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Current Status of ACE Format Libraries for MCNP at Nuclear Data Center of KAERI

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ABSTRACT

Background: The current status of ACE format MCNP/MCNPX libraries by NDC of KAERI is presented with a short description of each library.

Materials and Methods: Validation calculations with recent nuclear data evaluations ENDF/B-VII.0, ENDF/B-VII.1, JEFF-3.2, and JENDL-4.0 have been carried out by the MCNP5 code for 119 criticality benchmark problems taken from the expanded criticality validation suite supplied by LANL. The overall performances of the ACE format KN-libraries have been analyzed in comparison with the results calculated with the ENDF/B-VII.0-based ENDF70 library of LANL.

Results and Discussion: It was confirmed that the ENDF/B-VII.1-based KNE71 library showed better performances than the others by comparing the RMS errors and χ^2 values for five benchmark categories as well as whole benchmark problems. ENDF/B-VII.1 and JEFF-3.2 have a tendency to yield more reliable MCNP calculation results within certain confidence intervals regarding the total uncertainties for the k_{eff} values.

Conclusion: It is found that the adoption of the latest evaluated nuclear data might ensure better outcomes in various research and development areas.

Keywords: MCNP/MCNPX, ACE format library, Expanded criticality validation suite, Root mean square error, χ^2 value, Unresolved resonance probability table

Original Research

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Introduction

As the applicability of MCNP to various research and development areas has been expanded, the demands for high precision nuclear data have been increasing accordingly. Los Alamos National Laboratory (LANL) has provided many kinds of ACE (A Compact ENDF) format libraries for use with the MCNP/MCNPX Monte Carlo code packages. These libraries have been originally generated based on different releases of ENDF/B nuclear data evaluations, which contain evaluated cross sections induced by several types of nuclear reactions such as neutron, photoatomic, photonuclear, electron, and proton reactions. However, the up-to-date ACE format neutron data library called ENDF71x [1] included in the latest MCNP6.1/MCNP5-1.60/MCNPX-2.7.0 code package was only until 2013, which was almost two years after the Cross Section Evaluation Working Group (CSEWG) released the ENDF/B-VII.1. Furthermore, they had not even dealt with other evaluated nuclear data libraries such as Japanese Evaluated Nuclear Data Library (JENDL) from the Japan Atomic Energy Agency and Joint Evaluated Fission and Fusion File (JEFF) from the OECD/NEA (Nuclear Energy Agency of the Organisation for Economic Co-operation and Development).

The Nuclear Data Center (NDC) of the Korea Atomic Energy Research Institute (KAERI) has produced a lot of ACE format neutron data libraries for MCNP since the release of ENDF/B-VI.5 and disseminated them to domestic and foreign researchers. In this study, the current status of ACE format libraries by NDC of KAERI is presented with a short description of each library. Validation calculations with recent nuclear data evaluations ENDF/B-VII.0, ENDF/B-VII.1, JEFF-3.2 and JENDL-4.0 have been carried out by the MCNP5 code for 119 criticality benchmark problems taken from the expanded criticality validation suite [2] supplied by LANL. The overall performances of the ACE format libraries have been analyzed in comparison with the results calculated with the ENDF/B-VII.0-based ENDF70 [3] library of LANL.

Materials and Methods

1. Current status of ACE format libraries at NDC

The NDC of KAERI has been producing several kinds of cross section libraries for general purpose radiation transport/depletion programs such as MCNP/MCNPX, DANTSYS, DOORS, WIMS, and ORIGEN. The cross section libraries have been widely used in many research areas by domestic and foreign researchers. The MCNP/MCNPX code adopts ACE-formatted continuous-energy cross section libraries for the Monte Carlo radiation transport calculations. The ACE format libraries have been generated through NJOY [4] code processing with the corresponding source evaluated nuclear data files. The first ACE format library MCLIB-E6[1)] contained continuous-energy neutron data at 300 K, 600 K, and 900 K for 332 nuclides mainly from ENDF/B-VI.5. The library can be easily found on the OECD/NEA Data Bank Website.

