U.P.B. Sci. Bull., Series A, Vol. 86, Iss. 4, 2024 ISSN 1223-7027

COMPARATIVE ANALYSIS OF NUCLEAR DATA LIBRARIES IN A LIQUID METAL COOLED REACTOR

Andreea MOISE[1] , Daniel DUPLEAC[2]

Nuclear data libraries play a crucial role in accurate simulation, affecting reactor systems criticality, safety, and performance assessments. This article thoroughly evaluates diverse nuclear data collections through comparative analysis, highlighting their implications and impact on reactor performance in the context of a liquid-cooled reactor. The research underscores the importance of choosing the appropriate nuclear data library and its implications on reactor design, safety protocols, and operational decision-making.

Keywords: nuclear data libraries, liquid metal cooled reactor, Monte Carlo code.

1. Introduction

Gen IV liquid metal cooled reactors are essential components of the global nuclear energy landscape, encompassing reactors such as lead fast reactors (LFR) and sodium fast reactors (SFR). These reactors utilize liquid coolant, such as lead or sodium, to transfer heat generated in the core to produce electricity. Accurate modeling and simulation of these reactors are vital for safety, efficiency, and overall performance. The precise modeling of these reactors relies heavily on the quality and accuracy of nuclear data libraries, which provide essential information about nuclear processes, such as neutron cross-sections, decay data, and fission yields. These libraries serve as the foundation for reactor physics codes and play a pivotal role in predicting reactor behavior under various conditions [1].

The uncertainties associated with evaluated nuclear data represent a paramount source of uncertainty in reactor physics simulations. Improving these data is imperative for advancing reactor development, facilitating safety assessments, and navigating the licensing processes. This paper centers on investigating discrepancies in the effective multiplication factor (k_{eff}) induced by variations among cross-sections sourced from the major nuclear data libraries available [2]. To conduct this analysis, a benchmark neutronic calculation was used to determine the first criticality of the China Experimental Fast Reactor core configuration. This calculation utilized the Continuous-energy Monte Carlo Reactor Physics Burn-up Calculation Code, MCNP6.2 [3].

[1] Research, Institute for Nuclear Research Pitesti, e-mail: andreea.moise@nuclear.ro
[2] Prof., Department of Energy Generation and Use, National University of Science and Technology Politehnica of Bucharest, Romania, e-mail: Daniel.dupleac@upb.ro

In the ever-evolving landscape of scientific research, current work represents an extension of a previous study [4]. Even if building upon the foundational ideas and initial findings showcased prior, it introduces a series of enhancements, focusing on broadening the scope and depth of the analyses. Among these improvements are the inclusion of two additional nuclear data libraries, a widely validated calculation code, an extensive examination of multiple isotopes, and a different approach to isotopic substitution methodologies. These developments underscore the commitment to refining previous research methodologies and deepening the understanding of the subject matter.

2. Nuclear Data Libraries: An overview

Several nuclear data libraries, each with its strengths and limitations, are available, each based on different measurement techniques, evaluation methods, and data sources. These libraries are crucial for assessing reactor safety, fuel performance, and neutron behavior within the core. The most commonly used nuclear data libraries are:

- *ENDF/B (Evaluated Nuclear Data File):* Produced by a collaborative effort involving US and Canadian institutions, it offers evaluated data on neutron cross-sections, fission yields, decay data, and more for a wide range of elements and isotopes. The latest version, ENDF/B-VIII.0 [5], is considered a reference point.
- *JEFF (Joint Evaluated Fission and Fusion File):* An international library jointly maintained by OECD-NEA and the Radioprotection and Nuclear Safety Institute of France (IPSN). The latest version used here is JEFF-3.3 [6].
- *JENDL (Japanese Evaluated Nuclear Data Library):* Developed by Japan's Nuclear Data Center, JENDL-4.0 [7] provides data on neutron cross-sections, nuclear decay, and other properties.
- *CENDL (Chinese Evaluated Nuclear Data Library):* Tailored to Chinese nuclear facilities, CENDL-3.1 [8] was developed by the China Nuclear Data Center and the China Nuclear Data Coordination Network.
- **BROND Nuclear Data Library:** Coordinated by Russia's Institute for Physics and Power Engineering (IPPE), BROND-3.1 [9] offers extensive isotopic and energy range coverage.

