

Discussion on variety of cross-section candidate obtained by cross-section adjustment method

Sohei Odani^{1*}, Satoshi Takeda¹, and Takanori Kitada¹

¹ Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

Abstract. The cross-section adjustment method gives only one best-estimated cross-section set based on Bayesian theory. In this study, cross-section sets other than the best-estimated set were discussed. The cross-section sets were obtained by the random sampling method using a covariance matrix adjusted by the cross-section adjustment method. 1,000,000 cross-section sets were obtained by the random sampling method. From these cross-section sets, significant cross-section sets other than the best-estimated set were considered. 593,340 cross-section sets that accurately evaluate nuclear characteristics were obtained. The result of the cross-section adjustment method shows that the change due to U235 χ is the largest positive. However, k_{eff} is not changed to the positive side by U235 χ in 179,994 of the 593,340 cross-section sets obtained by the random sampling method. Although the best-estimated cross-section set is obtained by the cross-section adjustment method, the result suggests there are various candidates for the adjusted cross-section set.

1 Introduction

Accurate evaluation of nuclear characteristics is essential for the safe and efficient operation of nuclear reactors. Reduction of the uncertainties is important for higher evaluation accuracy. Among the uncertainties that lead to the uncertainty of nuclear characteristics, the uncertainty arising from the nuclear data is a major factor.

The cross-section adjustment method [1, 2] is one of the methods for reduction of the uncertainty arising from nuclear data. The cross-section adjustment method provides a best-estimate cross-section set whose calculated values reproduce experimental values well. However, it is pointed out that some of the results of the cross-section adjustment method have no nuclear physics justification [3]. In addition, it has been reported that there are various cross-section sets whose C/E (calculation/experiment) values are consistent with the results of the cross-section adjustment method due to the compensation effect [4, 5]. Some of these various cross-section sets may be more reliable than the result of the cross-section adjustment method. However, the significance of these various cross-section sets has not been assessed. Therefore, in this study, the significance of the various cross-section sets was discussed.

The random sampling method can generate cross-section sets based on covariance data and is used in the community of reactor physics [6-8]. In this study, the random sampling method was used to generate cross-section sets that accurately evaluate nuclear characteristics. Then, the significance of the cross-section set was assessed by comparison. The random sampling method is summarized in Sec. 2. A

comparison of the cross-section sets obtained by the random sampling method with that by the cross-section adjustment method is shown in Sec. 3. Finally, the conclusion is summarized in Sec. 4.

2 Random sampling using cross-section adjustment method

For random sampling, an adjusted cross-section set and an adjusted covariance matrix obtained by the cross-section adjustment method were used. Assuming that experimental error, calculation error, and cross-section error are independent of each other, the adjusted cross-section set is obtained by

$$\mathbf{t}_{adj} = \mathbf{t}_0 + \mathbf{M}\mathbf{G}^T(\mathbf{G}\mathbf{M}\mathbf{G}^T + \mathbf{V}_e + \mathbf{V}_m)^{-1}(\mathbf{R}_e - \mathbf{R}_c(\mathbf{t}_0)), \quad (1)$$

where \mathbf{t}_{adj} is the adjusted cross-section set, \mathbf{t}_0 is the original cross-section set, \mathbf{M} is the covariance matrix, \mathbf{G} is the sensitivity coefficient of the cross-section set, \mathbf{V}_e is the covariance matrix of the experimental error, \mathbf{V}_m is the covariance matrix of the calculation error, \mathbf{R}_e is the experimental value and \mathbf{R}_c is the calculated value. The adjusted covariance matrix \mathbf{M}_{adj} is obtained by

$$\mathbf{M}_{adj} = \mathbf{M} - \mathbf{M}\mathbf{G}^T(\mathbf{G}\mathbf{M}\mathbf{G}^T + \mathbf{V}_e + \mathbf{V}_m)^{-1}\mathbf{G}\mathbf{M}. \quad (2)$$

