The Calculation and Comparison of Criticality Benchmark Models with ENDF/B-VIII.0 and CENDL-3.2 Fe-56 Nuclear Data

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Abstract. In order to compare the ENDF/B-VIII.0 and CENDL-3.2 Fe-56 nuclear data, twenty-nine iron sensitive models were selected from the International Criticality Safety Benchmarking Experiments Evaluation Project(ICSBEP), including twenty-one highly enriched uranium models and eight plutonium metal models. The benchmark models were modeled in MC program and \( k_{eff} \) were calculated with complete ENDF/B-VIII.0, and with hybrid ENDF/B-VIII.0 with CENDL-3.2 Fe-56 substituted, respectively. For most models, the benchmarking criticality calculation results show that with hybrid ENDF/B-VIII.0 there are 381 pcm or less reduction in \( k_{eff} \), compared with complete ENDF/B-VIII.0. Besides, it shows improved agreement for plutonium metal models and a little worsened agreement for highly enriched uranium models with hybrid ENDF/B-VIII.0.

1 Introduction

With the development of science and technology, nuclear data have been broadly applied in a number of areas, including nuclear technology and engineering, medicine, irradiation breeding, resource exploration, aerospace and so on. In order to meet the growing demand of nuclear data, major international nuclear powers and regions had set up specialized nuclear data center to evaluate nuclear data and established database. Now, there are five major nuclear data centers in the world, including US National Nuclear Data Center(NNDC), Organization for Economic Cooperation and Development(NEADB), Russian Nuclear Data Center(CJID), Japan Atomic Energy Agency(NDC), China Nuclear Data Center(CNDC) and International Atomic Energy-Nuclear Data Section(IAEA-NDS). In addition, they have published their own evaluated nuclear data library, shown in Table 1. China evaluated data library CENDL-3.2[1] published in 2020 includes 272 nuclides, and data quality and category have made great improvement compared with previous version. US evaluated data library ENDF/B-VIII.0[2] published in 2018 includes 557 nuclides, and updated evaluation of light nuclides, structural material, etc.

In nuclear technology application and engineering construction, iron is one of the most common elements for structural material. Because Fe-56 is the dominant isotope of iron with a nature abundance of 91.8%, it is one of the important nuclides to evaluate the reaction cross section of medium heavy isotopes[2]. In order to verify the improvement of CENDL-3.2, various relevant calculation and analysis are required, such as influence on calculated result of shielded integral experiment[3]. Because the related research is rare, this paper aims to analyze the influence of CENDL-3.2 Fe-56 nuclear data through \( k_{eff} \) calculation with iron sensitive benchmarking models from ICSBEP by contrast with ENDF/B-VIII.0.

2 Models and Calculation

For selecting appropriate benchmarks, some previous works were surveyed. Finally, twenty-nine iron sensitive models, drawn from ENDF/B-VIII.0 integral data testing[2], CIELO and ENDF/B-VIII.0 validation[4] and ENDF/B-VIII.0 Fe-56 validation[5], were selected from ICSBEP[6]. There are twenty-one highly enriched uranium models and eight plutonium metal models, including metal, solution and compound models.

The effective multiplication factors \( k_{eff} \) were calculated with complete ENDF/B-VIII.0, and with hybrid ENDF/B-VIII.0 with CENDL-3.2 Fe-56 substituted, respectively. For each calculation, the total number of cycles included 50 inactive and 200 active cycles with 100000 neutrons per cycle corresponding to 25 million histories.

3 Analysis Methodology

To determine performance of complete ENDF/B-VIII.0 and hybrid ENDF/B-VIII.0, \( k_{eff} \) were taken in ratio to benchmark values to normalize, and absolute bias (\( \Delta k \)) was used to quantify the difference between normalized values and unity[7] and shown as

\[
\Delta k = \frac{C}{E} - 1, \tag{1}
\]

where \( C \) is the calculated \( k_{eff} \); \( E \) is the benchmark values. The average \( \text{Avg}_{\text{abs}} \Delta k \) and deviation \( \text{Std}_{\text{abs}} \Delta k \) of absolute bias and goodness of fit \( \chi^2 \) were applied to analyze the agreement of calculated \( k_{eff} \)[8]. They are defined as...
The main international evaluated nuclear data library