It is crucial to emphasize that nuclear data are subject to uncertainties. Experiments, inherently, come with imperfections. They introduce uncertainties due to the constraints of measurement procedures and the inherent statistical fluctuations that are beyond our control. Furthermore, the numerical values of physical parameters predicted by theoretical models also carry uncertainties. These uncertainties are scrutinized and evaluated to be incorporated into nuclear data evaluations using covariance matrices. Nevertheless, it is worth noting that uncertainty information is not uniformly available across all datasets.

3. Model description

This study chose a typical liquid metal cooled reactor model based on CEFR reactor to perform a comparative analysis of various nuclear data libraries applied within reactor simulation code MCNP6.2. In order to mitigate the impact of the inherent statistical nature of the Monte Carlo method on result variability, each MCNP6.2 calculation was executed with a substantial number of neutron histories: $5 \cdot 10^5$ neutron histories were employed per cycle, with 100 inactive cycles and an additional 300 active cycles. These specific calculation conditions were chosen to ensure a more robust and reliable assessment of results. As a result of this approach, the standard deviation was notably reduced to 5/6 pcm (percent mille or parts per million). This reduction in standard deviation signifies higher precision and confidence in the calculated outcomes, which is of utmost importance in nuclear physics simulations and reactor design studies.

MCNP6.2 model relies on the geometry descriptions provided in the technical specifications of the CRP. Each assembly is individually modeled, allowing for the creation of separate universes to represent different axial regions within each assembly. Some simplifications were made in less important regions of the active zone. For instance, in the case of fuel assemblies, the spacer wire mass was integrated into the cladding mass, and an equivalent radius for each cladding was calculated based on this assumption. Similarly, the spring within the fuel rod was modeled as a cylinder. A comparable approach was used for modeling control rods. As it does not impact neutronic calculations, nozzles were not modeled. The geometric details of various assemblies are illustrated in Fig. 1. It is important to note that when modeling the fuel assembly, the geometric details of the fuel pellet were retained.

