Sensitivity and Uncertainty Analyses for Similarity Coefficient Generation in Monte Carlo Calculations

Ho Jin Park [a*]
[a]*Kyung Hee Univerisity, 1732, Deogyeong-daero, Giheung-gu, Yongin-si, 17104, Korea*
[*]*Corresponding author: parkhj@khu.ac.kr*

1. Introduction

Recently, new-type of nuclear reactors and systems have been developed by various design methods and tools in various research institutes and industrial companies. In general, a new system design should provide enough safety margins to ensure that it is adequately subcritical under any condition. To calculate accurate safety margins, the uncertainties or bias for design methods and tools should be provided by comparing experimental and calculated safety parameters (i.e., criticality).

Accordingly, it is very crucial and important to select proper critical experiments for safety margin and bias estimations. For the selection of the critical experiments, the nuclear system designers and licensees should provide computational justification to regulating body. Some researchers quantified the degree of similarity between the critical experiments and target system for the justification [1-2]. There are already many studies about the similarity quantification. For example, the *TSUNAMI* code in the *SCALE* code package can calculate a correlation coefficient that is a quantitative measurement of the degree of similarity between an experiment and target system.

In this study, the estimation of the degree of similarity between critical experiment benchmarks [3] and SMART small modular reactor (SMR) target system [4] will be conducted by deterministic based sensitivity and uncertainty (S/U) methods and stochastic sampling (S.S.) methods.

2. Similarity Coefficient

2.1. Generation of S/U method-based similarity coefficients in MC calculations

The mean of a MC estimate on a nuclear parameter Q and its variance can be expressed by

$$\overline{Q} = \lim_{K\to\infty} \frac{1}{K}\sum_{k=1}^{K} Q_k \quad , \tag{1}$$

$$\sigma^2[Q] = \lim_{K\to\infty} \frac{1}{K}\sum_{k=1}^{K}\left(Q_k - \overline{Q}\right)^2 \quad , \tag{2}$$

where k and K is an index number and total number of MC calculations. If one assumes that the total uncertainty on Q comes from statistical uncertainties of MC calculations and cross section uncertainties, Eq. (2) can be rewritten as [5]

$$\sigma^2(Q) = \lim_{K\to\infty} \frac{1}{K}\sum_{k=1}^{K}\left(Q_k - < Q_k > + < Q_k > - \overline{Q}\right)^2 \tag{3}$$

The angular bracket in $< Q_k >$ means the operator implying the expected value of a quantity on it. By the first-order Taylor expansion for $< Q_k >$ about the mean values of nuclear reaction cross section, $< Q_k > - \overline{Q}$ can be expressed by

$$< Q_k > - \overline{Q} \approx \sum_i \sum_\alpha \sum_g \left(\left(x^i_{\alpha,g}\right)_k - \overline{x^i_{\alpha,g}}\right)\left(\frac{\partial Q}{\partial x^i_{\alpha,g}}\right) \tag{4}$$

$x^i_{\alpha,g}$ is the α -type microscopic cross section of isotope i for energy group g. Substituting Eq. (4) into Eq. (3), one can obtain

$$\sigma^2(Q) = \sigma^2_{SS}(Q) + \sigma^2_{XX}(Q) \tag{5}$$

where

$$\sigma^2_{SS}(Q) = \lim_{K\to\infty} \frac{1}{K}\sum_{k=1}^{K}\left(Q_k - < Q_k >\right)^2 , \tag{6}$$

$$\sigma^2_{XX}(Q) = \lim_{K\to\infty} \frac{1}{K}\sum_{k=1}^{K}\left(< Q_k > - \overline{Q}\right)^2 = \sum_{i,\alpha,g}\sum_{i',\alpha',g'} \mathrm{cov}\left[x^i_{\alpha,g}, x^{i'}_{\alpha',g'}\right]\left(\frac{\partial Q}{\partial x^i_{\alpha,g}}\right)\left(\frac{\partial Q}{\partial x^{i'}_{\alpha',g'}}\right) \tag{7}$$

