

An Evaluation of Eigenvalue Uncertainty Caused by Monte Carlo Uncertainties of Multi-group Cross Section

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1. Introduction

Multi-group cross sections have been produced by lattice code. In the case of complicate geometry like TRISO particles, it is noted that spatial approximations of lattice code could make biases of results [1]. Monte Carlo (MC) method have been tried to calculate multi-group cross sections [2]. The Boltzmann transport equation can be directly solved by MC particle transport method without spatial approximation. Therefore, MC method is advantageous when complicate geometries are modeled. Multi-group cross sections calculated by MC method involve statistical uncertainties. Hence, it is essential to analyze reactor characteristics caused by uncertainty of cross sections.

In this study, multi-group cross sections with uncertainties were calculated by MC method. Using uncertainty propagation theory, uncertainties of eigenvalue caused by statistical error of multi-group cross section were estimated.

2. Methods and Results

In the section 2.1, multi-group cross sections with uncertainties for a sample case are calculated by MC method. Two sets of multi-group cross section were produced to compare uncertainties. In section 2.2, using uncertainty propagation theory and multi-group cross sections, uncertainty of eigenvalue is calculated to estimate statistical error of cross section

2.1 Multi-group Cross Section Generated by Monte Carlo Method

To calculate microscopic multi-group cross sections, group reaction rates are divided by group flux as follows [3]:

$$\sigma_{g,a} = \frac{\int_V \int_{\Delta E} \int_{4\pi} \sigma_a(r,E) \phi(r,E,\Omega) d\Omega dE dr}{\int_V \int_{\Delta E} \int_{4\pi} \phi(r,E,\Omega) d\Omega dE dr} \quad (1)$$

where $\sigma_{g,a}$ is microscopic multi-group cross section of reaction a , ϕ is flux of position \mathbf{r} , energy E , and angle Ω . σ_a is continuous microscopic cross section of reaction a .

The standard deviation of multi-group cross section can be calculated as follows [4]:

$$S_{\bar{u}} = \frac{1}{N-1} \sum_{i=1}^N \left(u_i - \frac{\sum_{i=1}^N u_i}{N} \right)^2 \quad (2)$$

where $S_{\bar{u}}$ is standard deviation of expected multi-group cross section \bar{u} . N is total number of transported particles. u_i is calculated multi-group cross section of i^{th} particle transportation.

To generate multi-group cross section, a sample problem is made as shown in Fig. 1. Multi-group cross section of Uranium 235 was generated by using Eq.1. Detail information of the problem is given in Table I. Smart and User-friendly Monte Carlo Particle Transport Code (SUIT)[5], which has been developed in Hanyang Univ., was used to produce multi-group cross sections.

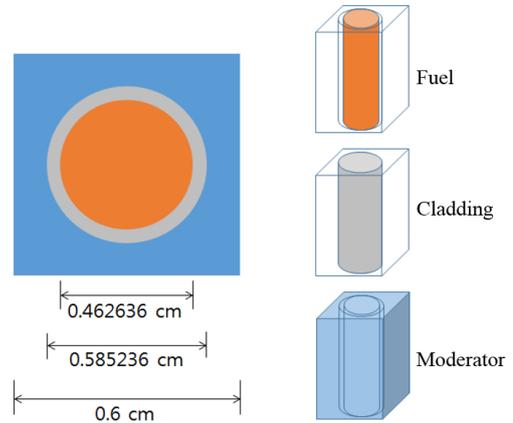


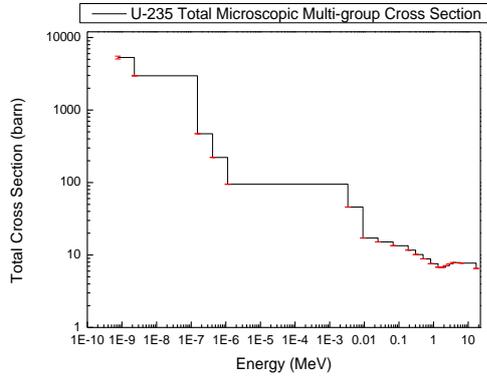
Fig. 1 Structure of Sample Problem

Table I: Detail Information of the Sample Problem

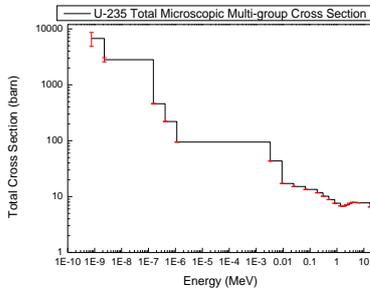
Fuel Material	Uranium Zircaloy
Density	7.86 g/cc
Enrichment	19.75w/o
Cladding Material	Zircaloy
Density	6.55 g/cc
Moderator Material	Water
Density	0.658 g/cc
Cross Section Library	ENDF-VII

Two set of total reaction multi-group cross sections were generated as following: Set #1 multi-group cross sections was generated with 300,000 particles to be used as the reference data in section 2.2; Set #2 multi-group cross section was calculated with 7,500 particles.

