Uncertainty Analysis of Few Group Cross Sections Based on Generalized Perturbation Theory

Tae Young Han*, Hyun Chul Lee, Jae Man Noh
Korea Atomic Energy Research Institute, 989-111, Daedeok-daero, Yuseong-gu, Daejeon, Korea
**Corresponding author: tyhan@kaeri.re.kr*

1. Introduction

For sensitivity and uncertainty analyses for general core responses, a two-step method is available and it utilizes the generalized perturbation theory (GPT) for homogenized few group cross sections in the first step and stochastic sampling method for general core responses in the second step. The uncertainty analysis procedure based on GPT in the first step needs the generalized adjoint solution from a cell or lattice code. For this, the generalized adjoint solver has been integrated into DeCART in our previous work [1].

In this paper, MUSAD (Modues of Uncertainty and Sensitivity Analysis for DeCART) [2] code based on the classical perturbation theory was expanded to the function of the sensitivity and uncertainty analysis for few group cross sections based on GPT. First, the uncertainty analysis method based on GPT was described and, in the next section, the preliminary results of the verification calculation on a VHTR pin cell problem were compared with the results by TSUNAMI of SCALE 6.1 [3].

2. Methods and Results

From the sandwich rule [4], the uncertainty of the homogenized few group cross section caused by the uncertainty of the nuclear data can be calculated by the product of the sensitivity of the group cross section and the covariance data inside the evaluated nuclear data. The sensitivity coefficient needs a generalized adjoint solution in a cell or lattice of interest. One can see the procedure for the generalized adjoint solution in the reference 1. After obtaining the solution, the sensitivity coefficient for the few group cross sections can be derived using the generalized perturbation theory.

2.1 Sensitivity Analysis based on GPT

The general response is commonly expressed as the following.

$$R = \frac{<H_1(\alpha)\phi(\alpha)>}{<H_2(\alpha)\phi(\alpha)>} \tag{1}$$

Here, α is an input parameter such as multi-group cross section and H_1 and H_2 are response functions such as few group cross sections in this study.

Neglecting over the second order term, the small perturbation of the general response, Eq.(1), can be approximated as the following

$$\delta R \cong \left\langle \left(\frac{\partial R}{\partial H_1}\frac{\partial H_1}{\partial \alpha} + \frac{\partial R}{\partial H_2}\frac{\partial H_2}{\partial \alpha} + \frac{\partial R}{\partial \phi}\frac{\partial \phi}{\partial \alpha} \right) \delta\alpha \right\rangle \tag{2}$$

Using the definition of the general response, Eq.(1), Eq.(2) can be rewritten as

$$\frac{\delta R}{R} \cong \frac{<\delta H_1\phi>}{<H_1\phi>} - \frac{<\delta H_2\phi>}{<H_2\phi>} + \frac{<H_1\delta\phi>}{<H_1\phi>} - \frac{<H_2\delta\phi>}{<H_2\phi>} \tag{3}$$

The first two terms can be easily calculated from their definitions, and the last two terms can be transformed to a simple form by the solution of the generalized adjoint equation.

For this, we need the first order perturbed equation for the eigenvalue problem as the following

$$(A - \lambda B)\delta\phi = -(\delta A - \lambda \delta B)\phi + \delta\lambda B\phi \tag{4}$$

As described in the reference 1, the generalized adjoint equation can be defined as the following

$$(A^* - \lambda B^*)\Gamma^* = S^* \equiv \frac{1}{R}\frac{\partial R}{\partial \phi} = \frac{H_1}{<H_1\phi>} - \frac{H_2}{<H_2\phi>} \tag{5}$$

Here, Γ^* is the generalized adjoint solution which can be appropriately determined according to the generalized adjoint source term in the right side.

Taking the inner product with the weight of Γ^* in Eq.(4) and the weight of $\delta\phi$ in Eq.(5), and using the definition of the adjoint operator and the auxiliary condition, $< \Gamma^* B\phi > = 0$ [1], the sensitivity of the general response can be readily rewritten as the following

$$S_{R,\alpha} = \frac{\delta R}{\delta \alpha}\frac{\alpha}{R} = \left(\frac{<\delta H_1\phi>}{<H_1\phi>} - \frac{<\delta H_2\phi>}{<H_2\phi>} - < \Gamma^*(\delta A - \lambda \delta B)\phi > \right) \frac{\alpha}{\delta\alpha} \tag{6}$$

