Performance of the CENDL-3.2 and other major neutron data libraries for criticality calculations

Authors: Zhang, Bin, Ma, Xu-Bo, Hu, Kui, Zhang, Teng, Ma, Xuan, Chen, Yi-Xue, Ma, Xu-Bo

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Abstract

Nuclear data are the cornerstones of reactor physics and shielding calculations. Recently, China released CENDL-3.2 in 2020, and the United States released ENDF/B-VIII.0 in 2018. Therefore, it is necessary to comprehensively evaluate the criticality computing performance of these newly released evaluated nuclear libraries. In this study, we used the NJOY2016 code to generate ACE format libraries based on the latest neutron data libraries (including CENDL-3.2, JEFF3.3, ENDF/B-VIII.0, and JENDL4.0). The MCNP code was used to conduct a detailed analysis of fission nuclides, including 235U, 233U, and 239Pu, in different evaluated nuclear data libraries based on 100 benchmarks. The criticality calculation performance of each library was evaluated using three statistical parameters: , , and . Analysis of the parameter showed that CENDL-3.1 and JENDL-4.0 both had >10 benchmarks that exceeded 3σ, whereas CENDL-3.2, ENDFB-VIII.0, and JEFF-3.3 had, 7, 5, and 4 benchmarks, respectively, exceeding 3σ. The ENDF/B-VII.1 library performed best, with only two benchmarks exceeding 3σ. Compared with CENDL-3.1, CENDL-3.2 offers an improvement in criticality calculations. Compared with the JEFF-3.3 and ENDF/B-VIII.0 libraries, CENDL3.2 performs better in the calculation of the 233U assemblies, but it performs poorly in the pusl11 series case calculation of the 239Pu assemblies, and thus further improvement is needed.

Full Text

Performance of CENDL-3.2 and Other Major Neutron Data Libraries for Criticality Calculations

Bin Zhang, Xu-Bo Ma*, Kui Hu, Teng Zhang, Xuan Ma, and Yi-Xue Chen
School of Nuclear Science and Engineering, North China Electric Power University, Beijing 102206, China
Corresponding author. E-mail address: maxb@ncepu.edu.cn

Abstract

Nuclear data are the cornerstones of reactor physics and shielding calculations. Recently, China released CENDL-3.2 in 2020, and the United States released ENDF/B-VIII.0 in 2018. Therefore, it is necessary to comprehensively evaluate the criticality computing performance of these newly released evaluated nuclear libraries. In this study, we used the NJOY2016 code to generate ACE format libraries based on the latest neutron data libraries (including CENDL-3.2, JEFF3.3, ENDF/B-VIII.0, and JENDL4.0). The MCNP code was used to conduct a detailed analysis of fission nuclides, including 235U, 233U, and 239Pu, in different evaluated nuclear data libraries based on 100 benchmarks. The criticality calculation performance of each library was evaluated using three statistical parameters: , , and . Analysis of the parameter showed that CENDL-3.1 and JENDL-4.0 both had >10 benchmarks that exceeded 3σ, whereas CENDL-3.2, ENDFB-VIII.0, and JEFF-3.3 had, 7, 5, and 4 benchmarks, respectively, exceeding 3σ. The ENDF/B-VII.1 library performed best, with only two benchmarks exceeding 3σ. Compared with CENDL-3.1, CENDL-3.2 offers an improvement in criticality calculations. Compared with the JEFF-3.3 and ENDF/B-VIII.0 libraries, CENDL3.2 performs better in the calculation of the 233U assemblies, but it performs poorly in the pusl11 series case calculation of the 239Pu assemblies, and thus further improvement is needed.

Key words: Criticality calculations, CENDL-3.2, ENDF/B-VIII.0, Neutron, ACE library

1. Introduction

Evaluated nuclear data libraries are the basis of reactor physics and shielding calculations. Currently, there are five major evaluated nuclear libraries in the world, which have recently released their latest versions. In 2020, the China Institute of Atomic Energy released CENDL-3.2 [1], which includes revised and updated data for most key nuclides in nuclear applications (e.g., U, Pu, Th, and Fe). In 2018, Brookhaven National Laboratory in the United States released ENDF/B-VIII.0 [2], which fully incorporates the new International Atomic Energy Agency standards, includes improved thermal neutron scattering data, and uses newly evaluated data from the CIELO project [3] for neutron reactions on 1H, 16O, 56Fe, 235U, 238U, and 239Pu. In 2017, the Nuclear Energy Agency officially released JEFF-3.3 [4], which thoroughly updated the neutron, decay data, fission yields, and neutron activation libraries in EAF format and provided neutron thermal scattering files for 20 compounds. In 2010, the Japan Atomic Energy Agency released JENDL4.0 [5], placing much emphasis on the improvement of fission products and minor actinoid data, with ENDF files of some nuclides updated as of 2016.

