Macroscopic Few Group Cross Section Adjustment in Reflector Region using GLS Method

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Keywords : two-step core analysis, cross section adjustment, uncertainty estimation of group constant, generalized least square method

1. Introduction

The generation of few-group constants (FGCs) plays a crucial role in ensuring the accuracy of two-step core analysis. Consequently, many lattice codes have employed various methods to preserve whole core characteristics within lattice geometry during calculations. Despite these efforts, producing 'appropriate' FGCs for whole core analysis, particularly in the reflector region, remains a challenging and important issue, given that it is known to have a significant impact on the core power distribution [1-2]. In such contexts, many core calculation codes have attempted to address this concern by treating the reflector region exceptionally, altering the cross sections themselves.

At this point, we aimed to reduce errors in the 2-step core calculation by adjusting the FGCs of the reflector region. There has been a consistent effort to adjust various types of cross sections to fit experimental integral data [3-4] using Monte Carlo codes with Generalized Least Square(GLS) data adjustment method, considering the uncertainties in cross section data arising from its measurement. Similar adjustments can be applied to the FGCs of the reflector region in order to fit the integral data in terms of the best estimate.

In this paper, the complete process for FGC adjustment will be introduced. Microscopic fine group covariance data are utilized to evaluate the covariance matrix of the FGCs [5], and then FGCs are adjusted using the GLS method to match the reference integral data set through nodal calculations. The integral data set and FGCs are generated using McCARD, and the nodal calculation is performed using an in-house nodal code.

2. Cross Section Adjustment with GLS and Covariance Generation of FGCs

In this section, the methodology of cross section adjustment based on GLS and the generation of the covariance matrix of FGCs are described.

2.1 Cross Section Adjustment using GLS

Evaluating posterior expectation of variable set $\vec{x}$ for nonlinear system $\vec{y} = f(\vec{x})$ can be performed by following GLS cost function:

$$\chi^2_{GLS} = (\vec{x} - \vec{x}_e)^T M_x^{-1} (\vec{x} - \vec{x}_e) + (\vec{y} - f(\vec{x}_e))^T M_y^{-1} (\vec{y} - f(\vec{x}_e)). \quad (1)$$

In this context, as we will be employing a nodal calculation system, $\vec{x}$ represents the FGCs, and $\vec{y}$ represents the established reference integral data. The subscript "*e*" denotes the expected value, and the matrice M_x and M_y correspond to the priori covariance matrix of $\vec{x}$ and the covariance matrix of $\vec{y}$, respectively. To minimize the cost function χ^2_{GLS}, following first order approximation is applied to the system:

$$f(\vec{x}) = f(\vec{x}_e) + S \cdot (\vec{x} - \vec{x}_e), \quad (2)$$

and the matrix S is sensitivity matrix of the system, having size $N_y \times N_x$, which is assumed constant due to the first order approximation.

$$S_{ij} = \frac{\partial f_i}{\partial x_j}. \quad (3)$$

The first order solution can then be derived,

$$\vec{x} = \vec{x}_e + M_x \cdot S^T \left(M_y + S \cdot M_x \cdot S^T \right)^{-1} \cdot (\vec{y} - f(\vec{x}_e)), \quad (4)$$

along with the posterior covariance matrix.

$$M_{x,post} = M_x - M_x \cdot S^T \left(M_y + S \cdot M_x \cdot S^T \right)^{-1} \cdot S \cdot M_x. \quad (5)$$

One point that needs to be noted is that our system (nodal calculation) is not inherently linear with respect to FGCs. Therefore, it is necessary to iterate the above process repetitively. Depending on the system used, applying under relaxation in Eq.(4) and Eq.(5) can provide significant assistance in convergence.

