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A Comparative Computational Analysis of the MCS and MCNP6 Monte Carlo Codes for MOX Critical Benchmark Problems

Ta Duy Long, Ser Gi Hong*, [a]Ho Choel Shin
Dept. Of Nuclear Engineering, Kyung Hee University, 1732 Deogyeong-daero, Giheung-gu, Yongin
[*]Corresponding author: sergihong@khu.ac.kr
[a]Core and Fuel Analysis Group, Korea Hydro & Nuclear Power Central Research Institute, Daejon

1. Introduction

The critical safety analyses with burnup credit are needed to ensure that the spent fuel storage or transportation systems meets sufficient sub-criticality with consideration of uncertainties and biases. The critical safety analyses with burnup credit for spent nuclear fuel are performed by using some computational methods to the spent nuclear fuel compositions and the effective multiplication factors (k_{eff}). Therefore, it is very important to estimate the biases and bias uncertainties associated with the computational methods. For the critical safety analysis, the bias and uncertainty are mainly classified into two different types: 1) uncertainty and bias related to the cross sections and computational methods in estimating k_{eff}, and 2) the ones related to the estimation of the spent fuel compositions. The former type bias and uncertainty are evaluated by applying the computational methods (or codes) including cross section library to a group of criticality benchmark problems. In particular, the criticality benchmark problems should be carefully selected such that they are as similar as possible to the applied model. In this work, we performed a comparative criticality calculation for four square lattice, mixed oxide plutonium-uranium critical benchmark problems to validate the MCS Monte Carlo code which has been developed by UNIST. The results can be used to determine the bias and uncertainty of the MCS code in the future. In addition, we applied MCNP6 code to these benchmark problems for comparison with MCS.

2. Methods and Results

2.1 Computer Code System

MCNP is a general purpose, continuous-energy, generalized-geometry Monte Carlo radiation transport code developed by Los Alamos national laboratory. The MCNP code can be used for neutron, photon, electron transport and it includes the capability to calculate eigenvalues for critical systems. MCS is a 3D continuous energy Monte Carlo code for particle transport, which was developed at Ulsan National Institute of Science and Technology (UNIST), Korea since 2013. The MCS have two options for criticality calculations and fixed source for shielding problems. In this work, the critical calculations were performed using both the MCNP6 and MCS codes with ENDF/B-VII.1 cross-section library.

2.2 Critical Benchmark Experiments

Four critical benchmark problems with mixed Plutonium-Uranium oxide were considered in this work to evaluate the applicability of MCS for critical safety analyses with burnup credit. These problems were listed in NUREG/CR-7109 [1] with the identification numbers from MIX-COMP-THERM-001 to MIX-COMP-THERM-004. They involve MOX fuel pins in square-pitched lattices that are moderated and reflected with water. The natural uranium is used in the MOX fuels.

Critical benchmark problems MIXED-COMP-THERM-001 considered mix oxide fuel with approximately 20 wt% of Plutonium with light water moderation and reflection in a water tank which has diameter of 120 cm. The plutonium vector is 86.2wt% ^{239}Pu, 11.5wt% ^{240}Pu, and 1.8wt% ^{241}Pu. The fuel rod has the total length of 237.744 cm and diameter of 0.5842 cm while the active fuel length is 91.44 cm surround by water, as shown in Fig 1a. The radial view of the pin array for the first configuration of this problem is shown in Fig 1b. In this problem, four experiment configurations have been accepted as critical benchmark experiments. These four configurations have different number of fuel pins, the different locations in the pin array and the different pitches between fuel pins in array.

