McCARD and MCNP6.2 Modern Criticality Experiment Benchmark Analyses and Geometric Uncertainty Analyses using Monte Carlo Perturbation Method

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1. Introduction

Up until the 1980s, numerous critical facilities and research reactors were constructed worldwide, and critical benchmark problems were developed based on the experimental results obtained from those facilities and reactors. The International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook compiles such benchmark problems together with experimental data and computational analysis results. Since the 1980s, several critical facilities have developed new critical benchmarks, which are often referred to as "modern benchmarks". Representative problems included in the modern benchmark suite are Kilowatt Reactor Using Stirling Technology (KRUSTY), Thermal/Epithermal eXperiments (TEX), and Godiva-VI. In this study, criticality analyses of these modern benchmarks will be performed to assess the performance of newly evaluated nuclear data libraries by McCARD Monte Carlo (MC) code. Moreover, geometric uncertainties or tolerances are generally provided for each critical benchmark problem. In this study, the MC geometric perturbation technique, which was proposed in previous work, will be applied to quantify the impact of such geometric uncertainties on criticality analysis results.

2. Modern Benchmark Analysis by McCARD with Various Evaluated Nuclear Data Libraries

The three benchmarks (i.e., KRUSTY, GODIVA-IV, and TEX) among the modern benchmarks were selected to perform the criticality analyses, and to evaluate geometric uncertainty analysis.

2.1 KRUSTY

The Kilopower Reactor Using Stirling TechnologY (KRUSTY) is a compact fast-spectrum critical assembly developed jointly by NASA and the U.S. Department of Energy to demonstrate the feasibility of nuclear thermal power for space applications. The system consists of a cylindrical annular core of uranium—molybdenum (U—Mo) alloy fuel surrounded by a thick beryllium oxide (BeO) reflector, with sodium heat pipes penetrating the core for heat removal in the full KRUSTY design. The initial critical experiment, reported in the ICSBEP handbook, was conducted with the reflector configured to achieve prompt criticality at

a compact core size of approximately 11 cm in height and diameter.

In this work, the KRUSTY benchmark model was constructed following the specifications of the initial critical experiment. The fuel region was modeled as a homogeneous annular cylinder of U–Mo alloy with 93 wt.% enrichment of ²³⁵U. The molybdenum fraction was explicitly included in the material definition. The reflector was modeled as a homogeneous BeO annular cylinder with a thickness of approximately 29 cm and a minimum density of 99.5 wt.%. Non-fuel structural components, such as the sodium heat pipe channels, cladding, and support hardware, were homogenized with the surrounding fuel material to simplify the geometry while preserving the average atom densities. Figure 1 shows a simplified KRUSTY model applying the above points.

Table 1 and Table 2 compared the effective multiplication factors by McCARD with those by MCNP6.2 with ENDF/B-VII.1 and ENDF/B-VIII.0, respectively. The effective multiplication factors by McCARD agree well with those by McNP6.2. Table 3 shows the effective multiplication factors calculated by McCARD with the ENDF/B-VIII.1, which is the most recently released version of the ENDF/B library. It is observed that ENDF/B-VIII.0 and ENDF/B-VIII.1 yield comparable results, which show the closest agreement with the experimental measurements.

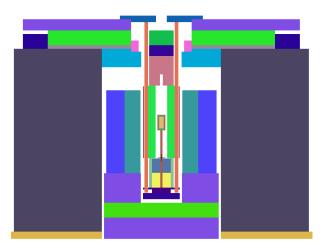


Figure 1: KRUSTY simplified modeling (Case 1)

Table 1: Effective multiplication factors of KRUSTY benchmark using ENDF/B-VII.1

CASE	Effective multiplication factor		
	MCNP6.2	McCARD	
1	1.00291±0.00002	1.00264 ±0.00002	
2	1.00585±0.00002	1.00548±0.00002	
3	1.00274±0.00002	1.00244±0.00002	
4	1.00282±0.00002	1.00240±0.00002	
5	1.00419±0.00002	1.00387±0.00002	

Table 2: Effective multiplication factors of KRUSTY benchmark using ENDF/B-VIII.0

