Evaluation of CENDL-3.2 and CENDL-TMSR-V1 on zero power experimental benchmark of Molten Salt Reactor Experiment

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Abstract

The 2019 edition of the International Handbook of Reactor Physics Evaluation Project (IRPhEP) includes the Molten Salt Reactor Experiment (MSRE) benchmark, which provides keff (effective multiplication factor) values from various nuclear data libraries, including ENDF/B-VII.1, derived from first criticality experiments and control rod worth calculations. This benchmark constitutes the first comprehensive reference case for molten salt reactor physics and has been widely used to assess the consistency and accuracy of Monte Carlo codes and nuclear data libraries in molten salt reactor modeling. Since 2011, the Shanghai Institute of Applied Physics, Chinese Academy of Sciences, has been developing the Thorium-based Molten Salt Reactor (TMSR) nuclear energy system to promote thorium resource utilization. To support this initiative, the China Nuclear Data Center developed the CENDL-TMSR-V1 library dedicated to the thorium-uranium fuel cycle. However, the validation status of the Chinese nuclear data libraries CENDL-3.2 and CENDL-TMSR-V1 for molten salt reactor applications remains unexplored. This work developed a high-fidelity MSRE model using OpenMC and performed a comparative analysis across four evaluated nuclear data libraries: ENDF/B-VII.1, ENDF/B-VIII.0, CENDL-3.2, and CENDL-TMSR-V1. Neutronics parameters were systematically evaluated, including reactivity coefficients, control rod differential worth, zero-power flux distribution, and 500-day burnup calculations. Key findings indicate that the relative deviation in keff between all databases and the IRPhEP benchmark values remains below 300 pcm (0.3% $\Delta k/k$). The maximum relative difference in power distribution predictions between the CENDL series libraries and ENDF/B-VII.1 is less than 2%. The keff deviation in burnup calculations stays within 0.2%. This study validates the applicability of the CENDL series libraries for neutronics simulations of molten salt reactors.

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Full Text

Evaluation of CENDL-3.2 and CENDL-TMSR-V1 on Zero-Power Experimental Benchmark of Molten Salt Reactor

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Abstract: The 2019 edition of the International Reactor Physics Evaluation Project (IRPhEP) Handbook incorporated the Molten Salt Reactor Experiment (MSRE) benchmark, providing keff (effective multiplication factor) values derived from first criticality experiments and control rod worth calculations for multiple nuclear data libraries including ENDF/B-VII.1. This benchmark constitutes the first comprehensive reference case for molten salt reactor physics, having been extensively utilized to assess the consistency and accuracy of Monte Carlo codes and nuclear data libraries in molten salt reactor modeling. Since 2011, the Thorium Molten Salt Reactor (TMSR) nuclear energy system has been under development at the Shanghai Institute of Applied Physics, Chinese Academy of Sciences to facilitate thorium resource utilization. In support of this initiative, the China Nuclear Data Center developed specialized CENDL-TMSR-V1 libraries tailored for thorium-uranium fuel cycles. Nevertheless, the verification status of Chinese nuclear libraries CENDL-3.2 and CENDL-TMSR-V1 in molten salt reactor applications remains unexplored. In this work, a high-fidelity MSRE model was developed using OpenMC, with comparative analyses conducted across four evaluated nuclear data libraries: ENDF/B-VII.1, ENDF/B-VIII.0, CENDL-3.2, and CENDL-TMSR-V1. A systematic evaluation of neutronic parameters was performed, encompassing reactivity coefficients, control rod differential worth, zero-power flux distribution, and 500-day burn-up calculations. Key findings reveal that the relative deviations in keff between all libraries and IRPhEP benchmark values remain below 300 pcm (0.3% Δk/k). The maximum relative discrepancy in power distribution predictions between CENDL-series libraries and ENDF/B-VII.1 is <2%. The keff deviations during burn-up calculations are maintained within 0.2% Δk/k. This study validates the applicability of CENDL-series libraries for molten salt reactor neutronic simulations.

