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Original Article

McCARD/MIG stochastic sampling calculations for nuclear cross section sensitivity and uncertainty analysis

Ho Jin Park

Kyung Hee University, 1732, Deogyeong-daero, Giheung-gu, Yongin-si, Gyeonggi-do, South Korea

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ABSTRACT

In this study, a cross section stochastic sampling (S.S.) capability is implemented into both the McCARD continuous energy Monte Carlo code and MIG multiple-correlated data sampling code. The ENDF/B-VII.1 covariance data based 30 group cross section sets and the SCALE6 covariance data based 44 group cross section sets are sampled by the MIG code. Through various uncertainty quantification (UQ) benchmark calculations, the McCARD/MIG results are verified to be consistent with the McCARD stand-alone sensitivity/uncertainty (S/U) results and the XSUSA S.S. results. UQ analyses for Three Mile Island Unit 1, Peach Bottom Unit 2, and Kozloduy-6 fuel pin problems are conducted to provide the uncertainties of k_{eff} and microscopic and macroscopic cross sections by the McCARD/MIG code system. Moreover, the SNU S/U formulations for uncertainty propagation in a MC depletion analysis are validated through a comparison with the McCARD/MIG S.S. results for the UAM Exercise I-1b burnup benchmark. It is therefore concluded that the SNU formulation based on the S/U method has the capability to accurately estimate the uncertainty propagation in a MC depletion analysis.

1. Introduction

In conventional nuclear reactor development, uncertainties or biases of nuclear core design and analysis codes are evaluated and provided by comparing calculated values with those measured from related experiments. Generally, the uncertainties of a nuclear core design and analysis code are calculated under conservative conditions and a nuclear core design engineer may additionally consider adequate margins to design parameters. However, the conservative calculation conditions can lead to extra cost in terms of the margin. Recently, the "Best Estimate Plus Uncertainty" (BEPU) method [1] has been widely investigated and utilized for the uncertainty quantification (UQ) of nuclear core design and analysis codes. In the BEPU method, the uncertainty of the nuclear core design and analysis code provides a combination of the best-estimate models under realistic conditions. Accordingly, the results by the BEPU method are reported with averages and their uncertainties, which can be calculated by the uncertainties of various input parameters. There are two streams for the UQ analysis in the BEPU method. One is the deterministic-based Sensitivity/Uncertainty (S/U) analysis method with the perturbation theory [2,3] and the other is the stochastic sampling (S.S.) method [4,5] by random sampling (RS) of input parameters according to their covariance data. In general, the deterministic-based S/U method offers great benefits in computing time compared with the S.S. method. Meanwhile, it is very easy and intuitive to implement the S.S. method into any code system. The uncertainties of all design output parameters from the outputs calculated by S.S. calculations can be estimated without additional efforts. Various applications of the BEPU method for a nuclear core design and analysis can be found in the literature. In the SCALE code system [4,6], the S/U UQ analysis for multiplication factors and other integral quantities was performed with TSUNAMI sequence for calculating sensitivity coefficients and uncertainties, based on first order perturbation theory. At the VTT technical research center of Finland [3], a classical S/U perturbation theory was implemented to CASMO-4 to estimate the uncertainties of the multiplication factor by propagating the uncertainty related to a neutron cross section. The XSUSA code [4], which was developed by Gesellschaft für Anlagen-und Reaktorsicherheit (GRS), has been widely used for S.S. UQ analysis. The XSUSA code can perform sampling of multi-group neutron cross sections with multi-group cross section covariance data. In the same manner, "Total Monte Carlo" (TMC) [5] is an application of the sampling process for input design parameters. The TMC is an S.S. based UQ analysis tool utilizing a set of perturbed TENDL evaluated

E-mail address: parkhj@khu.ac.kr.

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nuclear data libraries.

Meanwhile, Monte Carlo (MC) perturbation techniques such as differential operator sampling (DOS) with the fission source perturbation (FSP) method and the first-order MC adjoint-weighted perturbation (AWP) techniques [7] have been successfully applied for S/U analyses in the McCARD Monte Carlo code [8], which was developed by Seoul National University. Through the McCARD S/U calculations in the Godiva and Big-ten critical experiment benchmarks, it was shown that the first-order AWP method is equivalent to the first-order DOS method with the FSP.

In this study, a S.S. code system with the McCARD code will be newly established to quantify the uncertainties of output design parameters due to the cross section uncertainties. Section II presents an overview of the newly-established S.S. code system with the McCARD code and the MIG utility. In Section III, this McCARD/MIG S.S. code system is verified and validated through an UQ analysis for various benchmark problems. Section III also gives the results of a McCARD uncertainty propagation analysis for an uncertainty analysis modeling (UAM) [9] pin depletion benchmark (Exercise I-1b) by the S.S. method. The results by the S.S. method are compared with those by the SNU S/U formation [10]. The conclusions and summations are given in Section IV.

