Criticality Experiment Benchmark Selection and New Critical Assembly Design Based on Similarity Analyses for LEU+ i-SMR System

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1. Introduction

Various design methods and tools are employed in the development of new types of nuclear reactors and systems. Any design must provide sufficient safety margins to maintain subcriticality under all conditions. To achieve this, calculated safety parameters (e.g., multiplication factor) must be systematically compared with experimental data to quantify uncertainties or biases in the design methods and tools. Therefore, selecting proper criticality experiments that accurately represent the target system is a crucial step in ensuring the reliability of safety margin calculations. During this criticality experiment selection process, the similarity between the criticality experiment benchmark problems and the target system will be quantitatively evaluated.

In order to improve the economic performance of newly developed small modular reactors (SMRs), the use of LEU+ fuels has been proposed as a strategy to address acceptability concerns for light water SMRs. In the previous study [1], the design code was validated by applying LEU+ fuel to the innovative SMR (i-SMR) [2] currently under development in Rep. of Korea. For the verification of the Monte Carlo (MC) solutions, criticality experiments with uranium fuel having enrichment (i.e., 5 wt.% ~ 8 wt.%) comparable to LEU+ were analyzed, but discrepancies were observed between their neutron energy spectra and those of the i-SMR system. This finding indicates that simply matching parameters (i.e., enrichment) may be insufficient to ensure the representativeness of the benchmark problems.

In this study, motivated by these observations, a study and strategy are introduced to select a criticality experimental benchmark suitable for the i-SMR with LEU+ fuels based on similarity coefficients. First, the similarity coefficient between the i-SMR and various benchmark problems [3] included in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) was calculated and compared. Next, the validity of the similarity coefficient was verified by comparing the neutron energy spectra of the top candidates. At last, we evaluated EALF (Energy of Average Lethargy of Fission) as complementary tool. Finally, a critical assembly with high similarity to an i-SMR containing approximately ^{235}U 8 wt.% enrichment was designed, and the similarity was evaluated. All calculations were performed using deterministic based sensitivity and uncertainty (S/U) similarity analysis procedure using McCARD [4] MC code and SimTest [5] utility.

2. Similarity Coefficient Generation

2.1 Similarity Coefficient Generation using S/U method

For the selection of the criticality experiments, the nuclear system designers and licensees should provide computational justification to regulating body [6-7]. Some researchers quantified the degree of similarity between the criticality experiments and target system. The similarity coefficient between the criticalities in two systems, c_k for multiplication factor is defined as Eq (1). Equation 2 shows the covariance between criticalities for two systems.

$$c_k = \frac{cov\,[k_I, k_{II}]}{\sigma(k_I)\cdot\sigma(k_{II})} \quad (1)$$

where

$$cov\,[k_I, k_{II}] = \sum_{i,\alpha,g}\sum_{i',\alpha',g'} cov\,[x^{i}_{\alpha,g}, x^{i'}_{\alpha',g'}]\left(\frac{\partial k_I}{\partial x^{i}_{\alpha,g}}\right)\left(\frac{\partial k_{II}}{\partial x^{i'}_{\alpha',g'}}\right) \quad (2)$$

$\sigma(k)$ is the standard deviation of the multiplication factor for each system. The nuclear reaction cross-section covariance matrix, $cov\,[x^{i}_{\alpha,g}, x^{i'}_{\alpha',g'}]$ is obtained from an evaluated nuclear data library, and sensitivity coefficients can be taken from adjoint analyses for two systems. $x^{i}_{\alpha,g}$ is the α-type microscopic cross-section of isotope i for energy group g. For α-types nuclear data are elastic scattering (MT=2), inelastic scattering (MT=4), capture (MT=102), (n, 2n) reaction (MT=16), (n, 3n) reaction (MT=17), particle-induced fission (MT=18), and $\bar{\nu}$ (MT=452). The coefficient, c_k defined similarity to the Pearson correlation coefficient [8], quantifies the degree of correlation between system I and II. When the two systems contain identical materials, c_k provides a measure of how strongly they are related. Its value, ranging from -1 to 1, approaches 1 when the systems are highly positively correlated.

