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Benchmark Validation of Space Reactor Criticality Based on Different Evaluated Nuclear Data Libraries

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Date: 2024-03-15T00:00:00+00:00

Abstract

To enhance the reliability of space reactor neutronics simulations, based on the criticality benchmark experiments for space reactors documented in the International Criticality Safety Handbook (HMF005 benchmark experiment), Monte Carlo codes were employed to model the core configurations in the HMF005 benchmark experiment. Using different evaluated nuclear data libraries, the deviation between calculated and experimental k_{eff} values for six core configurations was computed, and an in-depth analysis was performed on the mean, standard deviation, 2 statistic, and root-mean-square error of the calculated-to-experimental ratios. The study found that the biases between the calculated core k_{eff} results from the ENDF/B-VII.1, CENDL-3.2, ENDF/B-VIII.0, and JEFF-3.3 libraries and the experimental values fall within three standard uncertainties, with ENDF/B-VII.1 yielding results closest to the experimental values and CENDL-3.2 exhibiting a marginally larger deviation. This larger deviation for CENDL-3.2 is primarily attributed to the molybdenum and beryllium nuclides in the evaluated library, with 92Mo exerting the most significant influence among molybdenum isotopes. Furthermore, sensitivity analysis reveals that the total reaction sensitivity coefficients for 92Mo and 9Be are predominantly associated with elastic scattering sensitivity coefficients, while the radiative capture sensitivity of 9Be shows substantial discrepancy between CENDL-3.2 and ENDF/B-VII.1, reaching a difference of 34.9%.

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Criticality Benchmark Testing of Space Reactors Based on Different Evaluated Nuclear Data Libraries

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Abstract

To improve the reliability of neutronics simulation for space reactors, this study models the core configurations of the HMF005 benchmark experiment from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) using a Monte Carlo program. By combining different evaluated nuclear data libraries, the deviation between calculated and experimental keff values for six core arrangements is computed, and the mean, standard deviation, ^{2}, and root mean square error (RMSE) of the calculated-to-experimental (C/E) ratios are thoroughly analyzed. The results show that the deviations of keff calculations from experimental values using the ENDF/B-VII.1, CENDL-3.2, ENDF/B-VIII.0, and JEFF-3.3 libraries are within three times the uncertainty, with ENDF/B-VII.1 showing the best agreement and CENDL-3.2 exhibiting slightly larger deviations. The larger deviation observed with CENDL-3.2 is primarily attributed to the molybdenum and beryllium nuclides in the library, with the molybdenum isotope 92Mo having the greatest impact. Sensitivity analysis reveals that the total reaction sensitivity coefficients of 92Mo and 9Be are mainly associated with elastic scattering sensitivity coefficients, while the radiative capture sensitivity of 9Be differs significantly between CENDL-3.2 and ENDF/B-VII.1, with a discrepancy of up to 34.9%.

Keywords: criticality calculations; effective multiplication factor; evaluated nuclear data libraries; Monte Carlo simulation
Classification: TL375.5 **Document code:** A

As global space exploration technology advances, space power systems based on solar and chemical energy are approaching their technical limits. With deepening space activities, conventional energy sources will struggle to meet the demands of deep-space exploration and special missions. Nuclear energy, characterized by its wide power range, high energy density, minimal environmental impact, and long lifespan, holds broad application prospects in space exploration. Currently, the United States, Russia, the European Union, and other nations regard space nuclear power technology as a core national frontier technology and have actively implemented strategic deployments for space applications and resource development [1-2]. Since digital reactor technology can shorten reactor development cycles and reduce costs, countries are now utilizing it for space reactor design. The accuracy of data in evaluated nuclear databases directly impacts space reactor design precision, making it crucial to assess the applicability of these databases for space reactor design. Although numerous space reactor studies exist domestically and internationally—such as the TOPAZ-I and TOPAZ-II series developed by the former Soviet Union in the 1960s [3], the kilowatt-scale Kilopower reactor tested by the United States in 2018 [4], the SPACE-R proposed by the China Institute of Atomic Energy [5], the ACMIR space reactor developed by Tsinghua University' s REAL team [6], another ACMIR reactor developed by the Reliability and Environmental Science Laboratory of the Beijing Institute of Spacecraft Environment Engineering [7], and the molten salt-cooled space reactor concept proposed by Li Ting et al. at Nanjing University of Aeronautics and Astronautics [8]—most current conceptual designs directly use evaluated nuclear databases for reactor physics calculations without validating their reliability for space reactor applications. Therefore, conducting macroscopic benchmark testing of nuclear data for space reactors is essential for design. Critical benchmark experiments are commonly used to evaluate the accuracy of physics calculation models, design methodologies, and nuclear databases; precise measurement of reactor keff enables macroscopic benchmark testing of key material nuclear data [9]. To validate the evaluated nuclear databases used in space reactor physics calculations, this study selects the HMF005 benchmark from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [10], employs the MCNP program with different evaluated nuclear databases to calculate core keff values corresponding to experimental conditions, and performs macroscopic in-reactor validation of nuclear data for space applications. By analyzing the differences between calculated and experimental keff values from various databases, the reliability of current evaluated nuclear databases is assessed.

