Validation of Uncertainty Propagation Formulation in Monte Carlo Burnup Analysis by Direct Stochastic Sampling Method

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

1. Introduction

As computational resource and technology develops, Monte Carlo (MC) depletion calculations have been widely used for a nuclear core design and analysis. In the MC depletion analysis, an uncertainty propagation is really important issues. Only a few studies [1-5] covered theoretical formulations to quantify the uncertainties of the MC tallies and their propagation behavior with the progress of the system depletion. Shim et al. [2,4] proposed a new formulation aimed at quantifying uncertainties of Monte Carlo (MC) tallies as well as nuclide number density estimates in MC depletion analysis. The new uncertainty propagation formulation is referred to as "SNU formulation". The SNU formulation is based on the Sensitivity/Uncertainty (S/U) analysis method with the perturbation techniques. It had incorporated into the Monte Carlo Code for McCARD.

In the previous study, the McCARD/MIG cross section random sampling (RS) code system [6] for Direct Sampling Method (DSM) in continuous energy MC calculations was successfully established. The DSM can be utilized as the useful and efficient verification and validation (V&V) tools for the S/U method. In this study, we perform the McCARD uncertainty propagation analysis for an uncertainty analysis modeling (UAM) pin depletion benchmark (Exercise I-1b) [7] by the SNU formulation based on the S/U method and the DSM. The SNU formulations are validated through comparison with DSM reference results.

2. Methodology

2.1 SNU Formulation for Uncertainty Propagation

A MC depletion analysis can be divided into MC transport simulation stage and depletion calculation stage. In the MC transport simulation stage, the uncertainties of MC tallies due to the statistical, nuclear data, and number density uncertainties cause those of the updated number densities. Meanwhile, the uncertainties of the updated number densities in the depletion calculation stage cause those of the MC tallies in the next MC simulation stage. With the progress of burnup, the MC tallies uncertainties of a burnup step propagate to the number density uncertainties for the next burnup step and to those of the next burnup step.

In the SNU uncertainty propagation formulation [4], the variance of Q, $\sigma_{SU}^2[Q]$, is estimated by

$$\sigma_{SU}^2[Q] = \sigma_{\mathrm{STATS}}^2[Q] + \sigma_{\mathrm{NN}}^2[Q] + \sigma_{\mathrm{XX}}^2[Q] + 2\sigma_{\mathrm{NX}}^2[Q] \tag{1}$$

$$\begin{aligned} \sigma_{\mathrm{NN}}^2[Q] &= \sum_{m,i}\sum_{m',i'} \mathrm{cov}\left[N_{m,i}^n, N_{m',i'}^n\right]\left(\frac{\partial Q}{\partial N_{m,i}^n}\right)\left(\frac{\partial Q}{\partial N_{m',i'}^n}\right), \\ \sigma_{\mathrm{XX}}^2[Q] &= \sum_{i,\alpha,g}\sum_{i',\alpha',g'} \mathrm{cov}\left[x_{\alpha,g}^i, x_{\alpha',g'}^{i'}\right]\left(\frac{\partial Q}{\partial x_{\alpha,g}^i}\right)\left(\frac{\partial Q}{\partial x_{\alpha',g'}^{i'}}\right), \\ \sigma_{\mathrm{NX}}^2[Q] &= \sum_{m,i}\sum_{i',\alpha',g'} \mathrm{cov}\left[N_{m,i}^n, x_{\alpha',g'}^{i'}\right]\left(\frac{\partial Q}{\partial N_{m,i}^n}\right)\left(\frac{\partial Q}{\partial x_{\alpha',g'}^{i'}}\right). \end{aligned} \tag{2}$$

$\sigma_{\mathrm{STATS}}^2$ indicates the contribution from the statistical uncertainties. And σ_{NN}^2 and σ_{XX}^2 are the contribution from the number density and cross section uncertainties, respectively. In the SNU formulation, the partial derivatives in Eq. (2) are calculated by

$$\frac{\partial Q}{\partial X} \cong \frac{Q\left(\bar{X} + \sigma[X]\right) - Q\left(\bar{X}\right)}{\sigma[X]} = \frac{\delta Q(X)}{\sigma[X]} \tag{3}$$

$\delta Q(X)$'s in Eq. (3) can be estimated by the differential operator sampling method [8] with the fission source perturbation [9].