2.2 Energy of Average Lethargy of Fission (EALF)

Energy of Average Lethargy of Fission (EALF) is a crucial concept in traditional criticality safety validation. In conventional criticality safety analysis, EALF is one of the physical characteristics used to evaluate system similarity between a criticality experiment and a target system. It provides an average measure of the neutron energy spectra where fissions predominantly occur. EALF is defined as Eq (4) using Eq (3).

$$\bar{u} = \frac{\sum_m \sum_g \left(\bar{u} \times \Sigma_{fg}^m \phi_g^m\right)}{\sum_m \sum_g \left(\Sigma_{fg}^m \phi_g^m\right)} \quad (3)$$

$$EALF = E_0 \,/\, e^{\bar{u}} \quad (4)$$

where

m = number of a physical zone inside core

$\bar{u}_g$= midpoint of the g th lethargy group, defined as lethargy of a neutron with energy $\bar{E}_g = \sqrt{E_g E_{g-1}}$

Σ_{fg} =group macroscopic fission cross section

ϕ_g= neutron flux within lethargy group g.

Lethargy u of a neutron with energy E is defined as $\ln(E_0/E)$, where E_0 is some maximum neutron energy, which here is 10 MeV.

3. Similarity Test between Relevant Criticality Experiments and LEU+ loaded i-SMR core systems

3.1 McCARD/SimTest Code System

The MC code system for similarity tests between relevant criticality experiments and target systems are performed using the McCARD code and SimTest code. Figure 1 shows the code flowchart for the deterministic S/U method based similarity coefficient generation. The McCARD code already has the capability of the MC perturbation technique for sensitivity coefficient generation due to the uncertainty of nuclear reaction cross section. The SimTest code can generate the S/U method based c_k using the sensitivity coefficients from the McCARD code and the cross-section covariance data from the evaluated nuclear data library.

3.2 Similarity Test based on S/U method between criticality experiments and i-SMR core system

Similarity tests can be conducted by comparing similarity coefficients, neutron energy spectra and EALF. First, the similarity coefficients between the selected criticality experiment benchmarks [2] and the target application (i.e., LEU+ loaded i-SMR system) were calculated using the S/U method. For the similarity tests, criticality benchmarks in the HMF, LMT, LST, and LCT categories of the ICSBEP benchmark handbook [3] were selected. The ENDF/B-VII.1 covariance data matrix with the LANL 30-group structure was employed for two major actinide isotopes (i.e., ^{235}U and ^{238}U).