The multivariate normal random number according to the adjusted covariance matrix is obtained by

$$\mathbf{z} = \mathbf{A}\mathbf{x} + \boldsymbol{\mu}, \quad (3)$$

* Corresponding author: s-odani@ne.see.eng.osaka-u.ac.jp

where \mathbf{z} is the vector whose elements are multivariate normal random numbers, \mathbf{x} is the vector whose elements are standard normal random numbers, and $\boldsymbol{\mu}$ is the mean vector. When the adjusted covariance matrix is a positive semidefinite matrix, the adjusted covariance matrix is expanded using \mathbf{A} as

$$\mathbf{M}_{\text{adj}} = \mathbf{A}\mathbf{A}^T. \quad (4)$$

To satisfy equation (4), \mathbf{M}_{adj} must be a positive semidefinite matrix. However, it has been reported that the covariance matrix may not be positive semidefinite [8-10]. This problem is caused by the distortion of eigenvalues due to rounding. In this study, when the covariance matrix is not positive semidefinite, the nearest covariance matrix, which is positive semidefinite matrix obtained by Higham's method [11], was used. In this case, the nearest covariance matrix \mathbf{M}_{near} is expanded using \mathbf{B} as

$$\mathbf{M}_{\text{near}} = \mathbf{B}\mathbf{B}^T. \quad (5)$$

When using the nearest covariance matrix, the random number is obtained by

$$\mathbf{z} = \mathbf{B}\mathbf{x} + \boldsymbol{\mu}. \quad (6)$$

3 Random sampling using two uranium benchmarks

3.1 Calculation condition

The cross-section adjustment method was performed using the criticality of light water-moderated uranium benchmarks summarized in ICSBEP [12]. The benchmark problems are HEU-SOL-THERM-001-001 (HST1-1) and LEU-COMP-THERM-001-001 (LCT1-1). HST1-1 is high-enriched uranium fuel system and LCT1-1 is low-enriched uranium fuel system. In addition, both systems do not contain plutonium. Sensitivity coefficients and covariance data were used from a package included in the MCNP6.2 [13] packages, WHISPER [14]. Sensitivity coefficients included in WHISPER were calculated with ENDF/B-VII.1 [15]. The calculations used 100,000 neutrons per cycle, 100 skip cycles, and 600 active cycles. Covariance data in WHISPER is the same data that is distributed with SCALE 6.1 and is 44-group energy structure [16]. Then, the two benchmark problems are assumed to be independent, \mathbf{V}_e and \mathbf{V}_m have zero covariance elements, and the diagonal elements are each variance.

3.2 Selection of target nuclide reactions

Due to computer memory utilization issues, not all cross-sections of nuclides included in the benchmark problem were adjusted using the cross-section adjustment method. The adjusted cross-section was selected by the contribution to the uncertainty of criticality. The uncertainty of criticality due to a particular reaction is obtained by

$$\sigma_\alpha^2 = \mathbf{G}_\alpha \mathbf{M}_\alpha \mathbf{G}_\alpha^T, \quad (7)$$

where σ_α is the standard deviation of criticality due to a particular reaction, \mathbf{G}_α is the sensitivity coefficient of the reaction, and \mathbf{M}_α is the covariance matrix of the reaction.

In this study, the threshold was set at 1/100 of the uncertainty of criticality due to all reactions. Therefore, the cross-section with $\sigma_\alpha > 0.005\%$ were adjusted by the cross-section adjustment method. The target nuclides for the cross-section adjustment method are summarized in Table 1.

Table 1. Target nuclides for the cross-section adjustment method

Nuclide	Reaction or parameter
U234	(n, γ)
U235	Elastic scattering, Inelastic scattering, (n,2n), (n, γ), ν , χ
U238	Elastic scattering, Inelastic scattering, (n,2n), (n, γ), ν , χ
H1	Elastic scattering, (n, γ)
N14	(n,p)
O16	Elastic scattering, Inelastic scattering
Al27	Elastic scattering, Inelastic scattering, (n, γ)
Cr52	Elastic scattering
Mn55	Elastic scattering
Fe56	Elastic scattering

3.3 Result and discussion

3.3.1 Results of cross-section adjustment method

The calculated and experimental values before the cross-section adjustment method are summarized in Table 2.

