MIG 1.5 Code for Random Sampling of Multiple Correlated Variables

Ho Jin Park [a*], Tae Young Han [a], Jin Young Cho[a]
[a]*Korea Atomic Energy Research Institute, 111, Daedeok-daero 989 Beon-gil, Daejeon, 34057*
[*]*Corresponding author: parkhj@kaeri.re.kr*

1. Introduction

The Korea Atomic Energy Research Institute (KAERI) uses McCARD [1], a Monte Carlo (MC) neutron-photon transport simulation code, as a tool of generating a reference solution for a wide range of nuclear reactors, and as a neutronics design analysis code for a research reactor such as Jordan Research Training Reactor (JRTR) [2]. McCARD has been equipped with various special features for a challengeable large-scale reactor calculation. As a part of efficiency-enhancement methods for MC nuclear reactor analysis, the B_1 theory-augmented MC method [3] for the generation of Few Group Constants (FGCs) was implemented into McCARD. Reference and branch calculations are essential for the tabularization of FGCs as a function of state parameters such as *burnup, soluble boron concentration, and various temperature*. To automate all procedures for FGC generation, MIG (McCARD Input Generator) and MOCHA (McCARD Output Converter into Homogenized FGC ASCII file) utility codes have been developed [3]. The latest MIG code, MIG 1.5, is capable of performing multiple-correlated sampling to estimate uncertainties of nuclear reactor core design parameters by means of a direct sampling method (DSM). In this study, multiple-correlated sampling methods [4], [5], such as the Cholesky decomposition method and the LDL^T decomposition method, are implemented into the MIG code, and the numerical results for the applications are provided.

2. Direct Sampling Methods and Validation

2.1 Direct Sampling Method

One can formally define the mean value and variance for a tally parameter, *Q*, as follows:

$$\overline{Q^i} \cong \frac{1}{K}\sum_{k=1}^{K} Q_k^i \tag{1}$$

$$\sigma^2(Q^i) \cong \frac{1}{K-1}\sum_{k=1}^{K}(Q_k^i - \overline{Q^i})^2, \tag{2}$$

where Q_k^i denotes the *i*-th parameter for a *k*-th sample. A covariance between the *i*-th and *j*-th parameters, $\mathrm{cov}[Q^i, Q^j]$, can be calculated by

$$\mathrm{cov}[Q^i, Q^j] \cong \frac{1}{K-1}\sum_{k=1}^{K}(Q_k^i - \overline{Q^i})(Q_k^j - \overline{Q^j}). \tag{3}$$

Suppose that $\mathbf{C}_Q$ is the covariance matrix defined by $\mathrm{cov}[Q^i, Q^j]$ and that a lower triangular matrix **B** is known through the Cholesky decomposition of $\mathbf{C}_Q$, then we have

$$\mathbf{C}_Q = \mathbf{B}\cdot\mathbf{B}^T \tag{4}$$

where $\mathbf{B}^T$ is the transpose matrix of **B**. Then, one can obtain a sample set by:

$$\mathbf{X}^\kappa = \overline{\mathbf{X}} + \mathbf{B}\cdot\mathbf{Z} \tag{5}$$

where $\overline{\mathbf{X}}$ is the mean vector defined by the mean values from Eq.(1), and **Z** is a random normal vector calculated directly from a random sampling of the standard normal distribution. In this study, **Z** is calculated using the Box-Muller method. If $\mathbf{C}_Q$ is symmetrical but not positive definite, then the Cholesky decomposition method will not be valid. In that case of a positive semi-definite matrix, LDL^T decomposition method can be utilized as an alternative method. In the LDL^T decomposition method, the covariance matrix can be expressed by lower-triangular (**L**) and diagonal (**D**) matrices as below:

$$\mathbf{C}_Q = \mathbf{L}\cdot\mathbf{D}\cdot\mathbf{L}^T \tag{6}$$

The multiple-correlated variables can be generated by

$$\mathbf{X}^\kappa = \overline{\mathbf{X}} + (\mathbf{L}\cdot\mathbf{D}^{1/2})\cdot\mathbf{Z}. \tag{7}$$

The LDL^T and Cholesky decomposition modules are implemented into the MIG 1.5 code.