<table>
<thead>
<tr>
<th>Nuclear Data Center</th>
<th>Evaluated Nuclear Data Library</th>
<th>Updated</th>
<th>Number Of Nuclide</th>
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<td>CNDC</td>
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<td>272</td>
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<tr>
<td>NNDC</td>
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<tr>
<td>CJD</td>
<td>BROND-3.1</td>
<td>2016</td>
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\[
Ave_{\Delta k} = \frac{\sum \Delta k_1}{n} \quad (2)
\]

\[
Std_{\Delta k} = \sqrt{\frac{\sum (\Delta k_1 - Ave_{\Delta k})^2}{n}} \quad (3)
\]

\[
\chi^2 = \frac{\sum (C - E)/\sigma_E)^2}{n} \quad (4)
\]

where \(\sigma_E\) is the uncertainty of benchmark values; \(n\) is the number of models.

4 Results and Analysis

Absolute bias of twenty-one highly enriched uranium models are shown in figure 1, where ENDF80 represents calculation with complete ENDF/B-VIII.0; CENDL32 represents hybrid ENDF/B-VIII.0. The largest uncertainty is 690 pcm for benchmark values, and is only 24 pcm for calculation.

Figure 1 shows that the largest absolute bias is 1955 pcm from the 21st model. The smallest is 1 pcm from the 6th model. Besides, absolute bias of CENDL32 is lower than ENDF80 for most models, and the maximum difference is 183 pcm. There are only four models that the absolute bias of CENDL32 are higher than ENDF80, and all of them have high \(k_{eff}\) compared with benchmark values. Further analysis indicates that the differences of \(k_{eff}\) between ENDF80 and CENDL32 are primarily due to the changes in elastic and inelastic cross section of CENDL32 Fe-56. If the effect on \(k_{eff}\) from CENDL-3.2 on the increase of elastic cross section is greater than on the decrease of inelastic cross section, the absolute bias due to CENDL32 Fe-56 cross section will increase. Otherwise, the absolute bias will reduce.

Absolute bias for the eight plutonium metal models are shown in figure 2, where ENDF80 represents calculation with complete ENDF/B-VIII.0; CENDL32 represents hybrid ENDF/B-VIII.0. The largest uncertainty of benchmark values is 310 pcm, and is 16 pcm for calculation.

In figure 2, the largest absolute bias is 2825 pcm from the 29th model which is intermediate model and different from others, and the smallest is 8 pcm from the 25th model. In addition, absolute bias of CENDL32 is lower than ENDF80 for all models, and the maximum difference is 381 pcm. The reason of differences between absolute bias of CENDL32 and ENDF80 is similar with highly enriched uranium models.

Table 2 shows the results of average and deviation of absolute bias and goodness of fit. There are a little difference in deviation of absolute bias and goodness of fit, but huge discrepancy in average of absolute bias. This huge discrepancy is caused by absolute bias that have positive and negative values. Apart from this, deviation of absolute bias and goodness of fit of ENDF80 are smaller for uranium models, and deviation of absolute bias and goodness of fit of CENDL32 are smaller for plutonium models. This indicates that ENDF80 has better agreement in calculation of uranium models, and CENDL32 is more adaptive for plutonium models.

5 Conclusion

In this paper, the \(k_{eff}\) of twenty-nine iron sensitive benchmarking models were calculated with complete ENDF/B-VIII.0, and with hybrid ENDF/B-VIII.0 with CENDL-3.2 Fe-56 substituted. The effect to criticality calculation from CENDL-3.2 Fe-56 nuclear data was presented through comparison.

For the majority of models, calculations of hybrid ENDF/B-VIII.0 show the reduction by not more than 400 pcm in \(k_{eff}\). Only four models show the increase of \(k_{eff}\), because the competition of \(k_{eff}\) influence between the changes of elastic and inelastic cross section of CENDL-3.2 Fe-56 nuclear data compared ones in ENDF/B-VIII.0. Additionally, it indicates a little better agreement in plutonium models but a little poorer agreement in uranium models with CENDL-3.2 Fe-56 nuclear data than with ENDF/B-VIII.0.

References


Figure 1. Absolute bias of highly enriched uranium models

Figure 2. Absolute bias of plutonium metal models

Table 2. Results of mean and standard deviation of absolute bias and goodness of fit

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Library</th>
<th>$\Delta k_{I}$</th>
<th>$\text{Avg}_k$</th>
<th>$\text{Std}_k$</th>
<th>$\chi^2$</th>
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<tr>
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