In addition, China’ s nuclear data measurement technology has progressed, providing effective support for CENDL library evaluation. Researchers at the Chinese Academy of Sciences [6] measured the neutron capture cross section of

197Au using the time-of-flight technique at the Back-n facility of the China Spallation Neutron Source in the 1 eV to 100 keV range, with results in good agreement with ENDF/B-VIII.0, CENDL-3.1, and other libraries in the resonance region and consistent with both neutron time-of-flight and GELINA experimental data in the 5–100 keV range. Researchers at Lanzhou University [7] measured cross sections of the (n,2n) reactions for Nd isotopes induced by 14-MeV neutrons using activation and relative methods, with results generally consistent with ENDF/B-VII.1, CENDL-3.1, and JENDL-4.0 data at neutron energies of 14.2 and 14.9 MeV.

An evaluated nuclear data library cannot be used directly and must be processed into a working nuclear library using a nuclear data processing code such as NJOY [8] or NECP-Atlas [9]. Working nuclear libraries are generally divided into multi-group cross-section libraries for deterministic codes and continuous point-wise cross-section libraries for stochastic codes. The ACE format [10] is a common continuous point-wise cross-section library storage format used in stochastic codes for reactor physics and shielding calculations.

From civil nuclear power plants to space reactors for aerospace and power reactors for submarines, many applications have high requirements for nuclear data libraries. Different evaluated nuclear data libraries employ different evaluations for some important reaction channels of key nuclides, making it necessary to conduct detailed tests on the quality of nuclear data from different libraries. The validation of nuclear data libraries generally includes criticality, shielding, and depletion tests. The criticality benchmark test is an important form of acceptance testing that can effectively test the data accuracy of key fission nuclides and provide effective guidance for thermal and fast reactor designs. A more detailed understanding of the criticality calculation performance of newly released evaluated nuclear data libraries is needed to provide a reference for library selection in thermal and fast reactor designs. Hence, it is very important to evaluate the quality of newly released nuclear libraries through criticality benchmark testing.

In this study, the MCNP [11] code was used to evaluate the performance of newly released evaluated nuclear data libraries for criticality calculations. Several criticality benchmarks from the ICSBEP manual [12] were selected to verify criticality calculation performance, with each library evaluated using three statistical parameters: , , and [13, 14]. The remainder of this paper is organized as follows: Section 2 introduces the methods for ACE library development, Section 3 describes numerical verification of the newly released libraries, and Section 4 presents our conclusions.

2. Methodology

To study the criticality calculation performance of newly released evaluated nuclear data libraries, ACE-formatted libraries for Monte Carlo code calculations were created based on CENDL-3.1 [15], CENDL-3.2, ENDF/B-VIII.0, ENDF/B-

VII.1 [16], JEFF-3.3, and JENDL-4.0 using the NJOY2016 code [8]. Based on criticality benchmarks in the ICSBEP manual, the criticality calculation performance of different evaluated nuclear data libraries was studied in detail using statistical analysis methods. Section 2.1 describes the methods used to develop ACE-formatted libraries, Section 2.2 describes the ICSBEP benchmark suite, and Section 2.3 describes the details of the statistical analysis methods.

2.1. ACE-formatted libraries and MCNP simulation details

The ACE library production and MCNP simulation processes are shown in Fig. 1. The NJOY program is a popular nuclear data processing program that can generate nuclear data in multiple formats for shielding and criticality calculations based on evaluated nuclear data libraries. The JOYPI code can generate NJOY inputs for ACE library development. The ACE format library is a continuous point-wise cross-section library for Monte Carlo program calculations that can be processed using the NJOY program. The main NJOY modules used to create the ACE library include RECONR, BROADR, THERMR, PURR, and ACER. The RECONR module performs point cross-section resonance reconstruction based on ENDF file data. The BROADR module performs temperature-related Doppler broadening. The THERMR module generates cross sections for free scatters in the thermal energy range. The PURR module calculates unresolved resonance probability tables, and the ACER module converts the previously generated data into a c-type ACE file for use in MCNP.

