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Criticality validation of SuperMC with ICSBEP

Binhang Zhang [a,b], Jing Song [a], Guangyao Sun [a], Chaobin Chen [a], Liqin Hu [a,b,*]

[a] Key Laboratory of Neutronics and Radiation Safety, Institute of Nuclear Energy Safety Technology, Chinese Academy of Sciences, Hefei, Anhui 230031, China
[b] University of Science and Technology of China, Hefei, Anhui 230027, China

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ABSTRACT

Monte Carlo transport codes are extensively used in neutronic analysis, especially in criticality safety analysis and shielding analysis. Super Monte Carlo Simulation Program for Nuclear and Radiation Process (SuperMC) is a CAD based Monte Carlo program for integrated simulation of nuclear systems. The aim of this paper was to show the capability of SuperMC on criticality calculation with different models. In this study 119 representative benchmarks from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) were used for validating the code. All the benchmark models and input files were built and completed by employing the models' conversion and construction function of SuperMC. The results showed that there was a good agreement between SuperMC and experimental data, and the discrepancies were mainly included in the statistical uncertainty.

1. Introduction

The development of advanced nuclear energy system raises great challenges to current simulation methods and tools on neutronics, fluids and heat transfer, materials, fuels, geometrical modeling and data visualization. In consideration of these existing challenges, 3D Monte Carlo (MC) transport codes for nuclear system have been widely used and fast developed in recent years. Aimed at supporting the demand of advanced nuclear energy system, a new Monte Carlo code named Super Monte Carlo Simulation Program for Nuclear and Radiation Process (SuperMC) is under the development of the FDS team in China (Wu et al., 2002, 2009a,b, 2015). It is mainly designed to perform radiation transport, isotope burn-up and material activation simulations. With the development of a software, the code validation is indispensable for evaluating the simulation system. Independent validation of Monte Carlo codes is necessary to enhance its reliability in neutronic transport calculation.

As a rule, criticality safety practitioners are required to validate the computational tools used in the work, which are the same with the code developers. The effective neutron multiplication factor k_{eff} determining how a nuclear chain reaction proceeds, is an important parameter for criticality calculation in reactor physics analysis. At present, Several MC codes verification and validation operations are mainly based on International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) (OECD, 2006; Mosteller et al., 2011) for criticality safety validation, such as MCNP (Marck, 2012), Serpent(Leppänen, 2007), McCARD (Shim et al., 2012) and TRIPOLI-4 (Jaboulay et al., 2014). Thus a validation suite was selected from ICSBEP to validate criticality safety calculation capacity and correctness of SuperMC, which gave a broad coverage of fissile materials, reflector materials and energy spectrum. Then the calculation results were compared and analyzed with experimental data and the other MC code.

The structure of this paper is as follows: Firstly, in Section 2, the function structure of SuperMC and validation suite are respectively introduced in details. Then Section 3 describes the simulation and analysis methods. And the calculation results and comparison between experimental data and codes are presented in Section 4. Section 5 is for the conclusion.

2. Code and validation suite

2.1. Computational code

The latest version SuperMC 2.1 can perform neutron, photon, coupled neutron and photon transportation, geometry and physics modeling, results and process visualization. The verification and validation (V&V) work of SuperMC is on process, which is carried out by the benchmark work and verification experiments and the results are presented in the related literature (Song et al., 2014). The code function of SuperMC is shown in Fig. 1.

* Corresponding author at: Key Laboratory of Neutronics and Radiation Safety, Institute of Nuclear Energy Safety Technology, Chinese Academy of Sciences, Hefei, Anhui 230031, China.
E-mail address: evanustc@mail.ustc.edu.cn (L. Hu).

