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Uncertainty Propagation of Fine-Group Cross Section Generated by Monte Carlo Method

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1. Introduction

Fine-group cross sections are used in transport calculation of lattice code such as Method Of Characteristics (MOC) code. As fine-group cross sections are used to calculate neutronics parameters such as eigenvalue, and few group constants. the fine-group cross sections are one of the most important factor to calculate neutronics parameters accurately. Commonly when fine-group cross sections are generated, the calculation was performed in an infinite and homogeneous medium [1]. Fine-group cross sections generated by this method are suitable in commercial reactors. However, this method can make a bias caused from complex geometry such as Very High Temperature Reactor (VHTR). In these days, using Monte Carlo (MC) method to generate group cross section [2] was therefore proposed to solve this problem.

Fine-group cross sections generated by MC method have statistical uncertainties. Statistical uncertainties can be reduced by central limit theorem [3]. For the efficient calculation, it is important to estimate effect of statistical error of fine-group cross sections on neutronics parameters.

The main purpose of this study is to figure out effects of fine-group cross sections uncertainties on the neutron multiplication factor. To achieve this goal, fine-group cross sections and their statistical uncertainties were calculated by MC method. Also, uncertainty of the multiplication factor was estimated by error propagation theories. To validate, the estimated uncertainty was compared to the uncertainty calculated by brute force method.

2. Methods and Results

In the section 2.1, the method to generate fine-group cross sections is introduced. Also, fine-group cross section was generated for a sample problem. In section 2.2, uncertainty propagation methods are introduced. Using those methods, uncertainty of fine-group cross sections on the neutron multiplication factor was estimated and validated.

2.1 Fine-group Cross Section Generated by Monte Carlo Method

To calculate fine-group cross sections, group reaction rates are divided by group flux as follows [4]:

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

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

The statistical error of fine-group cross sections can be represented as the standard deviation. The standard deviation of fine-group cross sections is calculated as follows [3]:

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

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

187 group total fine-group cross sections of uranium 235 were generated for a sample problem. The sample problem is illustrated in Fig. 1. Boundaries of the problem are reflected boundaries. Detailed information of the problem is given in Table I. To produce fine-group cross sections, Smart and User-frIendly Monte Carlo Particle Transport Code (SUIT) [5] was used.

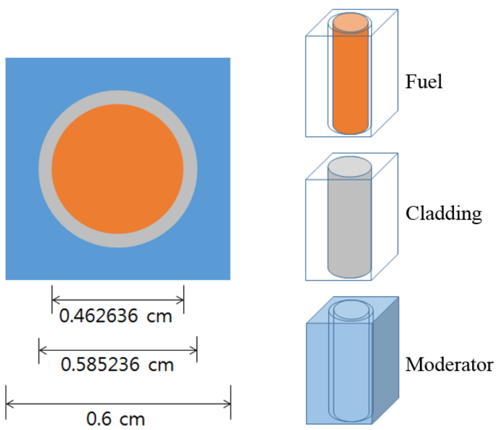

Fig. 1 Description of Sample Problem

Table I: Detail Information of the Sample Problem

Fuel Material Density Enrichment	Uranium Zircaloy 7.86 g/cm^3 19.75w/o
Cladding Material Density	Zircaloy 6.55 g/cm^3

Moderator Material Density	Water 0.658 g/cm^3
Cross Section Library	ENDF-VII

187 group total fine-group cross section of uranium 235 was generated as shown in Fig. 2. To make this cross section, 3,000 particles were transported. The red error bar represents two standard deviation of the cross section. It is shown that uncertainties of cross sections in resonance energy region were higher than those in other energy regions. These statistical error of fine-group cross sections can cause uncertainties of neutronics parameters. Therefore it is essential to estimate of effect of these uncertainties of cross section on calculation results.

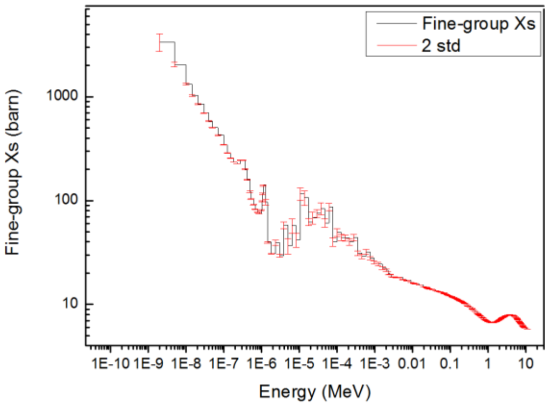

Fig. 2 187 group U-235 Total Fine-group Cross Section

2.2 Estimation Uncertainty of the Multiplication Factor Caused by Statistical Error of Fine-group Cross Section

As the neutron multiplication factor is a function of fine-group cross section, it can be expressed as follows [6]:

$$k_{eff} = f(xs_1, xs_2, xs_3, \dots, xs_n) \tag{3}$$

where k_{eff} is multiplication factor, xs_n is fine-group cross section of n^{th} energy group. Using the sandwich rule[7], variance of k_{eff} can be calculated by Eq. (4).

