Sensitivity and Uncertainty Analysis for UAM Pin-Cell Benchmark by McCARD

Ho Jin Park [a*], Jin Young Cho [a], Hyung Jin Shim [b]
[a]*Korea Atomic Energy Research Institute , 111, Daedeok-daero 989beon-gil, Daejeon, 305-353, Korea*
[b]*Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Korea*
[*]*Corresponding author: parkhj@kaeri.re.kr*

1. Introduction

Recently, there have been various approaches [1,2] to quantify uncertainty of design parameters such as k_{eff}, power distribution, and critical boron concentration (CBC) from covariance data of the cross section. The common approaches available for this interesting subject are the direct sampling method (DSM) often called the brute force method and the perturbation-theory based method. In the perturbation-theory based analysis, the uncertainty of the output is quantified from its sensitivities to the input parameters by the uncertainty propagation formulations.

In references 3 and 4, we present the uncertainty propagation equations in few group diffusion theory constants (FGCs) generation with the Monte Carlo (MC) code McCARD, and describe how to utilize them to determine uncertainties of the core design parameters by DSM for a two-step neutronics design calculation. Moreover, the formulation aimed at quantifying uncertainties of the reactor core design parameters in the direct MC calculation is presented in reference 5.

In this study, we perform an uncertainty qualification of FGCs for TMI-1 pin-cell benchmark, one of the OECD benchmarks for Uncertainty Analysis Modeling (UAM) [6] for the design, operation and safety analysis of LWRs by the uncertainty propagation equation and compare it with the results by the direct MC calculations.

2. Methods and Results

2.1 Verification of MC Perturbation for uncertainties of FGC

In order to calculate uncertainties of FGCs, the sensitivity coefficients for the change of the MC tallies, such as macroscopic reaction rate R and flux ϕ, due to the change of microscopic cross section data will be calculated by the MC perturbation technique. In this section, the prediction capability of the MC perturbation for δR or $\delta\phi$ caused by perturbations in microscopic cross section σ is assessed in the *Godiva* and TMI-1 PWR fuel pin problem. The fission and capture cross sections of U^{235} are assumed to be perturbed by as much as 5% in the whole neutron energy regions. To obtain reference solutions for these problems by direct subtraction, MC calculations are performed for 50 inactive and 10,000 active cycles on 100,000 histories per cycle while the MC perturbation analyses with 10,000 histories per cycle and 1,000 active cycles are performed for each case.

Table I: Comparison of δR_α for the 5% perturbation of U^{235} fission cross section in *Godiva* problem

Reaction Type(α)	δR_α ($\#/barn \cdot cm \cdot source\ neutron$)		
	Direct Subtraction	MC Perturbation	Diff.(%)*
fission	-2.25×10^{-6} $\pm$ 0.17%	-2.26×10^{-6}	0.72
(n,γ)	-3.52×10^{-7} $\pm$ 0.19%	-3.54×10^{-7}	0.69

*Diff=$\left(\delta R_\alpha^{MCPert}-\delta R_\alpha^{Direct}\right)/\delta R_\alpha^{Direct}\times100$

Table II: Comparison of δR_α for the 5% perturbation of U^{235} (n,γ) cross section in TMI-1 fuel pin problem

Reaction Type(α)	δR_α ($\#/barn \cdot cm \cdot source\ neutron$)		
	Direct Subtraction	MC Perturbation	Diff.(%)*
fission	-1.25×10^{-4} $\pm$ 1.92%	-1.26×10^{-4}	0.35
(n,γ)	-5.70×10^{-5} $\pm$ 2.61%	-5.72×10^{-5}	0.40

*Diff=$\left(\delta R_\alpha^{MCPert}-\delta R_\alpha^{Direct}\right)/\delta R_\alpha^{Direct}\times100$

Table III: Comparison of $\delta\phi$ for the 5% perturbation of U^{235} fission cross section in *Godiva* problem

$\delta\phi$ ($\#/barn \cdot source\ neutron$)		
Direct Subtraction	MC Perturbation	Diff.(%)*
-3.87×10^{-5} $\pm$ 0.18%	-3.89×10^{-5}	0.74

*Diff=$\left(\delta\phi^{MCPert}-\delta\phi^{Direct}\right)/\delta\phi^{Direct}\times100$

Table I and II show a comparison of δR_α calculated by the MC perturbation calculations while table III shows a comparison of $\delta\phi$. Overall, the MC perturbation predicts well the reference solution.

2.2 Uncertainties Quantification of FGCs

The S&U analysis module of McCARD and uncertainty propagation formulation is applied to the TMI-1 fuel pin problem, which is one of the UAM benchmarks. The nuclear cross section data including the covariance data files for computing both the two group constants and their uncertainties are obtained from ENDF/B-VII.1. The covariance data files of only the two major uranium isotopes U^{235} and U^{238} are used.