$\sigma^2_{SS}(Q)$ is the statistical contribution on the variance of Q whereas $\sigma^2_{XX}(Q)$ is commonly known as the sandwich equation for S/U analyses. In this study, we assumed that the statistical contribution on the variance of Q was negligible compared with the $\sigma^2_{XX}(Q)$.

$$\sigma^2(Q) \approx \sigma^2_{XX}(Q) \tag{8}$$

In some researches about similarity test between experiments and applications, the similarity coefficient between the criticalities in two systems, c_k, is defined as Eq. (9) using Eq. (8). Equation 10 indicates the covariance between criticalities for system I and II (i.e., k_I, k_{II}).

$$c_k = \frac{\mathrm{cov}\left[k_I, k_{II}\right]}{\sigma(k_I)\cdot\sigma(k_{II})} \tag{9}$$

where

$$\mathrm{cov}\left[k_I, k_{II}\right] = \sum_{i,\alpha,g}\sum_{i',\alpha,'g'} \mathrm{cov}\left[x^i_{\alpha,g}, x^{i'}_{\alpha',g'}\right]\left(\frac{\partial k_I}{\partial x^i_{\alpha,g}}\right)\left(\frac{\partial k_{II}}{\partial x^{i'}_{\alpha',g'}}\right) \tag{10}$$

$\mathrm{cov}[x^i_{\alpha,g}, x^{i'}_{\alpha',g'}]$ is the cross section covariance matrix from an evaluated nuclear data library. c_k is a kind of a Pearson correlation coefficient [6] and describes the correlation relationship between two systems (i.e. system I and system II). If two systems contain same materials, the c_k will help one identify how closely they are correlated each other. The similarity coefficient ranges from -1 to 1. If the similarity coefficient is close to 1, the two systems are strongly correlated.

2.2. Generation of S.S. method-based similarity coefficients in MC calculations

The similarity coefficients can be easily and directly generated by the S.S. method.

$$X^k = \left(\cdots, \left(x^i_{\alpha,g}\right)^k, \cdots\right) \tag{11}$$

$(x^i_{\alpha,g})^k$ is a *k*-th cross section sampled from a cross section covariance matrix and X^k mean the *k*-th cross section set. One can generate *K* sets of cross section samples using the *Cholesky* decomposition method from the standard normal distribution.

$$\sigma^2(k_I) = \frac{1}{K}\sum_{k=1}^{K}\left(k_I(X^k) - \overline{k_I(X^k)}\right)^2 \tag{12}$$

$$\sigma^2(k_{II}) = \frac{1}{K}\sum_{k=1}^{K}\left(k_{II}(X^k) - \overline{k_{II}(X^k)}\right)^2 \tag{13}$$

$$\mathrm{cov}\left[k_I, k_{II}\right] = \frac{1}{K}\sum_{k=1}^{K}\left(k_I(X^k) - \overline{k_I(X^k)}\right)\left(k_{II}(X^k) - \overline{k_{II}(X^k)}\right) \tag{14}$$

$k_I(X^k)$ and $k_{II}(X^k)$ mean k_{eff}'s calculated by the X^k cross section set for systems *I* and *II*, respectively. $k_I(X^k)$ and $k_{II}(X^k)$ can be calculated by the MC simulations with each sampled cross section set for the systems *I* and *II*. Finally, c_k can be calculated using Eq. (12) ~ Eq. (14).

In the same manner as show in Eq. (5), the contributions on the covariances can be separated into the statistical uncertainty term ($\mathrm{cov}_{SS}[k_I,k_{II}]$) and the cross section uncertainty term ($\mathrm{cov}_{XX}[k_I,k_{II}]$) as shown in Eq. (15).

$$\mathrm{cov}\left[k_I, k_{II}\right] = \mathrm{cov}_{SS}\left[k_I, k_{II}\right] + \mathrm{cov}_{XX}\left[k_I, k_{II}\right] \tag{15}$$