2. McCARD/MIG stochastic sampling code system

2.1. Stochastic sampling method

This section briefly explains the methodology of the stochastic sampling for multiple correlated parameters. The mean value of the uncertain input parameter u_i and the covariance between uncertain input parameters u_i and u_j are defined by

$$\overline{u_i} \cong \frac{1}{K}\sum_{k=1}^{K} u_i^k, \tag{1}$$

$$\mathrm{cov}[u_i, u_j] \cong \frac{1}{K-1}\sum_{k=1}^{K}\left(u_i^k - \overline{u_i}\right)\left(u_j^k - \overline{u_j}\right). \tag{2}$$

where K and k are the number of input parameters and the input index. Supposing that $\mathbf{C}_u$ is the covariance matrix defined by cov[u_i, u_j] and that a lower triangular matrix $\mathbf{B}$ is known through the Cholesky decomposition of $\mathbf{C}_u$, we then have

$$\mathbf{C}_u = \mathbf{B}\cdot\mathbf{B}^T \tag{3}$$

where $\mathbf{B}^T$ is the transpose matrix of $\mathbf{B}$. Then, if $\mathbf{C}_u$ is symmetrical and positive definite, one can obtain a sample set by

$$\mathbf{X}^i = \overline{\mathbf{X}} + \mathbf{B}\cdot\mathbf{Z} \tag{4}$$

where $\overline{\mathbf{X}}$ is the mean vector defined by the mean values from Eq. (1) and $\mathbf{Z}$ is a random normal vector calculated directly from a random sampling of the standard normal distribution using the Box-Muller method [11].

In S.S. calculations, a nuclear core design parameter MC tally Q or a number density N at each burnup step can be calculated by the MC code with each sampled input set, as shown in Fig. 1. The uncertainty of Q, $\sigma^2_{S.S.}[Q]$ and the uncertainty of N, $\sigma^2_{S.S.}[N]$ can be calculated by K sampled input sets as given below:

$$\sigma^2_{S.S.}[Q] \cong \frac{1}{K-1}\sum_{k=1}^{K}\left(Q^k - \overline{Q}\right). \tag{5}$$

$$\sigma^2_{S.S.}[N] \cong \frac{1}{K-1}\sum_{k=1}^{K}\left(N^k - \overline{N}\right). \tag{6}$$

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

2.2. Cross section sampling by MIG multiple correlated sampling code

To establish the UQ analysis code system based on the continuous energy McCARD MC code, we used the MIG utility code [12,13], which is capable of performing multiple-correlated sampling to estimate uncertainties of nuclear reactor core design parameters by means of the S.S. method. Fig. 2 plots a flowchart of the McCARD/MIG UQ analysis code system for MC S.S. calculations. The MIG code can generate $\overline{\mathbf{X}}$ and $\mathbf{B}$, as shown in Eq.(4), using a multi-group raw cross section covariance matrix from the evaluated nuclear data library. One generates K sets of cross section samples using K normal vectors from the standard normal distribution. The sampled cross section sets are provided in the form of the ratio to an average cross section. Continuous-energy McCARD calculations can then be performed utilizing each sampled cross section set in a multi-group representation. The MIG code creates a batch file for the entire process to automate the repetitive MC calculations for each sampled cross section set.

In this study, the raw cross section covariance matrix was generated by the ERRORR module of the NJOY code [14] using the ENDF/B-VII.1 evaluated nuclear data library and SCALE6 code package [6] data. The LANL 30 energy group structure for ENDF/B-VII.1 covariance data and the SCALE6 44 energy group structures were adopted for the cross section covariance matrix and the

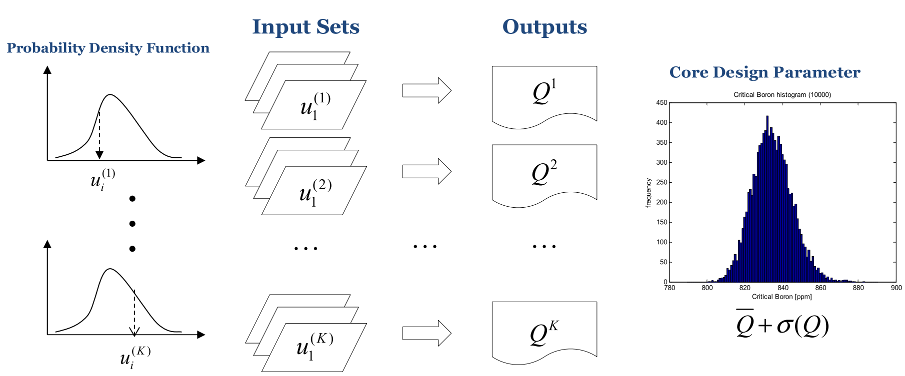

Fig. 1. Stochastic sampling method.

