

Validation of DeCART2D Criticality Calculations for LEU+ loaded SMR Systems

Min Ju Kim^a and Ho Jin Park^{a*}

^a Kyung Hee University, 1732, Deogyong-daero, Giheung-gu, Yongin-si, 17104, Korea

*Corresponding author: parkhj@khu.ac.kr

***Keywords :** LEU+, SMR, Criticality, STACY, McCARD, DeCART2D

1. Introduction

Small Modular Reactors (SMRs) are currently being actively researched worldwide as alternative energy sources. For light water SMRs, the smaller core results in reduced average core burnup due to increased neutron leakage. As a result, the volume of spent nuclear fuel, which is high-level radioactive waste, is greater compared to that produced by conventional large Light Water Reactors (LWRs). This poses a challenge to the acceptability of SMRs.

To address this issue, one of the strategies being considered is increasing nuclear fuel enrichment beyond LEU levels (i.e., 5 wt.%). Both Low Enriched Uranium Plus (LEU+) and High-Assay Low-Enriched Uranium (HALEU) are discussed in the context of SMRs and advanced nuclear reactors. To analyze and perform nuclear design analyses for LEU+ or HALEU-loaded SMR systems, it is necessary to verify the existing nuclear core design code system.

In this study, a two-step strategy was employed to validate and verify the existing nuclear core design code system for LEU+ loaded SMR analysis. Firstly, a Monte Carlo (MC) code capable of generating reference solutions for the new SMR system was validated by performing critical experiment benchmark analyses with ²³⁵U enrichment levels ranging from 5 wt.% to 10 wt.%. Next, a LEU+ loaded SMR system was analyzed using both the existing nuclear core design code and MC code. The validity of the existing design code will be assessed by evaluating the discrepancies between the two results.

In this study, the target SMR system for this analysis is the innovative SMR (i-SMR) [1] being developed in South Korea. The MC code for generating reference solutions is the McCARD neutron/photon transport code [2], and the design code is DeCART2D [3]/MASTER [4].

2. Validation of McCARD Solutions for 10 wt.% Criticality Benchmark Problem

2.1. ICSBEP STACY Critical Benchmark Experiments

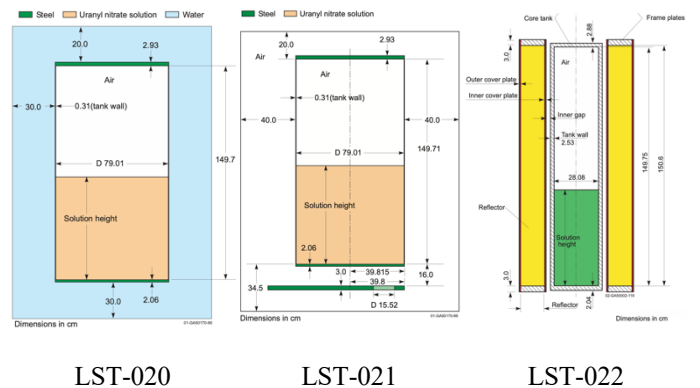
The low-enriched thermal uranium critical benchmark problems with 5 wt.% ~10 wt.% enrichment were selected from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [5].

Table I: Description of the selected ICSBEP LEU benchmark problems

No	Benchmark ID	Cases	Description
1	LST-020	4	Water-reflected uranyl nitrate solution in 80cm cylindrical water tank (10.0 wt.%)
2	LST-021	4	Unreflected uranyl nitrate solution in 80cm cylindrical water tank (10.0 wt.%)
3	LST-022	4	Borated concrete-reflected uranyl nitrate solution in 28cm thick slabs (10.0 wt.%)

Table I shows the description of the selected ICSBEP and the number of cases. Selected models are a series of experiments with the Static Experiment Critical Facility (STACY), they have the fuel as 10% uranyl nitrate solution. The enrichment of each fuel was similar to that of LEU+ nuclear fuels.

Figure 1 shows the elevation view of each benchmark model. LST-020 model consists of the fuel solution, the core tank, and the water reflector, and LST-021 model consists of the fuel solution, the core tank, the structure and devices that act as neutron reflectors. Also, LST-022 model consists of the fuel solution, the core tank, the concrete reflectors, and the reflector containers. LST-020 is a cylindrical structure, LST-021 is a cylindrical fuel tank structure in an air box, and LST-022 is a box structure. 4 cases exist in each model, the differences in each case in the model are the height of the structures, and the material composition of the fuel solution.