Received: December 29, 2023
Revised: March 7, 2024
Funding: National Natural Science Foundation of China (11875128)
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1. Critical Benchmark Experiment

The HMF005 series experiments were critical experiments conducted in 1987 by the Institute of Physics and Power Engineering in Obninsk, Russia. Based on different core material arrangements, six distinct core configurations were studied. All six reactor cores used highly enriched uranium metal as fuel. Due to its high reflectivity, high-temperature resistance, and corrosion resistance, some reactor designs employed metallic molybdenum as a reflector layer. In addition to molybdenum, some designs also used beryllium as a reflector material. These reactor designs provide excellent experimental data for validating evaluated neutron cross-section data for molybdenum and beryllium. The HMF005 benchmark includes six experiments, which are modeled in detail using the Monte Carlo program in this study. Table 1 lists the basic material compositions and atomic densities of various rod bundles used in the experiments. Five materials are involved: uranium blocks, reflector layers (top and bottom), molybdenum rods, beryllium rods, and empty tubes. These materials are assembled into different types of fuel or other rods, including U3, U6, U8, U11, molybdenum, beryllium, and empty tubes. The benchmark experiments construct six core experimental models by arranging and assembling fuel rods, reflector rods, and empty tubes, with specific core arrangements and compositions shown in Figures 1 [Figure 1: see original paper] through 6 [Figure 6: see original paper], with dimensions in centimeters.

Table 1 Material atomic densities in each region (1/barn · cm)

Material/Region	Density Values
Top and bottom reflector	3.3109$×10^{-4}, 3.2968×10{-2}, 1.4590×10^{-4}, 3.1467×10{-3}$
Molybdenum	3.0875$×10^{-3}, 5.3547×10{-2}, 5.3547×10^{-2}$
Beryllium	3.2912$×10^{-3}, 8.4596×10{-4}, 4.5748×10^{-4}, 5.6121×10{-5}, 4.5741×10^{-5}, 2.5489×10{-5}, 1.0624×10^{-3}, 3.0863×10{-3}$
Chromium	3.2273$×10^{-3}, 8.4596×10{-4}, 4.5748×10^{-4}, 5.6121×10{-5}, 4.5741×10^{-5}, 2.5489×10{-5}, 2.2461×10^{-5}$
Nickel	1.0962$×10^{-1}, 5.3293×10{-3}, 5.3293×10^{-3}, 3.2273×10{-3}, 1.3969×10^{-3}, 1.3969×10{-3}$
Manganese	8.4596$×10^{-4}, 7.5543×10{-4}, 7.5543×10^{-4}, 4.5748×10{-4}, 9.2673×10^{-5}, 9.2673×10{-5}$
Silicon	5.6121$×10^{-5}, 7.5532×10{-5}, 7.5532×10^{-5}, 4.5741×10{-5}, 4.2090×10^{-5}, 4.2090×10{-5}$
Titanium	2.5489$×10^{-5}, 3.7090×10{-5}, 3.7090×10^{-5}, 2.2461×10{-5}$
Carbon	2.2461$×10^{-5}$
Aluminum	1.0962$×10^{-1}$

Note: The table structure has been reconstructed from the original text data.