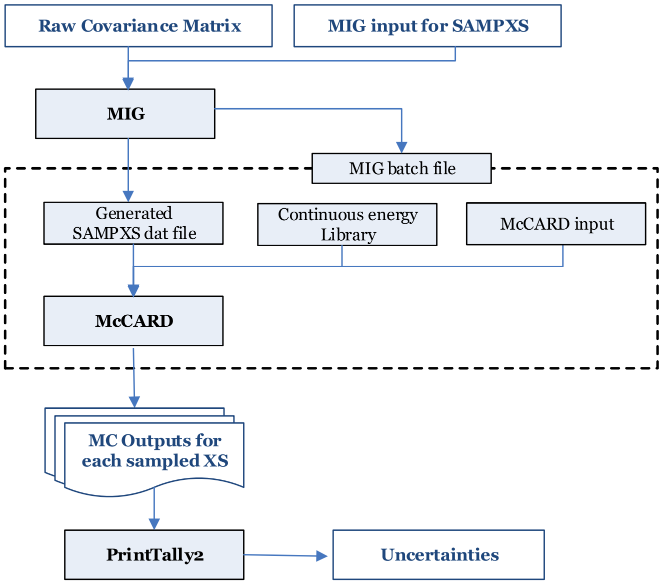

Fig. 2. Flowchart of McCARD/MIG UQ analysis code system for cross section stochastic sampling.

sampled cross section sets, respectively. Fig. 3 shows the correlation coefficient matrix of ^{235}U ν (mt452) from the raw cross section covariance data in the LANL 30 energy group structure and 1,000 random samples by the MIG cross section sampling process. Figs. 4 and 5 show the correlation coefficient matrix of ^{235}U considering three different cross section types (capture, elastic scattering, and inelastic scattering) in the LANL 30 group structure. Overall, the correlation coefficients sampled by the MIG code agree well with those from the raw cross section covariance.

Through the MIG cross section sampling process, the ENDF/B-VII.1 covariance data based 30 group and the SCALE6 covariance data based 44 group cross section sets for the two major actinide isotopes (i.e. ^{235}U and ^{238}U) and eight minor actinide isotopes (i.e. ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{244}Cm) were prepared for S.S. UQ calculations. In the cross section sampling, we considered the correlations between (n,γ), elastic scattering, inelastic scattering cross sections, and independently sampled the cross sections for the other reaction types (i.e. ν and fission).

3. Verification and validation of McCARD/MIG stochastic sampling code system

3.1. Uncertainty quantification of k_{eff} for critical experiment

To verify and validate the newly established McCARD/MIG stochastic sampling code system, a variety of critical experiment (CE) benchmarks were considered from the International handbook of Evaluated Criticality Safety Benchmark Experiment Problems (ICSBEP) [15] and the International handbook of Evaluated Reactor Physics Benchmark Experiment Problems (IRPhEP) [16]. Specifically, two ICSBEP benchmark problems, – Godiva and Jezebel, and one IRPhEP benchmark problem, KRITZ-LWR-RESR-003 (KRITZ-2:13), were selected. Godiva and Jezebel are the bare metallic uranium and plutonium sphere CE benchmark with the fast neutron spectra, whereas KRITZ-2:13 is the uranium fuel array CE benchmark with the thermal neutron spectra. The detailed specifications for each benchmark can be found in the references.

Table 1 compares the total uncertainties in k_{eff} for the three CE benchmarks by the S.S. and S/U codes: McCARD/MIG (S.S. method), McCARD (S/U method), XSUSA (S.S. method), and TSUNAMI (S/U method). The results by the XSUSA and TSUNAMI calculations were taken from the reference [17]. Figs. 6–8 show the uncertainties in k_{eff} of the Godiva, KRITZ-2:13, and Jezebel problem for each isotope and reaction type. To obtain nuclide-wise (e.g., ^{235}U, ^{238}U) and reaction-wise (e.g., ν, fission, capture, (n,2n) reaction) uncertainties in k_{eff}, the extra series of MC runs were performed respectively. For each individual and total case, 500 MC S S. runs were conducted. The statistical uncertainties in k_{eff} for a single MC calculation were less than 0.03%, respectively. Noted that the total uncertainty in k_{eff} for the Jezebel problem is less than the uncertainties in k_{eff} due to the uncertainties of ^{239}Pu inelastic cross sections, as shown in Fig. 8. The uncertainties in k_{eff} due to the uncertainties of ^{239}Pu elastic and inelastic cross sections are 0.45% and 0.82%, respectively. The strong negative covariance between ^{239}Pu elastic and inelastic scattering cross section leads to the negative contribution to the total uncertainty in k_{eff}. The confidence intervals of the total uncertainties were calculated by the bootstrapping method using 1,000 repeated