Keywords: Molten salt reactor experiment; zero-power experiment; OpenMC; CENDL-TMSR-V1; CENDL-3.2

1 Introduction

The Molten Salt Reactor Experiment (MSRE) was a liquid-fueled molten salt prototype reactor designed and constructed by Oak Ridge National Laboratory (ORNL) in the United States. It achieved first criticality in 1965 and operated until 1969. The MSRE used LiF-BeF2-ZrF4-UF4 molten salt fuel, accumulating over 13,000 hours of operation at 7.3 MWth[1-3]. It successfully validated core technologies including online refueling and fuel chemical stability, providing critical experimental data for subsequent molten salt reactor development. These data have served as a standard reference for developing and validating multiple MSR simulation tools[4,5].

Molten salt reactor technology has gained significant international attention in recent years as a crucial development direction for advanced nuclear energy systems. Since 2011, the Shanghai Institute of Applied Physics, Chinese Academy of Sciences (SINAP-CAS) has initiated the Thorium Molten Salt Reactor Nuclear Energy System (TMSR) research program. This program proposes an innovative technical pathway based on thorium-uranium fuel cycles. In molten salt reactor design, the accuracy of nuclear data directly impacts the reliability of neutronics calculations. Current mainstream evaluated nuclear databases include ENDF/B[6-8], JEFF[9,10], JENDL[11,12], and CENDL[13]. To address the specific requirements of efficient thorium utilization in the TMSR system, the China Nuclear Data Center developed the specialized library, CENDL-TMSR-V1, under the Chinese TMSR Strategic Pioneer Science and Technology Project. Multiple Chinese research teams have conducted comprehensive benchmark validations to verify its reliability. First, validations were performed on critical assemblies containing nuclides such as ^{233}U, ^{235}U, Th, Pu, F, Li and Be. The results indicated calculation errors below 0.5% for assemblies involving ^{233}U, ^{235}U, F, and Li. However, relative errors exceeding 0.5% were observed in Th/Pu assemblies and Be-containing configurations when comparing CENDL-TMSR-V1 with ENDF/B-VII.0[14]. Further validation utilized 1,245 sets of critical experiment data from the International Criticality Safety Benchmark Evaluation Project (ICSBEP). This analysis demonstrated that relative errors between calculated keff values and experimental values remained below 0.5% for the majority of benchmark configurations[15]. Additional simulations were performed on benchmark facilities including the LR-0 graphite-moderated reactor and FLiNa molten salt system using CENDL-TMSR-V1. These studies revealed that relative errors in the effective multiplication factor keff from experimental values consistently fell within statistical uncertainties[16].

Current validation efforts primarily rely on ICSBEP benchmarks and light water reactor experimental facilities, with no validation conducted using real molten salt reactor prototypes. This study selects the MSRE zero-power experimental benchmark to evaluate CENDL-3.2 and CENDL-TMSR-V1. First, an MSRE model was developed using OpenMC, with the model's accuracy verified through comparative calculations against the IRPhEP model. Subsequently, continuous-energy ACE-format cross-section libraries were generated using the CENDL series libraries for criticality calculations, power distribution predictions, and burnup analysis.

The paper is structured as follows: Section 2 details the core structural characteristics and modeling process of MSRE, emphasizing geometric differences between this model and the IRPhEP model. Section 3 comprehensively describes the CENDL-TMSR-V1 and CENDL-3.2 libraries, and briefly explains the production workflow of continuous-energy HDF5-format cross-section libraries for OpenMC calculations. Section 4 comparatively analyzes the performance of different libraries in the MSRE benchmark, including keff error distributions, radial power peaking factors, and burnup evolution characteristics. Section 5 presents conclusions, summarizing differences and findings of CENDL series libraries in MSR calculations.