LST-020

LST-021

LST-022

Fig. 1. Elevation view of STACY benchmark models

2.2 Results and discussions of STACY benchmarks

McCARD modeling is prepared for LST-020, LST-021, and LST-022 STACY benchmark problems. For the eigenvalue calculations in LST-020 and LST-021, 50 inactive and 1000 active cycles were used with 10,000 histories per cycle, while 50 inactive and 400 active cycles were used with 50,000 histories per cycle for LST022. All the McCARD calculations were performed with the ENDF/B-VII.1 evaluated nuclear data library. Table II shows the multiplication factors by McCARD, MCNP, and experimental results for LST-020, LST-021, and LST-022 STACY benchmark problems.

Table II: Comparisons of multiplication factors by McCARD and MCNP for LST-020, LST-021, and LST-022 STACY benchmark problems

Problem		Multiplication Factor			Δp [pcm]	
		Experiment (A)	McCARD ¹⁾ (B)	MCNP ²⁾ (C)	(A)-(B)	(C)-(B)
LST-020	1	0.99950 (0.00100)	0.99946	0.99989	4	43
	2	0.99960 (0.00100)	0.99902	0.99953	58	51
	3	0.99970 (0.00120)	0.99835	0.99886	135	51
	4	0.99980 (0.00120)	0.99956	1.00004	24	48
LST-021	1	0.99830 (0.00090)	0.99796	0.99787	34	9
	2	0.99850 (0.00100)	0.99755	0.99828	95	73
	3	0.99890 (0.00110)	0.99664	0.99758	227	95
	4	0.99930 (0.00120)	0.99871	0.99948	59	77
LST-022	1	0.99990 (0.00100)	1.00200	- ³⁾	210	-
	2	0.99940 (0.00100)	1.00185		245	-
	3	0.99930 (0.00100)	1.00204		274	-
	4	0.99940 (0.00100)	1.00255		314	-

- 1) Stochastic uncertainties (1σ) are less than 20 pcm.
- 2) Stochastic uncertainties (1σ) are less than 100 pcm.
- 3) There was no result of LST-022 by MCNP in Ref. [6].

In the LST-020 problems, the differences in reactivity between McCARD and MCNP codes ranged from 43 pcm to 51 pcm, and in LST-021 problems, from 9 pcm to 95 pcm. There are no significant differences between the reactivity results of the two codes and the experimental results.

Figures 2 through 4 compare neutron energy spectra between LST020 ~ 022 and i-SMR fuel assemblies (i.e., A1 and A5). Each spectrum showed a similar pattern, but the peak value differed due to geometry and materials. The ^{235}U fuel enrichments in A1 and A5 FAs were adjusted to 10 wt.% to consider neutronic conditions similar to a LEU+-based system. Because the STACY benchmark problem is based on the uranyl nitrate fuel solution in the water tank, it has a neutron spectrum that is more thermalized than 10 wt.% i-SMR FA problems.