Since then, the KAERI/NDC (KN)-series of ACE format libraries have been produced in accordance with the release of new evaluated nuclear data files ENDF/B, JEFF, and JENDL [5]. Basically, the libraries contain neutron cross section data at room temperature (293.6 K). The special purpose libraries at certain temperatures have been provided to the researchers upon request. Table 1 summarizes currently available KN-series libraries, which have been disseminated through the KAERI/NDC website (http://atom.kaeri.re.kr/NDVG/). The nuclides in an ACE format library are identified by their ZA identifiers (ZAID). Here, ZZZ is the atomic number, AAA is the atomic mass number, and nnC is the user-supplied suffix for the ACE format library in use. For a metastable nuclide, the atomic mass number is changed to (AAA+50) for distinction with its ground state one. The atomic mass number is set at '000' for a natural element.

Table 1. Current Status of ACE Format KN-Libraries

Library	Source Data	Number of Nuclides	ZA Identifier (ZZZAAA.nnC)
KNE62	ENDF/B-VI.2	89	.62C
KNE68	ENDF/B-VI.8	316	.80C
KNE70	ENDF/B-VII.0	392	.85C
KNE71	ENDF/B-VII.1	423	.86C
KNF30	JEFF-3.0	97	.70C
KNF31	JEFF-3.1	380	.71C
KNF311	JEFF-3.1.1	381	.72C
KNF312	JEFF-3.1.2	381	.73C
KNF32	JEFF-3.2	466	.74C
KNJ33	JENDL-3.3	335	.90C
KNJAC-08	JENDL/AC-2008	76	.91C
KNJ40	JENDL-4.0	356	.92C

2. Criticality benchmark problems

The expanded criticality validation suite is widely used to validate the MCNP code along with the nuclear data libraries. The suite includes 119 criticality benchmark problems taken from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP)[2)]. The benchmark problems have been chosen for testing a wide range of energy regions and a variety of fissile and reflector materials, although the benchmark suite could not cover all nuclides and energy spectra of interest. The problems can be classified as five categories according to the principal fuel, i.e., highly enriched uranium (HEU), intermediate enriched uranium (IEU), low enriched uranium (LEU), Pu, and ^{233}U systems. Table 2 shows the number of problems in each of these categories of the expanded validation suite.

Results and Discussion

The benchmark calculations were carried out by the MCNP5 code and the reference calculation results were ob-

1) Refer to "Gil CS. ZZ-MCLIB-E6, Continuous energy cross section library from ENDF/B-VI.5 for MCNP-4A, -4B, 300K, 600K, 900K. OECD Nuclear Energy Agency NEA-1601/01. 2002."

2) Refer to "OECD Nuclear Energy Agency. International handbook of evaluated criticality safety benchmark experiments. OECD Nuclear Energy Agency NEA/NSC/DOC(95)03. 2009."

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Table 2. Number of Benchmark Problems in Each of Categories

Category	Number of Benchmark Problems
HEU	40
IEU	17
LEU	8
Pu	36
^{233}U	18
Whole	119

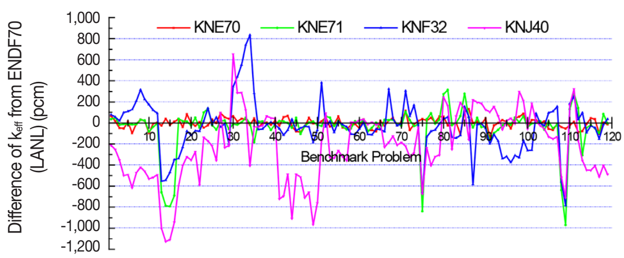

Fig. 1. Differences of calculated k_{eff} values with different KN-libraries from those with reference ENDF70 library.

tained with the ENDF/B-VII.0-based ENDF70 library of LANL. Validation calculations of KN-libraries have been carried out for the recent nuclear data evaluations ENDF/B-VII.0, ENDF/B-VII.1, JEFF-3.2, and JENDL-4.0. Figure 1 shows the differences of calculated k_{eff} values with these KN-libraries from those with the reference ENDF70 library. The KNE70 library shows good agreement with the reference calculation results while maintaining the differences within about ±100 pcm except for several benchmark problems. It could have granted us the validity of generation procedures for KN-libraries. Other libraries show relatively large differences in comparison with the reference one whether the differences are of benefit to the benchmark k_{eff} values or not.