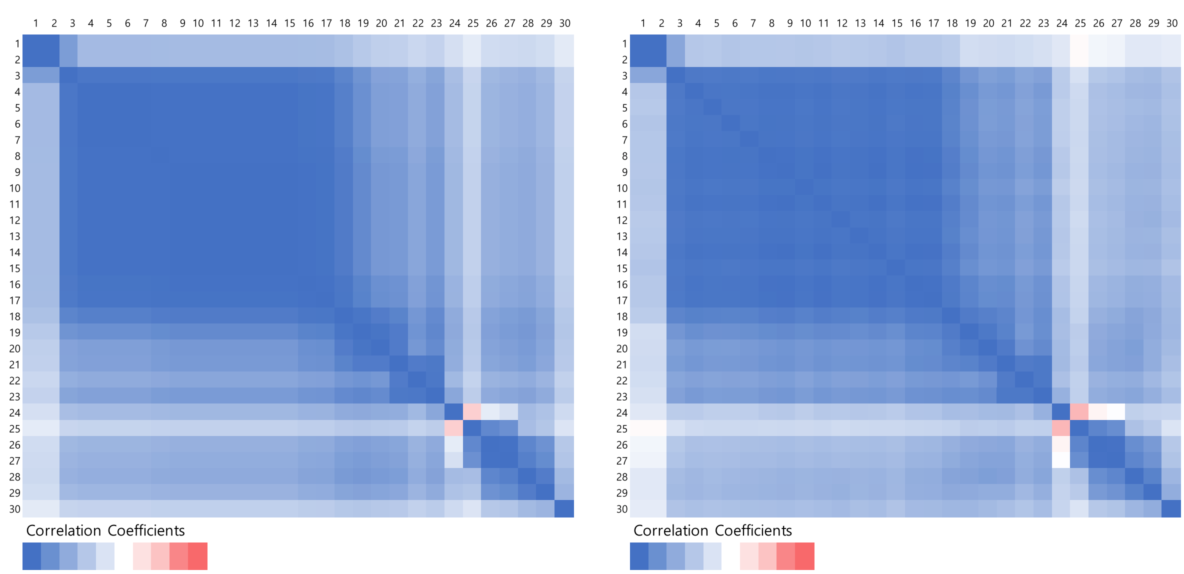

Fig. 3. Correlation coefficient matrix of ^{235}U ν (mt452) from raw cross section covariance data (left) and 100 random samples by MIG (right).

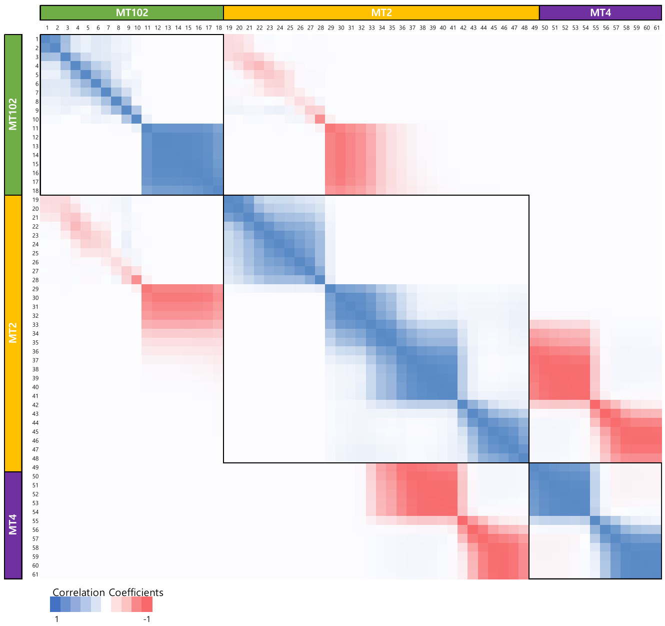

Fig. 4. Correlation coefficient matrix of ^{235}U considering three cross section types (capture, elastic and inelastic scattering) from raw cross section covariance data.

samplings. The uncertainties in k_{eff} by the S/U and S.S. UQ analysis were in good agreement.

3.2. UAM exercise I-1 benchmark problem

The expert group of the Nuclear Energy Agency (NEA), Organization for Economic Co-operation and Development (OECD) proposed the UAM benchmark problems at the UAM workshop meetings [9]. The main goal of the UAM benchmark is to determine the uncertainties in the nuclear reactor physics and thermal/hydraulic (T/H) calculations for light water reactor (LWR) design and

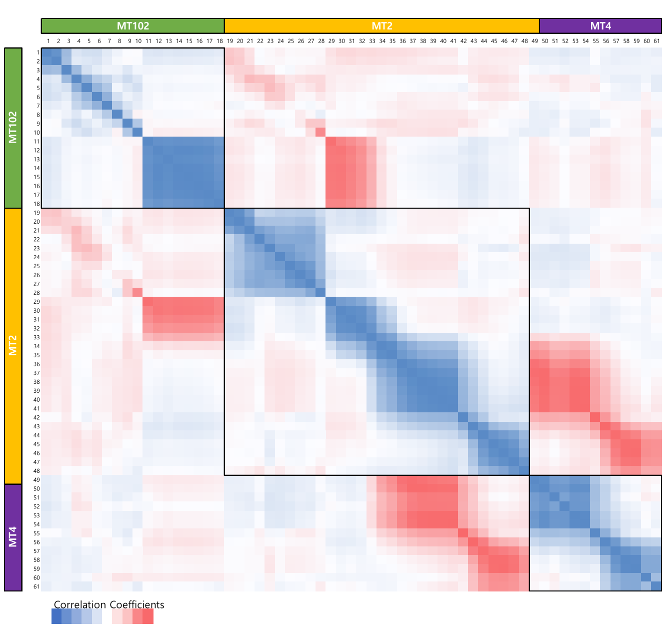

Fig. 5. Correlation coefficient matrix of ^{235}U considering three cross section types (capture, elastic and inelastic scattering) from 100 random samples by MIG.

Table 1
Uncertainties in k_{eff} for the critical experiment benchmarks.