In the ICSBEP manual benchmark suite, some benchmarks contain thermal neutron scattering materials, requiring processing of the corresponding thermal neutron scattering sub-library (TSL library). While new versions of ENDF/B-VIII.0, JENDL-4.0, and JEFF-3.3 have corresponding TSL libraries, CENDL-3.2 and CENDL-3.1 do not provide TSL libraries. To maintain consistency in verification across different evaluated nuclear data libraries, we used the verified and publicly available ACE thermal scattering library from JEFF-3.3 for criticality calculations of benchmarks with thermal neutron scattering materials. The purpose of this study is to verify the overall criticality calculation performance of neutron data libraries. The standard neutron ACE library used in this study was based on different data libraries and produced using the NJOY2016 program. If moderators are present in benchmark facilities, the TSL library must be considered in calculations, with the TSL library for benchmarks with moderators taken from the JEFF-3.3 ACE library.

For all assemblies calculated by MCNP, 3000 source neutrons were run per kcode cycle. For metal assembly benchmarks, 40 inactive cycles and 360 active cycles were run, while for solution assemblies, 40 inactive cycles and 760 active cycles were run. These numbers ensure sufficient active cycles to obtain good statistics for calculations [17]. All benchmarks use total nubar data in the MCNP input, with eigenvalue uncertainties < 70 pcm, approximately an order of magnitude lower than most benchmark uncertainties.

2.2. Description of the criticality benchmarks suite

A set of 100 criticality safety benchmarks was selected and established for the MCNP code from two reports: a suite of criticality benchmarks for validating nuclear data [17] and an expanded criticality validation suite for MCNP [18]. Among the 100 benchmark cases, 88 were from the first report and 12 from the second. Although all benchmark cases have standard ICSBEP names, the names are too long for chart display, so abbreviations consistent with those in the above two reports are used.

The fission nuclides 233U, 235U, and 239Pu produce the majority of fission products in reactors. The criticality benchmark suite in this study comprises five major categories based on major fission nuclides: critical assemblies utilizing 233U, intermediate-enriched 235U (IEU), highly enriched 235U (HEU), 239Pu, and mixed metal (MIX) assemblies. Within each category, there are bare, reflected, and solution assemblies. The classification of assemblies and the number of each classification are listed in Table 1. The ICSBEP benchmarks and their abbreviations and reference values used in this study are listed in Table A1 in Appendix A, and the calculated values and statistical errors of each data library are listed in Table A2.

2.3. Statistical analysis methods

The benchmark results were analyzed using statistical parameters , , and . is a statistical parameter used to determine which evaluated nuclear data library is most suitable for criticality calculations. measures the average difference between calculated and benchmark eigenvalues, while indicates the consistency between the evaluated library and benchmark value in each case.

We use the 3σ rule to evaluate benchmark calculation results. In statistics, the 3σ rule is a shorthand for remembering the percentage of values within an interval estimate in a normal distribution: 68%, 95%, and 99.7% of values lie within one, two, and three standard deviations of the mean, respectively. In empirical sciences, the 3σ rule expresses a conventional heuristic that nearly all values lie within three standard deviations of the mean, making it empirically useful to treat 99.7% probability as near certainty. Results can be considered identical if the relative difference between eigenvalues and benchmark values was within the $±3 $ interval. Values exceeding $±3 $ are bolded in each benchmark table to facilitate identification.

and are defined by 12* MERGEFORMAT () and 34* MERGEFORMAT (), where n is the benchmark number, is the benchmark experimental uncertainty, simulated eigenvalue and benchmark eigenvalue, respectively, and i and n are the specific benchmark and total number of benchmark cases, respectively. was used to provide a confidence level for benchmarks. The relative difference and relative combined statistical uncertainty are defined by 56* MERGEFORMAT () and 78* MERGEFORMAT (). and are lumped parameters that describe the overall performance of the data library in corresponding benchmark types, while can locate the performance of each data library in each benchmark.