2 High-Fidelity OpenMC Model of MSRE

The 2019 edition of IRPhEP includes a model of the MSRE first criticality experiment. Reactor physics parameters such as control rod worth calculated based on this model show good agreement with experimental values[17]. Based upon this model, researchers have employed SCALE, MCNP, and Serpent Monte Carlo codes with ENDF/B-VII.0, ENDF/B-VII.1 and ENDF/B-VIII.0 to calculate the effective multiplication factor. These studies compared the impacts of different Monte Carlo codes and evaluated nuclear data libraries on results[18]. Using OpenMC, the effective multiplication factors were calculated for both the IRPhEP model and the MSRE CAD model. The CAD model results showed approximately 1% lower values compared to the IRPhEP model, demonstrating closer alignment with experimental measurements[19]. The calculated effective multiplication factor for the IRPhEP model exceeded experimental values by 2%, representing an error six times larger than the experimental uncertainty[20]. The significant discrepancy observed between the MSRE benchmark results and experimental data is primarily attributed to substantial uncertainties in fuel composition. Although determining the exact causes of the error between historical MSRE benchmark calculations and experimental values remains challenging due to the time elapsed, the MSRE benchmark retains critical importance for nuclear data library validation.

The MSRE core active zone consists of tightly arranged graphite stringers[21] as shown in Fig. 3a [Figure 3: see original paper], with fuel salt flowing through channels formed by grooves on the sides of the graphite stringers. The central area of the graphite array contains three control rods and one sample basket, used for reactivity control and material irradiation testing, respectively. The core configuration during the MSRE first criticality experiment was: control rod 2 and control rod 3 fully withdrawn (129.54 cm), control rod 1 inserted to 3% of its integral worth (118.364 cm), with a nominal ^{235}U loading of 65.25 kg and fuel salt flow rate of 4.54 m^3/min. The IRPhE model simplifies the fuel salt as a static medium with uniform temperature distribution[17]. The fuel salt composition at first criticality is provided in Table 1 , with detailed MSRE model dimensions available in Reference [20].

Table 1 Fuel composition for MSRE first criticality experiment[20]

Component	Composition
^{235}U	0.79 mol %
^{7}LiF	64.88 mol %
BeF_2	29.27 mol %
ZrF_4	5.06 mol %
UF_4	(0.014$±$0.007) wt%
^{235}U	(1.408$±$0.007) wt%
^{234}U	(0.006$±$0.006) wt%

The axial and radial geometry of the present MSRE model is shown in Fig. 1 [Figure 1: see original paper], with control rod and sample basket modeling details illustrated in Fig. 2 [Figure 2: see original paper]. While maintaining consistency with the IRPhEP model[20] in primary dimensions, differences exist in structural details including graphite stringer top and horizontal graphite lattice.

The graphite stringer top in the MSRE core features a pyramidal shape[21] to prevent residual fuel salt accumulation during drainage, whereas the IRPhEP model simplifies this geometry to a conical shape. This model adopts the pyramidal configuration as shown in Fig. 3. The configuration of the horizontal graphite lattice is shown in Fig. 4a [Figure 4: see original paper][22], with a thickness of 2.54 cm and support rod holes of 2.642 cm diameter arranged in a cruciform configuration[20]. The IRPhEP model neglects the gap between lattice holes and support rods, whereas the model in this work accounts for these gaps (Fig. 4), achieving closer alignment with actual conditions.

OpenMC calculations employed 100,000 particles per generation, with 700 active and 50 inactive generations. As summarized in Table 2 , the keff discrepancy between this model and IRPhEP configurations is merely 4 pcm, well within standard deviation, indicating negligible reactivity impact from these modeling refinements.

