EPJ Web of Conferences **261**, 02004 (2022) https://doi.org/10.1051/epjconf/202226102004
ANPC 2021

Effect of Using Different Data Libraries and Simulation Codes on the Calculation of Spectra and Operational Quantities for the D_2O-^{252}Cf Source at PTB

Amer A. Al Qaaod[1*], *Marcel* Reginatto[1], *Andreas* Zimbal[1], and *Miroslav* Zbořil[1]

[1]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

Abstract. The neutron reference field produced by a heavy-water moderated ^{252}Cf source is used at PTB for calibrating neutron-measuring devices. Knowledge of the precise neutron spectrum is very important for the investigation of operational radiation protection quantities. Recently, new fission spectrum data of ^{252}Cf has been proposed based on the latest nuclear data library version. At PTB, earlier calculations for the D_2O moderated ^{252}Cf neutron source were carried out more than 20 years ago, thus updated and more detailed calculations are required. In this paper, a detailed simulation model of the PTB moderated ^{252}Cf source assembly has been prepared and investigated using new spectral data and two different Monte Carlo transport codes MCNP6.1 and PHITS3.22, with ENDF/BVIII.0, ENDF/B-VII.1, ENDF/B-V, and ENDL85 evaluated nuclear data libraries. The results show that the evaluated nuclear data libraries influence the calculated operational quantities by (3-5) %. The dosimetric quantities calculated with the PHITS code and the ENDF/B-VII.1 data library agree well with the MCNP6 results.

1 Introduction

The increasing use of radiation and neutron sources for research and industry applications makes it necessary to calibrate neutron measuring devices in well-characterized calibration fields [1], [2]. The International Organization for Standardization (ISO) recommends neutron reference radiations for calibrating neutron measuring devices [3], [4]. For routine calibrations, different types of radioactive neutron sources with wide-ranging neutron energy spectra should be used. An irradiation facility with ISO recommended radioactive neutron sources such as ^{252}Cf, unmoderated and moderated by heavy water (D_2O), and ^{241}Am-Be, is available at the Physikalisch-Technische Bundesanstalt (PTB), the National Metrology Institute of Germany, for calibrations of area monitors and personal neutron dosimeters [5]– [7].

* Corresponding author: amer.al-qaaod.ext@ptb.de

Earlier Monte Carlo simulations were performed at PTB for the irradiation facility some 20 years ago [5], [6]. In that study, a simple model for the facility with radionuclide neutron sources, D_2O moderated ^{252}Cf, ^{252}Cf bare and ^{241}Am-Be sources, was constructed to investigate the influence of the wall, the air, and the shadow object on the neutron fluence rate at the measurement position. Also, the different spectra were calculated and measured using a Bonner Sphere Spectrometer (BSS) [8]. The authors used a Maxwellian distribution with spectrum parameter T = 1.42 MeV to describe the probability density for a single neutron emission from the ^{252}Cf source. The Monte Carlo N-particle code (MCNP) version 4A with the ENDL85 cross section data library was used to calculate and evaluate the operational radiation protection quantities.

In this paper, a recent Monte Carlo calculation of the D_2O moderated ^{252}Cf neutron reference assembly at PTB is presented and discussed, taking into account the updated fission spectrum data [9], cross section library, more details of the source configuration, and using two different transport codes, MCNP6.1 [10] and the Particle and Heavy Ions Transport code System (PHITS) version 3.22 [11].

2 The D_2O- ^{252}Cf assembly description and simulation model

At PTB, the D_2O-^{252}Cf assembly consists of a ^{252}Cf source placed in a cylindrical capsule of height 11.3 mm and outer surface diameter 10.8 mm made of stainless steel. The source capsule is guided to the centre of the assembly with a stainless-steel tube of wall thickness 1 mm. The heavy water is enclosed in a spherical shell of stainless-steel thickness 1 mm and surrounded by a Cadmium (Cd) half-shell. The accurate diameter of the D_2O container is 299.2 mm, this value was used in the present calculations. The geometrical model is shown in Fig. 1.