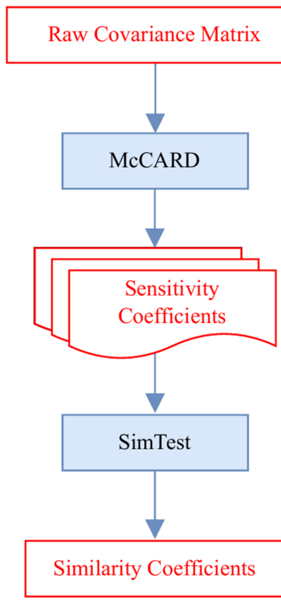

Fig 1. Flow chart of McCARD/SimTest code system

	2 wt.%	4 wt.%	6 wt.%	8 wt.%	10 wt.%	flattop25	GODIVA	HMF002c2	HMF032c1	IPENMB01	LCT001c1	LCT003c1	LMT007c2	LST002	LCT022c1	LST020c1	LST021c1	LST022c4	LCT085c1	LCT085c13
i-SMR 2wt.%	1.000	≈1.000	0.998	0.993	0.985	0.259	0.232	0.256	0.249	0.934	0.992	0.972	0.780	0.949	0.839	0.922	0.922	0.927	0.807	0.823
i-SMR 4wt.%	≈1.000	1.000	≈1.000	≈1.000	≈1.000	0.302	0.314	0.292	0.317	0.941	0.977	0.965	0.803	0.932	0.888	0.910	0.910	0.917	0.844	0.855
i-SMR 6wt.%	0.998	≈1.000	1.000	≈1.000	≈1.000	0.351	0.382	0.335	0.380	0.916	0.939	0.933	0.790	0.893	0.897	0.873	0.873	0.881	0.844	0.850
i-SMR 8wt.%	0.993	≈1.000	≈1.000	1.000	≈1.000	0.395	0.443	0.375	0.437	0.882	0.894	0.894	0.768	0.844	0.891	0.826	0.827	0.835	0.831	0.834
i-SMR 10wt.%	0.985	≈1.000	≈1.000	≈1.000	1.000	0.438	0.498	0.414	0.491	0.840	0.843	0.848	0.738	0.791	0.876	0.775	0.776	0.785	0.810	0.808
flattop25	0.259	0.302	0.351	0.395	0.438	1.000	0.758	0.991	0.930	-0.176	-0.223	-0.232	-0.293	-0.099	-0.069	-0.079	-0.080	-0.080	-0.173	-0.192
GODIVA	0.232	0.314	0.382	0.443	0.498	0.758	1.000	0.657	0.895	0.703	0.697	0.656	0.623	0.752	0.680	0.764	0.764	0.761	0.637	0.650
HMF002c2	0.256	0.292	0.335	0.375	0.414	0.991	0.657	1.000	0.887	-0.191	-0.210	-0.226	-0.335	-0.096	-0.117	-0.085	-0.087	-0.087	-0.219	-0.234
HMF032c1	0.249	0.317	0.380	0.437	0.491	0.930	0.895	0.887	1.000	-0.074	-0.220	-0.200	-0.077	-0.075	0.143	-0.021	-0.022	-0.020	0.045	0.016
IPENMB01	0.934	0.941	0.916	0.882	0.840	-0.176	0.703	-0.191	-0.074	1.000	0.947	0.959	0.986	0.914	≈1.000	0.923	0.925	0.931	≈1.000	≈1.000
LCT001c1	0.992	0.977	0.939	0.894	0.843	-0.223	0.697	-0.210	-0.220	0.947	1.000	≈1.000	0.997	0.952	≈1.000	0.951	0.952	0.959	≈1.000	≈1.000
LCT003c1	0.972	0.965	0.933	0.894	0.848	-0.232	0.656	-0.226	-0.200	0.959	≈1.000	1.000	≈1.000	0.894	≈1.000	0.892	0.893	0.902	≈1.000	≈1.000
LMT007c2	0.780	0.803	0.790	0.768	0.738	-0.293	0.623	-0.335	-0.077	0.986	0.997	≈1.000	1.000	0.718	≈1.000	0.748	0.750	0.759	≈1.000	≈1.000
LST002	0.949	0.932	0.893	0.844	0.791	-0.099	0.752	-0.096	-0.075	0.914	0.952	0.894	0.718	1.000	0.910	0.997	0.997	0.999	0.877	0.896
LCT022c1	0.839	0.888	0.897	0.891	0.876	-0.069	0.680	-0.117	0.143	≈1.000	≈1.000	≈1.000	≈1.000	0.910	1.000	0.720	0.722	0.732	0.969	0.957
LST020c1	0.922	0.910	0.873	0.826	0.775	-0.079	0.764	-0.085	-0.021	0.923	0.951	0.892	0.748	0.997	0.720	1.000	≈1.000	≈1.000	0.858	0.878
LST021c1	0.922	0.910	0.873	0.827	0.776	-0.080	0.764	-0.087	-0.022	0.925	0.952	0.893	0.750	0.997	0.722	≈1.000	1.000	≈1.000	0.860	0.880
LST022c4	0.927	0.917	0.881	0.835	0.785	-0.080	0.761	-0.087	-0.020	0.931	0.959	0.902	0.759	0.999	0.732	≈1.000	≈1.000	1.000	0.875	0.894
LCT085c1	0.807	0.844	0.844	0.831	0.810	-0.173	0.637	-0.219	0.045	≈1.000	≈1.000	≈1.000	≈1.000	0.877	0.969	0.858	0.860	0.875	1.000	0.986
LCT085c13	0.823	0.855	0.850	0.834	0.808	-0.192	0.650	-0.234	0.016	≈1.000	≈1.000	≈1.000	≈1.000	0.896	0.957	0.878	0.880	0.894	0.986	1.000