Table 2. The calculated and experimental values before the cross-section adjustment method

	Calculated value	Experimental value
HST1-1	0.9983 ± 0.0002	1.0000 ± 0.0025
LCT1-1	0.9996 ± 0.0001	0.9998 ± 0.0031

The changes in criticality for the two benchmark problems due to the cross-section adjustment method are summarized in Table 3. The amount of change in criticality due to each nuclide reaction in the adjusted cross-section set is summarized in Figure 1. Then, the

amount of change in criticality due to each nuclide reaction $\Delta k/k$ is obtained by

$$\frac{\Delta k}{k} = \sum_g \mathbf{G}_g \frac{\Delta t_g}{t_g} \quad (8)$$

where g is a certain energy group, \mathbf{G}_g is the sensitivity coefficient at a certain energy group, and $\Delta t_g/t_g$ is the change of cross-section at a certain energy group. As shown in Table 3, the difference between the adjusted and experimental values is small. Figure 1 shows that the C/E value is improved mainly by the adjustment of U235 χ .

Table 3. Changes in C/E-1 values of criticality with cross-section adjustment method

	Before adjustment	After adjustment
	C/E-1 [%]	C/E-1 [%]
HST1-1	-0.172	-0.016
LCT1-1	-0.021	0.016

C/E : Calculation/Experiment

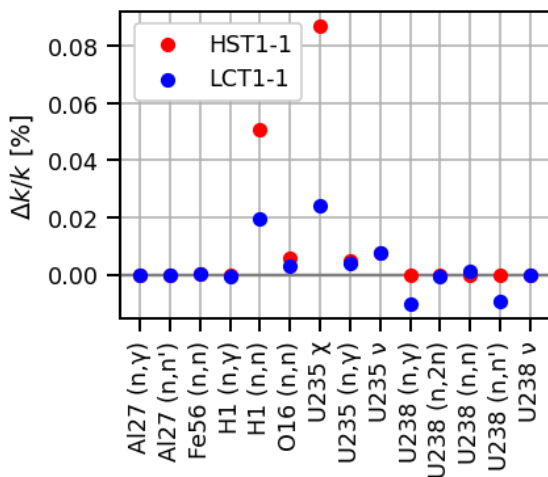


Figure 1. The amount of change in criticality due to each nuclide reaction by the cross-section adjustment method ($\Delta k/k > 1.0 \times 10^{-5} \%$)

As shown in Figure 1, the negative adjustments in U238 (n,γ) and (n,n') compensate the positive adjustments in H1 (n,n) and U235 χ . The compensation effects occurred in U238 (n,γ) and (n,n') because these reactions are sensitive only in LCT1-1, as shown in Figure 2.

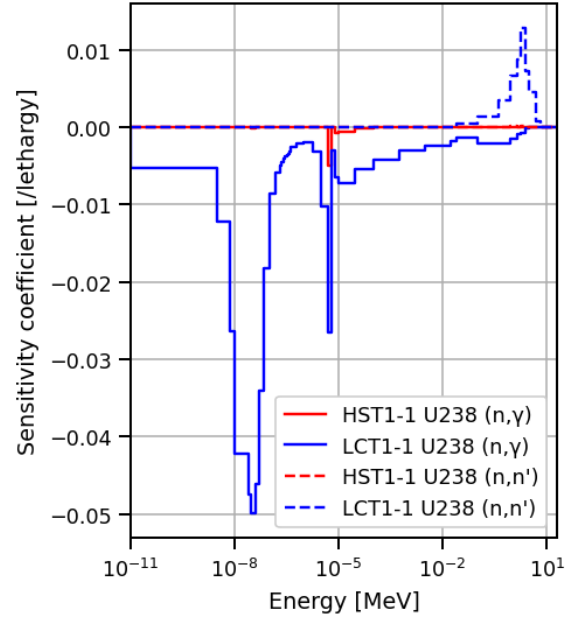


Figure 2. Sensitivity coefficients of U238 (n,γ) and (n,n')