In the same manner as above for the variance of Q, the variance of the number density in the depletion calculations can be calculated by

$$\sigma_{SU}^2\left[N_{m,i}^{n+1}\right] = \sigma_{\mathrm{NN}}^2\left[N_{m,i}^{n+1}\right] + \sigma_{\mathrm{RR}}^2\left[N_{m,i}^{n+1}\right] + 2\sigma_{\mathrm{NR}}^2\left[N_{m,i}^{n+1}\right] \tag{4}$$

$$\begin{aligned} \sigma_{\mathrm{NN}}^2\left[N_{m,i}^{n+1}\right] &= \sum_{i'}\sum_{i''} \mathrm{cov}\left[N_{m,i'}^n, N_{m,i''}^n\right]\left(\frac{\partial N_{m,i}^{n+1}}{\partial N_{m,i'}^n}\right)\left(\frac{\partial N_{m,i}^{n+1}}{\partial N_{m,i''}^n}\right), \\ \sigma_{\mathrm{RR}}^2\left[N_{m,i}^{n+1}\right] &= \sum_{j,\alpha}\sum_{j',\alpha'} \mathrm{cov}\left[r_{m,j,\alpha}^n, r_{m,j',\alpha'}^n\right]\left(\frac{\partial N_{m,i}^{n+1}}{\partial r_{m,j,\alpha}^n}\right)\left(\frac{\partial N_{m,i}^{n+1}}{\partial r_{m,j',\alpha'}^n}\right), \\ \sigma_{\mathrm{NR}}^2\left[N_{m,i}^{n+1}\right] &= \sum_{i'}\sum_{j,\alpha} \mathrm{cov}\left[N_{m,i'}^n, r_{m,j,\alpha}^n\right]\left(\frac{\partial N_{m,i}^{n+1}}{\partial N_{m,i'}^n}\right)\left(\frac{\partial N_{m,i}^{n+1}}{\partial r_{m,j,\alpha}^n}\right). \end{aligned} \tag{5}$$

The partial derivatives in Eq. (5) can be estimated with the direct subtraction method in the same way as Eq. (3). Reference 4 provided the detailed information for the SNU formulation.

2.2 Direct Sampling Method

In the DSM, the RS procedure of input parameters, such as cross sections and number densities, according to their covariance data are performed for uncertainty quantification (UQ). Suppose that $\mathbf{C}_u$ is the covariance matrix defined by cov[$x^i_{\alpha,g}, x^{i'}_{\alpha',g'}$] and that a lower triangular matrix **B** is known through the *Cholesky* decomposition of $\mathbf{C}_u$, then we have

$$\mathbf{C}_u = \mathbf{B} \cdot \mathbf{B}^T \quad (6)$$

where $\mathbf{B}^T$ is the transpose matrix of **B**.

$$\mathbf{X}^i = \overline{\mathbf{X}} + \mathbf{B} \cdot \mathbf{Z} \quad (7)$$

where $\overline{\mathbf{X}}$ is the mean vector and **Z** is a random normal vector, which can be calculated using the *Box-Muller* method. Using this RS procedure, the sampled input sets at the beginning of burnup cycle (BOC) can be prepared.

In the same manner, a stepwise MC tally Q or number density N for each sampled input set can be calculated. The uncertainty of Q, $\sigma^2_{DSM}[Q]$, and the uncertainty of N, $\sigma^2_{DSM}[N]$, at each burnup step can be calculated by K sampled input sets as below:

$$\sigma^2_{DSM}[Q] \cong \frac{1}{K-1}\sum_{k=1}^{K}(Q^k - \overline{Q}). \quad (8)$$

$$\sigma^2_{DSM}[N] \cong \frac{1}{K-1}\sum_{k=1}^{K}(N^k - \overline{N}). \quad (9)$$

where Q^k and N^k are the MC tally estimates and the number densities calculated by k-th sampled input set, respectively.