2. Analysis Methods

This study first utilizes the evaluated nuclear data libraries ENDF/B-VII.1 [11], CENDL-3.2 [12], ENDF/B-VIII.0 [13], and JEFF-3.3 [14] to generate continuous-point cross-section libraries for the MCNP program using the nuclear data processing code NJOY2016. The MCNP program is then used to calculate the effective multiplication factor keff and sensitivity coefficients for relevant nuclides.

Evaluation parameters include the mean and standard deviation of the calculated-to-experimental (C/E) ratios, with calculation formulas as described in the methodology. Additionally, the root mean square error (RMSE) is used to assess consistency between calculated and experimental results. The benchmark experiments were conducted at 300K, so the MCNP simulations are performed at 300K. For criticality calculations, 10,000 particles per generation are used, with 1,100 total generations and 100 inactive generations.

3. Results and Discussion

3.1 Effective Multiplication Factor

Figure 7 [Figure 7: see original paper] compares the calculated values with experimental values based on different evaluated nuclear databases. Table 2 presents the HMF005 benchmark calculation results including (C/E), RMSE, -1, and Δ. The experimental uncertainty for the benchmark is 360 pcm, while the maximum statistical error in the Monte Carlo calculations does not exceed 21 pcm. As shown in Figure 7, some calculated results fall within the 1σ confidence interval, and all results are within the 3σ confidence interval. According to the analysis method described in Section 2, the keff results for the six cores calculated using different evaluated nuclear databases are processed against the benchmark experimental values, with results shown in Table 2. It can be seen that calculations using ENDF/B-VII.1 and ENDF/B-VIII.0 libraries agree well with experimental values, while results based on CENDL-3.2 show significantly larger deviations compared to the other three libraries, with an RMSE approximately twice that of ENDF/B-VIII.0. Since the benchmark experiments extensively use molybdenum and beryllium nuclides as reflector materials, these differences may be caused by variations in the evaluated nuclear data for these reflector materials. To investigate the cause of the larger deviations with CENDL-3.2, the reflector materials in all six core configurations of the benchmark experiments were removed, and keff was recalculated using CENDL-3.2 and ENDF/B-VII.1. The results are shown in Table 3 . As shown in Table 3, after removing the reflector rods, the calculations from CENDL-3.2 and ENDF/B-VII.1 show excellent agreement, indicating that the deviations between CENDL-3.2 and other libraries primarily originate from differences in the evaluated nuclear data for reflector materials (molybdenum and beryllium rods).

HMF005_{04} contains only one molybdenum reflector rod and can be considered as having full beryllium rod reflection. Given the unique characteristics of HMF005_{01} (full molybdenum rod reflection) and HMF005_{04} (full beryllium rod reflection), these two benchmark experiments are investigated in depth. Based on CENDL-3.2 results, the molybdenum and beryllium data in CENDL-3.2 are replaced with data from ENDF/B-VII.1, and calculations for HMF005_{01} and HMF005_{04} are performed. The comparison of deviations between calculated and experimental values is shown in Table 4 . As shown in Table 4, after replacing the molybdenum nuclides in HMF005_{01} and beryllium nuclides in HMF005_{04} with ENDF/B-VII.1 sources, the deviation between keff calculated using CENDL-3.2 and experimental values is significantly reduced, with keff improvements of 643 pcm and 402 pcm, respectively. Following the principle of controlling a single variable, the natural isotopes of molybdenum in HMF005_{01} are individually replaced with nuclear database data to study the impact of each molybdenum isotope on keff. The calculation results are shown in Figure 8 [Figure 8: see original paper]. As shown in Figure 8, for the HMF005_{01} benchmark, among molybdenum isotopes, 92Mo has the greatest impact at 301 pcm; 100Mo has the smallest impact, while other isotopes have approximately 100 pcm impact.