Then, using Eqs. (5) and (15), Eq (9) can be arranged by

$$c_k \simeq \frac{\mathrm{cov}_{SS}\left[k_I, k_{II}\right] + \mathrm{cov}_{XX}\left[k_I, k_{II}\right]}{\sqrt{\sigma^2_{SS}(k_I) + \sigma^2_{XX}(k_I)}\cdot\sqrt{\sigma^2_{SS}(k_{II}) + \sigma^2_{XX}(k_{II})}}, \tag{16}$$

where

$$\mathrm{cov}_{SS}\left[k_I, k_{II}\right] = \frac{1}{K}\sum_{k=1}^{K}\left(k_I(X^k) - < k_I(X^k) >\right)\left(k_{II}(X^k) - < k_{II}(X^k) >\right) \approx 0, \tag{17}$$

$$\mathrm{cov}_{XX}\left[k_I, k_{II}\right] = \frac{1}{K}\sum_{k=1}^{K}\left(< k_I(X^k) > - \overline{k_I(X^k)}\right)\left(< k_{II}(X^k) > - \overline{k_{II}(X^k)}\right). \tag{18}$$

$$\gamma_I = \frac{\sigma_{SS}(k_I)}{\sigma_{XX}(k_I)} \tag{19}$$

$$\gamma_{II} = \frac{\sigma_{SS}(k_{II})}{\sigma_{XX}(k_{II})} \tag{20}$$

Using Eqs. (19) and (20), the c_k value considering statistical uncertainty effects can be estimated by

$$c_k(\gamma_I, \gamma_{II}) \simeq \frac{1}{\sqrt{1+\gamma_I^2}\cdot\sqrt{1+\gamma_{II}^2}} c_k. \tag{21}$$

3. Similarity Test between Relevant Critical Experiment Benchmarks and SMART

3.1. McCARD/MIG/SimTest code system

The MC code system for similarity tests between relevant critical experiment benchmarks and target application are established using the *McCARD* code [7] and the *MIG* multi-correlated input sampling code [8,9].

Figure 1 shows the code flowchart for the S/U and S.S. method-based similarity tests. The *McCARD* code already has the capability of the MC perturbation technique for sensitivity coefficient generation. *SimTest* code conduct the S/U method based c_k calculations using the sensitivity coefficients from the *McCARD*

code and the cross section covariance data from an evaluated nuclear data library.