CASE	Effective multiplication factor		
	MCNP6.2	McCARD	
1	1.00028±0.00002	1.00020±0.00002	
2	1.00311±0.00002	1.00301±0.00002	
3	1.00001±0.00002	0.99992±0.00002	
4	1.00014±0.00002	0.99996±0.00002	
5	1.00154±0.00002	1.00142±0.00002	

Table 3: Effective multiplication factors of KRUSTY benchmark using ENDF/B-VIII.1

CASE	Effective multiplication factor		
	Experiment	McCARD	
1	1.00050±0.00002	1.00029±0.00002	
2	1.00331±0.00002	1.00309±0.00002	
3	1.00001±0.00002	1.00004±0.00002	
4	1.00029±0.00002	1.00003±0.00002	
5	1.00169±0.00002	1.00149±0.00002	

2.2 GODIVA-IV

GODIVA-IV is a representative bare-metal highly enriched uranium (HEU) fast assembly designed to produce short bursts of intense neutrons and gamma rays for the testing of radiation detectors, criticality alarm systems, and related instrumentation. It was constructed and operated at Los Alamos National Laboratory as part of the GODIVA series of assemblies, and its detailed specifications are documented in the ICSBEP Handbook.

The core consists of metallic uranium enriched to 93.2 wt.% 235 U, configured without any external reflector. In the experimental system, the fuel was arranged in an annular cylindrical stack with a central safety block that directly influenced the reactivity. The benchmark consists of five primary configurations: four were reported with measured $k_{\rm eff}$ values of 1.0000 within negligible uncertainty, while the fifth configuration yielded $k_{\rm eff} = 1.0070 \pm 0.0003$.

In this study, the GODIVA-IV benchmark was modeled in McCARD according to the specifications outlined in the ICSBEP benchmark handbook. The uranium fuel was modeled as four annular columns to simplify the irregularities, and the detailed stack structure and minor irregularities were ignored. Figure 2

shows a simplified model of GODIVA-IV reflecting the above points.

Table 4 compares the multiplication factors of the Godiva-IV benchmark across different codes and nuclear data libraries. In the ENDF/B-VII.1 case, the multiplication factors from MCNP6.2 and McCARD showed agreement within the statistical uncertainties. There are no significant differences in multiplication factors among the ENDF/B versions.

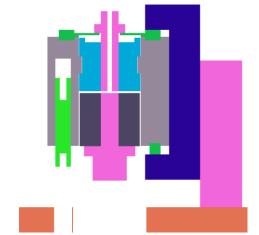


Figure 2: GODIVA-IV simplified modeling (Case 1)

2.3 TEX

The Thermal/Epithermal eXperiments (TEX) are a series of significant benchmark experiments developed as part of the United States Nuclear Criticality Safety Program (NCSP). These experiments were designed to establish baseline configurations using Pt/Al metal alloy plates with varying thicknesses of polyethylene moderator and a thin polyethylene reflector, covering five different fission energy regimes. The TEX experiments utilize Plutonium-Aluminum No-Nickel (PANN) plates, originally from the Zero Power Physics (ZPPR) program, Reactor to study fission characteristics across thermal, intermediate, and fast neutron energy regimes.

All five experimental configurations are accepted as benchmarks. In the experiments, the ZPPR plates composed of 98.9 wt.% plutonium were arranged in layers of 24 plates (a 6x4 array) on trays, resulting in an approximate footprint of 30cm by 30cm. To tune the neutron spectrum, varying thicknesses of polyethylene moderator were interspersed between the layers. Figure 3 shows a simplified model of TEX reflecting the above points.