3.2 Sensitivity Coefficient Analysis

To investigate the keff differences resulting from database replacement in HMF005_{01} and HMF005_{04}, the sensitivity coefficients for total reaction, elastic scattering, total absorption, and radiative capture reactions of 92Mo and 9Be in ENDF/B-VII.1 and CENDL-3.2 are studied. Table 5 shows the total sensitivity coefficients for 92Mo under four reaction channels in HMF005_{01}. Comparison reveals that the differences in total reaction sensitivity coefficients and total absorption cross-section sensitivity coefficients for 92Mo between CENDL-3.2 and ENDF/B-VII.1 are within 1%, while the deviations in elastic scattering and radiative capture sensitivity coefficients reach 7%. Figures 9 [Figure 9: see original paper] through 12 [Figure 12: see original paper] show the sensitivity coefficient distributions. As seen in these figures, the total reaction sensitivity coefficient for 92Mo is primarily determined by the elastic scattering sensitivity coefficient. The sensitivity coefficients for radiative capture and absorption cross-sections of 92Mo are relatively small. In the high-energy region (neutron energy $> 10^4$ eV), significant differences exist in the sensitivity coefficients of 92Mo between ENDF/B-VII.1 and CENDL-3.2, which may be the cause of the larger keff differences.

Table 6 shows the sensitivity coefficients for 9Be under four reactions in HMF005_{04}. Comparison shows that the differences in total sensitivity coefficients, elastic scattering coefficients, and total absorption coefficients for 9Be between CENDL-3.2 and ENDF/B-VII.1 are within 2%, but the radiative capture sensitivity coefficient shows a large difference. Figures 13 [Figure 13: see original paper] through 16 [Figure 16: see original paper] present the sensitivity coefficient distributions for total reaction, elastic scattering, absorption, and radiative capture cross-sections. As shown in these figures, the total reaction sensitivity coefficient for 9Be is mainly related to elastic scattering sensitivity. The radiative capture sensitivity of 9Be differs significantly between CENDL-3.2 and ENDF/B-VII.1, with a deviation of up to 34.9%. Although the radiative capture sensitivity difference is large, its absolute value is small, accounting for a minor portion of the absorption cross-section sensitivity coefficient, resulting in minimal difference in absorption cross-section sensitivity coefficients.

3.3 Normalized Neutron Flux Density

Normalized neutron flux densities for the six benchmark experiments are calculated based on different evaluated nuclear databases, with results shown in Figures 17 [Figure 17: see original paper] through 22 [Figure 22: see original paper]. The neutron flux densities use a 30-group energy structure, with details available in reference [10]. As shown in Figures 17-22, the normalized neutron flux densities calculated using ENDF/B-VII.1, CENDL-3.2, ENDF/B-VIII.0, and JEFF-3.3 show consistent trends across the six core configurations with minor differences. The moderating effect of beryllium reflectors on neutrons is clearly visible from HMF005_{02} to HMF005_{06} benchmark experiments, while Model 1 exhibits a harder neutron spectrum compared to other benchmark models.

Conclusions

Based on the International Criticality Safety Benchmark Evaluation Project benchmark (HMF005 experiment), macroscopic validation studies of evaluated nuclear data for space reactors were conducted. Using the MCNP program and four evaluated nuclear databases (ENDF/B-VII.1, CENDL-3.2, ENDF/B-VIII.0, and JEFF-3.3), keff values for six core configuration space reactor benchmark experiments were calculated. The main conclusions are: (1) Benchmark experimental values and Monte Carlo program results show that all calculation deviations from experimental results are within three standard deviations. ENDF/B-VII.1 shows the best agreement with experimental values, while CENDL-3.2 exhibits larger deviations. (2) The larger deviation of CENDL-3.2 results primarily originates from reflector material nuclear data for molybdenum and beryllium. Replacing molybdenum and beryllium nuclear data in CENDL-3.2 continuous-point cross-section libraries with data from ENDF/B-VII.1 improves keff by 643 pcm for HMF005_{01} (full molybdenum rod reflection) and 402 pcm for HMF005_{04} (full beryllium rod reflection). Detailed study of natural molybdenum isotopes reveals that changes in the 92Mo nuclide between CENDL-3.2 and ENDF/B-VII.1 cause the largest keff variation. (3) Sensitivity coefficient studies of 92Mo and 9Be in ENDF/B-VII.1 and CENDL-3.2 show that total reaction sensitivity coefficients for both nuclides are primarily associated with elastic scattering sensitivity coefficients. The radiative capture sensitivity of 9Be differs significantly between CENDL-3.2 and ENDF/B-VII.1, with a deviation of up to 34.9%. The neutron spectra from the six benchmark experiments demonstrate the clear moderating effect of 9Be.

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