3.1. Comparison of the calculation results

The calculated values were compared with reference values (Figs. 2–6). Most calculated values were close to the allowable error interval of experimental values. The analysis and discussion of each benchmark type are as follows:

(1) For 233U assemblies (Fig. 2), calculated values in most cases were in good agreement with experimental values, though the calculated values for the 23umt4b benchmark deviated significantly from experimental values.

(2) For IEU assemblies (Fig. 3), calculated values in most cases were in good agreement with experimental values. For the ieumt4 benchmark, all calculated results except JENDL-4.0 were overestimated compared to experimental values, while for the ieumt6 benchmark, all calculated results were underestimated.

(3) For HEU assemblies (Fig. 4), all calculated values were overestimated compared to experimental values in the umet3k benchmark. For the umet9b, usol13c, umet8, and umet15 benchmarks, all calculated values were underestimated.

(4) For 239Pu assemblies (Fig. 5), calculated values in most cases were in good agreement with experimental values. For the four pusl cases (pusl11a, pusl11b, pusl11c, and pusl11d), calculation results from CENDL-3.2 and CENDL-3.1 were overestimated compared to other data libraries. Comparing individual nuclides revealed that 239Pu from CENDL-3.2 caused the overestimation in pusl11 series cases.

(5) For MIX assemblies (Fig. 6), calculated values in most cases were in good agreement with experimental values, though the calculated values for mixmet8-7 deviated greatly from experimental values.

3.2. Discussion of the statistical results

The three statistical parameters of each data library (Tables 2–6) were compared, with analysis and discussion as follows:

(1) For 233U assemblies (Table 2), CENDL-3.1 exceeded 3σ in four benchmarks (23umt4a, 23umt4b, 23umt5a, and 23umt5b). JEFF-3.3 exceeded 3σ in the flat23 benchmark, and all databases exceeded 3σ in the 23umt4b benchmark. Analysis of and values indicates that CENDL-3.2 offers significant improvement compared to CENDL-3.1.

(2) For IEU assemblies (Table 3), CENDL-3.1 exceeded 3σ in benchmarks lst7-14 and ieumt1c, while six benchmarks exceeded 3σ in the JENDL-4.0 library. Analysis of and values showed that ENDFB-VIII.0 and JEFF-3.3 performed better than other libraries.

(3) For HEU assemblies (Table 4), CENDL-3.1 exceeded 3σ in benchmarks umet19 and ieumt1c. JEFF-3.3 exceeded 3σ in the umet4b benchmark, and five benchmarks exceeded 3σ in the JENDL-4.0 library. Analysis of and values indicated that CENDL-3.2 is not significantly improved compared to CENDL-3.1.

(4) For 239Pu assemblies (Table 5), CENDL-3.1 and CENDL-3.2 both exceeded 3σ in benchmarks pusl11c and pusl11d. For the pumet8b benchmark, all data libraries except ENDF/B-VII.1 exceeded 3σ. Analysis of and values showed that the ENDF/B-VII.1 library performs better than other data libraries.

(5) For MIX assemblies (Table 6), all libraries exceeded 3σ in benchmark mixmet8-7. The ENDF/B-VII.1 library performs better than other data libraries, and analysis of and values shows that CENDL-3.2 performs better than CENDL-3.1.

Based on calculated values for all benchmarks, chi-square and average errors were used to analyze overall performance of all data libraries in criticality calculations (Table 7). From the perspective of library updates, CENDL-3.2 has smaller chi-square and average deviations for all benchmarks than CENDL-3.1, reflecting that CENDL-3.2 is superior to the previous version for the benchmark types involved. The average deviation of ENDF/B-VIII.0 for all benchmarks is similar to ENDF/B-VII.1 (both near 230), though the chi-square is larger than ENDF/B-VII.1. Counting benchmarks exceeding 3σ shows that JENDL-4.0 and CENDL-3.1 have >10 benchmarks exceeding 3σ, while ENDF/B-VIII.0 and JEFF-3.3 have ~5.

In general, based on these 100 criticality benchmark calculation results, we conclude that CENDL-3.2' s criticality calculation performance is better than CENDL-3.1. Analysis of chi-square, average deviations, and number of benchmarks exceeding 3σ demonstrates that ENDF/B-VIII.0 and JEFF3.3 have equivalent overall criticality calculation performance, while ENDF/B-VII.1 performed best. Compared with JEFF-3.3 and ENDF/B-VIII.0, CENDL3.2 performs better in 233U assembly calculations but poorly in pusl11 series Pu device calculations, requiring further improvement.