Fig. 2 shows the generated two sets of total multi-group cross sections. Red lines represent error bar for 95 % confidence level. The results are tabulated in Table II.



(A) Set #1



(b) Set #2

Fig. 2 Calculated Total Multi-group Cross Section of Uranium 235

Table II: Summary of Calculated Multi-group Cross section of Uranium 235

Number of Groups	20
Average % Error of Set #1	0.17
Maximum % Error of Set #1	2.25
Average % Error of Set #2	1.10
Maximum % Error of Set #2	13.9

2.2 Uncertainty Estimation of Eigenvalue caused by Statistical error of multi-group cross section

As eigenvalue is a function of multi-group cross section, it can be expressed as follows [6]:

$$k_{eff} = f(cx_1, cx_2, cx_3, \dots, cx_n) \quad (3)$$

where k_{eff} is eigenvalue, cx_n is multi-group cross section of n^{th} energy group. By the uncertainty propagation theory, variance of k_{eff} is written as follows [6]:

$$\sigma(k_{eff})^2 \cong \mathbf{J}\mathbf{J}^T \quad (4)$$

where $\mathbf{J} = \left(\frac{\partial k_{eff}}{\partial cx_1}, \frac{\partial k_{eff}}{\partial cx_2}, \dots, \frac{\partial k_{eff}}{\partial cx_n} \right)$,

$$\{\mathbf{V}\}_{i,j} = cov(cx_i, cx_j)$$

Matrix \mathbf{J} of set #2 is calculated by correlated sampling method (CSM) [7], which is one of the MC perturbation method. Fig. 3 shows the component of matrix \mathbf{J} of set #2.

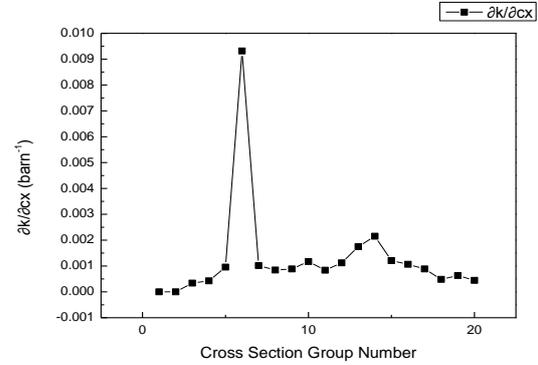


Fig. 3 Matrix \mathbf{J} of multi-group cross section for set #2

Using Eq. (4), eigenvalue uncertainty caused by uncertainties of set #2 was estimated with assumption that covariance between other groups were ignorable. The predicted uncertainty of eigenvalue ($\sigma(k)$) for set #2 was 301 pcm. To verify the predicted uncertainty, 43 multi-group cross sections with same condition of set #2 were produced. Fig. 4 and Table III show that almost all of biased eigenvalues were estimated to be in predicted confidence interval.

Standard deviation of 43 biased eigenvalue $\sigma(k_{bias})$ was 383 pcm. The difference of predicted $\sigma(k)$ and $\sigma(k_{bias})$ was 82 pcm. It shows that predicted $\sigma(k)$ can be used as useful information to generate multi-group cross section. It is recommended that the predicted $\sigma(k)$ should be lower than the purposed standard deviation of eigenvalue to make MC uncertainty of multi-group cross section ignorable.

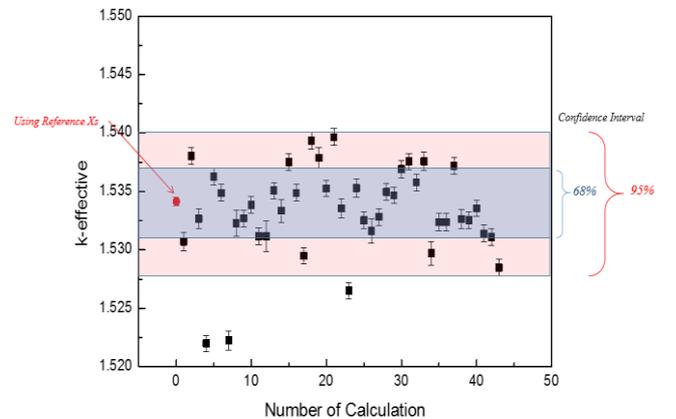


Fig. 4 Validation Calculation of Predicted $\sigma(k)$

Table III: Eigenvalue Comparison

* Predicted $\sigma(k)$: ± 301 pcm (65% interval), ± 602 pcm (95% interval)