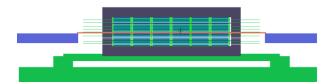


Figure 3: TEX simplified modeling (Case 1)

Table 4. Effective multiplication factors of GODIVA-IV benefithat Kini each code and evaluated factor data florary				
CASE	MCNP6.2	McCARD	McCARD	McCARD
	(ENDF/B-VII.1)	(ENDF/B-VII.1)	(ENDF/B-VIII.0)	(ENDF/B-VIII.1)
1	0.9893±0.00030	0.9894 ± 0.00030	0.98998±0.00030	0.98937±0.00030
2	0.9898±0.00030	0.9902±0.00030	0.99004±0.00030	0.98921±0.00030
3	0.9903±0.00030	0.9906 ± 0.00030	0.99061±0.00030	0.99019±0.00030
4	0.9907±0.00030	0.9910±0.00030	0.99138±0.00030	0.99177±0.00030

 0.9959 ± 0.00030

Table 4: Effective multiplication factors of GODIVA-IV benchmark for each code and evaluated nuclear data library

Table 5: Effective multiplication factors of TEX benchmark using ENDF/B-VII.1

CASE	Effective multiplication factor		
	MCNP6.2	McCARD	
1	1.00195±0.00008	1.00230±0.00008	
2	0.99781±0.00009	0.99788±0.00009	
3	1.00546±0.00009	1.00545±0.00009	
4	0.99869±0.00009	0.99869±0.00009	
5	1.00308±0.00009	1.00323±0.00009	

0.9961±0.00030

Table 6: Effective multiplication factors of TEX benchmark using ENDF/B-VIII.0

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CASE	Effective multiplication factor		
	MCNP6.2	McCARD	
1	1.00333±0.00008	1.00355±0.00008	
2	1.00059±0.00009	1.00094±0.00009	
3	1.01129±0.00009	1.01130±0.00009	
4	1.00363±0.00009	1.00393±0.00009	
5	1.00632±0.00009	1.00688±0.00009	

Table 7: Effective multiplication factors of TEX benchmark using ENDF/B-VIII.1

6			
CASE	Effective multiplication factor		
	Experiment	McCARD	
1	1.00027±0.00260	1.00268±0.00008	
2	1.00021±0.00236	0.99833±0.00009	
3	1.00088±0.00220	1.00773±0.00009	
4	1.00073±0.00287	1.00110±0.00009	
5	0.99917±0.00193	1.00493±0.00009	

Tables 5 and 6 compare the effective multiplication factors of five TEX benchmarks by MCNP6.2 and McCARD with the ENDF/B-VII.1 and ENDF/B-VIII.0 libraries, respectively. The effective multiplication factors by McCARD agree well with thos by MCNP6.2 within the statistical uncertainties. Table 7 compares the effective multiplication factors calculated by McCARD with ENDF/B-VIII.1 and the experimental values. Except for Case 5, the effective multiplication factors calculated by McCARD show no significant deviation from the experimental values.

3. Quantification of Criticality Uncertainty due to

Geometrical Tolerances for Modern Benchmark

Geometric perturbation analysis is based on MC Perturbation Formulation derived from the collision density equation [1]. All the regions of a given systems are divided into two regions. One is the non-perturbed region and the other is the perturbed region. The perturbed region is the region which was influenced by uncertainties of geometric parameters. The nonperturbed regions are modeled using the original geometric parameters while the perturbed regions are set using the perturbed geometric parameters excluding the non-perturbed regions as shown in Fig 4. In the perturbed regions, the variation of tally Q due to isotopic number density, $\delta Q(N)$ will be calculated by the 2-step procedure.

0.99674±0.00030

0.99701±0.00030

On step 1, in the perturbed region, all the isotopic number density of the non-perturbed region I, which is related with the uncertainty of geometric parameter, is perturbed to 100%. $\delta Q(N_I)$ will be calculated.

On step 2, in the perturbed region, all the isotopic number density of the non-perturbed region II is perturbed to -100%. $\delta Q(N_{II})$ will be calculated.