Compared with CENDL-3.1, CENDL-3.2 [1] includes more materials (272), with data for 134 nuclides being new or updated evaluations in the 10^{-5} eV to 20 MeV energy region. Data for most key nuclides in nuclear applications (e.g., U, Pu, Th, and Fe) have been revised, and covariance data for main reactions were added for 70 fission product nuclides.

Compared with ENDF/B-VII.1, ENDF/B-VIII.0 [2] employs major changes for neutron reactions on important isotopes (1H, 16O, 56Fe, 235U, 238U, and 239Pu) and other nuclides that impact nuclear criticality simulations. The number of materials increased from 423 to 557, with notable updates to neutron reactions on light nuclei, structural materials, minor actinides, fission energy release, decay data, charged particle reactions, and thermal neutron scattering data.

We expected ENDF/B-VIII.0' s criticality calculation performance to be better than ENDF/B-VII.1. However, for different benchmark experiments, the new evaluated library ENDF/B-VIII.0 results are not universally better than the previous version, such as in three Pu assembly benchmarks (pusl11a, pusl11b, and pumet21b). In these benchmarks, ENDF/B-VIII.0 results are 200–500 pcm smaller than ENDF/B-VII.1 results compared to experimental values. One goal of our work is to identify benchmarks not sensitive to newly evaluated libraries to provide references for subsequent evaluation work. Table 7 lists only the statistical performance of current benchmark cases and cannot definitively show that ENDF/B-VIII.0 results are better than ENDF/B-VII.1, requiring specific analysis based on specific issues.

3.3. Discussion of the anomalous benchmarks

From Section 3.2 discussion, the value of all data libraries exceeded 3σ in three benchmarks (23umt4b, pumet8b, and mixmet8-7), indicating large deviations between experimental and calculated values that need separate addressing.

The 23umt4b (u233-fast-met-004) benchmark is a spherical device with two layers: an inner layer containing 233U fuel and an outer reflective layer dominated by tungsten. The pumet8b (pu-met-fast-008b) benchmark is a spherical device with two layers: an inner layer containing Pu fuel and an outer reflection layer of 232Th. The mixmet8-7 (mix-met-inter-008-case-7) benchmark is based on a k∞ measurement, consisting of a rectangular plate with three rectangular normal-uranium plates above and three below, enclosed on all sides by a rectangular steel sheath.

Physically, is mainly dominated by fission nuclides, but the reflective layer also importantly influences . The average deviation between pumet8b and 23umt4b benchmarks and experimental values was ~600 pcm. Some benchmarks have deviations >600 pcm from experimental values, such as JEFF-3.3 calculation results for pumt21b. For mixmet8-7, the deviation between calculated values of all libraries and experimental values was within 1000–2000 pcm. Additionally, results of reference values from ENDF/B-VII.0 and ENDF/B-VI deviate from experimental values by >1000 pcm. The result of MCNP6.2 based on ENDF/B-VII.1, found in the LA-UR-17-25040 report [19], is 1.0192, deviating 1620 pcm from experimental value. Currently, no report explains the reason for the large deviation between calculated and experimental values for mixmet8-7, requiring further research.

From a nuclear data perspective, because benchmarks involve many nuclides, qualitative analysis cannot determine which nuclides have greater impact on . The commonly used method is to identify important reaction channels of key nuclides through sensitivity and uncertainty analyses. This work has not yet been completed and will be further studied in our future work.

4. Conclusion

A comprehensive suite of 100 criticality benchmarks has been established for validating nuclear data, including CENDL-3.2, ENDF/B-VIII.0, JEFF3.3, JENDL-4.0, CENDL-3.1, and ENDF/B-VII.1. The suite contains benchmarks for five major categories: critical assemblies utilizing 233U, IEU, HEU, 239Pu, and MIX assemblies.

(1) In these 100 calculation benchmark cases, calculated values for most cases were in good agreement with experimental values.

(2) Comprehensive device analysis and and values demonstrate that ENDF/B-VIII.0 and JEFF3.3 have basically equivalent overall criticality calculation performance, while ENDF/B-VII.1 offers the best performance. CENDL-3.2 is improved compared to CENDL-3.1 and is better than JENDL-4.0. CENDL-3.2 performed better in 233U assembly calculations but poorly in pusl11 series Pu device calculations, requiring further improvement.