3. Validation of the SNU Formulation

3.1 UAM PWR Pin-cell Burnup Benchmark

The object of the UAM pressurized-water reactor (PWR) pin-cell burnup benchmark problem – Exercise I-1b [6] is to evaluate the uncertainties in the depletion calculation due to the nuclear cross section covariance data. The benchmark represents the burnup uncertainty propagation analysis for a typical fuel rod from the TMI-1 PWR, 15x15 assembly with 4.85 w/o enrichment, as shown in Table I. Its final burnup is 61.28 GWd/MTU with the specific power of 33.58 kW/kgU. For UAM exercise I-1b problem, the McCARD analyses are conducted with the continuous-energy cross section libraries processed by NJOY from the ENDF/B-VII.1 neutron cross section libraries and their covariance data. The LANL 30-group covariance matrix from the raw ENDF/B-VII.1 covariance libraries are generated by the ERRORR module in the NJOY.

Table I: Configuration of UAM PWR Pin-cell Burnup Benchmark Problem (Exercise I-1b)

Fuel temperature	900.0	Kelvin
Cladding temperature	600.0	Kelvin
Moderator temperature	562.0	Kelvin
Pin pitch	1.4427	cm
Fuel pellet diameter	0.9391	cm
Cladding outer diameter	1.0928	cm
Cladding thickness	0.0673	cm

3.2 Uncertainty Propagation of MC tallies in MC Depletion Analysis

The MC burnup uncertainty propagation analyses were conducted by using the covariance data of 2 major actinide isotopes – ^{235}U and ^{238}U. All McCARD eigenvalue calculations were performed on 200 active cycles with 10,000 histories per cycle. The uncertainties by the DSM were estimated from 100 replicas with a different sequence of random number.

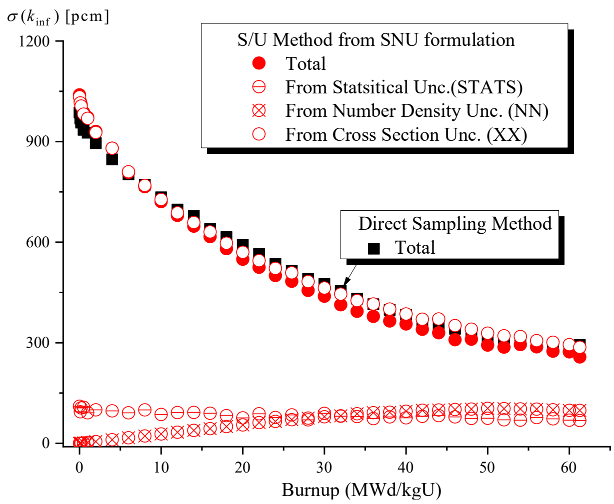

Fig. 1. Uncertainty propagation of k_{inf} for UAM PWR pin-cell Burnup Benchmark Problem with 2 covariance data

Figure 1 compares the uncertainties of k_{inf} by the DSM and the S/U method for UAM PWR pin-cell burnup benchmark problem with ^{235}U and ^{238}U covariance data. It is noted that the uncertainties of k_{inf} from the S/U method from SNU formulation agree excellent with those by the DSM. The S/U method give smaller difference in the uncertainties of k_{inf} than 53 pcm.

Table II compares the uncertainties of one-group absorption cross section for burnup calculation at BOC by the DSM and the S/U method. It is observed that there are no considerable differences in the one-group absorption cross sections between the two methods.

Table II: Comparison of One-group Absorption Reaction Rates for Burnup Calculation at beginning of burnup

Isotope	Relative Standard Deviation (Rel. SD) of One-group Absorption Reaction Rate		
	DSM (%)	S/U (%)	Diff*
^{235}U	1.30	1.36	-0.06
^{238}U	0.89	0.95	-0.06

* Diff = Rel. SD (DSM) – Rel. SD(S/U).

3.3 Uncertainty Propagation of Number Densities in MC Depletion Analysis

Figures 2 and 3 present the uncertainties of the number densities of ^{235}U and ^{238}U over burnup. It is observed that the uncertainties estimated by the S/U method are quite comparable to those by the DSM.