Finally, the uncertainties of tally Q can be calculated by Eq. (1).

$$\delta Q = \delta Q(N_{I}) + \delta Q(N_{II}) \tag{1}$$

One calculates the variance of the uncertainties of tally Q, $\sigma^2(\delta Q)$, by Eq. (2).

$$\sigma^{2}(\delta Q) = \sigma^{2}(\delta Q(N_{I})) + \sigma^{2}(\delta Q(N_{I}))$$

$$+2\text{cov}[\delta Q(N_{I}), \delta Q(N_{I})] \approx \sigma^{2}(\delta Q(N_{I})) + \sigma^{2}(\delta Q(N_{I}))$$
(2)

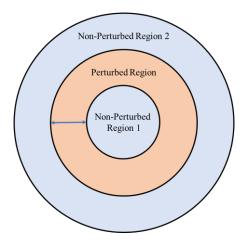


Figure 4: Separating perturbed and unperturbed regions

3.2 Application of Monte Carlo Geometric Perturbation for Modern Benchmark Problems

Table 8 shows the results of the geometrical uncertainty analyses for the three modern criticality experimental benchmark problems (i.e., KRUSTY-GODIVA-IV, and TEX) by the direct subtraction method and the MC perturbation method. In the KRUSTY benchmark, the fuel height and the radius of inner and outer reflectors were considered as the geometrical uncertain input parameters. Figure 5 shows the perturbed cells in step 1 and 2 in the criticality difference analysis according to fuel height. Meanwhile, in the GODIVA-IV benchmark, the safety block height, inner and outer radius of safety block have uncertain geometry input parameters. In the TEX benchmark, the heights in top reflector and lower plate have ± 0.1 cm uncertainty. It was noted that the MC perturbation method are in good agreements with the direct subtraction method, which can be considered as the reference solutions, except for the fuel height in the KRUSTY benchmark and the outer radius of safety block in the GODIVA-IV benchmark.

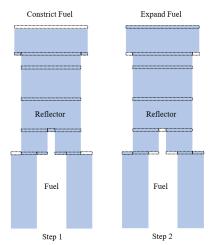


Figure 5: Step 1 and step 2 shapes (dashed lines indicate perturbed regions) of KRUSTY fuel height in the Monte Carlo perturbation method

4. Conclusion

In this study, criticality analyses were performed for modern criticality experiment benchmark problems, which are conducted in recent years, using the McCARD and MCNP6.2 with both the existing ENDF/B-VII.1 and the up-to-date ENDF/B-VIII.1 evaluated nuclear data libraries. It was confirmed that the effective multiplication factors by McCARD agree well with those by MCNP6.2 within a range of 20 to 30 pcm, with the exception of certain cases. Furthermore, across all three benchmarks, the new ENDF/B-VIII.1 library tended to match the experimental values more closely than the old ENDF/B-VIII.0 library.

Moreover, this study extended the MC perturbation technique based geometrical perturbation method to more complex modern criticality benchmarks (i.e., KRUSTY and TEX) in order to verify its applicability and efficiency. As mentioned in Section 3.2, in most cases, there are no significant differences between the direct subtraction method and the MC perturbation method. However, when the perturbed region was subdivided into a large number of cells (82 cells), particularly in the KRUSTY fuel region with highly segmented geometry, the perturbation method tended to deviate from the actual change in criticality. It was inferred that this discrepancy arises from the accumulation of statistical uncertainties across multiple cells and the diminished correlation between reference and perturbed tallies at numerous cell boundaries.

Despite these limitations, the method effectively calculates sensitivities of multiple parameters simultaneously, even for complex modern benchmarks. In the near future, the effect of cell resolution on perturbation accuracy will be examined. And the techniques will be improved to enhance multi-cell perturbations, further extending the applicability to real reactor systems.

Table 8: Geometric perturbation results for each modern benchmark using the direct subtraction method and the MC perturbation method.

Benchmark	Parameter	Deviation (cm)	Δk _{eff} (pcm)	
			Direct Subtraction	MC perturbation method*
KRUSTY	Fuel height	±0.109728	-405±3	-273±9
	Inner radius of inner reflector	±0.018288	-87±3	-98±15
	Outer radius of outer reflector	±0.036576	-50±3	-52±7
GODIVA-IV	Safety block height	-0.0508	-81±40	-74 <u>+</u> 4
	Outer radius of safety block	-0.0254	-176±40	-138±4
	Inner radius of safety block	+0.0254	-61±40	-42±3
TEX	Top reflector Height	±0.1	664±8	698±6
	Lower plate Height	±0.1	-75±8	-77±2

^{* 10000} particles/cycle and 1000 active cycles was used for MC perturbation calculations.

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