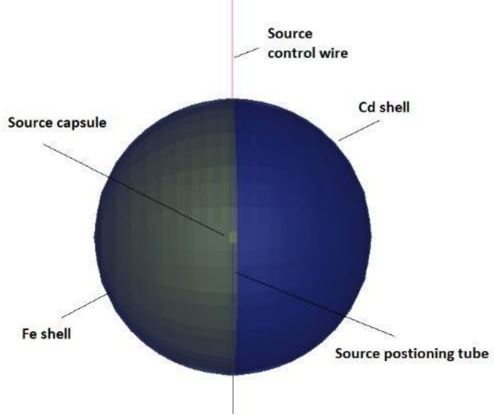

Fig. 1. 3D MCNP6 geometrical model of the D_2O-^{252}Cf assembly at PTB.

The codes MCNP version 6.1 and PHITS version 3.22 were used with the cross-section data libraries ENDF/B-VIII.0, ENDF/B-VII.1, ENDF/B-V, and ENDL85. The codes were run using a High-Performance Computing (HPC) Cluster in Berlin, which is a key facility for centralized scientific computing at PTB. Use of the cluster reduced the calculation time and allowed for a reduction in the uncertainty. The number of source-particle histories run in the problem was 10^9 so the relative error was kept under 0.07 %.

The materials composition of the assembly was described in detail in the model using values obtained from the "Compendium of Material Composition" [12]. Thermal neutron scattering treatment for the heavy water and iron at 293.6 K were considered in the material card in both codes. The D_2O-^{252}Cf assembly model assumes a free-space field, meaning that the source and moderator configuration are surrounded by vacuum (no air, walls, and equipment), and the spectral fluence for the direct neutron component was scored at 100 cm from the geometrical centre of the source at the Cd side using a point detector tally F5.

3 Results and discussion

The ENDF/B-VIII.0 neutron data which is used in the present investigation was released in 2018 [13]. It provides cross-section data for 557 nuclides and thermal scattering libraries for 33 different compounds in ENDF-6 files, whereas the earlier ENDF/B-VII.1 provides cross-section data for 423 nuclides. Also, the ENDF/B-VIII.0 library, in contrast to ENDF/BVII.1, has major changes for neutron reactions for the major actinides and other nuclides that impact simulations. The important isotopes ^{1}H, ^{16}O, ^{56}Fe, ^{235} U ,^{238}U, and ^{239}Pu have been the focus of the international CIELO collaboration and the resulting advances have been incorporated into ENDF/B-VIII.0 [14]. As an example of changes, we point out a previous renormalization of the *(n,α)* cross section downwards by 32 % for ENDF/B-VII which has now been removed in the new data library [13].

The aforementioned isotopes, specifically ^{16}O and ^{56}Fe, are major components of the D_2O^{252}-Cf assembly (see section 2) and the update of their cross-section data would be expected to influence the dosimetric parameters calculation. This is leading us to re-evaluate those parameters using different release cross section data libraries and discuss their impact. Another point to be taken into account is that the use of different codes in the analysis of a calibration problem is both an essential feature and a source of strong feedback for further improvements in data through mutual comparison of results.

For this purpose, MCNP6.1 and PHITS3.22 were used with four evaluated nuclear data libraries, ENDF/B-VIII.0, VII.1, V, and ENDL-85, to calculate the quantities of interest for the realistic model at PTB. The PHITS code used to simulate the D_2O-^{252}Cf assembly model incorporated the same dimensions, material densities, fission spectrum data and fluence-todose conversion coefficient used for the MCNP6 code. Tally [t-point] was chosen to score the fluence rate at 100 cm from the geometrical centre on the Cd side, which corresponds to the F5 tally in MCNP. For the neutron energy below 20 MeV, the PHITS code makes use of the cross-section data library when the option of using data library is turned on.

