Bias Evaluations in McCARD Criticality Analysis for Low-enriched Uranium Thermal Critical Experiment Benchmarks

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1. Introduction

In 2019, Korea Atomic Energy Research Institute (KAERI) and King Abdullah City for Atomic and Renewable Energy (K.A.CARE) established KAERI-K.A.CARE joint research and design (R&D) center at KAERI to continue the effective and close cooperation for the National Nuclear Laboratory (NNL) establishment in Saudi Arabia. This center has carried out various joint R&D projects which both parties are mutually interested.

As a part of the joint R&D projects, the "Application of a Monte-Carlo Neutron/Photon Transport Simulation Code (McCARD) for Advanced Shielding Design of Nuclear Reactors" project has been conducted. The main goal of this project is to train the K.A.CARE engineer for a nuclear core shielding design analysis and to validate the McCARD [1] Monte Carlo (MC) code to be used for advance shielding design and analysis of a new-type reactor.

Recently, the KAERI and K.A.CARE engineers performed the critical analysis by the McCARD code and the up-to-date evaluated nuclear data libraries (i.e. ENDF/B-VIII.0 [2], JENDL-5.0 [3], JEFF-3.3 [4], CENDL-3.2 [5] and TENDL-2021 [6]). As the benchmark problems, some low-enriched uranium (LEU) benchmark problems were selected from the International Handbook of Evaluated Criticality Safety Benchmark Experiment Problem (ICSBEP) [7]. The calculated k_{eff} results can be used as the bias value in the critical analysis of a pressurized water reactor (PWR)-type small modular reactor (SMR) fuel storage.

2. Methods and Results

2.1 ICSBEP LEU Critical Benchmark Experiments

Among the LEU benchmarks, the low-enriched uranium critical experiment benchmark problems with thermal spectrum and square lattice were selected. Table I shows the description of the selected ICSBEP LEU thermal spectrum problems and the number of its sub-cases. The number of its total sub-cases is 140, but the one-hundred sub-cases were prepared and utilized for the criticality analysis. To perform the McCARD critical analysis, its input files are prepared. Figures 1 and 2 present the X-Y cross sections of the prepared McCARD sample inputs. The cross sections were plotted by the McVIEW [8], McCARD input visualizer utility, which was developed by Seoul National University for user's friendliness and convenience.

Table I: Description of the selected ICSBEP LEU benchmark problems

No	Benchmark ID	Description
1	LCT-001	Water-Moderated UO_2 (2.35 w/o) Fuel Rods in Square-Pitched Arrays
2	LCT-002	Water-Moderated UO_2 (4.31 w/o) Fuel Rods in Square-Pitched Arrays
3	LCT-003	Water-Moderated UO_2 (2.35 w/o) Fuel Rods in Square-Pitched Arrays
4	LCT-004	Water-Moderated UO_2 (4.31 w/o) Fuel Rods in Square-Pitched Arrays
5	LCT-005	Critical Experiments with LEU Dioxide Fuel Rods in Water Containing Dissolved Gadolinium
6	LCT-006	Critical Lattice of Low Enriched UO_2 Fuel Rods with various Water-to-Fuel Volume Ratios
7	LCT-010	Critical Arrays of Water-Moderated UO_2 (4.31 w/o) Fuel Rods Reflected by Lead, Uranium, or Steel Walls
8	LCT-017	Critical Arrays of Water-Moderated UO_2 (2.35 w/o) Fuel Rods Reflected by Lead, Uranium , or Steel Walls

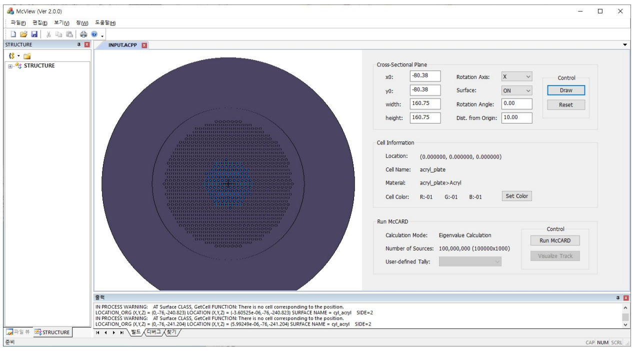

Fig. 1. X-Y cross section of LCT-004 ICSBEP case1 plotted by McVIEW visualizer utility

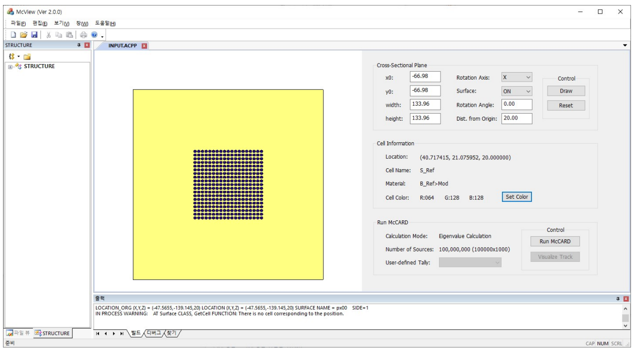

Fig. 2. X-Y cross section of LCT-006 ICSBEP case1 plotted by McVIEW visualizer utility