Problem	Relative uncertainties (%) in k_{eff}						
	Code	McCARD/MIG (S.S. method)		McCARD (S/U method)		XSUSA	TSUNAMI
	Cov.[a]	E71	SCALE6	E71	SCALE6	SCALE6	SCALE6
	Grp.[b]	30G	44G	30G	44G	44G	44G
Godiva		1.15±0.10	0.97±0.04	1.18	0.97	1.06	1.07
Jezebel		0.58±0.04	1.27±0.11	0.57	1.25	1.42	1.39
KRITZ-2:13		0.79±0.06	0.50±0.04	0.79	0.50	0.51	0.53

[a] Covariance Data. E71 and SCALE6 are the nuclear covariance data from the ENDF/B-VII.1 evaluated nuclear data library and the SCALE 6 code package, respectively.
[b] Group Structure. 30G and 44G indicate the LANL 30 energy group structure and the SCALE 44 energy group structure, respectively.

analysis. This benchmark is divided into three phases – "Neutronics Phase", "Core Phase", and "System Phase". In this study, the UQ analysis was performed for the "Neutronics Phase", which is focused on a stand-alone steady-state neutronics core calculation. Many participants at the UAM workshop meetings have already submitted their solutions to the UAM benchmark problems through the use of their own UQ analysis tools. We selected three types of LWR models among all "Exercise I-1" cell physics problems in the "Neutronics Phase" – Three Mile Island Unit 1 (TMI-1) of the Pressurized Water Reactor (PWR), Peach Bottom Unit 2 (PB-2) of the Boiling Water Reactor (BWR), and Kozloduy-6 (Koz-6) of the Russian VVER-1000 reactor. In this study, the three types of fuel pin benchmark calculations were performed at both hot zero power (HZP) and the hot full power (HFP) conditions using the ENDF/B-VII.1 covariance data based 30 group sampled cross section sets. The average values and uncertainties of k_{eff} and the microscopic and macroscopic cross sections for the TMI-1, PB-2, and Koz-6 problems by McCARD/MIG S.S. calculations are displayed in Tables 2-4

Tables 5-7 present the uncertainty breakdown of k_{eff} for the TMI-1, PB-2, and Koz-6 problems. These uncertainty breakdown tables show the top five reactions that contribute the most uncertainty to k_{eff} for each problem.

3.3. Validation of the uncertainty propagation formulation in Monte Carlo burnup analyses

As computational resource and technology develops, MC burnup calculations have been widely used for a nuclear core design and analysis. In the MC burnup analyses, an uncertainty propagation is really important issues. Only a few studies [10,18–20] covered theoretical formulations to quantify the uncertainties of the MC tallies and their propagation behavior with

Table 2
McCARD/MIG UQ Results for TMI-1 problem (ENDF/B-VII.1 covariance data).

Case	HZP		HFP	
	Value	RSD[a] (%)	Value	RSD[a] (%)
k_{eff}	1.43446	0.721	1.41709	0.726
$\sigma_{(n,\gamma)}(^{235}U)$	4.36E+01	0.836	4.26E+01	0.844
$\sigma_{(n,\gamma)}(^{238}U)$	9.07E-01	0.573	9.28E-01	0.596
$\sigma_{(n,f)}(^{235}U)$	3.54E+01	0.837	3.45E+01	0.845
$\sigma_{(n,f)}(^{238}U)$	1.02E-01	2.967	1.01E-01	2.987
$\Sigma_t(^{235}U)$	6.91E-02	0.672	6.84E-02	0.675
$\Sigma_t(^{238}U)$	4.20E-02	0.659	4.10E-02	0.662

[a] Relative Standard Deviation (%) = Standard Deviation / Value x 100.

Table 3
McCARD/MIG UQ Results for PB-2 problem (ENDF/B-VII.1 covariance data).

Case	HZP		HFP	
	Value	RSD[a] (%)	Value	RSD[a] (%)
k_{eff}	1.35197	0.754	1.23794	0.810
$\sigma_{(n,\gamma)}(^{235}U)$	6.07E+01	0.819	4.10E+01	1.023
$\sigma_{(n,\gamma)}(^{238}U)$	9.13E-01	0.535	8.49E-01	0.654
$\sigma_{(n,f)}(^{235}U)$	4.99E+01	0.821	3.30E+01	1.025
$\sigma_{(n,f)}(^{238}U)$	9.46E-02	3.147	8.86E-02	4.004
$\Sigma_t(^{235}U)$	6.25E-02	0.633	4.75E-02	0.747
$\Sigma_t(^{238}U)$	3.65E-02	0.619	2.48E-02	0.683

[a] Relative Standard Deviation (%) = Standard Deviation / Value x 100.

Table 4
McCARD/MIG UQ Results for Koz-6 problem (ENDF/B-VII.1 covariance data).

