), 161 112075, https://doi.org/10.1016/j.fusengdes.2020.112075

[9] Evaluated Nuclear Data File (ENDF), IAEA Nuclear Data Section, Vienna, Austria, https://www-nds.iaea.org/exfor/endf.htm

[10] Joint Evaluated Fission and Fusion (JEFF) Nuclear Data Library ,Nuclear Energy Agency (NEA) Data Bank, OECD, https://www.oecd-nea.org/dbdata/jeff/

[11] IAEA, Thermal Neutron Capture γ's database (CapGam), https://www-nds.iaea.org/capgam/index.htmlx