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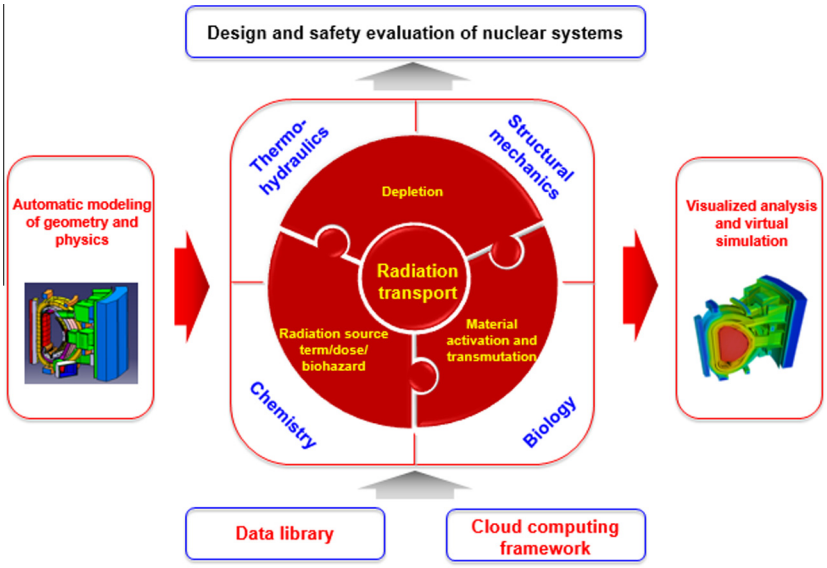

Fig. 1. Code function structure of SuperMC.

With continuous-energy cross-section libraries and mature physical models in broad energy range, criticality parameters of reactors and various fixed source can be simulated. Burn-up, activation and irradiation damage are used to meet different requirements of simulation. It has been recognized that direct geometry utilization of CAD model or automated translation is efficient and convenient to avoid manual modeling and enhance the ability for dealing with complicated geometry structure (Wilson et al., 2008). The methodology to build the geometry model was based on SuperMC/MCAM which was developed to improve the reliability of simulation model. Results and process of simulation can be visualized with 3D dataset directly. Advanced cloud computing framework makes the simulation more convenient as a network service. All those make SuperMC applicable for the accurate simulation of different nuclear systems and models.

2.2. Validation suite

The International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) is intended to validate calculational techniques used to establish minimum subcritical margins for operations with fissile materials and determine criticality alarm requirements (OECD, 2006). The data in the handbook are frequently used for validating the codes and cross section libraries in reactor physics simulation, especially in criticality safety analyses.

In order to validate the codes in criticality safety applications, a set of 119 representative benchmarks has been selected from the handbook. The validation suite covers a wide variety of fissile materials, reflector materials and energy spectrum. The physical forms of the fissile material include metal systems (MET), compound (COMP), solution (SOL) and miscellaneous systems (MISC). The benchmarks involve a variety of reflector materials e.g. C, Be, BeO, Al, W, Ni, W, Fe, as well as bare core and solution reactors. The benchmarks selected in the validation suite are divided into three categories by major isotopes: ^{233}U, ^{235}U, and ^{239}Pu. Further more, according to the enrichment of ^{235}U in fuel, the benchmarks in the ^{235}U category are divided into three categories: highly enriched uranium (HEU $\geqslant$ 60 wt.%), intermediate enriched uranium (10 wt.% < IEU < 60 wt.%) and low enriched uranium (LEU $\leqslant$ 10 wt.%). The suite also covers a wide range of neutron energy spectra and is categorized by fast, intermediate and thermal spectrum. The fast spectrum benchmarks are those the majority of fissions is caused by neutrons with energy higher than 100 keV. Thermal spectrum benchmarks are those the majority of fissions is caused by neutrons with energy lower than 0.625 eV. The intermediate spectrum benchmarks is those in which more than half of the fissions are caused by neutrons with energy between 0.625 eV and 100 keV. The LEU category only contains thermal cases because the systems cannot reach criticality with intermediate and fast spectrum. The plutonium benchmarks in the suite include cases with both Pu and mix identifiers. The cases of the validation suite in each of these categories are listed in Table 1.