$$\sigma^2(k_{eff}) \cong \boldsymbol{JVJ}^T \tag{4}$$

$$where \quad \boldsymbol{J} = \left(\frac{\partial k_{eff}}{\partial xs_1}, \frac{\partial k_{eff}}{\partial xs_2}, \dots, \frac{\partial k_{eff}}{\partial xs_n}\right),$$

$$\boldsymbol{V}(i,j) = cov(xs_i, xs_j).$$

The vector $\boldsymbol{J}$ is sensitivity of multiplication factor due to change of fine-group cross section, and the vector $\boldsymbol{V}$ is covariance matrix between fine-group cross sections. The sensitivity of multiplication factor can be calculated by Correlated Sampling Method (CSM) [8], which is one of the MC perturbation methods. Sensitivity of multiplication factor for the sample problem is calculated by SUIT code [5] with CSM as shown in Fig. 3. It is shown that multiplication factor is more sensitive in low energy and resonance energy region than other energy regions.

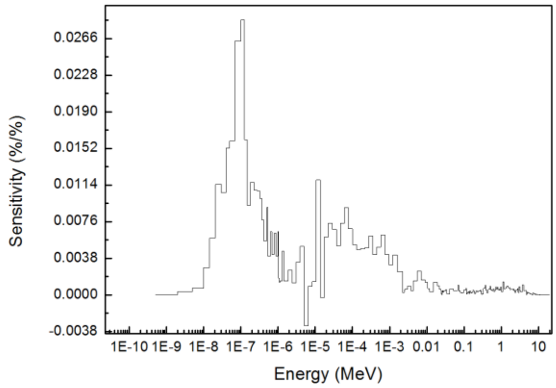

Fig. 3 187 Group Sensitivity of Multiplication Factor

The covariance of two fine-group cross sections is calculated as follows:

$$when \quad xs_t = xs_i + xs_j ,$$

$$\sigma^2(xs_t) = \sigma^2(xs_i) + \sigma^2(xs_j) + 2cov(xs_i, xs_j) \tag{5}$$

$$\therefore\ cov(xs_i, xs_j) = \frac{\sigma^2(xs_t) - \sigma^2(xs_i) - \sigma^2(xs_j)}{2} \tag{6}$$

where $\sigma^2(xs_t)$ is variance of sum of two fine-group cross sections. $cov(xs_i, xs_j)$ is covariance of fine-group cross section xs_i and xs_j. In this study, xs_t is calculated by tallying reaction rate and flux of each energy group as follow:

$$xs_t = xs_i + xs_j = \frac{rr_i}{fl_i} + \frac{rr_j}{fl_j} \tag{7}$$

Where rr_i and fl_i represents i^{th} energy group reaction rate and flux respectively. It is calculated while fine-group cross sections are generated by MC calculation. Using uncertainty propagation formula [2], variance of xs_t is expressed as follow:

$$\begin{aligned}\sigma^2(xs_t) = {} & \sigma^2(rr_i)\left(\frac{\partial xs_t}{\partial rr_i}\right)^2 + \sigma^2(fl_i)\left(\frac{\partial xs_t}{\partial fl_i}\right)^2 \\ & +\sigma^2(rr_j)\left(\frac{\partial xs_t}{\partial rr_j}\right)^2 + \sigma^2(fl_j)\left(\frac{\partial xs_t}{\partial fl_j}\right)^2 \\ & +2cov(fl_i, fl_j)\left(\frac{\partial xs_t}{\partial fl_i}\right)\left(\frac{\partial xs_t}{\partial fl_j}\right) \\ & +2cov(rr_i, rr_j)\left(\frac{\partial xs_t}{\partial rr_i}\right)\left(\frac{\partial xs_t}{\partial rr_j}\right) \\ & +2cov(fl_i, rr_i)\left(\frac{\partial xs_t}{\partial fl_i}\right)\left(\frac{\partial xs_t}{\partial rr_i}\right) \\ & +2cov(fl_i, rr_j)\left(\frac{\partial xs_t}{\partial fl_i}\right)\left(\frac{\partial xs_t}{\partial rr_j}\right) \\ & +2cov(fl_j, rr_i)\left(\frac{\partial xs_t}{\partial fl_j}\right)\left(\frac{\partial xs_t}{\partial rr_i}\right) \\ & +2cov(fl_j, rr_j)\left(\frac{\partial xs_t}{\partial fl_j}\right)\left(\frac{\partial xs_t}{\partial rr_j}\right)\end{aligned} \tag{8}$$