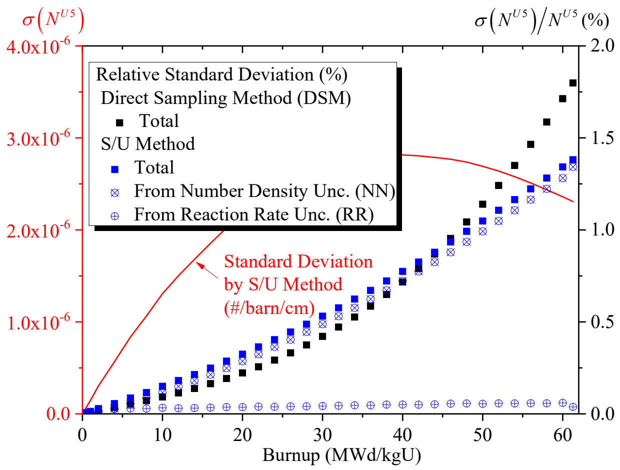

Fig. 2. Uncertainty propagation of ^{235}U number density for UAM PWR pin-cell Burnup Benchmark Problem with 2 covariance data

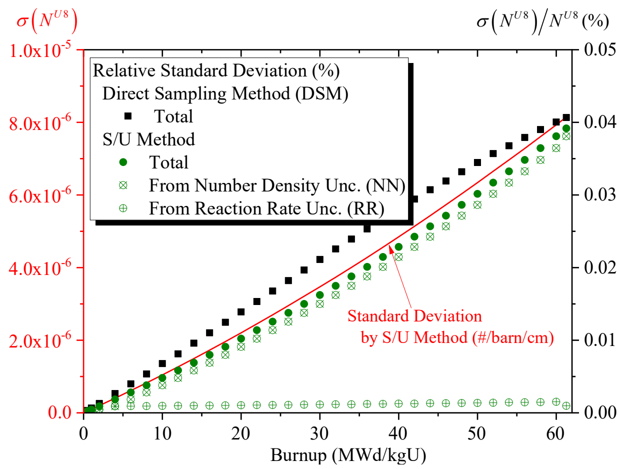

Fig.3. Uncertainty propagation of ^{238}U number density for UAM PWR pin-cell Burnup Benchmark Problem with 2 covariance data

As shown in Figs. 2 and 3, the uncertainties of the ^{235}U and ^{238}U number densities by the S/U method increase linearly whereas those by the DSM increase by quadratic functions. It is inferred that the difference in shapes between the S/U method and the DSM results comes from the first-order *Taylor* series approximation in the SNU formulations.

4. General Behavior of the Uncertainty Propagation in MC Depletion Analysis

A matter of primary concern or question for the uncertainty propagation in MC depletion analysis is that "*Are all uncertainties increasing steadily*?".

To observe the general behavior of the uncertainty propagation of MC tallies and number densities in PWR depletion analysis, a test case was considered using UAM exercise I-1b. In the test case, the calculation conditions were identical to those used in Section 3 except covariance data. For the test problem, we considered the covariance data of 10 actinide isotopes – ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, and ^{244}Cm. In this case, the ν (mt451), capture (mt102), fission (mt18), elastic (mt2), and inelastic (mt4) cross-sections for the 10 actinide isotopes have 1.0% cross section uncertainties over whole energy range.

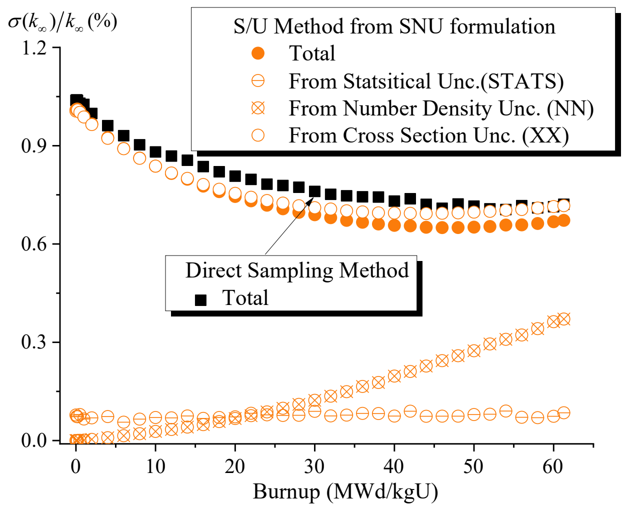

Fig. 4. Uncertainty propagation of k_{inf} for test problem considering constant cross section uncertainties (1.0%) for 10 actinide covariance data