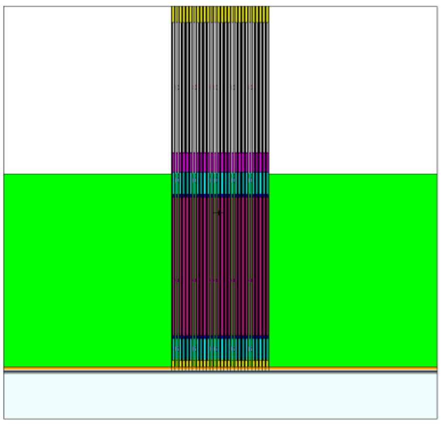

Fig. 1a: Benchmark problem 001 side-view configuration

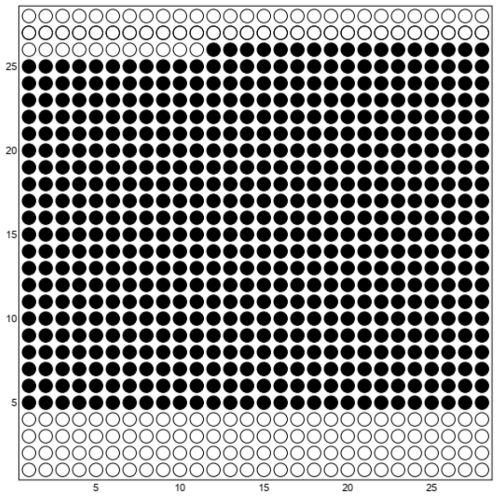

Fig. 1b: Benchmark problem 001 radial view of pin array

The next critical problem MIXED-COMP-THERM-002 consists of 6 sub-experiments with 2 wt% of PuO_2 in mixed oxide fuel named from PNL-30 to PNL-35. The plutonium vector is 91.8wt% ^{239}Pu, 7.8wt% ^{240}Pu, and 0.4wt% ^{241}Pu. In this benchmark problem, three configurations were considered with borated water moderator and the others were moderated by pure water. The active fuel length is 91.44 cm while the fuel rod has diameter of 1.4351 cm. The fuel loading map for the PNL-32 experiment is shown in Fig 2. The core tank in this benchmark problem has the radius of 91.44 cm while the sufficient thickness of water reflector is about 30 cm.

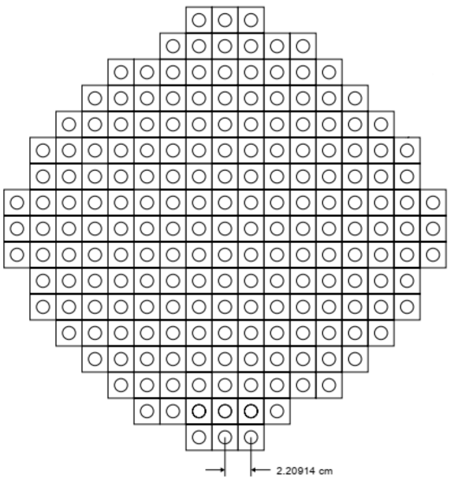

Fig. 2: Fuel loading map for subcase PNL-32 of problem number 002

The benchmark problem number 003 includes six mixed oxide fuel configurations with five different lattice pitches. In this problem, five subcases were performed with pure water moderator while the remaining one was performed with borated water. The mixed oxide fuel in this experiment consist of 6.6% PuO_2 in weight. The plutonium vector is 90.6wt% ^{239}Pu, 8.6wt% ^{240}Pu, and 0.8wt% ^{241}Pu. The active fuel length in this experiment is 92.964 cm while the total length of the fuel rod is 99.189 cm with the outer diameter of 0.99314 cm. The last critical benchmark problem MIXED-COMP-THERM-004 consider 11 configurations with 3.01 wt% PuO_2 – natural UO_2 fuel rods. The plutonium vector is 68.2wt% ^{239}Pu, 22.0wt% ^{240}Pu, and 7.3wt% ^{241}Pu. In these experiments, the criticality was determined by adjusting the water level in the tank. The water-to-fuel volume ratios in the lattice cell are ranged from 2.42 to 5.55 by changing the lattice pitch from 1.825 to 2.474 in different configurations. There are three different types of fuel array which include 23x23, 21x21 and 20x20 fuel patterns. A sample of side-view of these experiment configurations is shown in Fig 3. The thickness of radial water reflector was calculated and determine such that 30 cm of water reflector in thickness is sufficient for the calculation model.

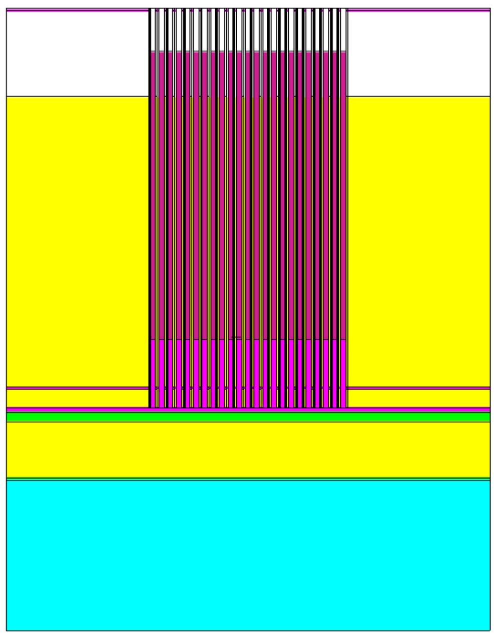

Fig. 3: Benchmark problem 004 side-view configuration

2.3 Results of Criticality calculations

This section presents the results of the criticality calculations for these four benchmark problems. Total 27 configurations were modelled by MCNP6 and MCS codes using ENDF/B-VII.1 cross-section library. Both MCNP6 and MCS are executed with 100 inactive cycles, 500 active cycle and 200,000 histories per cycle. The k-eff results for these configurations are presented in Table 1 below. As shown in the table, the results of MCS have very good agreements with those of MCNP6. The discrepancies between two codes are less than 30 pcm for all configurations while the standard deviations of all the Monte Carlo calculations are about 10 pcm. Therefore, the discrepancy between MCS and MCNP6 is nearly similar level of the statistical error of the Monte Carlo calculations. Also, it is noted that the maximum deviations from criticality are 633 and 613 pcm for MCS and MCNP6, respectively while MONK gives much higher deviation from criticality.