Table IV: TMI-1 fuel pin homogenized two group cross sections and their percentile relative errors (% RE)

Two Group Constants	$\Sigma_{\alpha,G}$ (cm^{-1})	% RE
$\Sigma_{\gamma 1}$	7.42×10^{-3}	0.12
$\Sigma_{\gamma 2}$	2.25×10^{-2}	0.38
$\nu\Sigma_{f1}$	8.67×10^{-3}	0.59
$\nu\Sigma_{f2}$	1.79×10^{-1}	0.70
$\Sigma_{s1\rightarrow2}$	1.69×10^{-2}	3.40
D_1	1.32×10^{0}	0.55
D_2	4.81×10^{-1}	0.10

Table V: Correlation coefficients matrix of TMI-1 fuel pin homogenized two group cross sections

	$\Sigma_{\gamma1}$	Σ_{f1}	$\nu\Sigma_{f1}$	$\Sigma_{\gamma2}$	Σ_{f2}	$\nu\Sigma_{f2}$
$\Sigma_{\gamma1}$	1.00	-0.59	-0.10	0.48	-0.36	-0.59
Σ_{f1}	-0.59	1.00	0.17	-0.07	0.22	0.04
$\nu\Sigma_{f1}$	-0.10	0.17	1.00	-0.01	0.04	0.43
$\Sigma_{\gamma2}$	0.48	-0.07	-0.01	1.00	-0.40	0.07
Σ_{f2}	-0.36	0.22	0.04	-0.40	1.00	0.17
$\nu\Sigma_{f2}$	-0.59	0.04	0.43	0.07	0.17	1.00

Tables IV represents the homogenized two group constants of TMI-1 fuel pin and their percentile relative errors (% RE) calculated by McCARD. The %RE is defined as $100\times\sigma(\mathrm{X})/\mathrm{X}$ in which X and σ(X) denote any member of the two group constants and its standard deviation (SD), respectively. The relative errors contain contributions from both statistical and U^{235} and U^{238} cross section uncertainties. As can be seen in Table IV, the fast and thermal group $\nu\times$fission cross sections have relatively higher %RE than the remaining types of the two group constants. Table V represents the correlation coefficients matrix between homogenized two group constants. The correlation coefficient matrix or covariance matrix between FGCs will be used for uncertainty quantification of design parameter in nodal whole core calculation.

2.3 Quantification Test for Uncertainties of FGCs

To perform a quantification test for the uncertainties of FGCs generated in the previous section, the uncertainties in k_∞ of a two-step calculation are calculated using the sensitivities of k_∞ by the two-group diffusion equations as shown in Eq.(1).

$$\begin{aligned}&\Sigma_{a1}\phi_1+\Sigma_r\phi_1=\frac{1}{k_\infty}\left(\nu\Sigma_{f1}\phi_1+\nu\Sigma_{f2}\phi_2\right)\\&\Sigma_{a2}\phi_2=\Sigma_r\phi_1\\&where\ \Sigma_r=\Sigma_{s1\rightarrow2}\end{aligned}\tag{1}$$

From the uncertainty propagation formulation, one can determine the variance of k_∞ as follow:

$$\begin{aligned}\sigma^2\left(k_\infty\right)&=\sum_{\alpha'',g''}\sum_{\alpha''',g'''}\mathrm{cov}[\Sigma_{\alpha'',g''},\Sigma_{\alpha''',g'''}]\cdot\frac{\partial k_\infty}{\partial\Sigma_{\alpha'',g''}}\cdot\frac{\partial k_\infty}{\partial\Sigma_{\alpha''',g'''}}\\&\cong\sum_{\alpha'',g''}\sum_{\alpha''',g'''}\rho[\Sigma_{\alpha'',g''},\Sigma_{\alpha''',g'''}]\cdot\delta k_\infty\left(\Sigma_{\alpha'',g''}\right)\cdot\delta k_\infty\left(\Sigma_{\alpha''',g'''}\right)\end{aligned}\tag{2}$$

The correlation coefficients between FGCs $\rho[X,Y]$ here are defined by $\mathrm{cov}[X,Y]/\sigma(X)\sigma(Y)$ with X or Y denoting $\Sigma_{\alpha'',g''}$ which is α -type macroscopic cross section of the g-group. The partial derivative in Eq (2) can be calculated by the following approximation.

$$\frac{\partial k_\infty}{\partial\Sigma_{\alpha,g}}\cong\frac{k_\infty\left(\overline{\Sigma_{\alpha,g}}+\sigma\left(\Sigma_{\alpha,g}\right)\right)-k_\infty\left(\overline{\Sigma_{\alpha,g}}\right)}{\sigma\left(\Sigma_{\alpha,g}\right)}=\frac{\delta k_\infty\left(\Sigma_{\alpha,g}\right)}{\sigma\left(\Sigma_{\alpha,g}\right)}\tag{3}$$

Table VI: Contribution of cross section uncertainties of Uranium isotopes to $\sigma^2(k_\infty)$ of TMI-1 fuel pin