2.2 Bias Evaluations Methodology

In a conventional critical safety analysis method [9], its bias and uncertainty should be provided for considering the uncertainties of calculation conditions, code, and library. Specially, the bias in critical safety analysis can be calculated by comparing calculated k_{eff} and experimental k_{eff} for various critical facility benchmark problems. Equation 1 explains how to calculate the final effective multiplication factor.

$$k_{eff}^{final} = \overline{k_{cal}} + \Delta k_{bias} + \Delta k_{unc} \qquad \ldots (1)$$

where $\overline{k_{cal}}$ is the calculated nominal k_{eff}, Δk_{bias} is the bias calculated from the criticality benchmark calculations, and is Δk_{unc} is the uncertainties caused from the uncertainty of the code systems and the design parameters.

In general, the bias value (Δk_{bias}) in the criticality analysis can be calculated by

$$\Delta k_{bias}^{i} = k_{\exp}^{i} - k_{cal}^{i}, \qquad \ldots (2)$$

$$\Delta k_{bias} = \frac{1}{N}\sum_{i=1}^{N} \Delta k_{bias}^{i}, \qquad \ldots (3)$$

$$\sigma(\Delta k_{bias}) = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(\Delta k_{bias}^{i} - \Delta k_{bias})^2}. \qquad \ldots (4)$$

$k_{\exp}$ and k_{cal} is the experimental and calculated k_{eff} for i^{th} benchmark problem, respectively. The number of the benchmark problem is *N*. A statistical uncertainty of the calculated bias value should be considered in the criticality safety evaluation. To apply 95% probability of uncertainty at the 95% confidence interval, one sided tolerance limit factor, which corresponds to the number of benchmark cases used in this analysis, shall be considered.

2.3 Bias Estimation in Critical Analyses with Various Evaluated Nuclear Cross Section Data Libraries

For the bias estimation in critical analysis of PWR-type SMR fuel storage, the McCARD eigenvalue calculations were performed with various evaluated nuclear cross section data libraries – ENDF/B-VII.1, ENDF/B-VIII.0, JENDL-4.0, JENDL-5.0, CENDL-3.2, JEFF-3.3, and TENDL-2021. In general, a regulating body has recommended the use of a newest evaluated nuclear data library in a nuclear core design and analysis. The ENDF/B-VIII.0 was released in 2018 with the major changes of the important isotopes (i.e. ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu) by the Collaborative International Evaluation Library Organization (CIELO). The JENDL-5.0 and JEFF-3.3 were released in 2021 and 2017. Lastly, TENDL-2021 is the 11st version of TENDL library and was most recently released (in December 2021). CENDL-3.2 was released in 2019 by the joint collaboration of CENDL working group. These evaluated nuclear data libraries were widely used around the world in the nuclear engineering field these days.

Figure 3 plots the difference between the calculated and experimental k_{eff} for the 100 ICSBEP benchmark problems with ENDF/B-VII.1, ENDF/B-VIII.0, JENDL-4.0, JENDL-5.0, CENDL-3.2, JEFF-3.3, TENDL-2021 evaluated nuclear data libraries. The differences in pcm were calculated by

$$\begin{aligned} diff(k_{eff}) &= \left(\rho_{cal} - \rho_{\exp}\right)\times 10^5 \\ &= \left(\frac{1}{k_{\exp}} - \frac{1}{k_{cal}}\right)\times 10^5. \end{aligned} \qquad \ldots (5)$$

Moreover, a chi square value (χ^2) can be utilized as an indicator to confirm the differences between experimental and calculated k_{eff}'s. A chi square value (χ^2) can be calculated by

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{k_{cal}^{i} - k_{\exp}^{i}}{\sigma_{\exp}^{i}}\right)^2. \qquad \ldots (6)$$

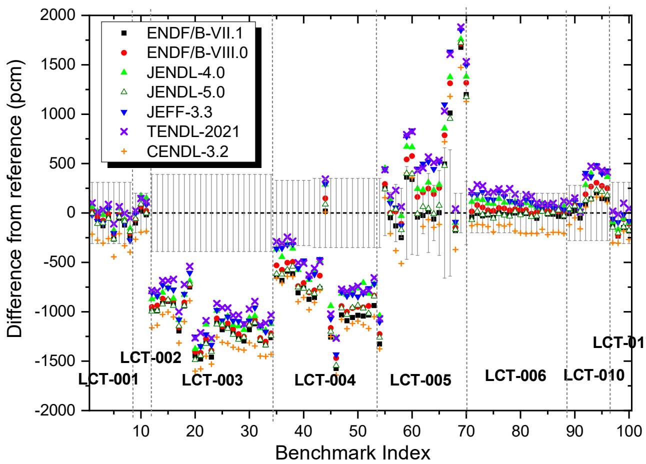

Fig. 3. Difference between the calculated and experimental (reference) k_{eff}'s for ICSBEP LCT benchmark problems