Table 2 keff of various model simplifications

<table>
<tr><th>Model configuration</th><th>keff</th></tr>
<tr><td>Conical top, no lattice gap (IRPhEP geometry)</td><td>1.02162$±0.00012||Conicaltop, withlatticegap|1</td></tr>
</table>

Table 3 compares the keff values between the model in this work, the IRPhEP model, and other MSRE zero-power benchmark Monte Carlo models. Using the same ENDF/B-VII.1 library as the IRPhEP model, the model in this work yields a keff value 34 pcm higher than the IRPhEP reference. Fig. 5 [Figure 5: see original paper] shows the core neutron energy spectra comparison between the model in this work and IRPhEP model. Fig. 6 [Figure 6: see original paper] and Fig. 7 [Figure 7: see original paper] present the axial neutron production

distribution and axial neutron flux distribution, respectively. The close agreement in core energy spectrum, axial neutron production, and flux distributions validates the fidelity of the model in this work. Geometric differences between the models induce localized discrepancy in axial neutron production profiles at horizontal graphite lattice interfaces and graphite stringer top regions.

Table 3 Comparison of calculated keff values for MSRE first criticality experiment

<table>
<tr><th>Model and Library</th><th>keff</th><th>100×(C-E)/E</th><th>100×(C-B)/B</th></tr>
<tr><td>SERPENT, ENDF/B-VII.1 (IRPhEP)</td><td>1.02132$±0.00010|2.15|−||SERPENT, JENDL−4.0(IRPhEP)|1.02061±0.00010|2.08|−0.07||SERPENT(CSG), ENDF/B−VIII.0(IRPhEP)|1.02355±0.00010|2.38|0.22||OpenMC(CSG), ENDF/B−VII.1|1.02142±0.00012|2.16|0.01||OpenMC(CSG), ENDF/B−VIII.0|1.02346±0.00012|2.37|0.21||OpenMC(CSG), JEFF3.3|1.02402±0.00012|2 VIII.0|1.00872±0.00012|0.89|−1.23||OpenMC(CSG), ENDF/B−VII.1(Thiswork)|1.02166±$0.00012</td><td>2.10</td><td>0.03</td></tr>
</table>

C: Calculated keff; E: Experimental keff
C: Calculated keff; B: Benchmark keff (IRPhEP: SERPENT, ENDF/B-VII.1)

3 CENDL Libraries and Cross-Section Processing

3.1 Introduction to CENDL Libraries

CENDL-3.2 is an Evaluated Nuclear Data Library independently developed in China, officially released on June 12, 2020. It adopts the internationally standardized ENDF-6 format, covering 272 nuclides with neutron incident energy ranging from 10^{-5} eV to 20 MeV. CENDL-3.2 updates nuclide data including U, Pu, Th, and Fe, while adding model-dependent covariance data for 70 fission product nuclides such as ^{137}Cs and ^{90}Sr. Validated against 1,261 critical benchmark experiments in ENDITS-1.0, CENDL-3.2 shows good consistency between calculated results and experimental data for various nuclear systems[13]. Compared to the JEFF-3.3 and ENDF/B-VIII.0 libraries, CENDL-3.2 performs better in the calculation of the ^{233}U assemblies[23].

To meet the requirements of nuclear design accuracy and thorium-uranium fuel cycle physics analysis, the China Nuclear Data Center has developed a specialized nuclear library for thorium-uranium cycles: CENDL-TMSR-V1. The library primarily sources its evaluated nuclear data from internationally established libraries (e.g., ENDF/B-VII.0, JENDL-4.0u, CENDL-3.2), with targeted improvements implemented for key isotopes including ^{6}Li, ^{7}Li, ^{232}Th, ^{232}U, and ^{233}U[16]. The library contains a total of 403 nuclides, including 16 light nuclei, 86 medium-heavy nuclei commonly found in structural materials, 224 medium-heavy nuclei in fission products, and 77 fission nuclides[14].