Fig 2. Similarity Coefficients for 20x20 benchmark matrix using ENDF/B-VII.1 30-group covariance matrix for ^{235}U and ^{238}U

Table I: Description of the selected 15 ICSBEP criticality experiment benchmark problems

Short Name (Benchmark ID)	Description
FLATTOP25 (HEU-MET-FAST-028)	^{235}U (93.24 wt.%) Sphere reflected by normal uranium
GODIVA (HEU-MET-FAST-001)	Bare, highly enriched uranium (94 wt.%) sphere
HMF002c2 (HEU-MET-FAST-002 case2)	Topsy 8-Inch-Tuballoy-Reflected Orally Assemblies (97.67 wt.%)
HMF032c1 (HEU-MET-FAST-032 case1)	^{235}U (94 wt.%) Spheres surrounded by natural-uranium reflectors
IPENMB01 (LEU-COMP-THERM-077 case1)	Water-moderated squared-pitched lattices UO2 (4.3486 wt.%)
LCT001c1 (LEU-COMP-THERM-001 case1)	Water-moderated UO2 (2.35 wt.%) Fuel Rods in 2.032 cm square-pitched arrays
LCT003c1 (LEU-COMP-THERM-003 case1)	Water-moderated UO2 (2.35 wt.%) Fuel Rods in 1.684 cm square-pitched arrays
LMT007c2 (LEU-MET-THERM-007 case2)	Water-Moderated and Water-Reflected 0.30 in. Diameter U (4.95 wt.%) metal rods in square-pitched arrays
LST002 (LEU-SOL-THERM-002)	174-liter spheres of low enriched (4.9 wt.%) uranium oxyfluorine solutions
LCT022c1 (LEU-COMP-THERM-022 case1)	Uniform water-moderated hexagonally pitched lattices of rods with UO2(10 wt.%) fuels
LST020c1 (LEU-SOL-THERM-020 case1)	Water-reflected uranyl nitrate solution in 80cm cylindrical water tank (10.0 wt.%)
LST021c1 (LEU-SOL-THERM-021 case1)	Unreflected uranyl nitrate solution in 80cm cylindrical water tank (10.0 wt.%)
LST022c4 (LEU-SOL-THERM-022 case4)	Borated concrete-reflected uranyl nitrate solution in 28cm thick slabs (10.0 wt.%)
LCT085c1 (LEU-COMP-THERM-085 case1)	Regular hexagonal lattices of low-enriched U (6.5 wt.%) fuel rods in light water
LCT085c13 (LEU-COMP-THERM-085 case13)	Regular hexagonal lattices of low-enriched U (6.5 wt.%) fuel rods in light water

Table I provides descriptions of the selected 15 criticality experiments. Flattop25, Godiva, ORNL1, and ORNL2 benchmarks represent highly enriched uranium (HEU) systems, whereas the others are low enriched uranium (LEU) system. Additionally, the LEU+ loaded i-SMR cores contain fuel assemblies with enrichments 2 wt.%, 4 wt.%, 6 wt.%, 8 wt.%, and 10 wt.% of ^{235}U and all pin pitch of the LEU+ i-SMR system is about 1.26 cm. Using the 15 ICSBEP benchmark problems and the 5 LEU+ loaded i-SMR core system, 20x20 benchmark matrix were established for the similarity analyses.

Figure 2 shows the similarity coefficients for 20x20 benchmark matrix including the criticality experiments and LEU+ loaded i-SMR core system using ENDF/B-VII.1 covariance data. All McCARD eigenvalue calculations are performed using 200 inactive cycles and 800 active cycles, with 80,000 histories per cycle. The similarity coefficients between HEU criticality experiment benchmarks and i-SMR core ranged from 0.232 to 0.498. However, those between LEU criticality experiment benchmarks and i-SMR core ranged from 0.738 to 0.992. It is noted that the U.S. nuclear regulatory commission (NRC) recommended that criticality safety analyses should be conducted using the criticality experiments with c_k value more than 0.90 [9]. Moreover, B. L. Broadhead et al. [6] suggested that a target application should have more than 20 experiments with c_k value greater than 0.80. Most benchmarks had sufficient similarity coefficients, but in some cases, the values were relatively low.