3. Simulation and analysis method

Each benchmark from ICSBEP has all of the evaluated experimental data, benchmark specifications containing geometry model, material data, temperature data and etc. In this paper, all the benchmark models were built with the SuperMC/MCAM referring to the benchmark specifications to complete the input files. The automatic function of the model' conversion and construction of SuperMC was used to greatly reduce the manual modeling and enhance the reliability of the calculation models (Li et al., 2007; Qiu et al., 1998; Wu et al., 1999, 2007, 2008, 2009, 2011). In the validation suite, there are a series of low enriched uranium reactor benchmarks with large amount of repeat structure description in the geometry model. Two processes are adopted in the validation work, which are the repeat structure construction of reactor cores based on the assigned parameters and the conversion between CAD models and MC calculation geometry models. Besides, physics attributes including materials, sources, tallies, and temperature

Table 1
Criticality validation suite from ICSBEP.

Principal fuel	Number of benchmarks by spectrum			
	Fast	Intermediate	Thermal	Total
LEU	0	0	8	8
IEU	10	2	6	18
HEU	29	5	6	40
^{233}U	10	1	7	18
Plutonium	21	1	13	35
Total	70	9	40	119

data were assigned graphically to form complete calculation input files.

For some simple benchmark models, such as Godiva, Stacy, Jezebel, a total of 3000 generations with 3000 histories per generation were used in the calculations and the calculation results were based on 9 million neutron histories. For complicated geometry and reactor benchmark models, a total of one hundred million neutron histories were used to achieve the desired accuracy. The results from the first 100 generations were excluded from the statistics. This was necessary if the initial source assumption was poor. The calculation was run in the *k*-eigenvalue criticality mode. The nuclear data library named Hybrid Evaluated Nuclear Data Library (HENDL) which can provide fine-group, coarse-group and point-wise nuclear data to fulfill the requirements of advanced reactor design and the relevant studies (Xu et al., 2010) was used for the code validation. The evaluated data in the nuclear library were selected from the international evaluated nuclear data source, such as ENDF, JENDL, and JEFF. The data library had also been extensively tested (Zou et al., 2010). All contrast simulation was done with the same nuclear data library and under the same computing configuration.

Discrepancies originating from the fundamental interaction data is eliminated with the same ACE format library files. In comparison with the benchmark experimental measurement data, the following equations are quoted to evaluate the deviations (Mosteller, 2004). The relative difference is defined by:

$$\Delta k = (k^{\text{benchmark}} - k^{\text{SuperMC}})/k^{\text{benchmark}} \quad (1)$$

where $k^{\text{benchmark}}$ and k^{SuperMC} are respectively the benchmark experimental data and the calculation results of SuperMC. The relative combined statistical uncertainty (σ) is defined by:

$$\sigma = \sqrt{(k^{\text{benchmark}} * \sigma^{\text{benchmark}}) + (k^{\text{SuperMC}} * \sigma^{\text{SuperMC}})^2} \quad (2)$$

where $\sigma^{\text{benchmark}}$ and σ^{SuperMC} are benchmark experimental uncertainties and statistical uncertainties of SuperMC results. σ is used to determine if the results of codes are statistically identical. The results may be considered identical if the relative difference is within a $\pm 3\sigma$ interval (i.e. 99.6% of confidence) (Jaboulay et al., 2014).

4. Calculation results and analysis

4.1. Calculation results and comparison

Using the first letter of ICSBEP name, the benchmark name can be abbreviated, for example, the case name HEU-MET-FAST-001 is simplified to hmf1. By comparison with the benchmark experimental data, the calculation results were analyzed to determine whether the code works well with broader examples. Using the same data library, the difference of k_{eff} between SuperMC and MCNP for this suite is displayed in Fig. 2. All the calculation results and statistics uncertainties of k_{eff} are collected and presented in Figs. 3–7. The MCNP calculation results with the ENDF/B-VII.0 data library are also presented in Figs. 3–7 to confirm whether the effects of different data libraries on calculation results (Mosteller et al., 2011; Marck, 2012). Considering the fact is statistical uncertainty of k_{eff} in SuperMC (0.00015–0.00090) and MCNP (0.00013–0.00083) are much less than the experimental uncertainty (0.0011–0.0110), the statistical uncertainty of calculation results are not presented in Figs. 3–7.