Case	HZP		HFP	
	Value	RSD[a] (%)	Value	RSD[a] (%)
k_{eff}	1.35559	0.751	1.33930	0.756
$\sigma_{(n,\gamma)}(^{235}U)$	5.92E+01	0.782	5.80E+01	0.790
$\sigma_{(n,\gamma)}(^{238}U)$	9.84E-01	0.567	1.01E+00	0.587
$\sigma_{(n,f)}(^{235}U)$	4.86E+01	0.785	4.75E+01	0.793
$\sigma_{(n,f)}(^{238}U)$	9.50E-02	2.870	9.47E-02	2.880
$\Sigma_t(^{235}U)$	6.81E-02	0.616	6.76E-02	0.619
$\Sigma_t(^{238}U)$	3.98E-02	0.615	3.90E-02	0.620

[a] Relative Standard Deviation (%) = Standard Deviation / Value x 100.

Table 5
Uncertainty Breakdown McCARD/MIG Results in k_{eff} for TMI-1 problem (ENDF/B-VII.1 covariance data).

Ranking	HZP		HFP	
	Case	VarFrac[a]	Case	VarFrac[a]
1	$\nu(^{235}U)$	6.96E-01	$\nu(^{235}U)$	6.79E-01
2	$\sigma_{(n,\gamma)}(^{238}U)$	1.59E-01	$\sigma_{(n,\gamma)}(^{238}U)$	1.67E-01
3	$\sigma_{(n,\gamma)}(^{235}U)$	9.27E-02	$\sigma_{(n,\gamma)}(^{235}U)$	9.26E-02
4	$\sigma_{(n,n')}(^{238}U)$	2.16E-02	$\sigma_{(n,n')}(^{238}U)$	2.39E-02
5	$\sigma_{(n,f)}(^{235}U)$	1.15E-02	$\sigma_{(n,f)}(^{235}U)$	1.16E-02

[a] Variance fractions (VarFrac) are the variance due to that parameter divided by the total variances.

the progress of the system depletion. Shim et al. [19] proposed a new formulation aimed at quantifying uncertainties of Monte Carlo (MC) tallies as well as nuclide number density estimates in MC depletion analysis. Moreover, this formulation can treat the stochastic uncertainties from MC simulations as the source of

Table 6
Uncertainty Breakdown McCARD/MIG Results in k_{eff} for PB-2 problem (ENDF/B-VII.1 covariance data).

Ranking	HZP		HFP	
	Case	VarFrac[a]	Case	VarFrac[a]
1	$\nu(^{235}U)$	6.67E-01	$\nu(^{235}U)$	5.06E-01
2	$\sigma_{(n,\gamma)}(^{238}U)$	2.14E-01	$\sigma_{(n,\gamma)}(^{238}U)$	2.77E-01
3	$\sigma_{(n,\gamma)}(^{235}U)$	6.56E-02	$\sigma_{(n,n')}(^{238}U)$	9.13E-02
4	$\sigma_{(n,n')}(^{238}U)$	2.92E-02	$\sigma_{(n,\gamma)}(^{235}U)$	6.32E-02
5	$\sigma_{(n,f)}(^{235}U)$	1.53E-02	$\nu(^{238}U)$	1.71E-02

[a] Variance fractions (VarFrac) are the variance due to that parameter divided by the total variances.

Table 7
Uncertainty Breakdown McCARD/MIG Results in k_{eff} for Koz-6 problem (ENDF/B-VII.1 covariance data).

Ranking	HZP		HFP	
	Case	VarFrac[a]	Case	VarFrac[a]
1	$\nu(^{235}U)$	6.78E-01	$\nu(^{235}U)$	6.61E-01
2	$\sigma_{(n,\gamma)}(^{238}U)$	2.08E-01	$\sigma_{(n,\gamma)}(^{238}U)$	2.16E-01
3	$\sigma_{(n,\gamma)}(^{235}U)$	6.94E-02	$\sigma_{(n,\gamma)}(^{235}U)$	6.95E-02
4	$\sigma_{(n,n')}(^{238}U)$	1.95E-02	$\sigma_{(n,n')}(^{238}U)$	2.14E-02
5	$\sigma_{(n,f)}(^{235}U)$	1.51E-02	$\sigma_{(n,f)}(^{235}U)$	1.38E-02

[a] Variance fractions (VarFrac) are the variance due to that parameter divided by the total variances.

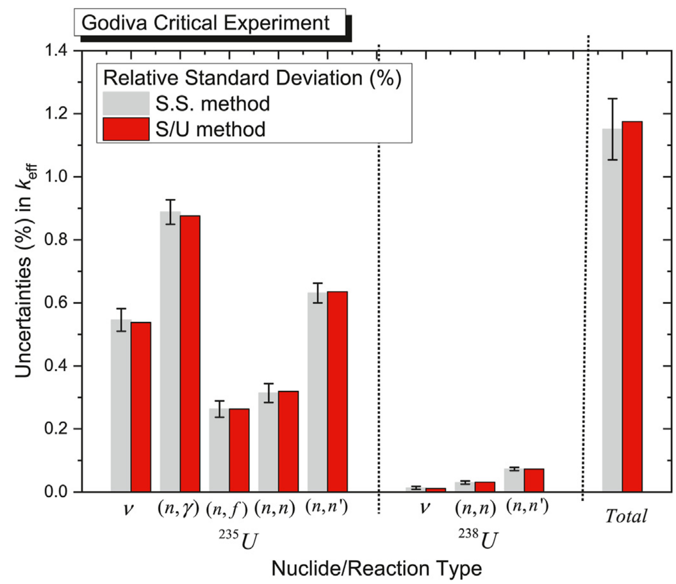

Fig. 6. Comparison between the uncertainties of k_{eff} by McCARD/MIG S.S. and McCARD S/U calculations for Godiva (100 samples for ENDF/B-VII.1 covariance data).