As the next step, the neutron energy spectra about several criticality experiment benchmarks were compared with those of the i-SMR core having different ^{235}U enriched uranium. Figure 3 shows the neutron energy spectra of LCT022c1, LCT085c13, and the i-SMR core system. ^{235}U enrichment of LCT022c1 is 10 wt.% and its similarity coefficient compared to i-SMR with 10 wt.% enrichment is 0.876. For LCT085c13, the enrichment is 6.5 wt.%, and the similarity coefficient compared to the i-SMR 6 wt.% enrichment is 0.85. Both cases are quite similar to the i-SMR core spectra.

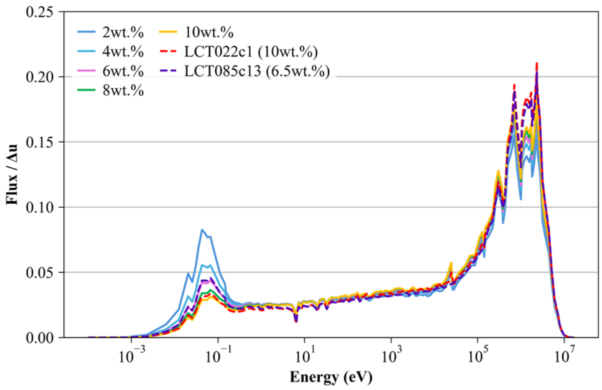

Fig 3. Neutron energy spectra of LCT benchmarks and i-SMR core system

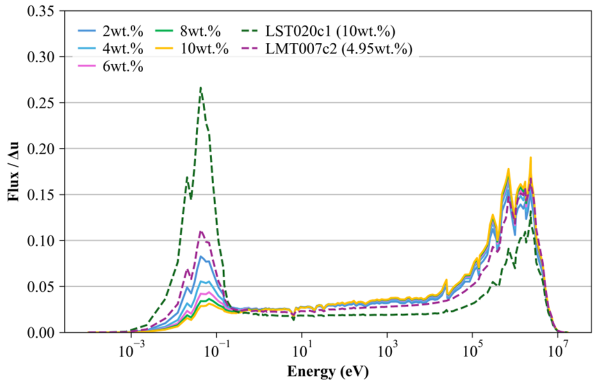

Fig 4. Neutron energy spectra of LST, LMT benchmarks and i-SMR core system

Figure 4 shows the neutron energy spectra of LST020c1, LMT007c2, and the i-SMR core system. Unlike the LCT benchmarks, the spectra of LST and LMT differ from those of i-SMR. The similarity coefficient between LST020c1 and i-SMR core (10 wt.%) is 0.775, and despite the enrichment being 10 wt.%, there was a significant difference in the spectra because the fuel was in solution form. For LMT007c2 (4.95 wt.%), similarity coefficients ranged from 0.738 to 0.803. When comparing the neutron energy spectra, there were differences between i-SMR and LMT007c2, but the differences were not as significant in the case of LST020c1. These results indicate that the similarity coefficients generally reflected the physical differences between the systems. However, the similarity coefficient of LST020c1 and i-SMR 2 wt.% was as high as 0.922, even though the physical properties of the two systems were different. The neutron energy spectrum of LST020c1 was thermalized due to the solution fuel and moderator, while that of i-SMR 2 wt.% was strongly moderated because of the low enrichment. Consequently, the similarity coefficient for the multiplication factor was high, since both systems are dominated by common nuclear data uncertainties. This highlights a limitation of using the similarity coefficient for multiplication factor, emphasizing the necessity to also considering physical property comparisons such as neutron energy spectrum and EALF.

Finally, we conducted EALF comparisons for criticality experiment benchmarks and the i-SMR core system. Figure 5 shows EALF values about LMT007c2, LST020c1, LCT022c1, LCT085c13, and i-SMR core according to enrichments.