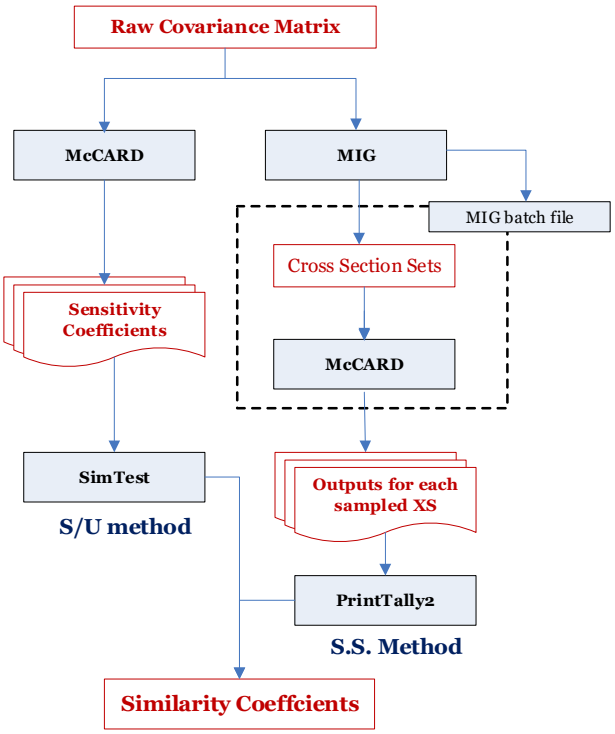

Fig. 1. Flow chart of McCARD/MIG/SimTest code system

Table I: Description of the selected eleven critical experiment benchmarks

Short Name (Benchmark ID)	Description
GODIVA (HEU-MET-FAST-001)	Bare, Highly Enriched Uranium (94 w/o) Sphere
FLATTOP25 (HEU-MET-FAST-028)	^{235}U (93.24 w/o) Sphere Reflected by Normal Uranium
HMF002c2 (HEU-MET-FAST-002 case2)	Tospy 8-Inch-Tuballoy-Reflected Orally Assemblies (97.67 w/o)
LCT001c1 (LEU-COMP-THERM-001 case1)	Water-Moderated UO_2 (2.35 w/o) Fuel Rods in 2.032 cm Square-Pitched Arrays
LCT002c1 (LEU-COMP-THERM-002 case1)	Water-Moderated UO_2 (4.31 w/o) Fuel Rods in 2.54 cm Square-Pitched Arrays
LCT003c1 (LEU-COMP-THERM-003 case1)	Water-Moderated UO_2 (2.35 w/o) Fuel Rods in 1.684 cm Square-Pitched Arrays
LCT004c1 (LEU-COMP-THERM-004 case1)	Water-Moderated UO_2 (4.31 w/o) Fuel Rods in 1.892 cm Square-Pitched Arrays
LCT005c1 (LEU-COMP-THERM-005 case1)	LEU (4.31 w/o) Dioxide Fuel Rods in Water Containing Dissolved Gadolinium (2.398 cm Square-Pitched Arrays)
LCT006c1 (LEU-COMP-THERM-006 case1)	LEU (1.5 w/o) Fuel Critical Lattice with various Water-to-Fuel Volume Ratios (1.849 cm Square-Pitched Arrays)
LCT010c9 (LEU-COMP-THERM-010 case9)	Water-Moderated UO_2 (4.31 w/o) Fuel Rods Reflected by Pb, U, or Steel Walls (2.540 cm Square-Pitched Arrays)
LCT017c13 (LEU-COMP-THERM-017case13)	Water-Moderated UO_2 (2.35 w/o) Fuel Rods Reflected by Pb, U, or Steel Walls (2.032 cm Square-Pitched Arrays)

	SMART	FLATTOP25	GODIVA	HMF002c2	LCT001c1	LCT002c1	LCT003c1	LCT004c1	LCT005c1	LCT006c1	LCT010c9	LCT017c13
SMART	1.000	0.325	0.340	0.326	0.986	0.989	0.991	0.997	0.992	0.994	0.990	0.986
FLATTOP25	0.325	1.000	0.959	0.999	0.204	0.223	0.231	0.288	0.242	0.251	0.227	0.204
GODIVA	0.340	0.959	1.000	0.956	0.225	0.243	0.251	0.306	0.262	0.270	0.247	0.225
HMF002c2	0.326	0.999	0.956	1.000	0.205	0.224	0.232	0.289	0.243	0.252	0.228	0.206
LCT001c1	0.986	0.204	0.225	0.205	1.000	0.999	0.999	0.993	0.998	0.998	0.999	0.999
LCT002c1	0.989	0.223	0.243	0.224	0.999	1.000	0.999	0.996	0.999	0.999	0.999	0.999
LCT003c1	0.991	0.231	0.251	0.232	0.999	0.999	1.000	0.997	0.999	0.999	0.999	0.999
LCT004c1	0.997	0.288	0.306	0.289	0.993	0.996	0.997	1.000	0.998	0.999	0.997	0.993
LCT005c1	0.992	0.242	0.262	0.243	0.998	0.999	0.999	0.998	1.000	0.999	0.999	0.998
LCT006c1	0.994	0.251	0.270	0.252	0.998	0.999	0.999	0.999	0.999	1.000	0.999	0.998
LCT010c9	0.990	0.227	0.247	0.228	0.999	0.999	0.999	0.997	0.999	0.999	1.000	0.999
LCT017c13	0.986	0.204	0.225	0.206	0.999	0.999	0.999	0.993	0.998	0.998	0.999	1.000

Fig. 2. Similarity Coefficients for 12x12 benchmark matrix using ENDF/B-VII.1 30-group covariance matrix for ^{235}U and ^{238}U

Meanwhile, the *MIG* code can generated the *K* sets of cross section sample files using random numbers and the cross section covariance data.