If the general response is a few group microscopic cross section for nuclide *i*, the sensitivity coefficient has the form as the following

$$S_{\sigma_R^i,\sigma_{xg}^i} = \frac{\sigma_{xg}^i < \frac{\delta\sigma_R^i}{\delta\sigma_{xg}^i}\phi >}{<\sigma_R^i\phi>} - \sigma_{xg}^i < \Gamma^* \left(\frac{\delta A}{\delta\sigma_{xg}^i} - \lambda \frac{\delta B}{\delta\sigma_{xg}^i} \right) \phi > = T_{0Rxg}^i + T_{1xgz}^i + T_{2xgz}^i + T_{3xgz}^i \tag{7}$$

$$T_{0Rxg}^{i} = \begin{cases} \frac{\sigma_{xg}^{i}\phi_g}{<\sigma_R^i\phi>} & if\ R = x \\ 0 & otherwise \end{cases}$$
$$T_{1xgz}^{i} = -\Sigma_{xg}^{i} V_z \sum_l \sum_m \frac{2l+1}{4\pi} \phi_{glm}\Gamma_{glm}^{*}$$
$$T_{2xgz}^{i} = \frac{1}{4\pi}\frac{1}{k} V_z \bar{\nu}_g^i \Sigma_{fg}^{i} \phi_g \sum_{g'} \left(\chi_{g'}^{i}, \Gamma_{g'}^{*}\right)$$
$$T_{3xgz}^{i} = V_z \sum_{g'} \sum_l \frac{2l+1}{4\pi} \Sigma_{sgg'}^{il} \sum_m \phi_{glm}\Gamma_{g'lm}^{*}$$

Here, l is the Legendre order and m is flux moments corresponding to l. They are similar to the sensitivity coefficients of the classical perturbation theory [2] except T_{0Rxg}^{i} term that is caused by the perturbation of the general response, σ_R^i.

2.2 Uncertainty Quantification

The uncertainty of the general response caused by the nuclear data can be obtained using the sandwich rule as the following.

$$u_{\sigma_R^k}^2 = S_{\sigma_R^k,\sigma_x^i} C_{\sigma_x^i \sigma_y^j} S_{\sigma_R^k,\sigma_y^j}^T \tag{8}$$

Here, $C_{\sigma_x^i \sigma_y^j}$ is the relative covariance matrix for x, y reaction pair of i, j nuclide and $S_{\sigma_R^k,\sigma_x^i}$ is the sensitivity coefficient vector for the R reaction response of k nuclide caused by x reaction of i nuclide.

2.3 Calculation Results

For the verification of MUSAD based on GPT, the results of the code on PMR200 pin cell designed by KAERI as a VHTR core were compared to them of TSUNAMI. In the calculations, TSUNAMI used the covariance data of SCALE 44 group built in SCALE 6.1 and MUSAD used the covariance data of ENDF/B-VII.1 with 238 group structure which is obtained using ERRORR(J) of NJOY, the multi-group cross section with 238 group structure processed by McCARD, and the forward and generalized adjoint solution from TSUNAMI not DeCART for the coincidence of the group structure. As is known in the reference 1, two codes, however, generate the similar generalized adjoint solution.

Table I shows the comparisons of the uncertainty for the one group microscopic capture cross section of U238 induced by the perturbed cross sections of U235 and U238. Except the uncertainty by the scattering cross section, two codes produced similar results. The discrepancy of the uncertainty by the scattering cross section between MUSAD and TSUNAMI may be related to differences in the order of flux moment. TSUNAMI uses 3rd order flux moment and MUSAD, however, uses only 0th order generalized adjoint flux moment in this study. In addition, the difference affects T_{1xgz}^{i} term in Eq.(7) and causes the small error of the uncertainty calculation by the capture and the fission cross section of U235 in particular. In case of U238, the uncertainty is dominantly dependent on T_{0Rxg}^{i} that is determined by the cross section and flux. Thus, the two results of the uncertainty caused by the U238 capture and capture variance are in a good agreement.

Table I : Uncertainty of U238 Capture XS

Nuclide	Cov. XS	TSUNAMI σ_{xx} (%)	MUSAD σ_{xx} (%)
Cov. Data		SCALE 44G	ENDF/B-VII.1 238G
U238	capture, capture	0.928	0.911
	capture, scattering	0.089	0.060
	scattering, scattering	0.074	0.021
U235	capture, capture	0.053	0.048
	capture, fission	*0.019	*0.018
	capture, scattering	0.002	0.002
	fission, fission	0.026	0.038
Total		0.937	0.921

* means negative covariance.

3. Conclusions

In this paper, the methodology of the sensitivity and uncertainty analysis code based on GPT was described and the preliminary verification calculations on the PMR200 pin cell problem were carried out. As a result, they are in a good agreement when compared with the results by TSUNAMI. From this study, it is expected that MUSAD code based on GPT can produce the uncertainty of the homogenized few group microscopic cross sections for a core simulator.

REFERENCES

[1] T. Y. Han, et al., "Implementation of Generalized Adjoint Equation Solver for DeCART," Korean Nuclear Society Spring Meeting, Gyeongju, Korea, October 24-25, 2013.
[2] T. Y. Han, et al., "Verification of Sensitivity and Uncertainty Analysis Code with the GODIVA and VHTR fuel," Korean Nuclear Society Spring Meeting, Gwangju, Korea, May 30-31, 2013.
[3] B.T. Rearden, et al., "Applications of the TSUNAMI Sensitivity and Uncertainty Analysis Methodology," Proceedings of the 7th International Conference on Nuclear Criticality Safety (ICNC2003), October, 2003, Tokai-Mura, Japan (2003).
[4] Cacuci, D.G., "Sensitivity and Uncertainty Analysis," vol. 1. Chapman & Hall/CRC, (2003).