3.2 Workflow of HDF5 Data Library

This study develops a continuous-energy cross-section library for OpenMC calculations based on CENDL-3.2 and CENDL-TMSR-V1, with the processing workflow illustrated in Fig. 8 [Figure 8: see original paper]. OpenMC provides the openmc.data module in its Python API. The IncidentNeutron.from_{njoy}() method can create OpenMC instances, and the export_{{{to}}_{{hdf5}}}() function then efficiently processes cross-section libraries into HDF5 format. The library processing employs identical temperature points to those in the ACE database released by Los Alamos National Laboratory (LANL) for MCNP simulations, specifically: 293.6K, 600K, 900K, 1200K, 2500K, 0.1K, and 250K[24]. Since CENDL-3.2 and CENDL-TMSR-V1 lack thermal scattering cross sections for graphite and hydrogen in water, this work utilizes thermal scattering data from ENDF/B-VII.1.

Fig. 8 Workflow for generating HDF5-format continuous-energy cross-section libraries using OpenMC' s Python API

4 Results

4.1 keff of First Criticality

Results with different nuclear data libraries are presented in Table 4 . The OpenMC simulations used 100,000 particles per generation, with 700 active generations and 50 inactive generations. Sections 4.2 and 4.3 maintained identical particle population settings, yielding keff standard deviation around 12 pcm. The CENDL-3.2 library produces keff values 72 pcm lower than ENDF/B-VII.1, while CENDL-TMSR-V1 shows a 56 pcm reduction compared to ENDF/B-VII.1. Both CENDL libraries demonstrate good agreement with ENDF/B-VII.1 in keff calculations.

Table 4 keff results from ENDF/B and CENDL libraries

<table>
<tr><th>Library</th><th>keff</th><th>100×(C-E)/E</th><th>100×(C-B)/B</th></tr>
<tr><td>IRPhEP ENDF/B-VII.1</td><td>1.02132$±0.00130|2.15|−||$ThisworkENDF/B−VII.1$|1.02166±0.00012|2.19|0.03||$ENDF/B−VIII.0$|1.02338±0.00012|2.36|0.20||$CENDL−$3.2|1.02094±0.00012|2.12|−0.07||$CENDL−TMSR−V1$|1.02110±$0.00012</td><td>2.03</td><td>-0.05</td></tr>
</table>

C: Calculated keff; E: Experimental keff
C: Calculated keff; B: Benchmark keff (IRPhEP: SERPENT, ENDF/B-VII.1)

4.2 Control Rod Worth

The differential and integral worths of control rod 1 were calculated at the initial critical uranium concentration with control rods 2 and 3 in fully withdrawn positions, and compared against IRPhEP model predictions and experimental measurements. Experimental differential worth curves were obtained by normalizing measured control rod 1 worths at various concentrations to the initial critical uranium concentration, while integral worth curves resulted from integrating experimental differential worth data[25].

Differential worth calculations require vertical movements of the control rod. Fig. 9 [Figure 9: see original paper] and Fig. 10 [Figure 10: see original paper] display control rod 1' s differential worth profiles at displacement distances of 5.08 cm and 10.16 cm, respectively. Calculated differential and integral worth curves from this study show good agreement with experimental data. For 5.08 cm displacements, the CENDL-TMSR-V1 library yielded the minimal average error (1.085 pcm) between calculated and experimental differential worth curves. At 10.16 cm displacements, CENDL-3.2 achieved the lowest average error (0.8 pcm), while CENDL-TMSR-V1 produced an average error of 1.258 pcm.

In integral worth comparisons, the IRPhEP model exhibited the maximum error (92 pcm) at 48.3 cm rod position, whereas CENDL-TMSR-V1 showed the maximum error (66 pcm) at 114.3 cm position, both within acceptable agreement ranges, as shown in Fig. 11 [Figure 11: see original paper].

Fig. 9 Differential worth of control rod 1 at 5.08 cm displacement: (a) differential worth, (b) absolute error from experiment

Fig. 10 Differential worth of control rod 1 at 10.16 cm displacement: (a) differential worth, (b) absolute error from experiment

Fig. 11 Integral worth of control rod 1: (a) integral worth, (b) absolute error from experiment

In the control rod shadowing experiments, control rod 1 served as the regulating rod under two compensation scenarios: first, control rod 2 acted as the shim rod with control rod 3 fully withdrawn; second, control rods 2 and 3 functioned as a coordinated shim rod bank at identical positions. This study analyzed shadowing effects for three uranium loadings (67.94 kg, 69.94 kg, 71.71 kg) using the rod position search method from reference[17], where the keff error during position searches was controlled within 20 pcm. Calculated results in Fig. 12 [Figure 12: see original paper] demonstrate good agreement with experimental data.