(3) Most benchmark case values in different data libraries were within the 3σ interval with 99.7% confidence. A few benchmark cases (e.g., 23umet4b, pumet8b, and mixmet8-7) have values exceeding the 3σ interval for all libraries. The reason for the large deviation between mixmet8-7 calculated values and experimental values requires further study.

Author contributions: All authors contributed to study conception and design. Material preparation, data collection, and analysis were performed by Xu-Bo Ma, Kui Hu, and Teng Zhang. The first draft was written by Bin Zhang, and all authors commented on previous versions. All authors read and approved the final manuscript.

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Appendix A

Table A1. ICSBEP benchmark abbreviation and reference value

Abbreviation	ICSBEP Benchmark	Reference
Abbreviation	ICSBEP Benchmark	Reference
23umt1	233U-MET-FAST-001	1.0000$±0.00100

||23umt2a|233U−
MET − FAST −
002Case1|1.0000±0.00100||23umt2b|233U−
MET − FAST −
002Case2|1.0000±0.00110||23umt3a|233U−
MET − FAST −
003Case1|1.0000±0.00100||23umt3b|233U−
MET − FAST −
003Case2|1.0000±0.00100||23umt4a|233U−
MET − FAST −
004Case1|1.0000±0.00070||23umt4b|233U−
MET − FAST −
004Case2|1.0000±0.00080||23umt5a|233U−
MET − FAST −
005Case1|1.0000±0.00300||23umt5b|233U−
MET − FAST −
005Case2|1.0000±0.00300||23umt6|233U−
MET − FAST −
006|1.0000±0.00140||23usl1a|233U−
SOL−THERM−
001Case1|1.0000±0.00310||23usl1b|233U−
SOL−THERM−
001Case2|1.0005±0.00330||23usl1c|233U−
SOL−THERM−
001Case3|1.0006±0.00330||23usl1d|233U−
SOL−THERM−
001Case4|0.9998±0.00330||23usl1e|233U−
SOL−THERM−
001Case5|0.9999±0.00330||23usl8|233U−
SOL−THERM−
008|1.0006±0.00290||bigten1|F−
10 −
1(InCSEWG)|0.9960±0.00300||bigten2|F−
10 −
2(InCSEWG)|0.9960±0.00300||flat23|F−
24(InCSEWG)|1.0000±0.00100||ieumt1a|IEU−
MET − FAST −
001Case1|0.9989±0.00100||ieumt1b|IEU−
MET − FAST −
001Case2|0.9997±0.00100||ieumt1c|IEU−
MET − FAST −
001Case3|0.9993±0.00050||ieumt1d|IEU−
MET − FAST −
001Case4|1.0002±0.00050||ieumt2|IEU−
MET − FAST −
002|1.0000±0.00300||ieumt3|IEU−
MET − FAST −
003|1.0000±0.00170||ieumt4|IEU−
MET − FAST −
004|1.0000±0.00300||ieumt5|IEU−
MET − FAST −
005|1.0000±0.00210||ieumt6|IEU−
MET − FAST

Table A2. values and statistical errors of different libraries

Benchmark	CENDL-3.1	CENDL-3.2	ENDF/B-VII.1	ENDF/B-VIII.0	JEFF-3.3	JENDL-4.0
23umt1	0.99987$±0.00055	0.99962±0.00059	0.99915±0.00067	0.99901±0.00070	0.99907±0.00057	0.99940±0