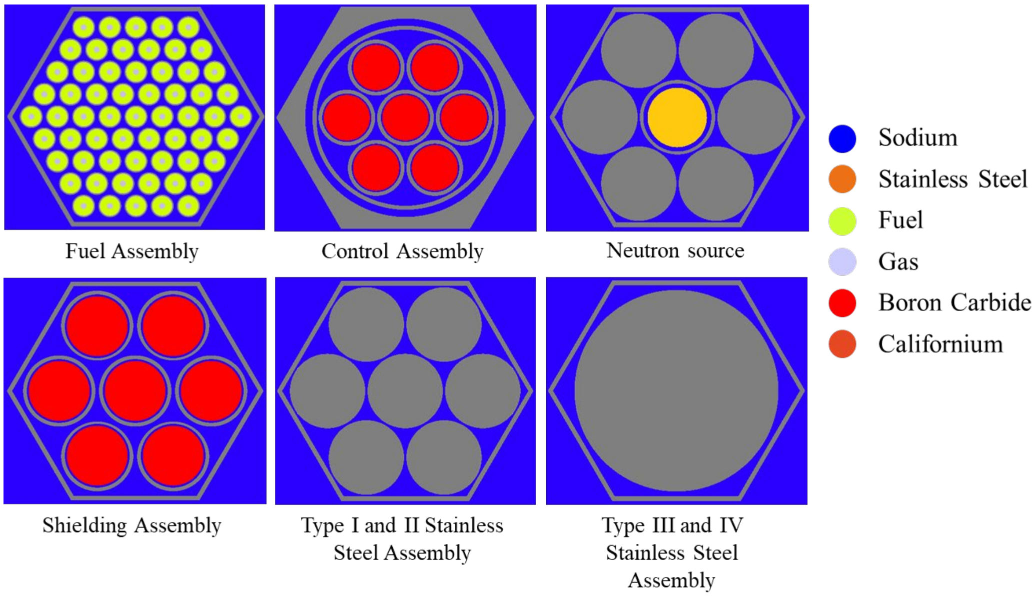

Fig. 1: Radial view of different assemblies of CEFR.

Details regarding the material characteristics and geometry of each assembly in their installation state (at 20°C) can be found in Reference [10]. The assessments considered both radial and axial thermal expansion at the cold-state temperature of 250 °C.

4. Results and Discussion

The main objective of this study is to conduct a comparative analysis of nuclear data libraries to identify and quantify discrepancies within these libraries, explicitly focusing on fast spectra, particularly for a small-sized sodium-cooled reactor.

This investigation aims to facilitate the design and advancement of reactors with similar characteristics. The study offers insights into the extent of variability inherent in the data validation process for the specific type of reactor under consideration. These insights play a key role in assessing the uncertainties introduced on reactivity and serve as a preliminary step toward more rigorous analyses.

The nuclear data libraries that have been taken into account in this study encompass ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0, CENDL-3.1, and BROND-3.1. The study assesses the impact of these nuclear data libraries on the multiplication factor obtained for the criticality calculation during the initial start-up of the CEFR reactor, and the comparative results are presented in Table 1.

Table 1

The multiplication factor obtained with different nuclear data libraries.

Nuclear data library	k_{eff}	Std. dev. [pcm]	$\Delta\rho$ [pcm]
ENDF/B-VIII.0	1.00078	6	78
JEFF-3.3	1.00221	5	221
JENDL-4.0	1.00583	5	583
CENDL-3.1	1.01291	6	1291
BROND-3.1	1.00433	5	433
(Expected) Experimental	1.00000	-	-

Previous studies [11], [12], have shown the better performance of the ENDF/B-VIII.0 library, particularly in fast spectra. ENDF/B-VIII.0 integrates the latest CIELO project evaluations, including isotopes like ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U, and ^{239}Pu [13]. However, given the influence of these new evaluations, further investigations are required, considering more isotopes and addressing different nuclear systems [4]. Substituting isotopes across nuclear data libraries can be a valuable qualitative tool to identify influential isotopes and elements contributing to system discrepancies.

In this study, ENDF/B-VIII.0 is the reference library to assess various isotopic impacts on reactivity. Each simulation is performed by replacing specific isotope data in ENDF/B-VIII.0 with corresponding data from the designated nuclear data library. Compared to the reference, the resulting reactivity differences are summarized in Table 2. It is worth noting that the presented data carry a statistical uncertainty of 5-6 pcm each.

Table 2

The reactivity induced by the isotopic substitution in ENDF/B-VIII.0.

Isotope	JEFF-3.3	JENDL-4.0	CENDL-3.1	BROND-3.1
^{10}B	-7.99	10.98	4.99	-3.00
^{11}B	6.99	2.00	0.00	6.99
^{12}C	-2.00	6.99	10.98	-5.99
^{16}O	153.52	192.33	169.45	130.62
^{23}Na	174.42	380.95	374.01	80.81
^{29}Si	0.00	-2.00	6.99	0.00
^{54}Fe	3.99	-3.99	-3.99	3.99
^{56}Fe	-125.96	10.98	-287.38	11.98
^{57}Fe	115.69	88.78	103.73	-73.94
^{58}Fe	9.98	-6.99	-3.99	3.00
^{58}Ni	267.86	62.86	-8.99	178.40
^{60}Ni	232.10	76.82	15.97	40.92
^{61}Ni	-9.99	-2.00	-1.00	-6.99
^{62}Ni	-6.99	-10.98	-27.96	5.99
64Ni	184.37	-3.99	10.98	-6.99
^{235}U	-529.97	-385.88	178.40	42.91
^{238}U	177.41	-63.94	-36.96	28.95
U	-377.84	-440.25	130.62	61.87