By utilizing the same cross section data, any differences in results can be directly attributable to differences in the codes

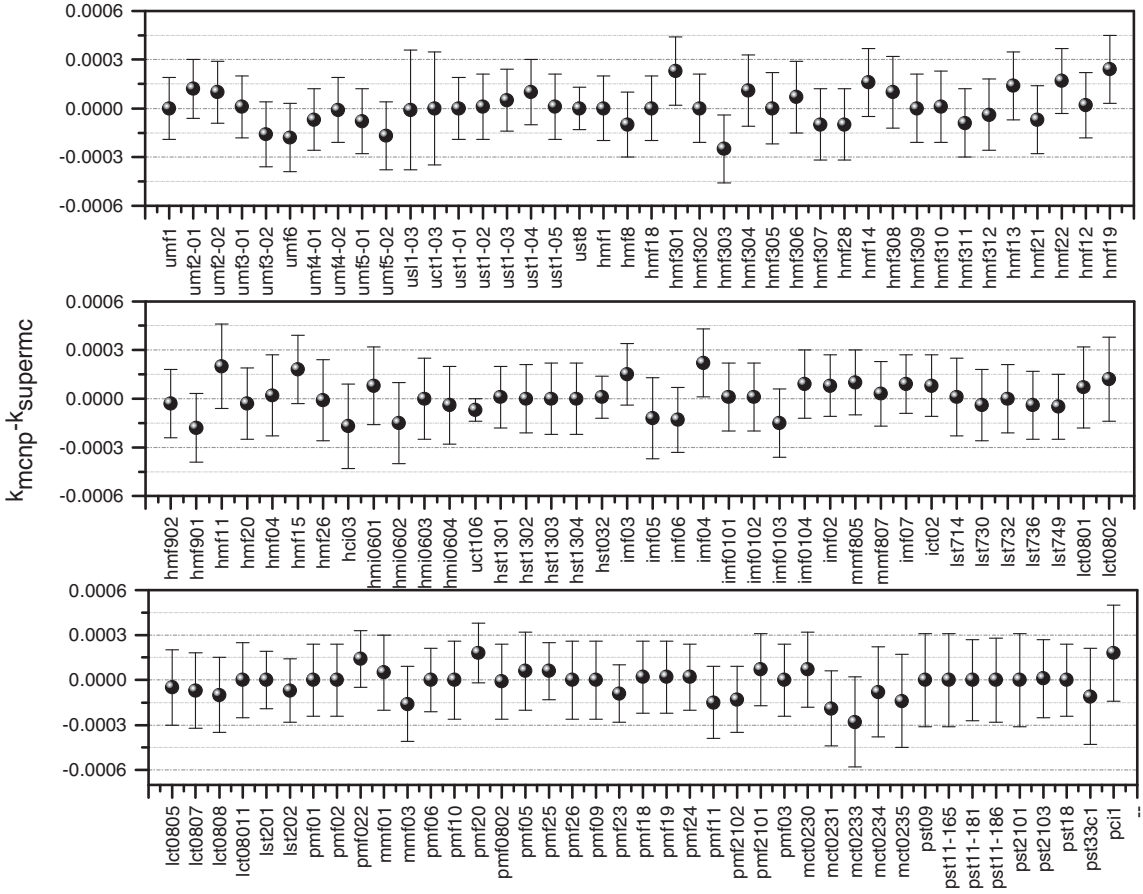

Fig. 2. Comparison between SuperMC and MCNP with the same data library.