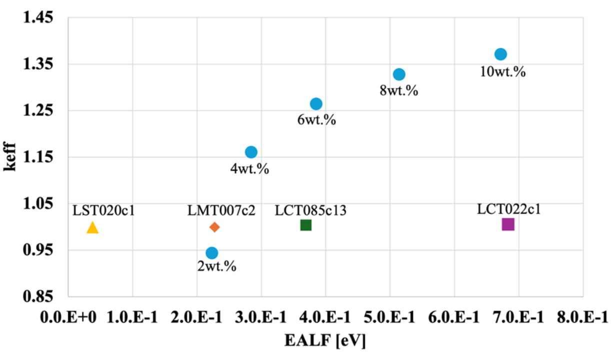

Fig 5. EALF of benchmarks and i-SMR core system

LCT022c1, with similarity coefficient of 0.876, was very similar to the i-SMR 10 wt.% core. However, LST020c1, with similarity coefficient of 0.775, differed significantly from the i-SMR 10 wt.% core.

4. Design of Critical Assemblies similar to LEU+ loaded i-SMR Core System

4.1 Draft Design of Critical Assemblies

Based on the similarity tests performed above, we aimed to directly design critical assemblies (CA) with high similarity to the LEU+ loaded i-SMR core. The critical assemblies were constructed using the i-SMR A1 assembly, with enrichment of 8 wt.% and 10 wt.%. Table II indicates simple specifications about the designed critical assemblies. Designed critical assemblies are composed of fuel, water, air, and SS304. Figures 6 and 7 show cross-section and elevation view of the critical assembly in case of 8 wt.% enrichment.

Table II: Specifications of LEU+ i-SMR critical assembly

Parameter	Value (8 wt.%)	Value (10 wt.%)	Unit
# of Assemblies	5	5	#
Reflector Outer Radius	75.708	75.708	cm
SS304 Thickness	10	10	cm
Total Radius	85.708	85.708	cm
Fuel Height	40	40	cm
Air Height	24.395	28.575	cm
Moderator Height	**30.605**	**26.425**	cm
Bottom Reflector Height	5	5	cm
Total Height	60	60	cm

For these models, eigenvalue calculation was performed under the conditions of 200 inactive cycles, 800 active cycles, and 80,000 histories per cycle using McCARD with the ENDF/B-VII.1 evaluated nuclear data library. As a result, the multiplication factor of the 8 wt.% critical assembly is 1.00001, and that of the 10 wt.% critical assembly is 1.00004. In both cases, the stochastic uncertainty (1σ) is less than 10 pcm.

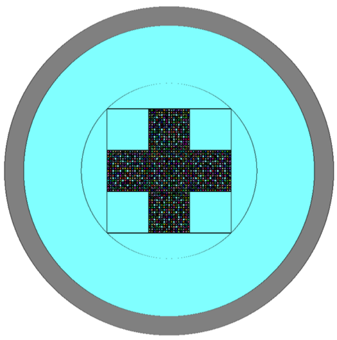

Fig 6. Cross-section of Critical Assembly (8 wt.%)

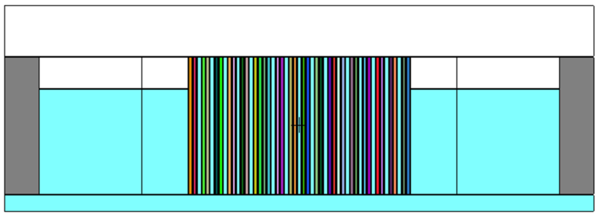

Fig 7. Elevation view of Critical Assembly (8 wt.%)

4.2 Similarity Test of Critical Assemblies with i-SMR core system

We evaluated the similarity tests between the designed assemblies and the LEU+ loaded i-SMR core. At first, similarity coefficient of critical assembly 8 wt.% (with i-SMR 8 wt.%) was 0.84570, and the value of critical assembly 10 wt.% (with i-SMR 10 wt.%) was 0.87425. These can be seen that the systems are highly similar, with a similarity coefficient of 0.8 or higher.