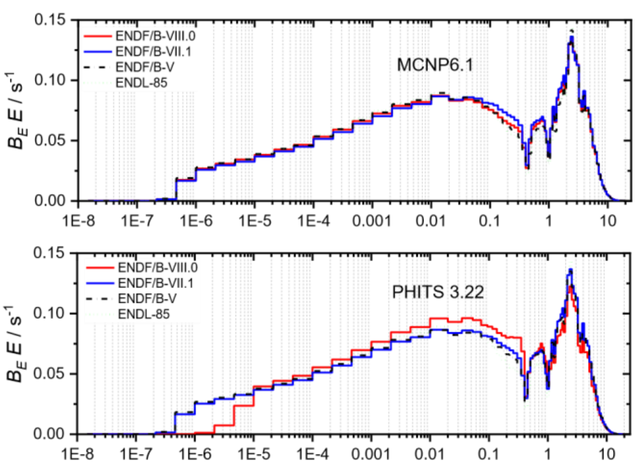

Fig. 2. A comparison of neutron spectra of the D_2O-^{252}Cf source assembly at 100 cm distance in vacuum for different released cross section data libraries, using the MCNP6.1 and PHITS3.22 codes.

The neutron spectrum for the assembly at 100 cm is shown in Fig. 2 for both codes and different cross section data. The MCNP6.1 calculation result shows a slight difference between the evaluated nuclear data libraries used in this comparison, especially in the case of ENDF/B-VII.1 in the energy range from 70 keV to 2 MeV. Also, one can observe a discrepancy in the dosimetric parameter values in Table 1, the ambient $h^*(10)$ and personal h_p (10, 0) conversion coefficient in the case of ENDL85 and ENDF/B-V are 108.34, 113.14 and 110.30 and 115.17 pSv cm^2 respectively, lower than the ENDF/B-VIII.0 values which are 113.78 and 118.81 pSv cm^2 respectively. Moreover, the discrepancy between ENDF/BVIII.0 and ENDF/B-VII.1 for calculated ambient and personal conversion coefficient was about 3 %, this is due to the higher values of the spectrum in the energy range between 0.07 and 2 MeV when using ENDF/B-VII.1 with MCNP6, as shown in Fig. 2 (top).

The ENDF/B-VIII.0 showed large deviation compared to the other evaluated nuclear data libraries when used with the PHITS code, the differences between the two codes MCNP6.1 and PHITS3.22 with same data library ENDF/B-VIII.0, ENDF/B-VII.1, ENDF/B-V, and ENDL85 are presented in Fig. 3a, b, c, and d respectively. The neutron spectrum calculated by PHITS code matches the MCNP6 spectrum when the ENDF/B-VII.1 and ENDL85 nuclear data library are used as shown in Figs. 3b and 3d, also the dosimetric parameters are in good agreement as can be seen in Table 1. For the ENDF/B-VIII.0 library the dose quantities are very similar in both codes although the fluence values and the spectral shapes are different. This is due to the dependence of the ambient and personal dose conversion coefficient on the neutron energy. As we can see from Figure 3a, the fluence for energies lower than 0.4 MeV is much higher when using PHITS than MCNP6.1, but these neutrons do not make a significant contribution to the dose quantities as do neutrons with energies greater than 1 MeV.