As can be observed from Table 1, all nuclear data libraries tend to overestimate experimental outcomes. The closest agreement between calculations and experiments is achieved using the ENDF/B-VIII.0 library, while the most significant deviations are when using the CENDL-3.1 library.

The substitution of certain isotopes, as presented in Table 2, highlights significant differences in reactivity. For instance, ^{235}U from JEFF-3.3 and JENDL-4.0 results in disparities of ~530 pcm and ~390 pcm, respectively, that can be attributed to the different evaluations of fission cross-sections and neutron spectrum in fast reactors. Even minor differences in this isotope's cross-sections data can lead to substantial changes in predicted reactivity, underscoring the sensitivity of fast reactor calculations to nuclear data. The ^{23}Na from JENDL-4.0 and CENDL-3.1 shows a difference of ~380 pcm, which emphasizes the importance of accurate neutron scattering data, particularly in the inelastic scattering channel. Sodium, as a coolant, relies on precise inelastic scattering cross-sections for effective energy moderation within the core. Variations in these cross-sections can significantly alter the neutron energy spectrum, thereby affecting the overall reactivity. The substitution of ^{58,60}Ni from JEFF-3.3 leads in a divergence of ~250 pcm, influenced by neutron absorption and scattering cross-sections in structural materials, especially in the resonance region. Nickel isotopes are often used in structural materials within reactors and their neutron interaction properties are essential for maintaining neutron economy and controlling the neutron spectrum. Furthermore, ^{56}Fe from CENDL-3.1 presents a deviation of ~290 pcm, likely due to variations in elastic and inelastic scattering cross-sections, which are essential for determining the neutron energy spectrum in the reactor. Iron, being a common structural material, interacts extensively with fast neutrons and inconsistencies in its nuclear data can significantly influence the calculated multiplication factor and overall reactor behavior.

The comparative analysis reveals reactor behavior and safety parameter variations based on the selected nuclear data library. Differences in cross-section data are observed, leading to corresponding disparities in reactor predictions. For instance, specific libraries may yield more conservative safety margins, while others may predict higher reactor performance. Selecting a certain library can significantly influence reactor control strategies, fuel management, and safety assessments.

5. Conclusions

This article underscores the role of nuclear data libraries in the accurate simulation and analysis of liquid metal cooled reactors. Engineers, researchers, and reactor operators must carefully consider the choice of a library when performing reactor modeling and safety assessments.

Accurate nuclear data is essential for making precise predictions regarding reactor behavior. However, extrapolating data beyond its initially evaluated scope can introduce additional sources of error. This becomes particularly critical when dealing with advanced reactor designs that diverge from conventional light-water reactors in terms of neutron spectrum and materials used.

In the process of compiling nuclear data libraries, individual isotopes of an element inherently carry uncertainties stemming from the difficulty of attributing specific behaviors to each isotope. While a dataset for a particular element may align well with critical experimental results, these compensating errors among isotopes remain reliable primarily within the energy spectrum range and material compositions represented by the experiments used during the data evaluation process. When venturing beyond this reference framework, errors may no longer offset each other, necessitating a characterization of these uncertainties for design and analysis purposes.

This study's primary focus was on nuclear data relevant to a small-sized sodium-cooled fast reactor, providing insights into the extent of variability associated with the data validation process for such reactor types.

Five nuclear data libraries were considered: ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0, CENDL-3.1, and BROND-3.1. These libraries were employed to simulate the attainment of achieving the first criticality in the CEFR reactor using the Monte Carlo code MCNP6.2. Initial simulations revealed reactivity differences between the experiment and simulations ranging from ~80 to ~1200 pcm.