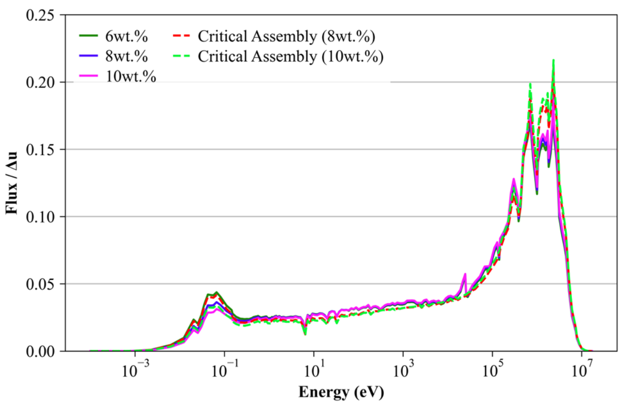

Fig 8. Neutron energy spectra of critical assembly and i-SMR core system

Figure 8 shows the neutron energy spectra of critical assembly 8 wt.% and 10 wt.%, i-SMR 6 wt.%, 8 wt.%, and 10 wt.% core. The spectra appear to be quite similar to those of the i-SMR core system.

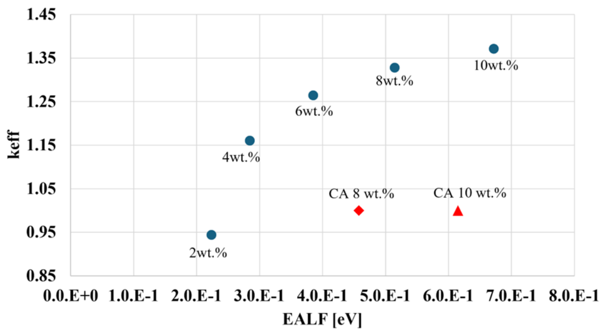

Fig 9. EALF of critical assembly and i-SMR core system

Figure 9 shows the comparison of EALF between 8 wt.%, 10 wt.% critical assemblies and i-SMR core systems. The EALF of the new LEU+ critical assemblies fell within the interval between the i-SMR 6 wt.% and 10 wt.% cores. Therefore, it was confirmed that the new LEU+ critical assembly was correctly developed via the similarity tests. In other words, the new LEU+ critical assembly adequately represents the neutronic characteristics of the LEU+ i-SMR system.

3. Conclusions

In this study, similarity analyses were conducted in two ways to select the proper criticality experiments for the validation and verification in the LEU+ loaded i-SMR core design [2] and to design a new critical assembly representative of the LEU+ i-SMR core.

First, the similarity coefficients for multiplication factors between various criticality experiment benchmarks and the LEU+ loaded i-SMR cores were calculated by the McCARD/SimTest code system. It was observed that the LEU+ benchmarks show higher similarity to the i-SMR core than some LEU (Low Enriched Uranium) benchmarks and nearly all HEU (Highly Enriched Uranium) benchmarks. In this study, benchmarks with similarity coefficients of 0.80 or higher, indicating high similarity to the i-SMR core, were identified. Moreover, the validity of the similarity coefficient was then verified by comparing the neutron energy spectra and the EALF. The LCT benchmarks in the ICSBEP benchmark showed a spectrum shape similar to that of the i-SMR core, whereas the LST and LMT benchmarks showed relatively large differences. These differences were also observed in the EALF. This suggests that relying solely on the similarity coefficient for multiplication factor to assess the representativeness of a system has limitations, and that physical characteristics, such as the energy spectrum and EALF, must also be considered.

Second, beyond the validation and verification for in the core design, the similarity coefficient can be directly used to design a new critical assembly similar to the i-SMR core. New critical assemblies using fuel enriched to 8 wt.% and 10 wt.% were designed and their high similarity to the i-SMR core was verified through comparisons of the similarity coefficient, neutron energy spectrum, and EALF. This result suggests that the potential of similarity analyses extends beyond selecting existing experiments and could serve as a valuable tool in the design process of new critical assemblies for the next-generation reactors.

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