In this study, three statistical approaches have been introduced to test the overall performances of the ACE format libraries. The root mean square (RMS) error, which is defined in equation 1, represents the sample standard deviation of the differences between calculated values and experimental values. Here, $k_{C,i}$ and $k_{E,i}$ are the calculated and experimental k_{eff} values for the i^{th} problem respectively and N is the total number of problems in each benchmark category. As shown in Figure 2, the RMS errors relative to the benchmark k_{eff} values were compared among the different ACE format libraries. For the reference ENDF70 library, the RMS errors are distributed around 0.5% except for the LEU systems. As a whole, the RMS errors for the KNE71 and KNF32 libraries are getting better than the others. The obvious changes by the

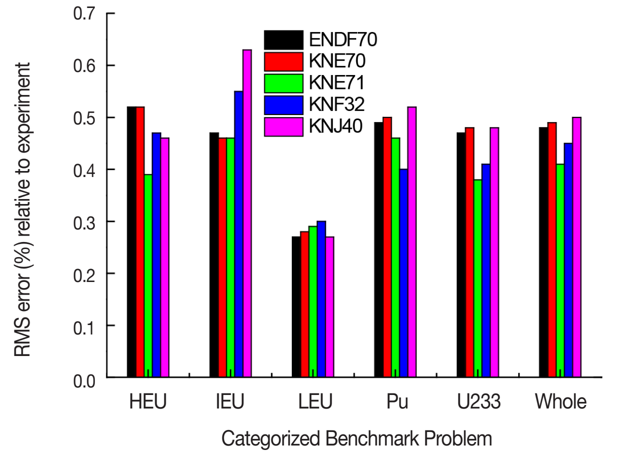

Fig. 2. Comparison of RMS errors relative to benchmark k_{eff} values among different ACE format libraries.

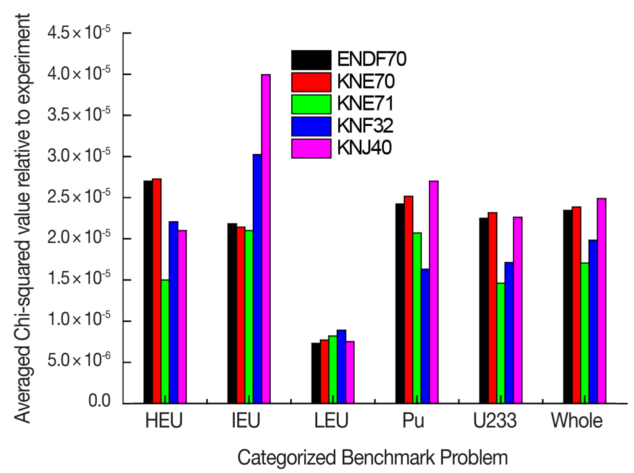

Fig. 3. Comparison of averaged χ^2 values relative to benchmark k_{eff} values among different ACE format libraries.

KNE71 library come into view in the HEU and ^{233}U systems when compared with the ENDF70 library.

$$RMS(\%) = \sqrt{\frac{\sum_{i=1}^{N}\left(k_{C,i} - k_{E,i}\right)^2}{N}} \quad (1)$$

The second statistical approach is the introduction of the χ^2 value, which is defined in equation 2. The χ^2 value can be considered as an effective indicator to determine whether there is a significant difference between the calculated and experimental data. As shown in Figure 3, a comparison of the averaged χ^2 values relative to the benchmark k_{eff} values for each benchmark category is quite similar to those of the RMS errors. In contrast, the χ^2 values tend to show more drastic changes between the calculated and experimental k_{eff}

Table 3. Number of Benchmark Problems that Belong to Certain Confidence Intervals for Different ACE Format Libraries

Confidence Interval	ENDF70	KNE70	KNE71	KNF32	KNJ40
< 1σ	71	68	78	73	50
1σ~2σ	27	30	28	31	36
2σ~3σ	13	13	8	11	18
> 3σ	8	8	5	4	15

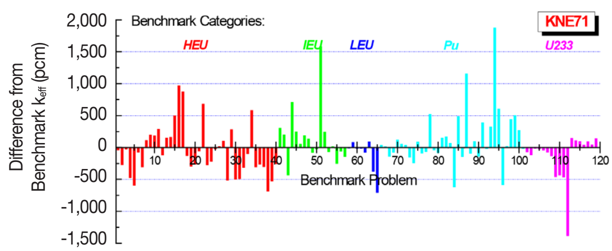

Fig. 4. Differences of ENDF/B-VII.1-based calculation results from benchmark k_{eff} values.

values than the RMS errors. In the HEU and ^{233}U systems, the KNE71 library shows the largest improvements of more than 35% when compared with the ENDF70 library. The improvement in the Pu system is remarkable for the KNF32 library. The deteriorations in the IEU system for the KNF32 and KNJ40 libraries should be improved for the future releases of JEFF and JENDL.