3.3.2 Effect of using the nearest covariance matrix

As mentioned in Sec. 2, the nearest covariance matrix was used to generate multivariate normal random number. To evaluate the effect of using the nearest covariance matrix, the uncertainty of criticality arising from cross-section was compared.

First, the nearest covariance matrix was compared to the original covariance matrix by the uncertainty of the criticality of each benchmark problem. The difference in standard deviations of the criticality in each benchmark problem $\Delta\sigma_b$ is obtained by

$$\Delta\sigma_b = \sqrt{\mathbf{GM}_{\text{near}}\mathbf{G}^T} - \sqrt{\mathbf{GM}_{\text{org}}\mathbf{G}^T}, \quad (9)$$

where \mathbf{M}_{org} is the original covariance matrix. The differences in each benchmark problem are summarized in Table 4. As shown in Table 4, the difference between the nearest covariance matrix and the original covariance matrix is small, so we concluded the effect of using the nearest covariance matrix is small.

Table 4. The relative uncertainty differences for each benchmark problem

Benchmark	Difference [%]
HST1-1	5.84×10^{-4}
LCT1-1	2.40×10^{-3}

Even if each matrix element in the nearest covariance matrix is significantly different from the original covariance matrix, the differences shown in Table 4 could be underestimated due to cancellation of positive and negative values. Therefore, the focus was on the variance of the each cross-section in all energy groups for all nuclide reactions. The difference due to each cross-section $\Delta\sigma_{tg}$ is obtained by

$$\Delta\sigma_{ig} = \sqrt{\mathbf{G}_{ig}^2 \mathbf{V}_{ig}^{\text{near}}} - \sqrt{\mathbf{G}_{ig}^2 \mathbf{V}_{ig}^{\text{org}}}, \quad (10)$$

where i is the nuclide reaction, g is the energy group, $\mathbf{V}_{ig}^{\text{near}}$ is the variance of the nearest covariance matrix, and $\mathbf{V}_{ig}^{\text{org}}$ is the original variance. The maximum difference due to each cross-section in each benchmark problem is summarized in Table 5. As shown in Table 5, the difference due to each cross-section is also small. Considering the above, the effect of using nearest covariance matrices was determined to be small.

Table 5. The maximum difference in standard deviations due to each cross-section

Benchmark	Maximum difference [%]
HST1-1	4.75×10^{-15}
LCT1-1	8.20×10^{-15}

3.3.3 Result of random sampling and discussion

The nearest covariance matrix was used to generate 1,000,000 random cross-section sets. From these random cross-section sets, the focus was on cross-section sets that accurately evaluate criticality. In this study, accurate evaluation of criticality means that the adjusted criticality is in the range shown in Table 6. This range was determined by the uncertainty of the experimental and calculated values, as shown in Table 2. At this time, statistical uncertainty and experimental uncertainty are assumed to be independent. As a result, 593,340 cross-section sets were in this range.

Table 6. The range of C values that accurately evaluate criticality

Benchmark	Range of C value
HST1-1	$0.9973 \leq C \leq 1.0027$
LCT1-1	$0.9966 \leq C \leq 1.0030$

The 593,340 cross-section sets were compared to the adjusted cross-section set obtained by the cross-section adjustment method. As shown in Figure 1, the cross-section adjustment method shows the largest positive change in criticality by U235 χ . The frequency of the change in criticality by U235 χ in the 593,340 cross-section sets in HST1-1 is shown in Figure 3. Figure 3 shows that the results of the cross-section adjustment method are included in the most frequent bin. However, in 179,994 of the 593,340 cross-section sets, criticality is not changed to the positive side by U235 χ . This result indicates that there are significant candidates for the cross-section set that accurately evaluate criticality, other than the results of the cross-section adjustment method.

