# Verification and Validation of McCARD using ZPR/ZPPR Benchmarks

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## 1. Introduction

The main objective of the PGSFR (Prototype Gen IV Sodium-cooled Fast Reactor) project is to demonstrate the transmutation technology of transuranic (TRU) elements for reducing the long-lived radiotoxicity of spent fuels from light water reactors [1]. The initial core of the PGSFR will load the U-Zr metal fuel, and the U-TRU-Zr fuel will gradually replace the U-Zr fuel through the transition cores. One of the issues in the TRU-loaded PGSFR is the uncertainty quantification of the reactor physics parameters calculated by the design and analysis codes because there is no suitable experimental benchmark for the metal-TRU-fuel loaded fast reactor. To address this issue, a series of experimental benchmarks were reviewed to select relevant benchmarks [2]. The computational modelling was performed using the Monte Carlo (MC) particle transport simulation code McCARD [3] and code-to-measurement comparisons were performed for the uncertainty analysis of the selected benchmarks

As a part of the above work, a translating Python script mcnp2mccard was developed to convert the MCNP [4] input models of the ZPR (Zero Power Reactor) and the ZPPR (Zero Power Physics Reactor) benchmarks provided in the benchmark book[5],[6] to the McCARD input models. Code-to-code comparisons were performed to verify the conversion between the McCARD and the MCNP6.1 models. Since the fundamental algorithms of particle tracking of random walk are same for the two codes, the criticality is expected to agree within 3σ range for a given nuclear data library if there is no error in the script. However, there exist non-negligible reactivity differences (less than 22 pcm) compared to the statistical uncertainty of the MC calculation.

This paper briefly introduces the ZPR/ZPPR benchmarks and provides the list of benchmarks for the verification and validation (V&V) of the McCARD with the ENDF/B-VII.1 library [7] for the fast reactor analysis with U-Pu mixed fuel. The identified cause of the reactivity discrepancy between the MCNP6.1 and the McCARD is due to a minor error in the fission nuclide sampling algorithm of the McCARD. The revised McCARD shows excellent agreements in the criticality with the MCNP6.1. In comparison to the experimental measurements, the reactivity difference calculated by the revised McCARD with the ENDF/B-VII.1 library ranged from -138 pcm to 231 pcm with the root-mean-square (RMS) difference of 98 pcm, where the differences fell well within the 2-sigma range of the overall uncertainty.

## 2. ZPR/ZPPR Benchmarks

The ZPR and ZPPR were split-table critical facilities operated from 1955 to 1990 by Argonne National Laboratory (ANL) to develop fast reactor technology. Valuable experimental measurements were acquired during the ZPR/ZPPR experimental programs including the criticality, reaction rate distribution, sodium void worth, expansion reactivity, control rod worth, kinetics parameters, and etc.

Table 1 shows the selected list of ZPR/ZPPR benchmarks for the validation of the McCARD with the ENDF/B-VII.1 library. For these benchmarks, the MCNP input models are provided in the benchmark documents. The mcnp2mccard script was used to convert the MCNP model to the McCARD model. The radial configuration of the McCARD model for ZPPR-10A was drawn by the McCARD plotter [8] and compared with the MCNP model in Figure 1.

Table 1. List of ZPR/ZPPR benchmarks for V&V of McCARD for fast reactor analysis with U-Pu mixed fuel.