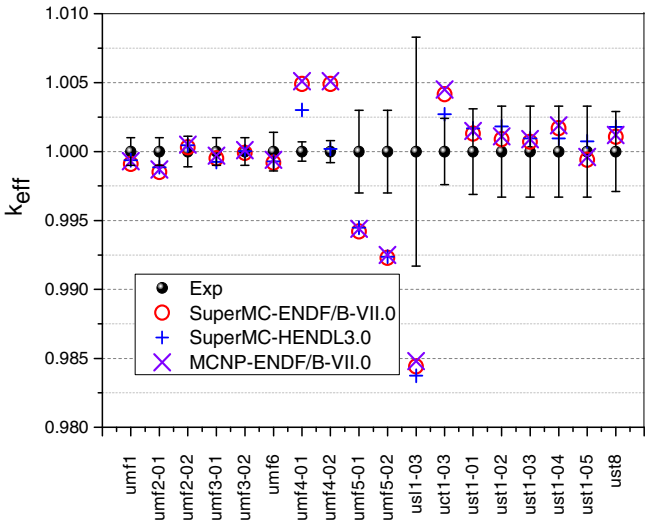

Fig. 3. Results for the ^{233}U benchmarks.

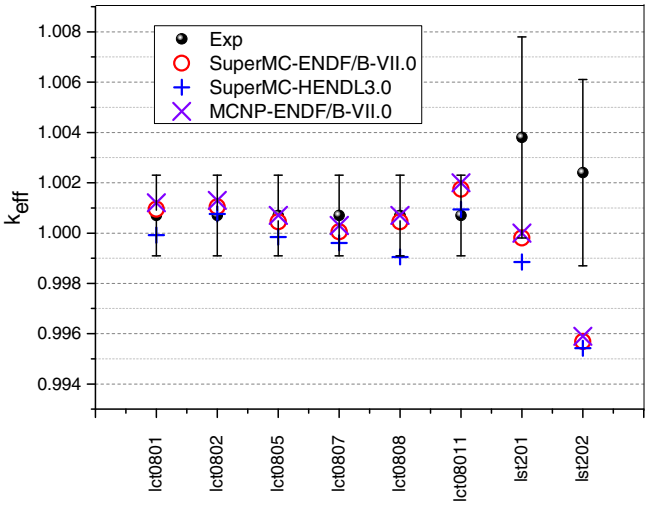

Fig. 6. Results for the LEU benchmarks.

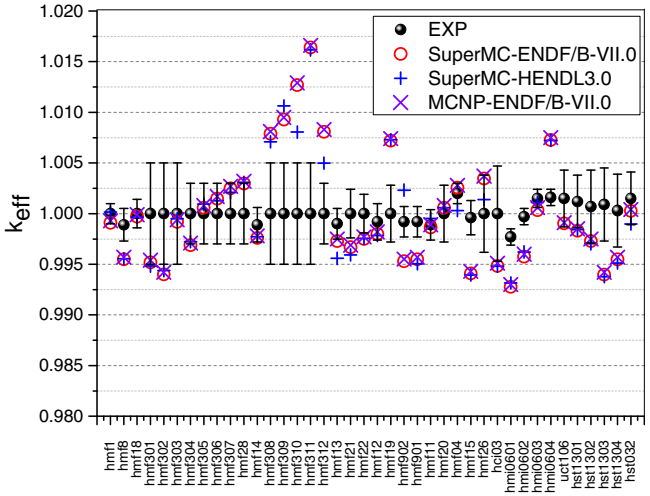

Fig. 4. Results for the HEU benchmarks.