Figure 4 shows the relative uncertainties of k_∞ by the DSM and the S/U method as a function of the pin-wise burnup. It is observed that the relative uncertainties of k_∞ gradually decreases to approximately 0.7% until the middle of burnup cycle (MOC). Subsequently, the relative uncertainties of k_∞ remain steady until the end of burnup cycle (EOC). Figure 5 shows the relative uncertainties of ^{235}U one-group microscopic reaction rates for burnup analysis over burnup. In the same manner, the change of the relative uncertainties of ^{235}U one-group microscopic reaction rates due to burnup is not considerably large. In contrast, the relative uncertainties ^{235}U number densities increases monotonically with burnup as shown in Fig 6. The relative uncertainties for ^{238}U and ^{239}Pu also increases linearly as shown in Fig. 7. The relative uncertainties for the other seven nuclides are less than 3.0% after MOC.

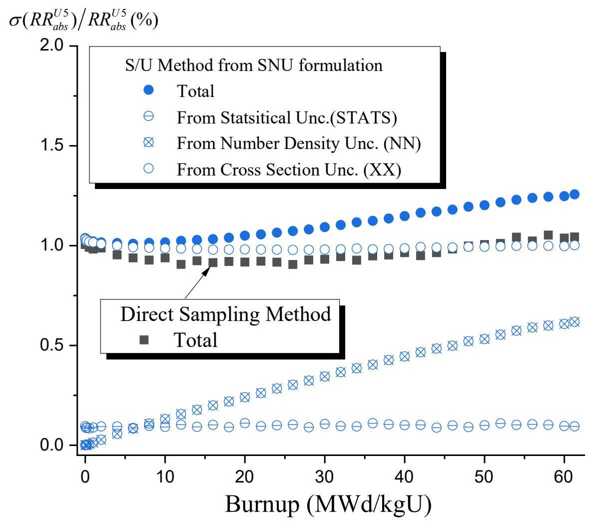

Fig. 5. Uncertainty propagation of ^{235}U one-group absorption microscopic reaction rate for the test problem (1% cross section uncertainty for 10 actinides)

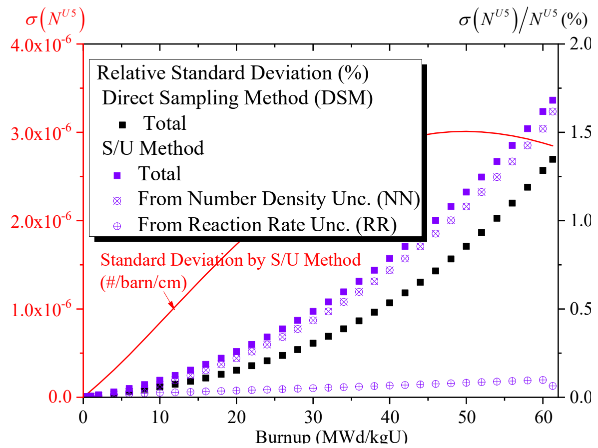

Fig. 6. Uncertainty propagation of ^{235}U number density for the test problem (1% cross section uncertainty for 10 actinides)

5. Conclusions

In this study, the SNU formulations for uncertainty propagation in MC depletion analysis are validated by comparing with the DSM reference results for an uncertainty analysis modeling pin depletion benchmark. The uncertainties of the MC estimates and number densities over burnup by the S/U method are in good agreement with those by the DSM. Therefore, it is concluded that the SNU formulation based on the S/U method have the accurate capabilities to estimate the uncertainty propagation in a MC depletion analysis.