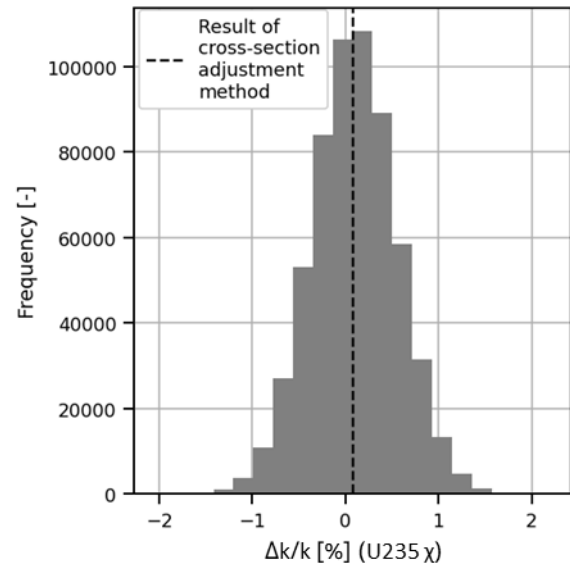


Figure 3. The frequency of the change in criticality by U235 χ for the 593,340 cross-section sets (HST1-1)

The 179,994 cross-section sets whose criticality is negatively adjusted by U235 χ were investigated. Focusing on the fourth most frequent bin in Figure 3, the amount of adjustment due to reactions other than U235 χ was investigated. The average amount of change in criticality due to all reactions is shown in Figure 4. The fourth most frequent bin is in the range of -0.35% to -0.14% of criticality change due to U235 χ . Then, the results shown in Figure 4 are the average of the criticality adjustments for the 84,120 cross-section sets in this range. Figure 4 shows that the negative adjustment due to U235 χ is mainly compensated by H1(n,n).

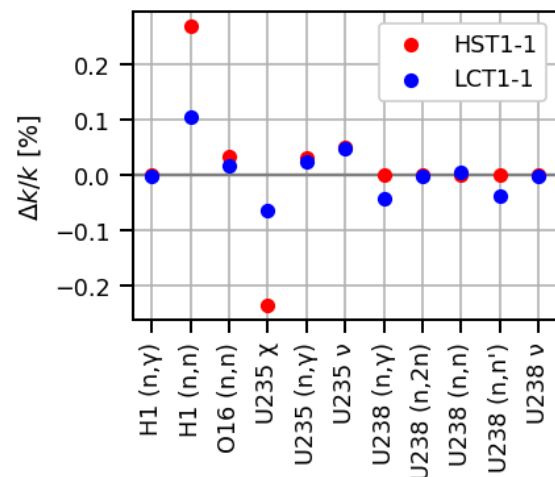


Figure 4. The average amount of criticality adjustment due to each nuclide reaction by 84,120 cross-section sets ($\Delta k/k > 1.0 \times 10^{-3} \%$)

The standard deviations of criticality obtained by substituting the nearest covariance matrix into equation (7) are shown in Table 7. As shown in Table 7, the standard deviation arising from U235 χ is larger than 0.09% (the amount of change in criticality by the cross-section adjustment method). Therefore, the negative adjustment by U235 χ is consistent with the covariance data. Furthermore, it is also consistent with the

covariance data that criticality is adjusted by H1 (n,n), which is the second largest when criticality is not adjusted by U235 χ .