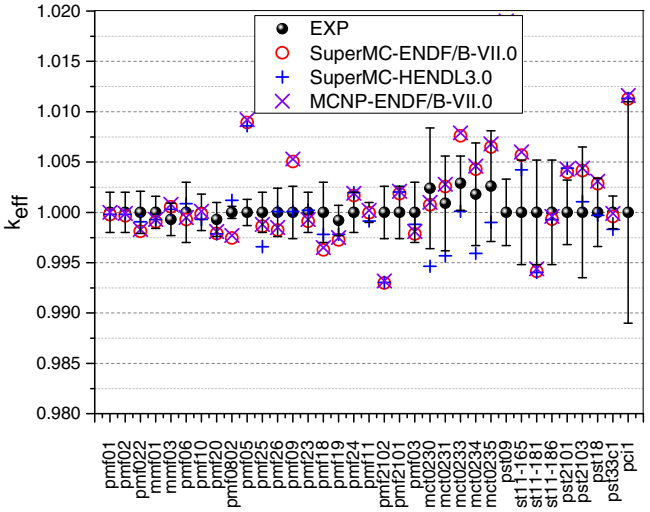

Fig. 7. Results for the Pu benchmarks.

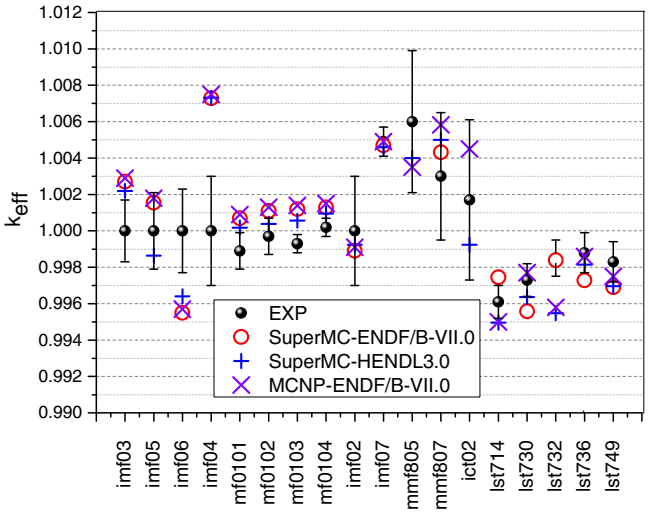

Fig. 5. Results for the IEU benchmarks.

themselves. As shown in Fig. 2, the criticality safety results of SuperMC is consistent with MCNP within 30 pcm. The calculation results are satisfying and depict that the average deviations from the experimental data of less than 100 pcm in Figs. 3–7. The evaluations of the main isotopes, especially for ^{233}U, ^{235}U, ^{239}Pu, could therefore be considered to be good quality. For instance, as for the fast spectrum benchmark categories, the average deviations from benchmark values are small, especially in the Pu and HEU categories. Overall, according to the equations in Section 3, the relative differences varied between −0.9% and 0.9% and are mainly within $\pm 3\sigma$ interval (around 92%), closing to the 99.6% theoretical value.

Although the results of SuperMC for most cases are consistent with experimental data using different data libraries in Figs. 3–7, some results of the benchmark series in this suite differ from the benchmark data for more than 100 pcm. Figs. 3–7 show that the calculation results with two data libraries are higher than experimental data, i.e. umf04, pmf05, hmf03 and pmf23 with amount of non-fissile elements are 300–400 pcm above the experimental data, on one side; on the other side, some results are relatively lower than experimental data, i.e. mct02-case-pnl-30, pnl-31,

Table 2
The suite containing significant amounts of selected elements.