Figures

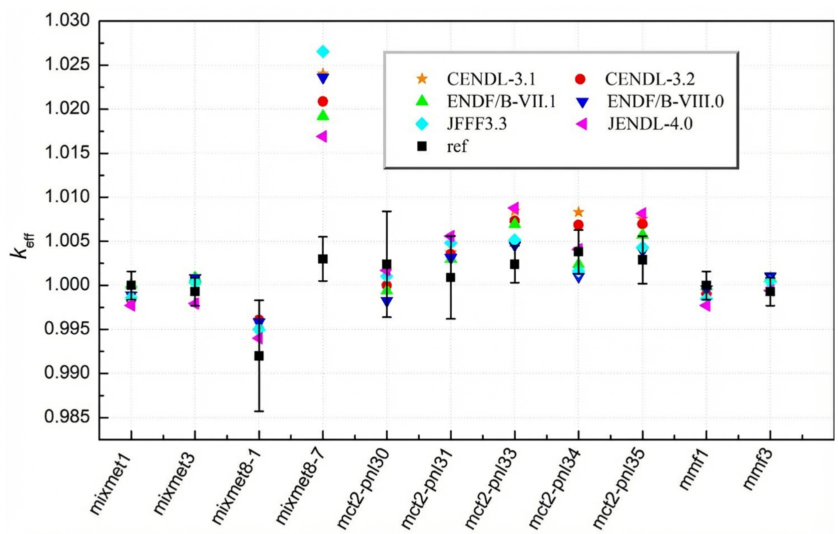

Figure 1: Figure 1

Source: ChinaXiv —Machine translation. Verify with original.