Table 7. The standard deviation of criticality arising from each reaction obtained from the nearest covariance matrix

Nuclide	Reaction or parameter	Standard deviation of criticality [%]
U235	χ	0.47
H1	Elastic scattering	0.44
U235	ν	0.26
U235	(n, γ)	0.19
O16	Elastic scattering	0.18

In the cross-section adjustment method, the best-estimated cross-section set is obtained, where criticality is adjusted mainly by U235 χ due to the largest standard deviation. However, the results obtained by using the random sampling method indicate that the cross-section sets that adjust criticality mainly in H1(n,n) is also significant.

4 Conclusion

In this study, the significance of various cross-section sets that accurately evaluate nuclear characteristics was assessed. The random sampling method was used to obtain various cross-section sets. The random cross-section sets, which accurately evaluate nuclear characteristics, were compared to the cross-section set obtained by the cross-section adjustment method. The comparison indicated that there are other significant candidates that are consistent with the covariance data. By using the random sampling method, significant candidates can be obtained without changing the benchmark problems used for the cross-section adjustment method. Therefore, it may be useful when the result of the cross-section adjustment method is unreliable.

References

- J. B. Dragt, J. W. M. Dekker, H. Guppelaar, et al., "Methods of adjustment and error evaluation of neutron capture cross sections; application to fission product nuclides", Nucl. Sci. Eng., **62**, 117-129 (1977).
- T. Takeda, A. Yoshimura, T. Kamei, "Prediction uncertainty evaluation methods of core performance parameters in large liquid-metal fast breeder reactors", Nucl. Sci. Eng., **103**, 157-165 (1989).
- E. Bauge, D. A. Rochman, "Cross-observables and cross-isotopes correlations in nuclear data from integral constraints", EPJ Nucl Sci Technol., **4**, 35 (2018).
- G. Palmiotti, M. Salvatores, K. Yokoyama, et al., "Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files", EPJ Web Conf., **239**, 13001 (2020).
- M. Salvatores, G. Palmiotti, G. Aliberti, et al., "Methods and Issues for the Combined Use of Integral Experiments and Covariance Data: Results of a NEA International Collaborative Study", Nuclear Data Sheets, **118**, 38-71 (2014).
- T. Watanabe, T. Endo, A. Yamamoto, et al., "Cross section adjustment method based on random sampling technique", J Nucl Sci Technol., **51**, 590-599 (2014).
- T. Endo, A. Yamamoto, T. Watanabe, "Bias factor method using random sampling technique", J Nucl Sci Technol., **53**, 1494-1501 (2016).
- L. Plevnik, G. Žerovnik, "Computer code ENDSAM for random sampling and validation of the resonance parameters covariance matrices of some major nuclear data libraries", Annals of Nuclear Energy, **94**, 510-517 (2016).
- M. Herman, P. Oblozinsky, C.M. Mattoon, et al., "AFCI-2.0 Neutron Cross Section Covariance Library", Brookhaven National Laboratory, BNL-94830-2011 (2011).
- R. Vanhanen, "Computing Positive Semidefinite Multigroup Nuclear Data Covariances", Nucl. Sci. Eng., **179**, 411-422 (2015).
- N. Higham, "Computing a Nearest Symmetric Positive Semidefinite Matrix", Linear Algebra Appl., **103**, 103-118 (1988).
- OECD/NEA, "International Handbook of Evaluated Criticality Safety Benchmark Experiments", OECD/NEA, NEA/NSC/DOC(95)03 (2016).
- C. J. Werner (editor), "MCNP Users Manual - Code Version 6.2", Los Alamos, LA-UR-17-29981 (2017).
- B. C. Kiedrowski, F. B. Brown, J. L. Conlin, et al., "Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits", Nucl. Sci. Eng., **181**, 14-47 (2015).
- M. B. Chadwick, M. Herman, P. Obložinský, et al., "ENDF/B-VII.1: Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data", Nucl. Data Sheets, **112**, 2887-2996 (2011).
- B. L. Broadhead, I. A. Kodeli, "ZZ SCALE6.0/COVA-44G, 44-group cross section covariance matrix library extracted from SCALE6.0", NEA Data Bank, USCD1236/03 (2011).