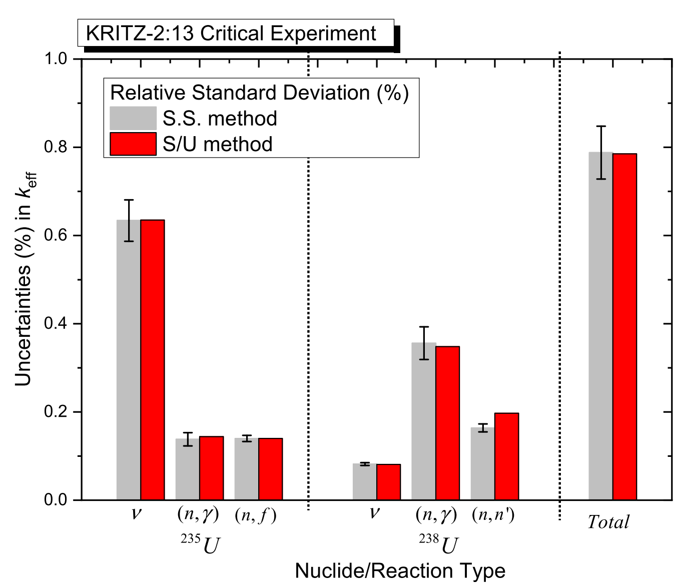

Fig. 7. Comparison between the uncertainties of k_{eff} by McCARD/MIG S.S. and McCARD S/U calculations for KRITZ-2:13 (100 samples for ENDF/B-VII.1 covariance data).

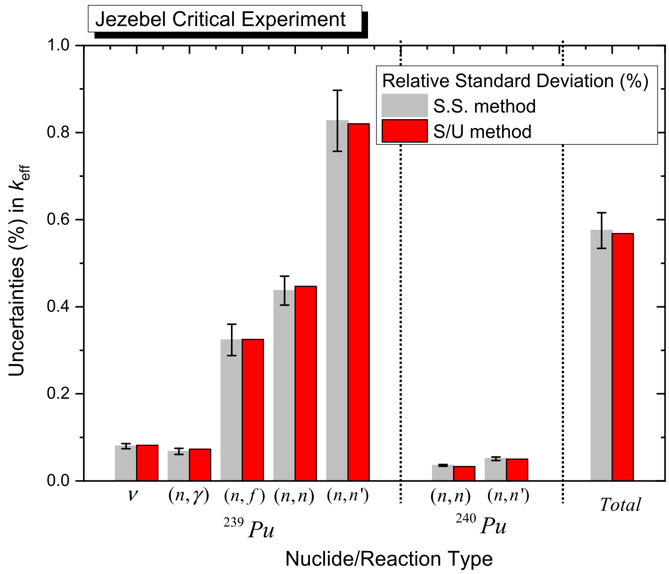

Fig. 8. Comparison between the uncertainties of k_{eff} by McCARD/MIG S.S. and McCARD S/U calculations for Jezebel (100 samples for ENDF/B-VII.1 covariance data).

Table 8
Configuration of UAM Exercise I-1b benchmark problem.

Parameter	Value	Unit
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

uncertainties in design parameters. The new uncertainty propagation formulation is referred to as SNU S/U formulation. This SNU formulation is based on the S/U analysis method with the perturbation techniques. It had already incorporated into the Monte Carlo Code for McCARD [10].

The basic aim in this section is to validate the SNU S/U formulation through comparison with the reference results by the

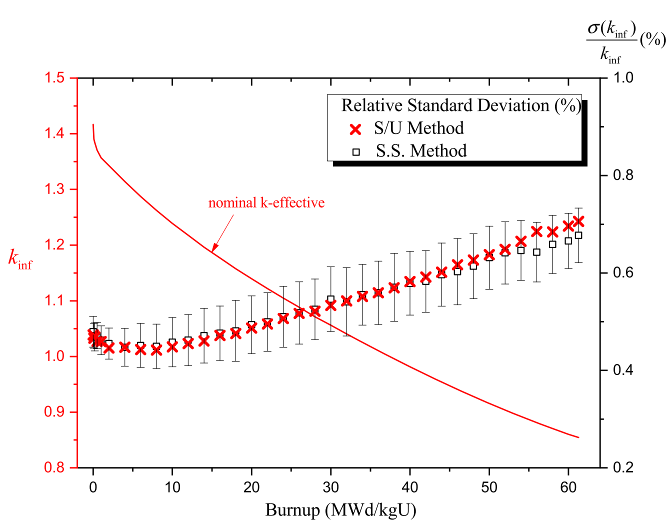

Fig. 9. Uncertainty propagation of k_{inf} for UAM Exercise I-1b Benchmark Problem with SCALE6 44 group covariance data.