Isotope	Reaction Type	$\sigma^2(k_\infty)$	
		Two-Step	Direct MC
U^{235}	fission	0.00084	0.00112
	(n,γ)	0.00289	0.00295
	ν	0.00855	0.00853
U^{238}	fission	0.00053	0.00022
	(n,γ)	0.00379	0.00416
	ν	0.00117	0.00102
Total		0. 00980	0.01016

Table VI shows the uncertainties of k_∞ by a two-step calculation and direct MC calculations for a TMI-1 fuel pin, respectively. In the direct MC calculation, we estimated the uncertainty of k_∞ using the sensitivities of k_∞ with respect to nuclear cross section data uncertainties from the direct McCARD calculation. Figure 1 shows the computational flow chart for the

quantification test of the uncertainties of FGCs by two-step calculation.

The contribution to $\sigma^2(k_\infty)$ arising from ν data uncertainties of U^{235} is dominant. It was noted that the uncertainties of k_∞ from the two-step calculation and the direct MC calculation are very similar.

3. Conclusions

In this study, an uncertainty quantification analysis of FGCs for a TMI-1 fuel pin, one of the UAM benchmarks is performed by McCARD. In order to examine the effectiveness of the uncertainty of FGCs, the uncertainty of k_∞ by the approximated two-group diffusion equations are calculated and compared with that by MC direct calculation counterparts. The uncertainty of k_∞ by the two-step calculation is comparable to that by the direct MC calculation. Because the uncertainty of FGCs contains both statistical and nuclear cross section data uncertainties and are influenced by the uncertainty propagation in the FGCs generation procedure, the uncertainty of k_∞ by the two-step calculation are slightly different from that by the direct MC calculation.

As the next step of this study, an uncertainty quantification analysis of the core parameter for the UAM benchmarks will be conducted by the McCARD/MASTER-based two-step neutronic design system [4]. In this system, we have adopted the DSM which involves a random sampling of a finite number of FGCs sets.

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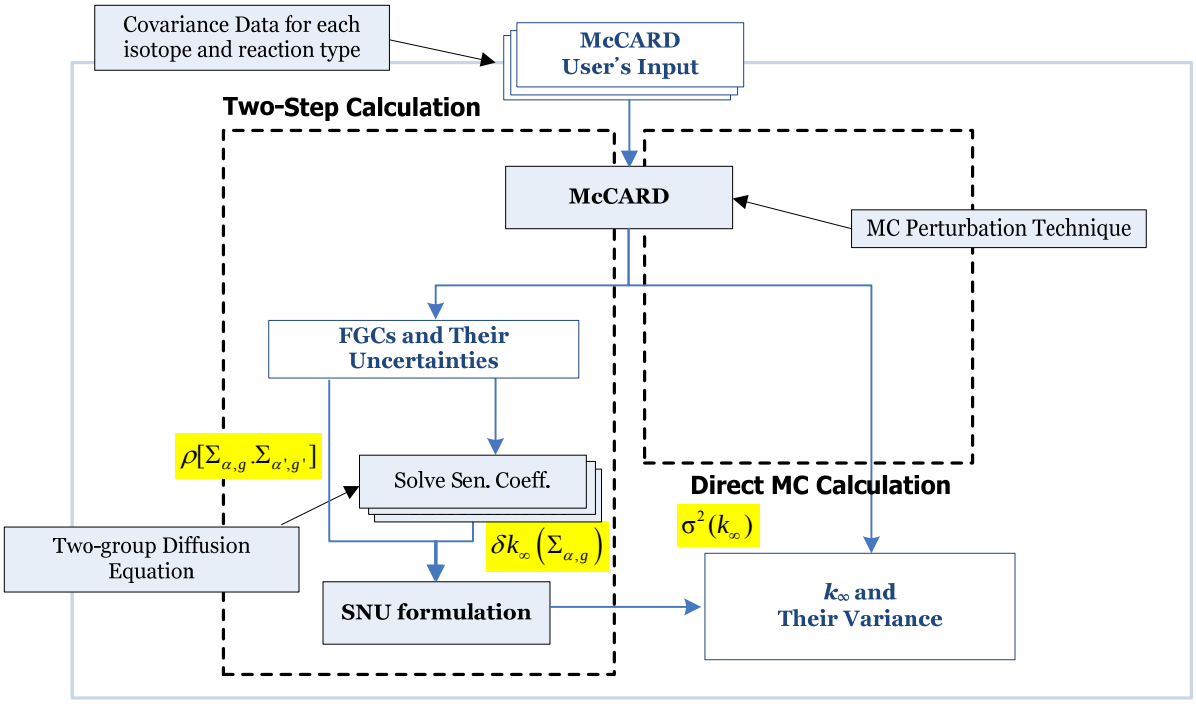

Fig. 1. Computational Flow chart for Quantification Test of Uncertainties of FGCs