The variance of xs_t can be derived by substituting derivation of Eq. (7) into Eq.(8) as show Eq. (9)

$$\begin{aligned}\sigma^2(xs_t) = \sigma^2(rr_i) \times \left(\frac{1}{fl_i}\right)^2 + \sigma^2(fl_i) \times \left(\frac{rr_i^2}{fl_j^4}\right) \\ + \sigma^2(rr_j) \times \left(\frac{1}{fl_j}\right)^2 + \sigma^2(fl_j) \\ \times \left(\frac{rr_j^2}{fl_j^4}\right) + 2cov(rr_i, fl_i) \times \left(-\frac{rr_i}{fl_i^3}\right) \\ + 2\,cov(fl_i, fl_j) \times \left(\frac{1}{fl_i fl_j}\right) \\ + 2\,cov(rr_i, fl_j) \times \left(-\frac{rr_i}{fl_i fl_j^2}\right) \\ + 2cov(fl_i, rr_j) \times \left(-\frac{rr_i}{fl_i^2 fl_j}\right) \\ + 2cov(fl_i, fl_j) \times \left(\frac{rr_i rr_j}{fl_i^2 fl_j^2}\right) \\ +2cov(rr_j, fl_j) \times \left(-\frac{rr_j}{fl_j^3}\right) \qquad (9)\end{aligned}$$

Using Eq. (9), the variance of sum of two fine-group cross sections is calculated. The relative covariance between two energy groups of total fine-group cross section for the sample problem was calculated as illustrated in Fig. 4.

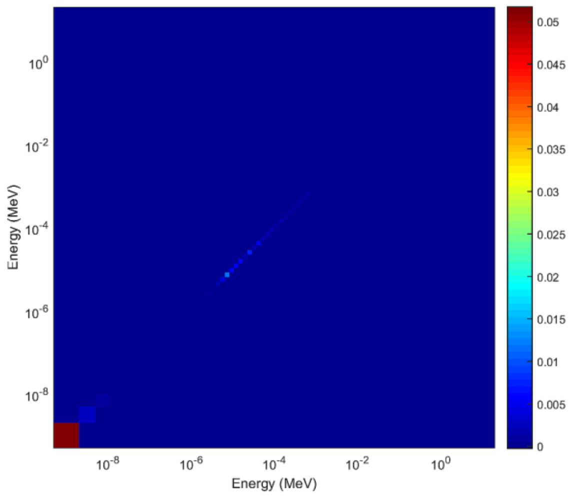

Fig. 4 Relative Covariance Matrix between Uranium 235 Total Fine-group Cross sections

Fig. 4 shows that when a total fine-group cross section is calculated by MC method, it is almost not interfered by fine-group cross section of another energy group. This is quite different result comparing evaluated nuclear covariance data.

Finally, by Eq. (4), standard deviation of multiplication factor for the sample problem was calculated to be 220 pcm. To validate this propagated uncertainty value, benchmarks were performed.

By MC method, 100 fine-group cross section files were generated only changing random number seed for using brute force method. Using these 100 cross sections, 100 multiplication factors were calculated. The standard deviation of these multiplication factors was 213 pcm. In this standard deviation, it contains MC uncertainties of multiplication factors. After removing MC uncertainties, the standard deviation is 206 pcm.

Fig. 5 shows propagated uncertainty value and brute force results. The error of predicted value has good agreement within 7.1% compared to the validation result.

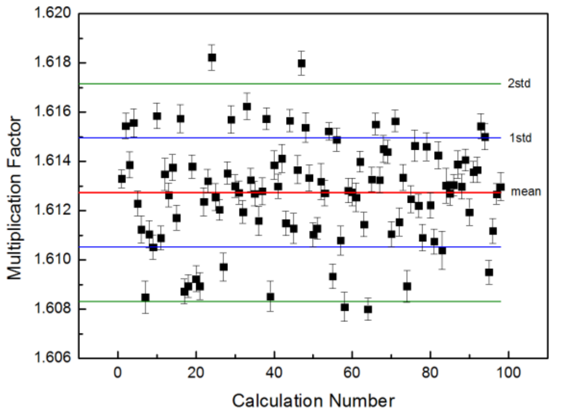

Fig. 5 propagated uncertainty value and brute force results

3. Conclusions

In this study, uncertainty of multiplication factor caused by statistical error of fine-group cross sections was estimated. Uncertainty propagation theories and MC perturbation method were used to analyze uncertainty propagation of statistical error. Using introduced method in this study, it is possible to predict uncertainty of multiplication factor propagated from statistical error of fine-group cross sections. Therefore, it is expected that efficient and accurate generation of fine-group cross sections is possible using results of this study.

4. Acknowledgement

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