As shown in Fig. 3, the k_{eff}'s were significantly overestimated by the McCARD for LCT-005 whereas those were underestimated for LCT-003 and LCT004. Overall, the calculated k_{eff} with JEFF-3.3 and TENDL-2021 were higher than the others. CENDL-3.2 predicted the smaller k_{eff}'s than the other evaluated nuclear data libraries for the LCT benchmark problems. It is noted that the statistical uncertainties of k_{eff}'s in MC simulations were less than 30 pcm where the uncertainties of k_{exp} from the reference the 640 pcm. In Fig. 3, error bars indicate the uncertainties of the experimental k_{eff}'s. Table II shows the bias values in McCARD criticality analysis with the seven evaluated nuclear data libraries. The biases were ranged from 0.00146 to 0.00499 whereas k_{cal}'s were from 0.99476 to 0.99830. The uncertainties of the average k_{cal} and biases were all 123 pcm.

Table II: Bias values in McCARD criticality analysis with various evaluated nuclear data libraries

Evaluated nuclear data library	$\overline{k_{cal}}$	Bias (Δk_{bias})	Uncertainty $2\sigma(\Delta k_{bias})$
ENDF/B-VII.1	0.99662	0.00313	0.01270
ENDF/B-VIII.0	0.99585	0.00391	0.01225
JENDL-4.0	0.99751	0.00224	0.01243
JENDL-5.0	0.99610	0.00366	0.01220
JEFF-3.3	0.99774	0.00201	0.01313
CENDL-3.2	0.99476	0.00499	0.01248
TENDL-2021	0.99830	0.00146	0.01286
Avg.	0.99670± 0.00123	0.00306± 0.00123	0.01258± 0.00034

Table III compared the chi square values for each evaluated nuclear data library. The χ^2 were ranged from 1.97 to 2.34. It was observed that there was no significant difference of the performance for the LEU benchmark criticality analysis.

Table III: Comparison of chi square values for each evaluated nuclear data library

Evaluated nuclear data library	χ^2
ENDF/B-VII.1	2.08
ENDF/B-VIII.0	2.14
JENDL-4.0	1.97
JENDL-5.0	2.10
JEFF-3.3	2.04
CENDL-3.2	2.34
TENDL-2021	1.99

2.4 Comparison with MCNP results

For the verification, the McCARD results were compared with the MCNP results, which were obtained from the reference [2] for LCT-001, LCT-002, LCT-005, LCT-006, LCT-010, and LCT-017 benchmark problems. Figure 4 shows the difference between k_{eff}'s by the McCARD and MCNP calculations. Table IV provides the root mean square (RMS) difference between McCARD and MCNP results. The RMS difference for ENDF/B-VII.1 was 54 pcm whereas that for ENDF/B-VIII.0 was 33 pcm. Considering the statistical uncertainties of the MCNP results were less than 100 pcm, it was concluded that the McCARD agree well with the MCNP.

Table IV: RMS difference between k_{eff} results by McCARD and MCNP calculations

Evaluated nuclear data library	RMS difference of k_{eff} (pcm)
ENDF/B-VII.1	54
ENDF/B-VIII.0	33

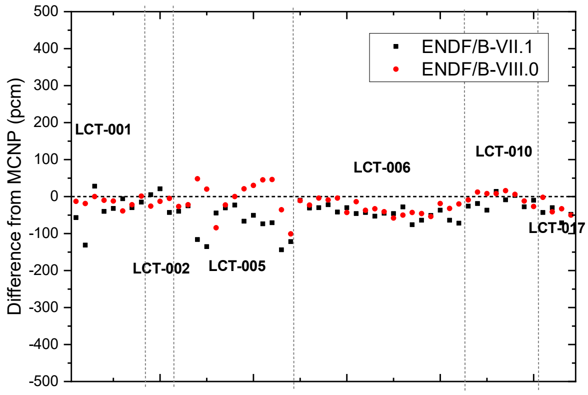

Fig. 4. Difference between k_{eff}'s by McCARD and MCNP calculations for ICSBEP LCT benchmark problems

3. Conclusions

In this study, the bias values in criticality analysis were estimated by the McCARD MC calculations for the selected ICSBEP LCT benchmark problems with the up-to-date evaluated nuclear data libraries. From the results, it was confirmed that the bias values are sensitive to the evaluated nuclear data library. A nuclear core shielding designer shall consider the sensitivity of the bias due to evaluated nuclear data libraries as uncertainty or margin. The calculated bias values may be usefully utilized as the reference for the design of a conventional PWR-type fuel storage.

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