| Case Name | Core Configuration | Fuel Type | Temp [K] | Model |
|---|---|---|---|---|
| ZPPR-10A/L007 | Reference Criticality | MOX | 293 | As-Built |
| ZPPR-9/L013 | Reference Criticality | MOX | 293 | As-Built |
| ZPPR-13A/L024 | Reference Criticality | MOX | 293 | As-Built |
| ZPPR-12/L009 | Reference Criticality | MOX | 293 | As-Built |
| ZPPR-2/L090 | Reference Criticality | MOX | 293 | As-Built |
| ZPR-6-7A/L012 | Reference Criticality | MOX | 293 | RZ Simplified |
| ZPR-6-7A/L099 | Reference Criticality | MOX | 293 | As-Built |
| ZPR-3-48/L047 | Reference Criticality | Pu-U-Mo Alloy | 300 | XYZ Simplified |
| ZPR-3-48B/L006 | Reference Criticality | Pu-U-Mo Alloy | 300 | XYZ Simplified |
| ZPR-3-56B/L017 | Reference Criticality | MOX | 300 | XYZ Simplified |
| ZPPR-15C/L166 | Reference Criticality | Pu-U-Zr Metal | 293 | As-Built |
| ZPPR-15C/L167 | Sodium Void Reference | | 293 | As-Built |
| ZPPR-15C/L168 | 8 inch Sodium Void | | 293 | As-Built |
| ZPPR-15C/L169 | 18 inch Sodium Void | | 293 | As-Built |
| ZPPR-15D/L184 | Sodium Void Reference | U-Zr Metal | 293 | As-Built |
| ZPPR-15D/L185 | Reference Criticality | | 293 | As-Built |
| ZPPR-15D/L189 | 8 inch Sodium Void | | 293 | As-Built |
| ZPPR-15D/L190 | 18 inch Sodium Void | | 293 | As-Built |

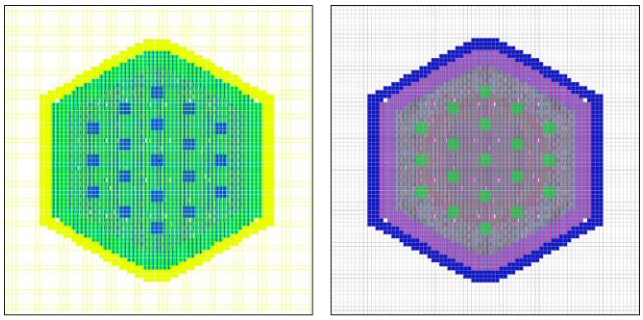


Figure 1. Radial configurations of MCNP and McCARD models for ZPPR-10A.

## 3. Results

The calculational conditions for each MC calculation are 250K particles/cycle, 100 inactive cycles, and $N_{active}$ active cycles which leads to the sample standard deviation of 3 pcm. Figure 2 shows the reactivity differences of the McCARD against the MCNP6.1. Overall, there exists a trend that the original McCARD slightly underestimates the criticality. The maximum discrepancy occurs in ZPR-6-7A/L099 case with an absolute difference of 22 pcm. One can define a combined statistical error of the reactivity difference as $\sigma_{real} = \kappa_{real/app}\sqrt{\sigma_{sample}^{2,MCNP} + \sigma_{sample}^{2,McCARD}}$ where the inter-cycle correlation correction factor $\kappa_{real/app}$ is determined as 1.4 for ZPR-6-7A benchmarks. Since the discrepancy of 22 pcm exceeds the $3\sigma_{real}$ of 18 pcm, it is inferred that there exists a systematic difference in the calculation results.

After an intensive inspection of the code-to-code comparisons, the fission nuclide sampling algorithm of McCARD was corrected. In the McCARD, the number of fission neutrons is determined by the collision estimator of $\left\lfloor W \times \sum_{i=1}^{I} N_i \nu\sigma_{f,i} \,/\, \sum_{i=1}^{I} N_i \sigma_{t,i} + \xi \right\rfloor$, where $W$ is the statistical weight of the particle entering the collision and $\xi$ is a uniform random number, and $N_i$ is the nuclide number density for nuclide $i$. Then, for each sampled fission neutron, the fission nuclide $i$ is sampled by the probability of $P(i) = N_i\sigma_{f,i} / \sum_{i=1}^{I} N_i\sigma_{f,i}$ which should be $P(i) = N_i\nu\sigma_{f,i} / \sum_{i=1}^{I} N_i\nu\sigma_{f,i}$. Once the fission nuclide is sampled, the energy of the fission neutron will be determined by the fission spectrum of the sampled nuclide. Therefore, the fission nuclide sampling algorithm of the original McCARD slightly biases the fission neutron spectrum.

Given the facts that 1) the ν value of Pu is higher than that of U and 2) the prompt fission spectrum of Pu is more hardened than that of U, the original McCARD can slightly underestimate the criticality of the fast reactor with the U-Pu mixed fuel due to the slightly softened prompt fission spectrum, especially in cases where a significant amount of Pu is loaded. In Figure 2, the revised McCARD shows excellent agreements in the criticality with the MCNP6.1.