The test calculations based on the UAM exercise I-1b were conducted to confirm the general behavior of the uncertainty propagation of MC tallies and number densities in a common PWR depletion analysis. The behaviors of the uncertainty propagation in the test problem can be summarized as follow:

I. Among the three contributors (σ_{STATS}, σ_{NN}, σ_{xx}) to $\sigma(k_\infty)$, to $\sigma_{xx}(k_\infty)$ arising from the cross section uncertainties is dominant at each burnup point. In other words, the $\sigma_{NN}(k_\infty)$ from number density uncertainties is less than $\sigma_{xx}(k_\infty)$.
II. Correlation coefficients between cross section and number densities is commonly negative. $\sigma^2_{NX}(k_\infty)$ is less than 0.
III. Relative number density uncertainties are not large.

It is concluded that the uncertainty propagation is not significantly affected for the uncertainties of the MC tallies over burnup.

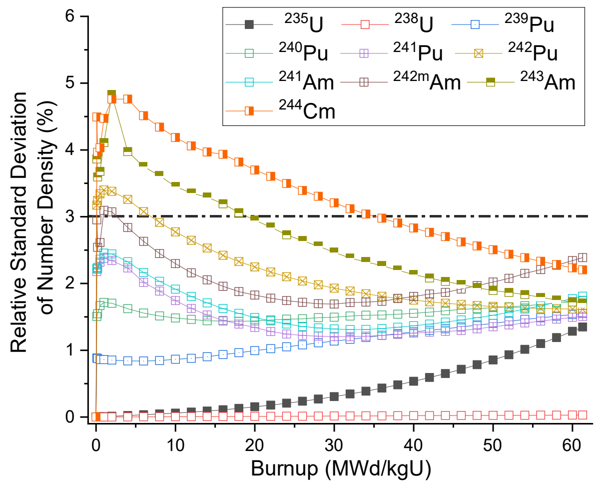

Fig. 7. Relative uncertainties of number densities for test problem by DSM (1% cross section uncertainty for 10 actinides)

REFERENCES

[1] T. Takeda, N. Hirokawa, and T. Noda, Estimation of Error Propagation in Monte-Carlo Burnup Calculations, J. Nucl. Sci. Technol., Vol.36, p.738, 1999.
[2] H. J. Shim and C. H. Kim, Error Propagation Module Implemented in the MC-CARD Monte Carlo Code, Trans. Am. Nucl. Soc., Vol.86, p. 325, 2002.
[3] N. Garcia-Herranz et al., Propagation of Statistical and Nuclear Data Uncertainties in Monte Carlo Burnup Calculations, Ann. Nucl. Energy, Vol.35, p. 714, 2008.
[4] H. J. Park, H. J. Shim, and C. H. Kim, Uncertainty Propagation in Monte Carlo Depletion Analysis, Nucl. Sci. Eng., Vol.167, p. 196, 2011.

[5] H. J. Park, H. J. Shim, and C. H. Kim, Uncertainty Propagation Analysis for PWR Burnup Pin-Cell Benchmark by Monte Carlo Code McCARD, Science and Technology of Nuclear Installations, Vol.2012, Article ID 616253, 2012.
[6] H. J. Park, T. Y. Han, and J. Y. Cho, Implementation of Cross Section Random Sampling Code System for Direct Sampling Method in Continuous Energy Monte Carlo Calculations, Transactions of the Korean Nuclear Society Virtual Spring Meeting, July 9-10, 2020.
[7] K. Ivanov, M. Avramova, S. Kamerow et al., Benchmark for uncertainty analysis in modeling (UAM) for design, operation and safety analysis of LWRs, volume I: specification and support data for the neutronics cases (Phase I), NEA/NSC/DOC, Nuclear Energy Agency, 2012.
[8] H. Rief, Generalized Monte Carlo Perturbation Algorithms for Correlated Sampling and a Second-order Taylor Series Approach, Ann. Nucl. Eng., Vol.11, p. 455, 1984.
[9] Y. Nagaya and T. Mori, Impact of Perturbed Fission Source on the Effective Multiplication Factor in Monte Carlo Perturbation Calculations, J. Nucl. Sci. Technol., Vol.42, p. 428, 2005.