2.2 Generating Covariance Matrix

Considering $\Sigma_{\alpha,G}$, which represents macroscopic cross section for the reaction type α and few group G, as a function of macroscopic reaction rate $R_{\alpha,G}$ and group flux ϕ_G, the covariance of macroscopic cross section can be expressed as Eq.(6)[5].

$$\begin{aligned}\mathrm{cov}\left[\Sigma_{\alpha,G},\Sigma_{\alpha',G'}\right] \cong\ & \mathrm{cov}\left[R_{\alpha,G},R_{\alpha',G'}\right]\left(\frac{\partial\Sigma_{\alpha,G}}{\partial R_{\alpha,G}}\right)\left(\frac{\partial\Sigma_{\alpha',G'}}{\partial R_{\alpha',G'}}\right) \\ & + \mathrm{cov}\left[\phi_G,\phi_{G'}\right]\left(\frac{\partial\Sigma_{\alpha,G}}{\partial\phi_G}\right)\left(\frac{\partial\Sigma_{\alpha',G'}}{\partial\phi_{G'}}\right) \\ & + \mathrm{cov}\left[R_{\alpha,G},\phi_{G'}\right]\left(\frac{\partial\Sigma_{\alpha,G}}{\partial R_{\alpha,G}}\right)\left(\frac{\partial\Sigma_{\alpha',G'}}{\partial\phi_{G'}}\right) \\ & + \mathrm{cov}\left[\phi_G,R_{\alpha',G'}\right]\left(\frac{\partial\Sigma_{\alpha,G}}{\partial\phi_G}\right)\left(\frac{\partial\Sigma_{\alpha',G'}}{\partial R_{\alpha',G'}}\right)\end{aligned} \quad (6)$$

And the derivative term in Eq.(6) can be induced as follow:

$$\frac{\partial\Sigma_{\alpha,G}}{\partial R_{\alpha,G}}=\frac{\partial\left(\frac{R_{\alpha,G}}{\phi_G}\right)}{\partial R_{\alpha,G}}\cong\frac{1}{\phi_G},\ \frac{\partial\Sigma_{\alpha,G}}{\partial\phi_G}=\frac{\partial\left(\frac{R_{\alpha,G}}{\phi_G}\right)}{\partial\phi_G}\cong-\frac{R_{\alpha,G}}{{\phi_G}^2} \quad (7)$$

Next, considering that there is no uncertainty for the number densities in reflector region, we can establish that $R_{\alpha,G}$ and ϕ_G are functions of only fine group microscopic cross sections of nuclide i, $\sigma^i_{\alpha,g}$. Accordingly, the covariance terms in equation (6) can be written as Eq.(8), Eq.(9), and Eq.(10) respectively.

$$\begin{aligned}\mathrm{cov}\left[R_{\alpha,G},R_{\alpha',G'}\right] \cong\ & \mathrm{cov}_S\left[R_{\alpha,G},R_{\alpha',G'}\right] \\ & + \sum_{i,g\in G,\alpha}\sum_{i',g'\in G',\alpha'}\mathrm{cov}\left[\sigma^i_{\alpha,g},\sigma^{i'}_{\alpha',g'}\right]\left(\frac{\partial R_{\alpha,G}}{\partial\sigma^i_{\alpha,g}}\right)\left(\frac{\partial R_{\alpha',G'}}{\partial\sigma^{i'}_{\alpha',g'}}\right),\end{aligned} \quad (8)$$

$$\begin{aligned}\mathrm{cov}\left[\phi_G,\phi_{G'}\right] \cong\ & \mathrm{cov}_S\left[\phi_G,\phi_{G'}\right] \\ & + \sum_{i,g\in G,\alpha}\sum_{i',g'\in G',\alpha'}\mathrm{cov}\left[\sigma^i_{\alpha,g},\sigma^{i'}_{\alpha',g'}\right]\left(\frac{\partial\phi_G}{\partial\sigma^i_{\alpha,g}}\right)\left(\frac{\partial\phi_{G'}}{\partial\sigma^{i'}_{\alpha',g'}}\right),\end{aligned} \quad (9)$$

$$\begin{aligned}\mathrm{cov}\left[R_{\alpha,G},\phi_{G'}\right] \cong\ & \mathrm{cov}_S\left[R_{\alpha,G},\phi_{G'}\right] \\ & + \sum_{i,g\in G,\alpha}\sum_{i',g'\in G',\alpha'}\mathrm{cov}\left[\sigma^i_{\alpha,g},\sigma^{i'}_{\alpha',g'}\right]\left(\frac{\partial R_{\alpha,G}}{\partial\sigma^i_{\alpha,g}}\right)\left(\frac{\partial\phi_{G'}}{\partial\sigma^{i'}_{\alpha',g'}}\right),\end{aligned} \quad (10)$$

where subscript "S" denotes the sample covariance which can be obtained from McCARD calculation. The derivative terms in above Eq.(8), Eq.(9), and Eq.(10) can be induced in the same manner as for Eq.(7).