Figure 3 shows the reactivity differences between the revised McCARD and the experimental measurement. The reactivity difference is in the range of -138 pcm to 231 pcm with the RMS difference of 98 pcm which shows a good agreement within $2\sigma_{comb}$ of the combined uncertainty.

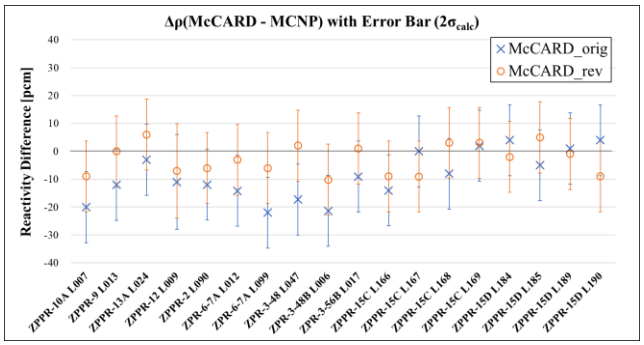


Figure 2. Reactivity differences [pcm] of McCARD against MCNP6.1 with error bar indicating $2\sigma_{calc}$; $\sigma_{calc}$ is the root-sum-square of the sample standard deviations of two codes.

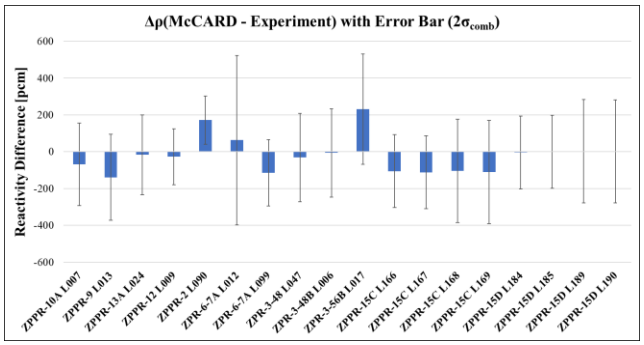


Figure 3. Reactivity differences [pcm] of McCARD against experimental criticality with error bar indicating $2\sigma_{comb}$; $\sigma_{comb}$ is the root-sum-square of the sample standard deviation of McCARD and the experimental uncertainty.

## 4. Summary

Using the ZPR/ZPPR benchmarks, the MC particle transport simulation code McCARD was verified by the code-to-code comparison with MCNP6.1 and validated by the experimental criticality for the fast reactor analysis with the U-Pu mixed fuel. During the code-to-code comparisons, a minor error in the fission nuclide sampling algorithm of the McCARD was corrected. In comparison to the experimental measurements, the criticality calculated by the McCARD with the ENDF/B-VII.1 shows errors in the range of -138 to 231 pcm with the RMS error of 98 pcm in the selected ZPR/ZPPR benchmarks. These results will be useful to quantify the reactivity uncertainty for the design and analysis of the PGSFR.

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**REFERENCES**

[1] J. Yoo, et al., "Overall System Description and Safety Characteristics of Prototype Gen IV Sodium Cooled Fast Reactor in Korea," Nuclear Engineering and Technology, Vol. 48(5), pp. 1059-1070 (2016).
[2] J. Yoo, J Choe, J.Y. Lim, "Status of nuclear data sensitivity and uncertainty analysis technologies for fast reactor validation," KAERI/AR-1461/2022, KAERI (2022).
[3] H. J. Shim, et al., "McCARD: Monte Carlo code for advanced reactor design and analysis," Nuclear Engineering and Technology, Vol. 44(2), pp. 161-176 (2012).
[4] T. Goorley, et al., "Features of MCNP6," Annals of Nuclear Energy, Vol. 87, pp. 772-783 (2016).
[5] L. G. LeSage, "An Overview of the Argonne National Laboratory Fast Critical Experiments 1963-1990," ANL-NT-175, Argonne National Laboratory, April 2001.
[6] International Handbook of Evaluated Reactor Physics Benchmark Experiments 2021 Edition," NEA/NSC/DOC(2006)1, OECD/NEA, 2008.
[7] M.B. Chadwick, et al., "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data," Nuclear Data Sheets, Vol. 112, pp. 2887-2996 (2011).
[8] H. Lee, "McCARD geometry visualization capability," Private Communication, KAERI, 2022.