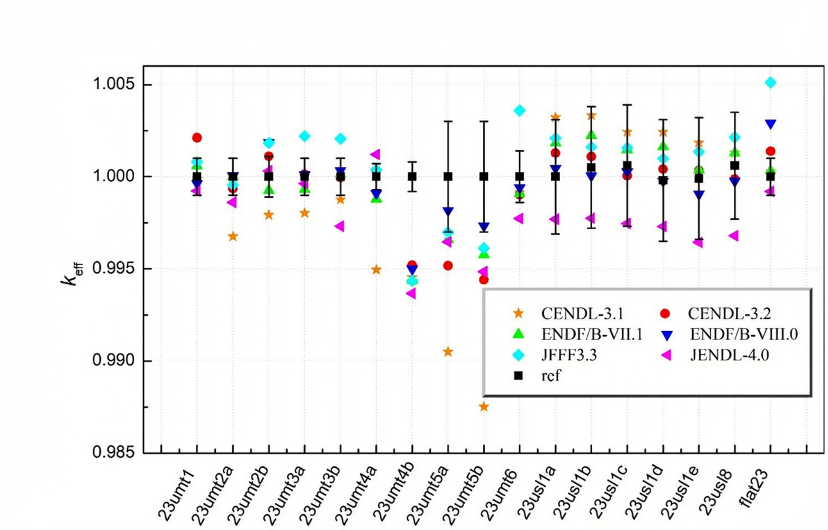

Figure 2: Figure 2

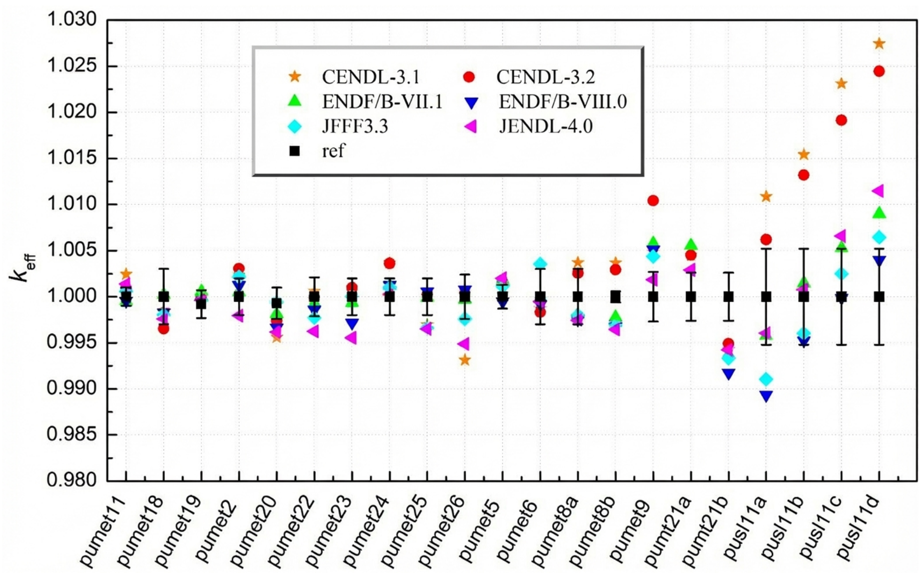

Figure 3: Figure 3

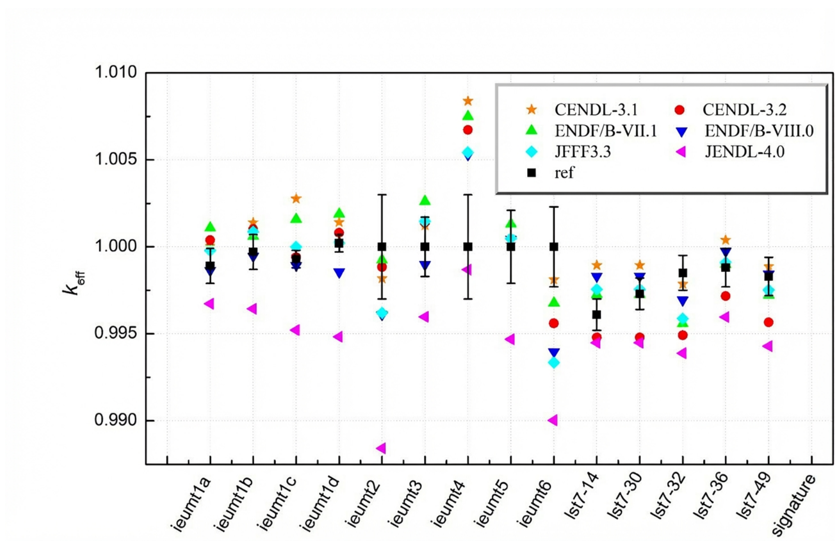

Figure 4: Figure 4

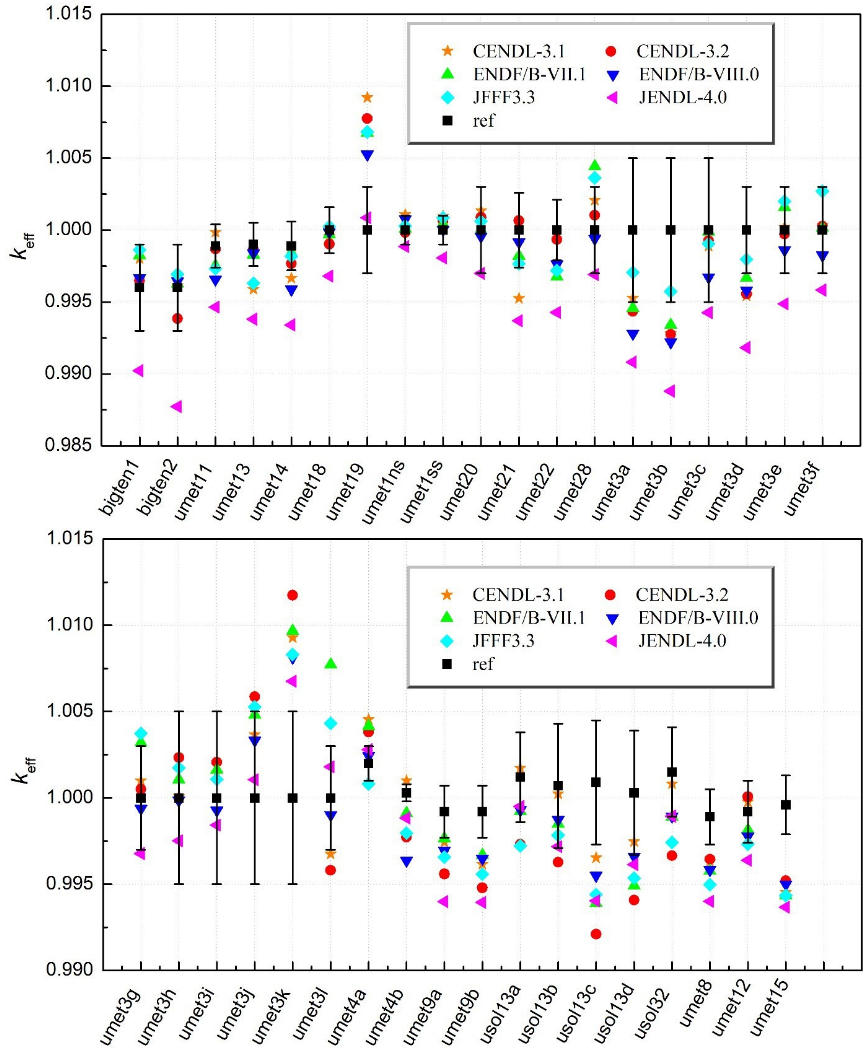

Figure 5: Figure 5