2.2 Verification and Validation for Direct Sampling Module

To verify the newly implemented LDL^T and Cholesky decomposition modules, test problems using two 3x3 covariance matrices are considered; the relevant matrices are as follows:

$$\mathbf{C}_{P1} = \begin{bmatrix} 1.0 & 0 & 0 \\ 0 & 1.0 & 0 \\ 0 & 0 & 1.0 \end{bmatrix} \tag{8}$$

$$\mathbf{C}_{P2} = \begin{bmatrix} 1.0 & 0.2 & 0.0 \\ 0.2 & 1.0 & -0.2 \\ 0.0 & -0.2 & 1.0 \end{bmatrix} \quad (9)$$

In Table I, covariance values calculated from 10^6 samples are presented; the values were obtained using the *Cholesky* and LDL^T decomposition modules in the MIG code. Here, a_{ij} denotes the element in the *i*-th row, the *j*-th column of the covariance matrix. It is noted that the sampled covariance agree well with the reference.

Table I: Comparison of covariance from 10^6 samples generated by MIG with reference

case		Reference	Sampled covariance	
			Cholesky	LDL^T
P1	a_{11}	1.000	1.002	1.002
	a_{12}	0.000	~0.000	~0.000
	a_{13}	0.000	~0.000	~0.000
P2	a_{11}	1.000	1.002	1.002
	a_{12}	0.200	0.199	0.199
	a_{23}	-0.200	-0.199	-0.208

3. Application of Direct Sampling Method by MIG

3.1 Uncertainty Propagation Analysis in Two-Step Procedure Based on the MC method

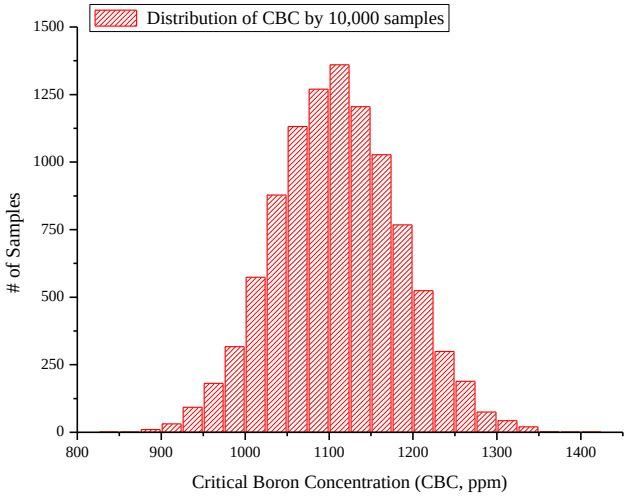

Fig. 1. Distribution of critical boron concentration from the 10,000 samples by two-group constants input sets for YGN4

Recently, there have been various studies [5,6] conducted that utilize DSM calculations that are based on a two-step procedure code system. In the study study of the McCARD/MASTER two-step code system [5], the authors prepare the covariance matrix between the FGCs of any pair of fuel assemblies (FAs) comprising the core. Using the covariance matrix, MIG can produce FA FGCs input sets by random multiple-correlated sampling. Using the sampled FA FGCs input sets, MASTER can perform direct sampling core calculations. Figure 1 shows a distribution of critical boron concentration (CBC) measured in ppm from a total of 1,000 MASTER computations with 1,000 randomly sampled two-group constant sets for Yonggwang Nuclear Unit 4 (YGN4) PWR core, generated by MIG code [5].