Subsequently, the study delved into the impact of individual isotopes by substituting isotope data within the reference library, ENDF/B-VIII.0, with data from the other four libraries of interest. The most significant reactivity difference observed was approximately ~530 pcm for ^{235}U data from the JEFF-3.3 library. Other notable discrepancies included ^{235}U data from JENDL-4.0, $^{58,60}Ni$ data from JEFF-3.3, ^{23}Na data from JEFF-3.3, JENDL-4.0, and CENDL-3.1, as well as ^{16}O data from all four libraries.

The CEFR contribution to advancing the understanding of fast reactor physics and its role in the IAEA's collaborative research project underlines its role in the nuclear research community and development efforts. Combining experimental data with sophisticated computational models, the CEFR and associated research drive advancements in nuclear safety and reactor design, thereby contributing to the broader global nuclear community's knowledge base.

In summary, this comparative analysis emphasizes the need for continuous improvement and validation of nuclear data libraries, ensuring their reliability in supporting the safe and efficient operation of a liquid-cooled reactor within the dynamic nuclear energy domain.

Acknowledgements

As part of the coordinated research initiative "Neutronics Benchmark of CEFR Start-Up Tests", this research effort recived support of the International Atomic Energy Agency.

R E F E R E N C E S

[1] IAEA "Liquid Metal Coolants for Fast Reactors Cooled by Sodium, Lead, and Lead-Bismuth Eutectic", IAEA Nuclear Energy Series, technical report, 2012.
[2] *P. Romojaro et al.* "Nuclear Data Uncertainty Analysis to Meet the Target Accuracy Requirements on the MYRRHA k_{eff}", EPJ Web of Conferences, 2023.
[3] "MCNP® USER'S MANUAL Code Version 6.2," Los Alamos National Laboratory report LA-UR-17-29981.
[4] *A. Moise and I. Visan*, "Neutronic Calculation of CEFR core using different nuclear data libraries," in The 22nd International Conference on Fast Reactors and Related Fuel Cycles: Sustainable Clean Energy for the Future, Viena, 2022.
[5] *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," Nuclear Data Sheets, vol. 148, pp. 1-142, 2018.
[6] *A. J. M. Plompen et. al..,* "The joint evaluated fission and fusion nuclear data library, JEFF-3.3," The European Physical Journal A, vol. 56, nr. 181, 2020.
[7] *K. Shibata et al.,* "JENDL-4.0: A new library for nuclear science and engineering," Journal of Nuclear Science and Technology, vol. 48, nr. 1, pp. 1-30, 2011.
[8] *Z. G. Ge et al.,* "The Updated Version of Chinese Evaluated Nuclear Data Library (CENDL-3.1)," Journal of the Korean Physical Society, vol. 56, nr. 2, pp. 1052-1056, 2011.
[9] *A.I. Blokhin et al.,* "New version of neutron evaluated data library BROND-3.1," Yad.Reak.Konst, nr. 2, p. 62, 2016.
[10] *H. Xingkai et al*., "Technical specifications for neutronics benchmark of CEFR start-up tests (CRP-I31032) V7.0," CIAE, unpublished data.
[11] *M. Griseri et al.,* "Nuclear data uncertainty propagation on a sodium fast reactor," Nuclear Engineering and Design, vol. 324, pp. 122-130, 2017.
[12] *S. Ohki and T. Jin* "Dependence of fast reactor fuel burn-up characteristics on nuclear data libraries," Journal of Nuclear Science and Technology, vol. 42, nr. 4, p. 390–397, 2005.
[13] *M.B. Chadwick et al.,* "CIELO Collaboration Summary Results: International Evaluations of Neutron Reactions on Uranium, Plutonium, Iron, Oxygen and Hydrogen," Nuclear Data Sheets, vol. 148, 2018.