$$\frac{\partial R_{\alpha,G}}{\partial\sigma^i_{\alpha,g}}=\frac{\partial\left(\sum_i\left(\sum_{g\in G}\sigma^i_{\alpha,g}\phi_g\right)N_i\right)}{\partial\sigma^i_{\alpha,g}}\cong\phi_g N_i, \quad (11)$$

$$\frac{\partial\phi_G}{\partial\sigma^i_{\alpha,g}}=\frac{\partial\sum_{g\in G}\phi_g}{\partial\left(\frac{r^i_{\alpha,g}}{\phi_g}\right)}\cong-\frac{{\phi_g}^2}{r^i_{\alpha,g}}=-\frac{\phi_g}{\sigma^i_{\alpha,g}}, \quad (12)$$

where $r^i_{\alpha,g}$ is microscopic reaction rate for the reaction reaction type α, fine group g, and nuclide i, and N_i is number density of nuclide i.

After obtaining covariance terms of microscopic cross section in Eq.(8), Eq.(9), and Eq.(10) using ERRORJ[6], the covariance matrix of FGCs can be evaluated from Eq.(6~12).

3. Calculation Result

We selected the first cycle of the SHINKORI-1 reactor for our simulation. Two-group assembly-wise homogenized constants for fuel assemblies with B1 critical spectrum are generated using McCARD. In-house nodal code performs a two-group nodal calculation to obtain the assembly-wise power distribution, which serves as integral data. The reference integral data and its covariance are configured based on the results of the McCARD whole core calculation. The core description is presented in Figure 1.

The FGCs and their covariance matrix for the reflector cells, categorized into four types based on the baffle structure have been computed. It is observed that, irrespective of the reflector type, there exists a positive correlation coefficient ranging from approximately 0.2200 to 0.2237 between the macroscopic absorption cross sections of the fast and thermal groups. The covariance between the macroscopic scattering and absorption cross sections is assumed to be zero, based on prior data indicating no correlation between the two at the microscopic level.

The radial power distributions and k_{eff} are used as integral data in the adjustment procedure. Figure 3 and 4 respectively illustrate the radial power distribution error before and after the adjustment. The root mean square (RMS) error for the radial power distributions has significantly decreased from 1.21% to 0.78%, while the error in k_{eff} has slightly increased from 40 pcm to 44 pcm. This is simply a result of the relatively small partition of k_{eff} in the objective function.

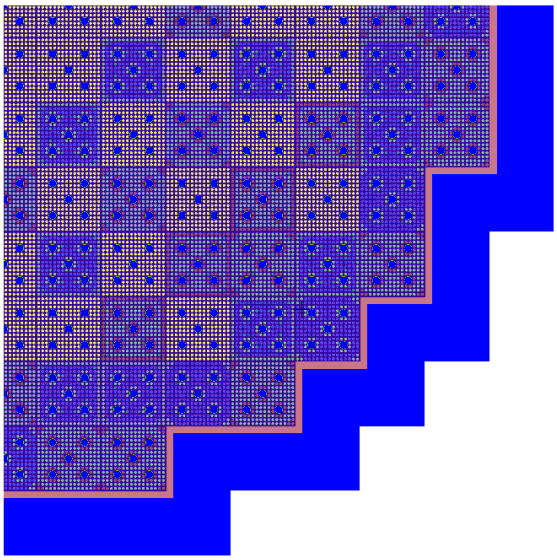

Fig 1. Discription of the first cycle of SHINKORI-1 core is displayed above.