3.2. S/U method based similarity test between critical experiment benchmarks and SMART

The similarity coefficients between the selected critical experiment benchmarks [3] and the target application – SMART SMR system [4] – were calculated by the S/U method. The ENDF/B-VII.1 covariance data matrix with LANL 30-group structure was used for two major actinide isotopes (i.e., ^{235}U and ^{238}U). Table I shows the description of the selected 11 critical experiments. Godiva, Flattop-25, and HMF-002 case 2 benchmarks are highly enriched uranium (HEU) system whereas the others are low enriched uranium (LEU) system. Meanwhile, the SMART core has fuel assemblies including 2.8 w/o and 4.8 w/o enriched UO_2 fuel rods, and its pin pitch is about 1.26 cm.

Figure 2 shows the similarity coefficients for 12x12 benchmark matrix including the critical experiments and SMART SMR target system using the ENDF/V-VII.1 covariance data. The similarity coefficients between HEU experiment benchmarks and SMART ranged from 0.325 to 0.340 whereas those between the LEU experiment benchmarks and SMART from 0.986 to

0.997. The U.S. nuclear regulatory commission (NRC) recommended that critical safety analyses should be conducted using the critical experiments with c_k value in excess of 0.90 [10]. The studies suggested that a target application should have more than 20 experiments with c_k value greater than 0.80 [1]. Therefore, it is worth to mention that the 8 LEU critical experiments benchmarks (i.e., LCT001c1, LCT002c1, LCT003c1, LCT004c1, LCT005c1, LCT006c1, LCT010c9, and LCT017c13) produced the very high-level similarity coefficients to the SMART SMR target application.

3.3. Similarity coefficient generation by the S.S. method and studies on statistical uncertainty effect

The similarity coefficients between four criticality experiments by the S.S. method were generated using the END/B-VII.1 covariance data with the LANL 30-group energy group structure. Table II compared the similarity coefficients for the two fast and two thermal spectrum criticality experiment benchmarks by the S/U and S.S. method each other. In the S.S. method, the 95% confidence intervals of the uncertainties of the requested outputs were calculated by 5 repetitions of one-hundred McCARD runs with different sampled cross section sets. The uncertainties of similarity coefficients from the 100 McCARD S.S. runs agree within two standard deviation with the McCARD S/U results. From the results, it was concluded that the S.S. method works well.

Table II: Comparison between similarity coefficients by the S/U and S.S. method (ENDF/B-VII.1)

S.S.[1] / S/U[2]	GODIVA	FLATTOP 25	LCT001c1	LCT002c1
GODIVA	-	0.93±0.04	0.22±0.12	0.23±0.12
		0.96	0.23	0.24
FLATTOP 25	0.93±0.04	-	0.24±0.08	0.26±0.08
	0.96		0.20	0.22
LCT001c1	0.22±0.12	0.24±0.08	-	0.98±0.02
	0.23	0.20		0.99
LCT002c1	0.23±0.12	0.26±0.08	0.98±0.02	-
	0.24	0.22	0.99	

1) S.S. = similarity coefficients by the S.S. method
2) S/U = similarity coefficients by the S/U method

Figure 3 shows the c_k values between Flattop-25 and the other experiments due to the stochastic uncertainties of k_{eff} in a MC calculation. In Fig. 3, the dots mean the results sampled by the mean and standard deviation for each k_{eff}, whereas the lines indicate the results estimated by Eq. (21). As a statistical uncertainty of k_{eff} increase, the similarity coefficient decreases. However, in this study, the uncertainty of k_{eff} in a single MC calculation is about 50 pcm. According to it, γ_I and γ_{II} are less than 0.065. Therefore, the impact on the c_k value from statistical uncertainties in MC eigenvalue calculations is not significant. Moreover, it is noted that the c_k value estimated by Eq. (21) agree very well with the reference.