Fig. 12 Calculated change in critical position of rod No. 1 as shim rods No. 2 and 3 are inserted into the core

Calculations using different libraries evaluated control rod bank worths in the current model under three ^{235}U loadings. Two configurations were analyzed: (1) control rods 1 and 2 grouped with control rod 3 fully withdrawn; (2) control rods 1, 2, and 3 grouped together. Results are shown in Fig. 13 [Figure 13: see original paper]. The ENDF/B-VII.1 implementation shows good agreement with IRPhEP model predictions, though both the current model's Rod 1-2 bank worth and IRPhEP results fall below the experimental range at 71.71 kg ^{235}U loading. Comparative analysis reveals that CENDL-TMSR-V1 yields lower bank worths than CENDL-3.2, while ENDF/B-VIII.0 produces smaller values than ENDF/B-VII.1. The error between CENDL-TMSR-V1 and ENDF/B-VII.1 calculations remains within 100 pcm.

Fig. 13 Rod bank worth

4.3 Neutron Flux and Power Distribution

The radial neutron flux distribution and relative power distribution calculated using ENDF/B-VII.1 in the current MSRE model are shown in Fig. 14 [Figure 14: see original paper]. Fig. 15 [Figure 15: see original paper] through Fig. 17 [Figure 17: see original paper] present the errors of radial flux distributions from other libraries relative to ENDF/B-VII.1. The CENDL-TMSR-V1 library demonstrates a maximum relative error of 4.4% in radial neutron flux compared to ENDF/B-VII.1, while CENDL-3.2 shows up to 4.6% error.

Fig. 14 Spatial flux distribution (left) and power distribution (right) in the x-y plane as computed by ENDF/B-VII.1

Fig. 15 Spatial flux distribution in the x-y plane as computed by ENDF/B-VIII.0 (left) and the relative error in flux between ENDF/B-VIII.0 and ENDF/B-VII.1 (right)

Fig. 16 Spatial flux distribution in the x-y plane as computed by CENDL-3.2 (left) and the relative error in flux between CENDL-3.2 and ENDF/B-VII.1 (right)

Fig. 17 Spatial flux distribution in the x-y plane as computed by CENDL-TMSR-V1 (left) and the relative error in flux between CENDL-TMSR-V1 and ENDF/B-VII.1 (right)

Fig. 18 [Figure 18: see original paper] displays power distributions for the central 29 fuel assemblies marked by the red box in Fig. 14. CENDL-TMSR-V1 maintains within 2% relative error from ENDF/B-VII.1 in these assemblies, whereas CENDL-3.2 exhibits error below 0.5% compared to ENDF/B-VII.1.

Fig. 18 Power distribution of central cells: (a) power distribution, (b) relative error from ENDF/B-VII.1

4.4 Customized MSRE Depletion Case

A customized burnup problem was established for the MSRE model. The burnup calculations duration was set at 500 days with a core thermal power of 8 MW. The primary loop molten salt volume measured approximately 1.96 m^3, including a lower plenum mixture (90.8% fuel salt and 9.2% INOR-8) of 0.35 m^3[3]. Shorter time steps were applied during initial burnup stages. Logarithmic coordinates were adopted on the horizontal axis to enhance visualization clarity. The keff evolution curve (Fig. 19 [Figure 19: see original paper]) demonstrates a maximum discrepancy of ~158 pcm between CENDL-TMSR-V1 and ENDF/B-VII.1 results throughout the burnup period. Fig. 20 [Figure 20: see original paper] through Fig. 27 [Figure 27: see original paper] present nuclide quantity comparisons and the relative error from ENDF/B-VII.1 across different libraries.