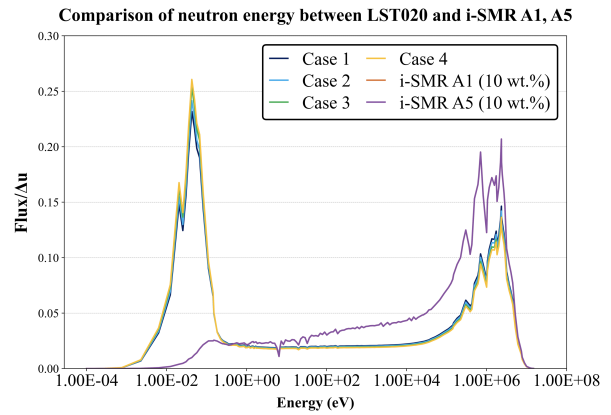


Fig. 2. Neutron energy spectra of LST-020 and i-SMR A1, A5

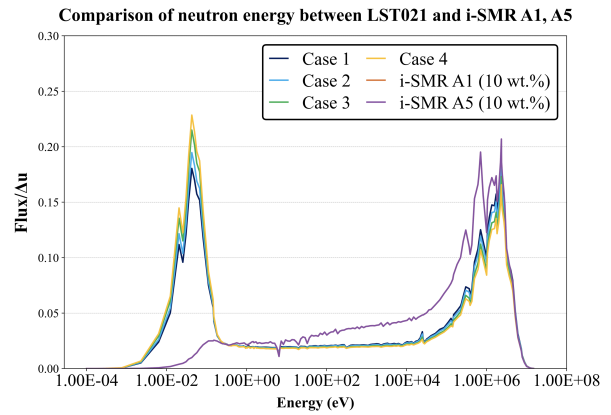


Fig. 3. Neutron energy spectra of LST-021 and i-SMR A1, A5

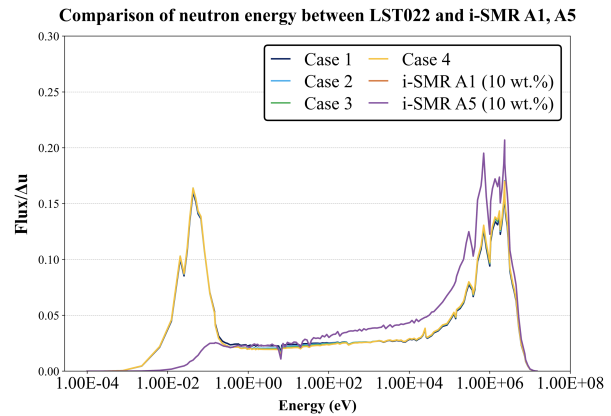


Fig. 4. Neutron energy spectra of LST-022 and i-SMR A1, A5

3. Validation of DeCART2D Solutions for LEU+ Loaded i-SMR System with ENDF/B-VII.1

3.1 Comparison of DeCART2D and McCARD codes in i-SMR 2D Fuel Assembly Problem

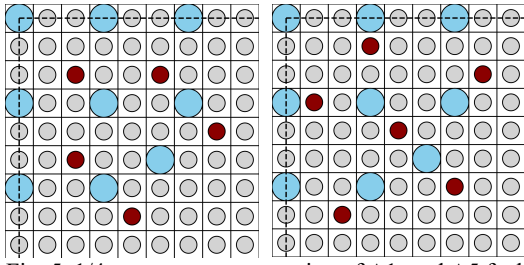


Fig. 5. 1/4 symmetry cross section of A1, and A5 fuel assembly

To validate the DeCART2D/MASTER code system for the LEU+ system, LEU+ FA problems based on the i-SMR system are introduced [1]. The A1 and A5 FA problems of i-SMR were selected for comparison. Figure 5 is a 1/4 symmetry cross-section of the A1 and A5 17x17 FAs. The multiplication factors were calculated by DeCART2D and McCARD for 6 cases: ^{235}U enrichments of 2 wt.%, 4 wt.%, 6 wt.%, 8 wt.%, 10 wt.%, and 12 wt.%. The McCARD eigenvalue calculations have been made on 200 inactive and 700 active cycles with 20,000 histories per cycle. McCARD and DeCART2D were calculated using ENDF/B-VII.1 evaluated nuclear data library [7].

Table III: Comparison in reactivity of A1 assembly by DeCART2D and McCARD

Enrichment	DeCART2D	McCARDx	$\Delta\rho$ [pcm]
2 wt.%	0.87594	0.87804	274
4 wt.%	1.09691	1.09916	187
6 wt.%	1.20580	1.20889	212
8 wt.%	1.27239	1.27616	232
10 wt.%	1.31806	1.32311	290
12 wt.%	1.35155	1.35849	378

Table IV: Comparison in reactivity of A5 assembly by DeCART2D and McCARD

Enrichment	DeCART2D	McCARD	$\Delta\rho$ [pcm]
2 wt.%	0.81037	0.81216	272
4 wt.%	1.03266	1.03553	269
6 wt.%	1.14635	1.15023	294
8 wt.%	1.21737	1.22229	331
10 wt.%	1.26674	1.27281	376
12 wt.%	1.30328	1.31153	483

Tables III and IV show the multiplication factors of A1 and A5 by DeCART2D and McCARD, respectively. The stochastic uncertainties of McCARD calculations were less than 10 pcm. It is observed that the reactivity differences between DeCART2D and McCARD ranged from a minimum of 187 pcm to a maximum of 483 pcm. Each table has the smallest value of reactivity differences at 4 wt.%. Meanwhile, as the ^{235}U enrichment increases,

the reactivity differences between DeCART2D and McCARD increase. The maximum reactivity differences of A1 and A5 FAs are 378 pcm and 483 pcm for 12 wt.% of ^{235}U enrichment case. Furthermore, 187 pcm and 269 pcm were observed at each 4 wt.% enrichment's reactivity differences. It is inferred that the DeCART2D cross-section library [7] was optimized for 2~4 wt.% ^{235}U enrichments considered in a typical LWR system, not the i-SMR system. Accordingly, it can be concluded that the new nuclear reaction cross section library generation for the new target system (i.e. i-SMR) will be needed.

Figures 6 and 7 show neutron energy spectra of A1 and A5 FAs due to the change of the ^{235}U enrichment. Both exhibited similar spectra between McCARD and DeCART2D at the same enrichment case.