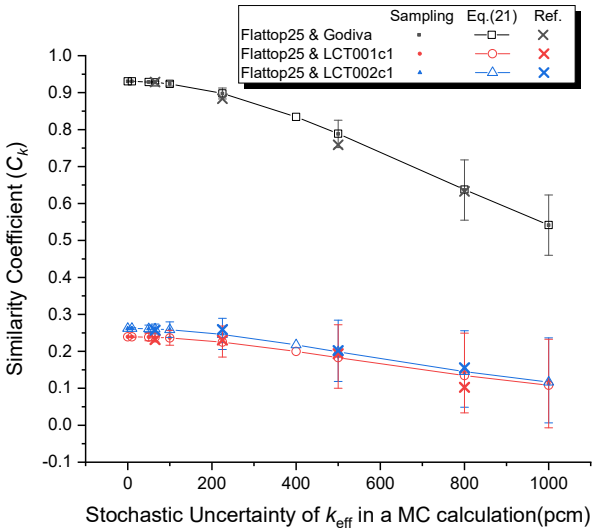

Fig. 3. S.S. method-based similarity coefficients due to stochastic uncertainties of k_{eff} in a MC calculation

4. Conclusion

In this study, the McCARD/MIG/SimTest code system for the S/U and S.S. method-based similarity test was successfully established. To verify and validate the similarity test code system, the c_k similarity coefficients among the relevant eleven critical experiments and the SMART SMR target application were generated by the ENDF/B-VII.1 covariance data with the LANL 30-group energy group structure. From the results, the c_k similarity coefficients between the LEU critical experiments and SMART ranged from 0.986 to 0.998. These results are very helpful for a licensee to justify the determination of the critical experiment benchmarks for computational bias estimations of the SMART target applications.

In the near future, the similarity tests among various critical experiment benchmarks and target applications (i.e., new-type nuclear system) will be conducted using up-to-date covariance data and cross section library.

REFERENCES

[1] B. L. Broadhead et al. Sensitivity- and Uncertainty-Based Criticality Safety Validation Techniques, Nuclear Science and Engineering, Vol 146, pp. 340-366, 2004.
[2] C. M. Perfetti and B. T. Rearden, Estimating Code Biases for Criticality Safety Applications with Few Relevant

Benchmarks, Nuclear Science and Engineering, Vol 193, pp. 1090-1128, 2019.
[3] "International Handbook of Evaluated Criticality Safety Benchmark Experiments," OECD Nuclear Energy Agency report NEA/NSC/COD(95)03, 1998.
[4] K. H. Lee et al. The Nuclear Design Report for SMART Standard Design Cycle 1, KAERI/TR-4522/2012, Korea Atomic Energy Research Institute, 2012.
[5] H. J. Park, H. J. Shim, and C. H. Kim. Uncertainty Propagation in Monte Carlo Depletion Analysis, Nuclear Science and Engineering, Vol 167, pp. 196-208, 2011.
[6] K. Pearson, Notes on Regression and Inheritance in the Case of Two Parents, Proc. R. Soc. London, Vol 58, pp. 240, 1895.
[7] H. J. Shim et al., McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis, Nuclear Engineering and Technology, Vol.44, p 161-176, 2012.
[8] H. J. Park, McCARD/MIG Stochastic Sampling Calculations for Nuclear Cross Section Sensitivity and Uncertainty Analysis, Nuclear Engineering and Technology, https://doi.org/10.1016/j.net.2022.06.012.
[9] H. J. Park, T. Y. Han, and J. Y. Cho, Implementation of Cross Section Random Sampling Code System for Direct Sampling Method in Continuous Energy Monte Carlo Calculations, Transactions of the Korean Nuclear Society Virtual Spring Meeting, July 9-10, 2020.
[10] Justification for Minimum Margin of Subcriticality for Safety, FCSS ISG-10, Rev. 0, U.S. Nuclear Regulatory Commission, Office of Nuclear Material Safety and Safeguards, Division of Fuel Cycle Safety and Safeguards, 2006.