Table 1: Criticality calculations results for Critical benchmark problems

Critical problem	Subcases	MONK results UKNDL/JEFF2.2	MCS ENDF/B-VII.1	MCNP6 ENDF/B-VII.1	Deviation from criticality (pcm)		Diff. between MCS and MCNP (pcm)
					MCS	MCNP6	
MIX-COMP-THERM-001	1	0.9917 ± 0.0010	1.00191 ± 0.00009	1.00191 ± 0.00008	191	191	0
	2	0.9934 ± 0.0010	1.00096 ± 0.00009	1.00111 ± 0.00008	96	111	-15
	3	0.9952 ± 0.0010	0.99962 ± 0.00009	0.99958 ± 0.00008	-38	-42	4
	4	0.9969 ± 0.0011	1.00188 ± 0.00009	1.00189 ± 0.00008	188	189	-1
MIX-COMP-THERM-002	1	-	1.00060 ± 0.00008	1.00053 ± 0.00007	60	53	7
	2	-	1.00181 ± 0.00008	1.00184 ± 0.00007	181	184	-3
	3	-	1.00212 ± 0.00008	1.00218 ± 0.00007	212	218	-6
	4	-	1.00633 ± 0.00008	1.00613 ± 0.00008	633	613	20
	5	-	1.00359 ± 0.00008	1.00357 ± 0.00007	359	357	2
	6	-	1.00572 ± 0.00007	1.00585 ± 0.00007	572	585	-13
MIX-COMP-THERM-003	1	0.9943 ± 0.0010	1.00154 ± 0.00009	1.00141 ± 0.00008	154	141	13
	2	0.9979 ± 0.0010	1.00207 ± 0.00009	1.00205 ± 0.00008	207	205	2
	3	0.9957 ± 0.0010	1.00156 ± 0.00009	1.00155 ± 0.00008	156	155	1
	4	0.9976 ± 0.0010	1.00057 ± 0.00009	1.00051 ± 0.00009	57	51	6
	5	0.9980 ± 0.0010	1.00068 ± 0.00009	1.00068 ± 0.00008	68	68	0
	6	0.9974 ± 0.0010	1.00264 ± 0.00008	1.00262 ± 0.00008	264	262	2
MIX-COMP-THERM-004	1	0.9992 ± 0.0010	0.99647 ± 0.00009	0.99620 ± 0.00008	-353	-380	27
	2	1.0002 ± 0.0010	0.99696 ± 0.00008	0.99704 ± 0.00007	-304	-296	-8
	3	0.9998 ± 0.0010	0.99716 ± 0.00008	0.99703 ± 0.00007	-284	-297	13
	4	0.9986 ± 0.0010	0.99697 ± 0.00008	0.99687 ± 0.00007	-303	-313	10
	5	1.0020 ± 0.0010	0.99782 ± 0.00007	0.99780 ± 0.00007	-218	-220	2
	6	1.0014 ± 0.0010	0.99783 ± 0.00008	0.99760 ± 0.00007	-217	-240	23
	7	1.0023 ± 0.0010	0.99779 ± 0.00007	0.99771 ± 0.00007	-221	-229	8
	8	0.9987 ± 0.0010	0.99829 ± 0.00007	0.99818 ± 0.00007	-171	-182	11
	9	0.9998 ± 0.0010	0.99867 ± 0.00007	0.99874 ± 0.00007	-133	-126	-7
	10	1.0006 ± 0.0010	0.99831 ± 0.00007	0.99843 ± 0.00007	-169	-157	-12
	11	0.9988 ± 0.0010	0.99842 ± 0.00007	0.99841 ± 0.00006	-158	-159	1

3. Conclusions

In this work, we modeled four critical benchmark problems using squared lattice mixed oxide Plutonium-Uranium fuel with total of 27 configurations and performed the criticality calculations by using MCS and MCNP6. This work was performed to determine the applicability of MCS to criticality safety analyses with burnup credit by comparing the validated Monte Carlo code MCNP6. The criticality calculations showed a good agreement of k_{eff} results between these two codes with the maximum different less than 30 pcm. The deviation from criticality then will be used to determine other biases such as from fission products and minor actinide nuclides in spent nuclear fuel before using the same computational method for spent nuclear fuel critical analyses.

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