3.2 Estimation of Axial Peaking Factor Uncertainties from Covariance Matrix for Fuel Mass Distribution

The DSM method was utilized as a way to quantify uncertainties of nuclear design parameters such as peaking factors, power distribution, and k_{eff} through MC calculations. At KAERI, the Fuel Design Team provide axial uranium mass distributions, which they obtained from raw fuel rod samples and in which they used a new-type fuel rod [7]. Such a distribution is typically caused by tolerance errors from the manufacturing process for mixed metallic-uranium pellets. Using Eqs. (2) and (3), the covariance matrix can be calculated with the samples. Regarding the correlation coefficients matrix for an axial metallic-uranium mass distribution [8] shown in Fig. 2, one can see that the mass of a fuel has a strong correlation with the axial position of the fuel. MIG can generate the input sets from the covariance matrix. Using the sampled input sets, the axial peaking factor and k_{eff} can be obtained.

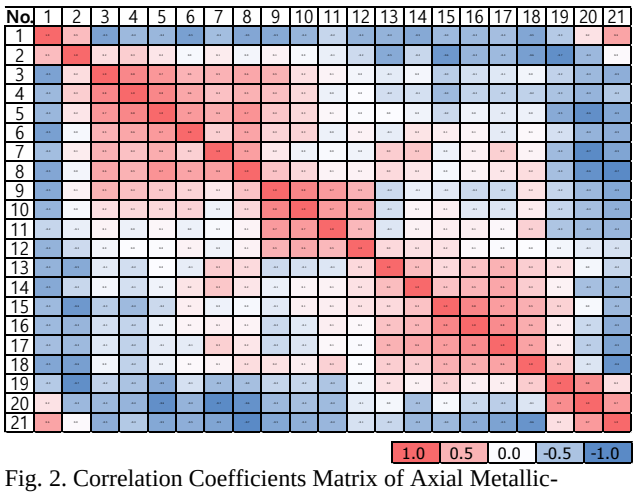

Fig. 2. Correlation Coefficients Matrix of Axial Metallic-Uranium Mass Distribution for New-type Fuel Pin

3.3 Estimation of k_{inf} Uncertainties by the Tolerance Errors of the Geometric Data

MIG can perform an uncertainty analysis for a design parameter according to the tolerance error of a geometric value provided by vendors. Figure 3 shows a 1/6 symmetric FA of a small modular reactor (SMR) in operation on ice-breakers [9]. The FA consists of a

bundle of fuel pins, burnable absorber rods, zirconium rods, and a cylindrical zirconium alloy tube. The whole of the FA can be assembled within the core by screwing tightly. Because the screwing process may causes the errors with regard to the rotation angle, it is necessary for a vendor to provide its tolerance errors. As shown in Fig. 3, the fuel rods may be shifted by the rotation angle.

In order to generate input sets for a shifted FA, it is necessary to know the center locations of the shifted fuel rods and surface equations. Equation (10) represents the center location (x_{new},y_{new}) of a fuel rod shifted by a rotation angle θ.

$$\begin{pmatrix} x_{new} \\ y_{new} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x_{org} \\ y_{org} \end{pmatrix} \tag{10}$$

$$a_{org}x + b_{org}y + cz = d \tag{11}$$

Equation (11) represents the equation of a plane surface, which is used in the common MC code. In the case of a rotation in the x-y plane, the equation of the plane surface and the coefficients of the shifted surface, a_{new} and b_{new}, can be calculated by

$$a_{new}x + b_{new}y + cz = d, \tag{12}$$

$$\begin{pmatrix} a_{new} \\ b_{new} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} a_{org} \\ b_{org} \end{pmatrix} \tag{13}$$

where “org” and “new” denote “original” and “shifted” (value), respectively.