To optimize computational efficiency, OpenMC calculations used reduced particle counts: 30,000 particles per generation, 300 active generations, and 50 inactive generations, achieving a standard error of ~30 pcm.

Nuclide quantity variations and library errors were analyzed for ^{85}Kr, ^{135}Xe, ^{149}Sm, ^{233}U, ^{239}Pu, ^{241}Am, ^{242}Am, and ^{244}Cm. CENDL-TMSR-V1 maintained the relative error within 5% from ENDF/B-VII.1 for all nuclides except ^{241}Am, ^{242}Am, and ^{244}Cm. These three isotopes exhibited initial relative errors of 49.84%, 57.94%, and 60.26% respectively, with errors decreasing as burnup progressed. The larger discrepancies likely stem from their lower absolute quantities during early burnup stages.

Similar error patterns (high initial values decreasing with burnup) were observed in CENDL-3.2 for ^{241}Am, ^{242}Am, and ^{244}Cm. However, CENDL-3.2 showed sustained relative errors exceeding 15% for ^{233}U concentrations compared to ENDF/B-VII.1 throughout the burnup period.

Fig. 19 Variation of keff during burnup calculations: (a) variation of keff with time, (b) absolute error from ENDF/B-VII.1

Fig. 20 ^{85}Kr atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

Fig. 21 ^{135}Xe atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

Fig. 22 ^{149}Sm atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

Fig. 23 ^{233}U atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

Fig. 24 ^{239}Pu atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

Fig. 25 ^{241}Am atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

Fig. 26 ^{242}Am atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

Fig. 27 ^{244}Cm atom quantities and relative error from ENDF/B-VII.1 in burnup calculations across different libraries

5 Conclusions

This study developed a new MSRE model using OpenMC based on existing research, and evaluated the applicability of CENDL-3.2 and CENDL-TMSR-V1 nuclear libraries for molten salt reactor benchmark calculations. The work expands the IRPhEP' s evaluation results for MSRE benchmarks using Chinese CENDL libraries. Results demonstrate that CENDL-3.2 and CENDL-TMSR-V1 are suitable for analyzing reactivity, control rod worth, and burnup. Their accuracy is generally comparable to ENDF/B-VII.1, with some outcomes surpassing those from the IRPhEP model using ENDF/B-VII.1.

The MSRE model incorporates realistic geometric features such as graphite stringer tops and gaps between support rods and horizontal graphite lattice. Compared to the IRPhEP model using ENDF/B-VII.1, the new model shows a 34 pcm error in keff. Neutron energy spectra, axial flux distributions, and neutron production match well with IRPhEP results. Integral control rod worth deviates by less than 40 pcm from experimental measurements, while control rod bank worth errors remain within 100 pcm. Calculated control rod shadowing effects match both experimental data and IRPhEP results, validating the model' s accuracy.

Detailed evaluations of CENDL-3.2 and CENDL-TMSR-V1 were conducted using the new MSRE model. Compared to ENDF/B-VII.1, both libraries yield keff values approximately 70 pcm lower. Radial flux errors stay below 5%, and power distribution errors in 29 central fuel cells remain less than 2%. Control rod bank worth discrepancies are within 100 pcm.

A customized MSRE burnup problem revealed maximum keff errors of 200 pcm for CENDL libraries relative to ENDF/B-VII.1. Relative errors for ^{85}Kr, ^{135}Xe, ^{149}Sm, and ^{239}Pu quantities stay below 5%. For ^{241}Am, ^{242}Am, and ^{244}Cm, initial errors exceed 45% but decrease with burnup progression. Notably, CENDL-3.2 shows sustained errors greater than 15% in ^{233}U concentrations throughout burnup, whereas CENDL-TMSR-V1 matches ENDF/B-VII.1 accuracy, demonstrating superior performance to CENDL-3.2 in burnup calculations.

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Note: Figure translations are in progress. See original paper for figures.