Multi-group Xs	k_{eff}	STD	$\Delta k(\text{pcm})$
Reference Xs	1.53402	0.00035	-
Comparison Xs 1	1.53071	0.00039	331
Comparison Xs 2	1.53804	0.00035	-402
Comparison Xs 3	1.53267	0.00041	135
Comparison Xs 4	1.52199	0.00035	1203
Comparison Xs 5	1.53626	0.00035	-224
Comparison Xs 6	1.53487	0.00036	-85
Comparison Xs 7	1.52225	0.00041	1177
Comparison Xs 8	1.53228	0.00057	174
Comparison Xs 9	1.5327	0.00036	132
Comparison Xs 10	1.53384	0.00036	18
Comparison Xs 11	1.53116	0.00036	286
Comparison Xs 12	1.53117	0.00066	285
Comparison Xs 13	1.53507	0.00035	-105
Comparison Xs 14	1.53334	0.00049	68
Comparison Xs 15	1.53751	0.00036	-349
Comparison Xs 16	1.53487	0.00036	-85
Comparison Xs 17	1.52948	0.00035	454
Comparison Xs 18	1.53933	0.00036	-531
Comparison Xs 19	1.53786	0.00045	-384
Comparison Xs 20	1.53524	0.00035	-122
Comparison Xs 21	1.53965	0.00036	-563
Comparison Xs 22	1.53354	0.00041	48
Comparison Xs 23	1.5265	0.00035	752
Comparison Xs 24	1.53529	0.0004	-127
Comparison Xs 25	1.53253	0.00035	149
Comparison Xs 26	1.53161	0.00052	241
Comparison Xs 27	1.53281	0.00036	121
Comparison Xs 28	1.53496	0.00036	-94
Comparison Xs 29	1.53465	0.00035	-63
Comparison Xs 30	1.53691	0.00037	-289
Comparison Xs 31	1.53756	0.00035	-354
Comparison Xs 32	1.53577	0.00036	-175
Comparison Xs 33	1.53757	0.00039	-355
Comparison Xs 34	1.5297	0.00051	432
Comparison Xs 35	1.53238	0.00038	164
Comparison Xs 36	1.53238	0.00038	164
Comparison Xs 37	1.53718	0.00035	-316
Comparison Xs 38	1.53264	0.0004	138
Comparison Xs 39	1.53253	0.00035	149
Comparison Xs 40	1.53356	0.00035	46
Comparison Xs 41	1.5314	0.00036	262
Comparison Xs 42	1.5311	0.00035	292
Comparison Xs 43	1.52848	0.00035	554

3. Conclusions

In this study, multi-group cross sections were generated by MC method. To estimate uncertainty of eigenvalue caused by MC uncertainties of multi-group cross section, uncertainty perturbation theory and MC perturbation method were used. Predicted uncertainty of eigenvalue was evaluated. It is shown that the bias caused by MC uncertainty of cross section can be predicted by uncertainty propagation. It is expected that using this study results, the reference statistical error of multi-group cross section can be calculated to get accurate multi-group cross section efficiently.

4. Acknowledgement

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REFERENCES

- [1] Ho Jin Park, Generation of Few-Group Diffusion Theory Constants by Monte Carlo Code McCARD, NUCLEAR SCIENCE AND ENGINEERING; 172, 66-77, 2012
- [2] Everett Lee Redmond II, Multigroup Cross Section Generation Via Monte Carlo Methods, Ph.D Thesis, 1997 Massachusetts Institute of Technology
- [3] R. E. MacFarlane, A. C. Kahler, Methods for Processing ENDF/B-VII with NJOY, Nuclear Data Sheets, Vol. 111, Pages 2739-2890, Los Alamos National Laboratory Unclassified Report LA-UR-10-04652, July 2010
- [4] X-5 Monte Carlo Team, MCNP – A General Monte Carlo N-Particle Transport Code, Version 5 Volume I: Overview and Theory, LA-UR-03-1987, 24 April, 2003
- [5] Song Hyun Kim, et al, “Smart and User-friendly Monte Carlo Particle Transport Code User Manual”, HYU-NURAL-001-2016, 2016
- [6] Walter Bich, “Uncertainty Evaluation by means of a Monte Carlo Approach”, BIPM Workshop 2 on CCRI (II) Activity Uncertainties and Comparisons, Sevres, 17-18 September, 2008
- [7] Yasunobu NAGAYA, Takamasa MORI, Impact of Perturbed Fission Source on the Effective Multiplication Factor in Monte Carlo Perturbation Calculation, Journal of NUCLEAR SCIENCE and TECHNOLOGY, Vol. 42, No. 5, p. 428-441, May 2005
- [8] J. Eduard Hoogenboom, Vladimir A. Khotylev, John M. Tholammakkil, Generation of Multi-group Cross Sections and Scattering Matrices with the Monte Carlo Code MCNP5, Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications, April 15-29, 2007
- [9] G. Ilas, N.H Hudson, F. Rahnama, et al, On the few-group cross-section generation methodology for PBR analysis, Annals of Nuclear Energy Vol. 33 pages 1058-1070, 2006