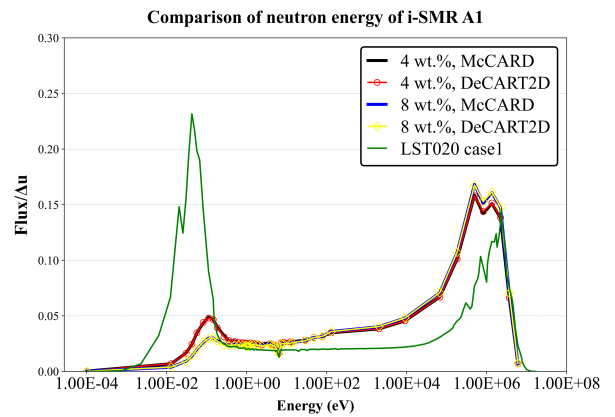


Fig. 6. Neutron energy spectra of A1 with enrichment of 4wt.%, 8wt.%

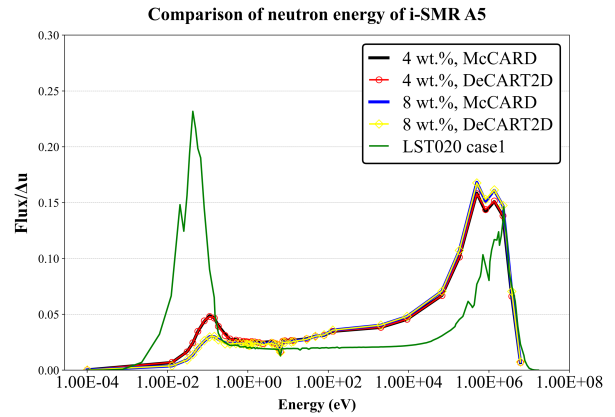


Fig. 7. Neutron energy spectra of A5 with enrichment of 4wt.%, 8wt.%

4. Conclusions

In this study, the preliminary suitability tests of the existing LWR core design code system (i.e., DeCART2D and MASTER) for LEU+ fuel-based SMRs were performed. The McCARD code provided a reference solution for an arbitrary system with LEU+ fuel. The ENDF/B-VII.1-based McCARD code capability was successfully validated by the LST-020, LST-021, and LST-022 STACY benchmark analyses.

To validate the DeCART2D/MASTER code system, LEU+ FA problems based on the i-SMR system are introduced. A comparison of DeCART2D and McCARD was also performed to verify the DeCART2D criticality capability for LEU+ fuel-based i-SMR FA problems. There are significant differences in reactivity between DeCART2D and McCARD because the current DeCART2D library [7] was optimized for typical ^{235}U enrichment. According to it, to reduce the errors of the DeCART2D library, improvements to the DeCART2D cross-section library will be conducted in the near future.

Moreover, it is observed that there are significant differences in neutron energy spectrum between the STACY benchmarks and the i-SMR FA. According to it, similarity analyses [8] between the STACY benchmarks and the i-SMR system will be conducted and the other similar benchmark problems will be searched.

Acknowledgement

This work was partly supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science and ICT) (No. RS-2024-00422848) and the 2024 University Innovation Support Project funded by the Ministry of Education (MOE).

REFERENCES

- [1] J. S. Kim, Optimization of Small Modular Reactor with Boron-Free Operation using Enriched Gadolinia, Master's thesis, Hanyang University, 2023.
- [2] H. J. Shim, B.S. Han, J. S. Jung, H. J. Park, C. H. Kim, McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis, Nuclear Engineering and Technology, Vol. 44, pp. 161-176, 2012.
- [3] J. Y. Cho et al, DeCART2D v1.1 User's Manual, KAERI/UM-40/2016.
- [4] J. Y. Cho et al, MASTER v4.0 User's Manual, KAERI/UM-41/2016.
- [5] International Handbook of Evaluated Criticality Safety Benchmark Experiments, OECD Nuclear Energy Agency Report NEA/NSC/DOC(95)03, OECD Nuclear Energy Agency: Paris, France, 1998.
- [6] D. A. Brown et al, ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data, Nuclear Data Sheets, Vol. 148, pp. 1-142, 2018.
- [7] H. J. Park et al., "An improved DeCART library generation procedure with explicit resonance interference using continuous energy Monte Carlo calculation," *Ann. Nucl. Eng.*, Vol. 105, pp. 95-105, 2017.
- [8] H. J. Park and J. W. Park, "Similarity Coefficient Generation Using Adjoint-Based Sensitivity and Uncertainty Method and Stochastic Sampling Method," *Energies*, Vol. 17, 827, 2024.