$$\chi^2 = \sum_{i=1}^{N} \frac{\left(k_{C,i} - k_{E,i}\right)^2}{k_{E,i}} \qquad (2)$$

The reliability of the MCNP calculation results to the benchmark k_{eff} values could be verified by comparing the number of benchmark problems that belong to certain confidence intervals regarding the total uncertainties for the k_{eff} values. It is assumed that the total uncertainty in this approach comes from the experiment and MCNP calculation. Table 3 shows the outcome of the reliability checkup for the different ACE format libraries. The ENDF/B-VII.1 and JEFF-3.2 tend to yield more reliable MCNP calculation results below 2 standard deviations (STD) than those of the ENDF/B-VII.0 and JENDL-4.0. An outstanding achievement is seen in ENDF/B-VII.1 in comparison to the previous ENDF/B-VII.0.

Figures 4 and 5 show differences in the calculated k_{eff} values with the KNE71 and KNE70 libraries from the benchmark k_{eff} values, respectively. It was also confirmed that the overall calculation results with the KNE71 library have been enhanced noticeably by comparing the two figures. For

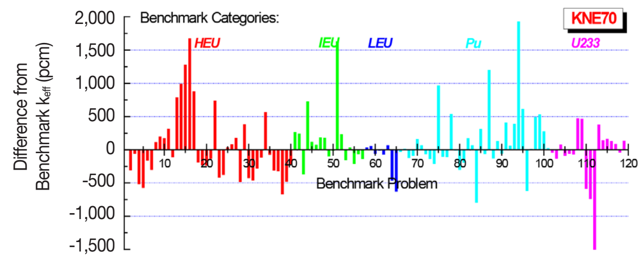

Fig. 5. Differences of ENDF/B-VII.0-based calculation results from benchmark k_{eff} values.

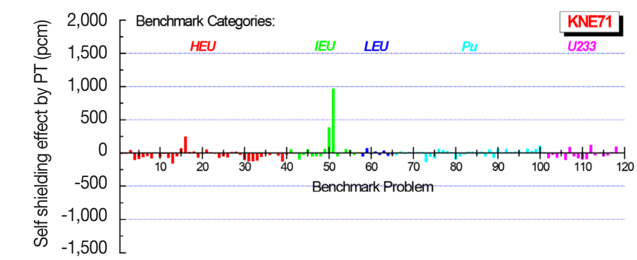

Fig. 6. Self-shielding effects by unresolved resonance probability tables in ENDF/B-VII.1-based calculation.

KNE71, the differences are generally maintained within about ± 500 pcm except for some benchmark problems.

The probability table has been introduced to correct the self-shielding effect resulting from the unrealistic averaged cross sections in the unresolved resonance (UR) energy region [5]. This methodology has been applied to the Monte Carlo calculations since the MCNP version 4C. In this study, the self-shielding effect is estimated as the difference of k_{eff} values calculated with and without using the UR probability tables. Figure 6 shows the self-shielding effects by the UR probability tables in the ENDF/B-VII.1-based benchmark calculation. The effects are generally small, less than about ± 100 pcm except for a few benchmark problems. The tungsten carbide (WC)-reflected TOPSY experiment and the BIG TEN experiment show the effects of 244 pcm and 380 pcm, respectively. The ZEBRA 8H experiment is the only IEU benchmark in the validation suite with an intermediate spectrum. Therefore, the benchmark shows the largest self-shielding effect of 966 pcm for ENDF/B-VII.1.

Conclusion

ACE format KN-libraries for MCNP/MCNPX by NDC of KAERI have been introduced. KN-libraries have been vali-

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dated through 119 criticality benchmark problems taken from the expanded criticality validation suite for MCNP. The validity of the generation procedures for KN-libraries has been confirmed by comparing the results calculated with two ENDF/B-VII.0-based ACE format libraries, KNE70 and ENDF70. Three statistical approaches have been applied to the performance test of the ACE format libraries. The analyses of the RMS errors and χ^2 values for the benchmark categories concluded that the ENDF/B-VII.1-based KNE71 library showed better performances than the others. In addition, the ENDF/B-VII.1 and JEFF-3.2 brought more reliable MCNP calculation results within certain confidence intervals regarding the total uncertainties for the k_{eff} values. This implies that the adoption of the latest evaluated nuclear data might ensure better outcomes in various research and development areas.

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