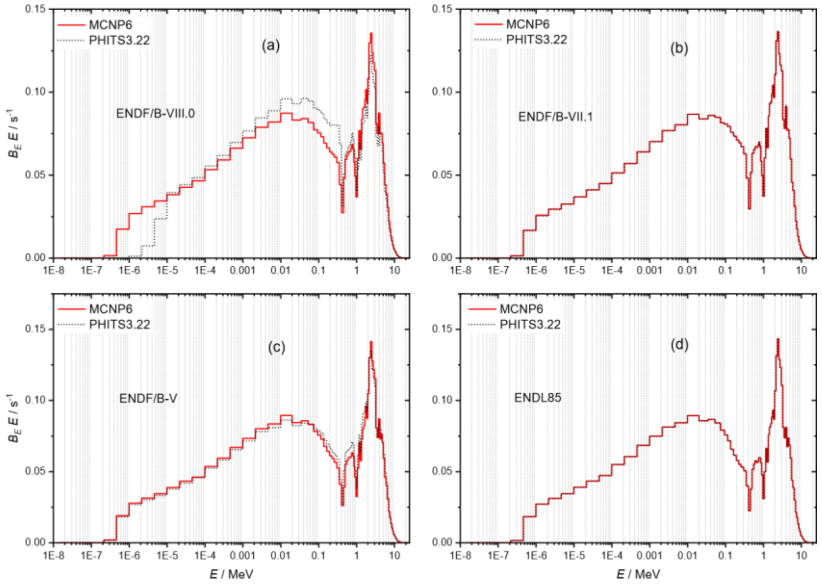

Fig. 3. Neutron spectra of the D_2O-^{252}Cf assembly at 100 cm distance calculated with MCNP6.1 and PHITS3.22 using four different data libraries (a) ENDF/B-VIII.0, (b) ENDF/B-VII.1, (c) ENDF/B-V and (d) ENDL-85.

Table 1. The fluence rate (Φ), fluence-average energy ($\bar{E}_\Phi$), ambient dose-average ($\bar{E}_H$), ambient $h^*(10)$ and personal h_p (10, 0) conversion coefficient at 100 cm from the source, variation with cross section data libraries for the D_2O-^{252}Cf assembly of PTB using the codes MCNP6 and PHITS. The relative uncertainty in the fluence rate and dose quantities was below 0.07 %.

Data library	**Code**	**Φ /cm^{-2}**	**$\bar{E}_\Phi$ / MeV**	**$\bar{E}_H$ / MeV**	**$h^*(10)$ / pSv cm^2**	**h_p (10, 0) / pSv cm^2**
ENDF/B-VIII.0	*MCNP*	6.99×10^{-6}	0.57	1.99	113.78	118.81
	PHITS	7.76×10^{-6}	0.58	1.98	113.71	118.66
ENDF/B-VII.1	*MCNP*	7.02×10^{-6}	0.58	1.98	117.20	122.44
	PHITS	7.00×10^{-6}	0.58	1.98	117.86	123.01
ENDF/B-V	*MCNP*	6.99×10^{-6}	0.56	2.04	110.30	115.17
	PHITS	7.00×10^{-6}	0.58	2.00	115.28	120.33
ENDL-85	*MCNP*	6.97×10^{-6}	0.55	2.04	108.34	113.14
	PHITS	6.96×10^{-6}	0.55	2.04	108.52	113.33

4 Conclusions

In this paper, a numerical investigation of the heavy water moderated ^{252}Cf source at PTB was carried out taking into consideration the latest fission spectrum data of ^{252}Cf, different evaluated nuclear data libraries and two recent versions of simulation codes, MCNP6.1 and PHITS3.22. The results of the calculation showed that the evaluated nuclear data libraries influence the calculated ambient and personal dose conversion coefficient for the D_2O-^{252}Cf assembly, and a significant difference in the calculated parameters between the latest released ENDF/B-VIII.0 and ENDF/B-VII.1, ENDF/B-V and ENDL85 has been found when the calculations are done with the same code MCNP6.1. ENDF/B-VIII.0 does not work properly with the PHITS code, a large deviation in the neutron spectrum and fluence rate with MCNP6.1 has been reported, and further validation should be performed for ENDF/B-VIII.0 considering single isotopes to figure out the source of the discrepancy. In general, the PHITS code proved its reliability and accuracy to simulate a heavy water moderated ^{252}Cf neutron source using ENDF/B-VII.1, where the results agree well with MCNP6.1 which contains the same cross section data library.

In future work, a comparison between the dosimetric quantities of the ISO and PTB moderator model using the previous (ISO 8529-1 2001) and a new proposed ^{252}Cf fission spectrum data (ISO 8529-1 2021) will be discussed. Furthermore, a realistic calculation including details of the calibration facility at PTB will be performed and evaluated taking into consideration the room return neutron components.