Element	Benchmark
Be	pmf19, pmf21, umf5
B	lct8,lct16
C	hmi6, pmf23
Gd	lct3, lct4, lct14,hst18
W	pmf5,hmf60
Cu	lct9,pmf13

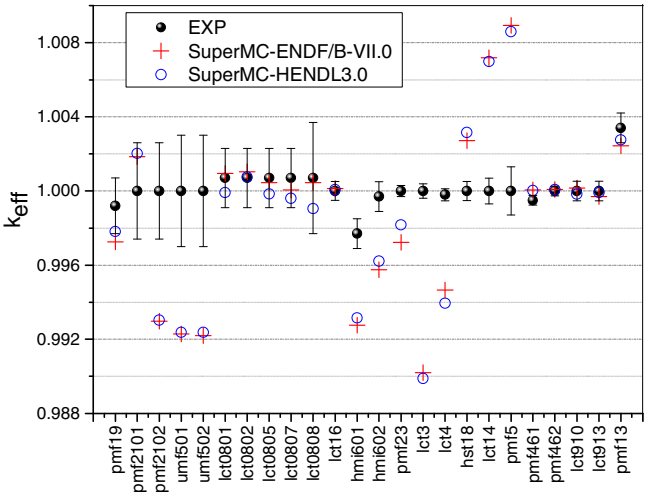

Fig. 8. Results for the benchmarks of the selected element.

pnl-32, pnl-33, and pnl-35 have large amount of repeat structure description in the geometry model and structural materials. The biggest discrepancy lied in the thermal spectrum benchmark pst09 with the two libraries. As shown in Fig. 7, the calculation results in SuperMC for pst09 are 1.01869 and 1.02118 with a statistical uncertainty of 0.00086 and 0.00087, with two data libraries. The experimental data is 1.0 with an uncertainty of 0.0033, and MCNP result with ENDF/B-VII.0 is 1.01900 with an uncertainty of 0.0020. All the simulation results are more than 1800 pcm above experimental data. These discrepancies will be discussed in Section 4.2.

4.2. Preliminary analysis for selected elements

Selected from the validation suite and handbook, Table 2 gives a list of selected elements, together with cases in which these selected elements are presented in significant amounts. This may be its location, its atomic density, or its mass in the benchmark model. The presence of these selected elements in these cases can have a obvious impact on the calculation results for analysis. Fig. 8 shows the calculation results of SuperMC with two data libraries for these elements.

The beryllium nuclide data have been received much attention and study for many years (Kahler et al., 2011). It remains a problem to make a data file consistent with all available data. The results for beryllium containing benchmarks are similar with different data libraries, but do not have a good consistence with experimental data as shown in Fig. 8. Two cases of benchmark pmf21 with Be and BeO as the reflector, have been performed, respectively. The difference of the results of two case is noticeable. Although the two cases are very similar in geometry and materials except the nuclide composition of the reflector, the difference between the results for the two cases are more than 1000 pcm. Also it shows in this validation suite that the results for beryllium containing benchmarks are mixed and inconclusive. More detailed discussions on beryllium are included in the related literature (Kahler et al., 2011).

Lct08 is a series of low enriched uranium reactor benchmarks and the results for boron benchmarks are mostly similar for the different data libraries and experimental data. And also lct16 performs well for two libraries (see Fig. 8). As a moderator in hmi6 and pmf23, the results of C are lower than the experimental data. The results of SuperMC with the HENDL data library are closer to the experimental data than those with the ENDF/B-VII.0. The reason may be that the capture cross section is increased and more accurate in HENDL data library.

Fig. 8 shows that the gadolinium benchmarks have no good consistence with experimental data. The benchmark lct3 and lct4, containing gadolinium as an impurity in water, the calculation results are lower than the experimental data. The cases lct14 and hst18 appear a trend that the results of cases without gadolinium or with low concentrations of gadolinium are lower than the cases with higher concentration. Further study of these results is necessary. And for other elements such as W and Cu, the results are consistence with experimental data as shown in Fig. 8. All these cases in the suite and handbook suggest that future optimization for nuclear data of non-fission elements may lead to improvements of the calculation results.

5. Conclusions

This paper aimed at the validation of SuperMC for the criticality calculations. ICSBEP and 119 representative benchmarks were adopted to validate the criticality calculation function and the correctness of SuperMC. The results showed good agreement with experimental data and discrepancies mainly lied in statistical uncertainties. The criticality safety calculation capacity and the correctness of SuperMC2.1 were shown.

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