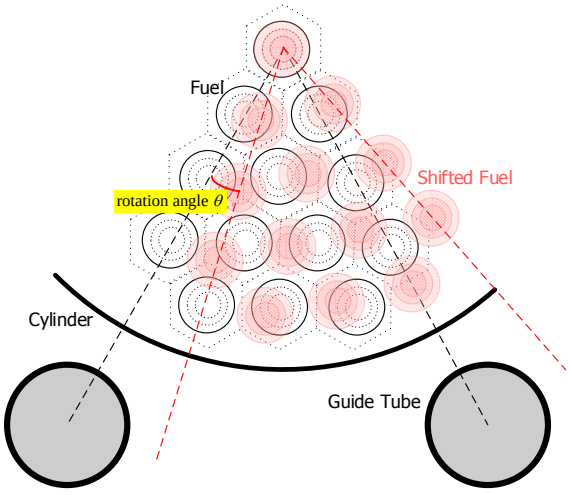

Fig. 3. Shift of fuel rods in a 1/6 symmetric FA of an ice-breaker SMR by the tolerance errors of rotation angle

Figure 4 shows the distribution of k_{inf} from 60 samples that were generated under the assumption that the standard deviation of the rotation angle is 10 degrees.

3. Conclusions

In this study, the LDL^T and Cholesky decomposition modules for DSM calculations were implemented into the latest MIG code, MIG 1.5, and verified by means of test problems as shown in Table I. The modules were used to quantify uncertainties of nuclear design parameters such *peaking factors*, *power distribution*, and k_{eff}. Owing to the versatility of the multiple-correlated variables sampling capability of the MIG code, one can usefully utilize for a variety of applications, reasons, or computer software.

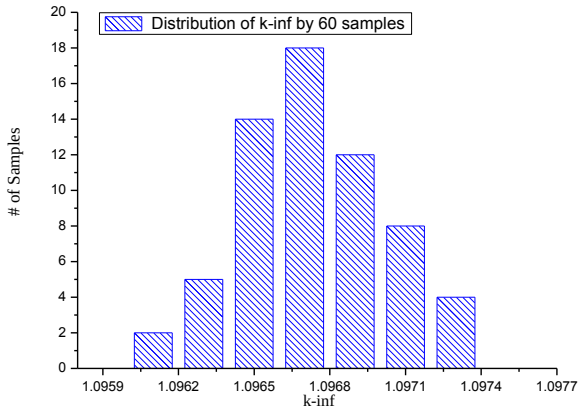

Fig. 4. Distribution of k_{inf} from the 60 samples which are generated by the tolerance errors of rotation angle

REFERENCES

[1] H. J. Shim et al., “McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis,” Nuclear Engineering and Technology, Vol. 44, p. 161, 2012.
[2] “Jordan Research & Training Reactor Final Safety Analysis Report,” Jordan Atomic Energy Commission, 2014.
[3] H. J. Park et al., “Generation of Few-Group Diffusion Theory Constants by Monte Carlo Code McCARD,” Nuclear Science and Engineering, Vol. 172, p. 66, 2012.
[4] W. H. Press et al., “Numerical Recipes in C: The Art of scientific Computing,” 2nd Edition, Cambridge, 1992.
[5] H. J. Park et al., “Uncertainty Propagation Analysis for Yonggwang Nuclear Unit 4 by McCARD/MASTER Core Analysis System,” Nuclear Engineering and Technology, Vol. 46, p. 291, 2014.
[6] T. Y. Han et al., “Core Parameter Uncertainty Analysis on HTGR UAM Benchmark with DeCART/MUSAD/CAPP,” Transactions of the Korean Nuclear Society Autumn Meeting, Gyeongju, Korea, October 26-27, 2017.
[7] J. Y. Oh, Nuclear Fuel Technology Development Group, Korea Atomic Energy Research Institute, Private Communication.
[8] H. J. Park et al., “Estimation of Axial Peaking Factor Uncertainty by Fuel Fabrication Error using Multiple Correlation Sampling,” Proceedings of the Reactor Physics Asia 2015 (RPHA15) Conference, Jeju, Korea, Sept. 17-18, 2015

[9] M. Bolshukin, et al., "Development and Verification of Full-Scale Model of Small Modular Reactor Core for Burnup Calculations by Monte-Carlo Method," PHYSOR2018: Reactor Physics paving the way towards more efficient systems, Cancun, Mexicom April 22-26, 2018.