This work was supported by the Philipp Schwartz Initiative of the Alexander von Humboldt Foundation and the Federal Foreign Office of Germany which made available a scholarship for Amer Al-Qaaod. Special thanks to Désirée Radeck for formulating and guiding the work of this project and for her crucial contributions to the results. We thank Sebastian Fässer, Sven Koch, and Sebastian Reinert for assistance with the calibration facility. Our thanks to all staff in the HPC in PTB Berlin for their support regarding the use of the computer cluster.

References

1. V. Gressier, V. Lacoste, A. Martin, and M. Pepino, “Characterization of a measurement reference standard and neutron fluence determination method in IRSN monoenergetic neutron fields”, Metrologia, 51, no. 5, p.431, 2014.
2. M. Ginjaume, “Active methods & instruments for personal dosimetry of external radiation : present situation in Europe and future needs,” *Current trends in radiation protection,* EDP Sciences, 65–82, 2021.
3. J. Böhm *et al.*, “ISO recommended reference radiations for the calibration and proficiency testing of dosemeters and dose rate meters used in radiation protection,” *Radiat. Prot. Dosimetry,* vol. 86, no. 2, pp. 87–105, 1999.
4. D. Thomas, R. Bedogni, R. Méndez, A. Thompson, and A. Zimbal, “Revision of ISO 8529-Reference neutron radiations,” *Radiat. Prot. Dosimetry,* vol. 180, no. 1–4, pp. 21–24, 2018.
5. H. Kluge, “Irradiation facility with radioactive refernce neutron sources: Basic principles,” *PTB-Report*, PTB-N-34, 1998.
6. S. Jetzke and H. Kluge, “Characteristics of the ^{252}Cf neutron fields in the irradiation facility of the PTB,” *Radiat. Prot. Dosimetry*, vol. 69, no. 4, pp. 247–256, 1997.
7. H. Kluge, W. Rasp, J.B. Hunt, “An intercomparison of the D_2O-moderated ^{252}Cf reference neutron sources at PTB and NPL,” *Radiat. Prot. Dosimetry*, vol. 11, no. 1, p. pp.61–63, 1985, [Online]. Available: https://doi.org/10.1093/oxfordjournals.rpd.a079446.
8. H. Kluge, A.V. Alevra, S. Jetzke, K. Knauf, M. Matzke, K. Weise and J. Wittstock, “Scattered neutron reference fields produced by radionuclide sources,” *Radiat. Prot. Dosimetry*, vol. 70, no. 1–4, pp. 327–330, 1997.
9. R. Méndez, J. M. Gómez-Ros, D. J. Thomas, A. K. Thompson, and R. Bedogni, “Revision of the ^{252}Cf and D_2O-moderated ^{252}Cf reference neutron fields for use in radiation protection dosimetry,” *Radiat. Phys. Chem.*, vol. 184, p. 109433, Jul. 2021, doi: 10.1016/j.radphyschem.2021.109433.
10. T. Goorley *et al.*, “Features of MCNP6,” *Ann. Nucl. Energy*, vol. 87, pp. 772–783, 2016, doi: 10.1016/j.anucene.2015.02.020.
11. T. Sato *et al.*, “Features of Particle and Heavy Ion Transport code System (PHITS) version 3.02,” *J. Nucl. Sci. Technol.*, 2018, doi: 10.1080/00223131.2017.1419890.
12. R.J. McConn Jr, C.J. Gesh, R.T. Pagh, R.A. Rucker, R.G. Williams III , “Compendium of Material Composition Data for Radiation Transport Modeling,” 2011, [Online]. Available: www.pnnl.gov/main/publications/external/technical_reports/pnnl-15870rev1.pdf.
13. 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, doi: 10.1016/j.nds.2018.02.001.
14. M. B. Chadwick *et al.*, “The CIELO collaboration: neutron reactions on ^{1}H, ^{16}O, ^{56}Fe, ^{235,238}U, and ^{239}Pu,” *Nucl. Data Sheets*, vol. 118, p. pp.1–25, 2014, [Online]. Available: https://doi.org/10.1016/j.nds.2014.04.002.