	Reference	Before Adjustment	After Adjustment
k_{eff}	1.03881	1.03921	1.03925
Difference(pcm)	-	+40	+44
Max. Error of Radial Power (%)	-	-2.91	-1.16
RMS Error of Radial Power (%)	-	1.21	0.78

Fig 2. The results of the two-step calculation before and after the adjustment were compared. Increment of k_{eff} error and decrement of power error can be observed through adjustment of FGCs.

0.08	-0.26	-0.74	0.94	-0.77	-1.11	-0.54	-2.81
-0.26	-0.46	1.19	-0.80	1.28	-0.99	-0.23	-2.84
-0.74	1.19	-0.55	1.57	-0.38	1.07	0.41	-1.61
0.94	-0.80	1.57	-0.21	1.65	-0.54	0.43	
-0.77	1.28	-0.38	1.65	1.25	1.47	0.28	
-1.11	-0.99	1.07	-0.54	1.47	1.30		
-0.54	-0.23	0.41	0.43	0.28			
-2.81	-2.84	-1.61					

Fig 3. Radial power distribution before adjustment are displayed. The maximum and RMS power error is -2.81%, and 1.21% respectively.

-0.37	-0.70	-1.14	0.63	-0.84	-0.71	0.61	-0.34
-0.70	-0.90	0.76	-1.14	1.13	-0.76	0.67	-0.68
-1.14	0.76	-0.99	1.13	-0.73	0.90	0.55	-0.47
0.63	-1.14	1.13	-0.74	1.03	-1.16	-0.21	
-0.84	1.13	-0.73	1.03	0.37	0.34	-0.68	
-0.71	-0.76	0.90	-1.16	0.34	-0.50		
0.61	0.67	0.55	-0.21	-0.68			
-0.34	-0.68	-0.47					

Fig 4. Radial power distribution after adjustment are displayed. The maximum and RMS power error is -1.16%, and 0.78% respectively, which is significantly improved compared to before.

4. Conclusion

Regarding the reduction of errors in integral data, we observed the effectiveness of FGCs adjustment. While this paper employed transport calculation results as integral data, the described procedure can be applied to a wide range of 2-step calculation codes that tailor themselves to on-site experimental integral data.

The errors in two-step calculations are likely not solely the result of FGCs' uncertainty but are also influenced by the computational methodology employed in the code. Given that the adjustment of FGCs can operate differently depending on the calculation code used, these adjusted FGCs can assume a role akin to customization of the system. This allows them to closely replicate desired scenarios from the perspective of a specific code. Such an approach can act as an alternative for codes grappling with excessive methodological alterations to align with specific experimental data.

ACKNOWLEGMENT

This work was supported by KOREA HYDRO & NUCLEAR POWER CO.. LTD(22-TECH-02).

REFERENCES

[1] Y. Perin et al., Challenge of PWR new core design simulation: A focus on uncertainties due to nuclear data and reflector modelling, Progress in Nuclear Energy, Vol 84, p.89-96, Sep 2015.
[2] Pavel Suk, Jan Frýbort, Reflector macroscopic cross-section data uncertainties effect on the nodal code full-core calculation, Nuclear Engineering and Design, Vol 366, 110743, Sep 2020.
[3] C. De Saint Jean et al., Evaluation of Cross Section Uncertainties Using Physical Constraints: Focus on Integral

Experiments, Nuclear Data Sheets, Vol 123, p.178-184, Jan 2015.
[4] Dong Hyuk Lee., Establishment and Applications of Monte Carlo Sensitivity and Uncertainty Analysis Framework Based on Continuous-Energy Covariance Data, Ph.D. dissertation, Dept. Nuc.Eng., SNU, 2021.
[5] Ho Jin Park., Generation of Assembly-Homogenized Few Group Constants and Estimation of Their Uncertainties by Monte Carlo Method, Ph.D. dissertation, Dept. Nuc.Eng., SNU, 2011.
[6] Go Chiba, "ERRORJ, A Code to Process Neutron-Nuclide Reaction Covariance, Version 2.3," JAEA-Data/Code 2007-007, March 2007.