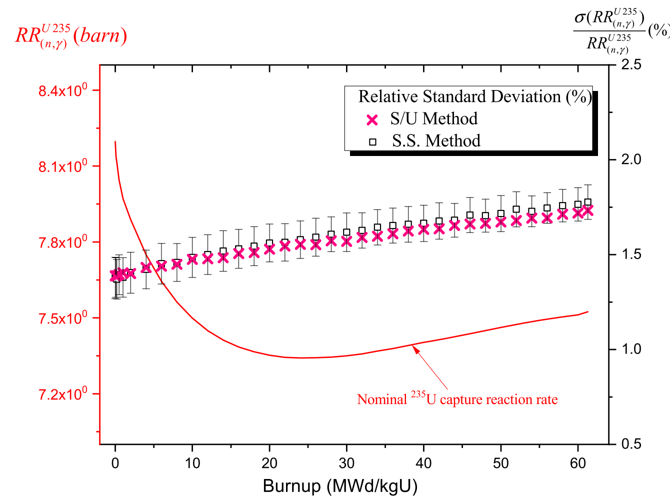

Fig. 10. Uncertainty propagation of ^{235}U capture reaction rate for UAM Exercise I-1b Benchmark Problem with SCALE6 44 group covariance data.

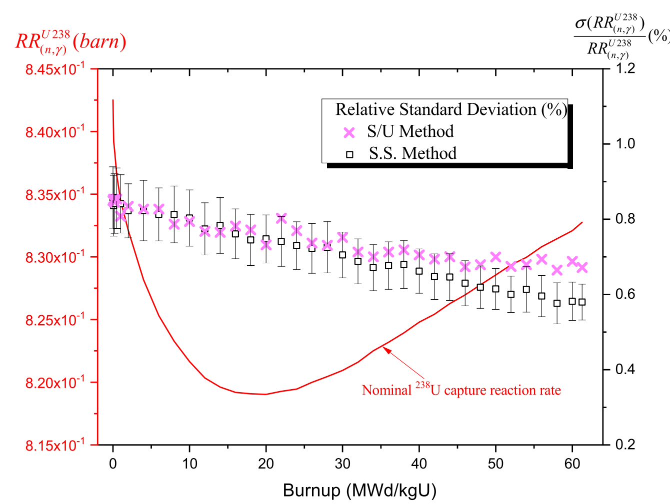

Fig. 11. Uncertainty propagation of ^{238}U capture reaction rate for UAM Exercise I-1b Benchmark Problem with SCALE6 44 group covariance data.

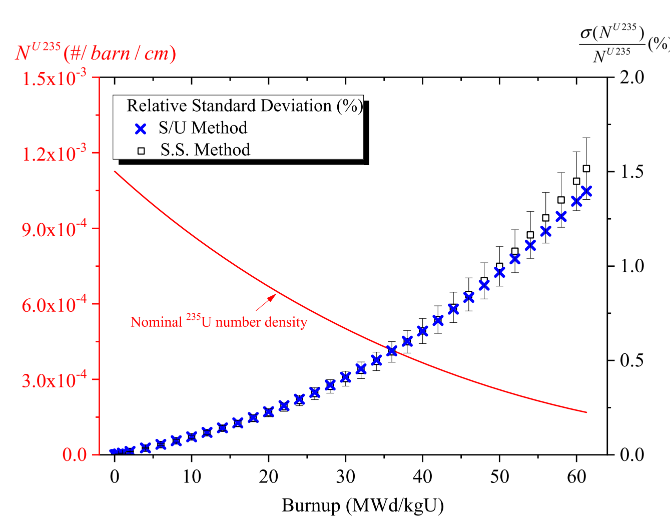

Fig. 12. Uncertainty propagation of ^{235}U number density for UAM Exercise I-1b Benchmark Problem with SCALE6 44 group covariance data.

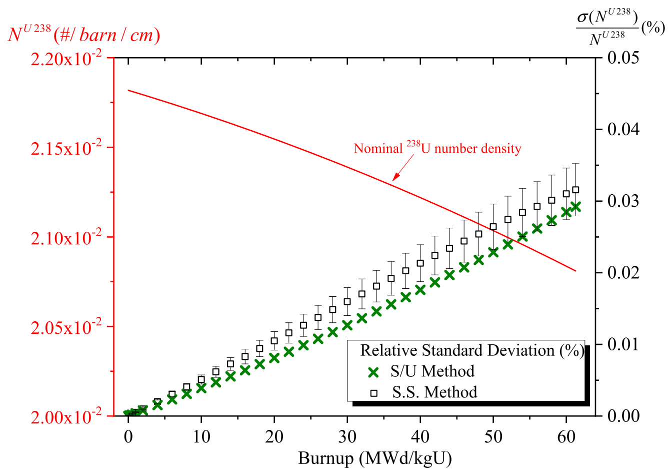

Fig. 13. Uncertainty propagation of ^{238}U number density for UAM Exercise I-1b Benchmark Problem with SCALE6 44 group covariance data.

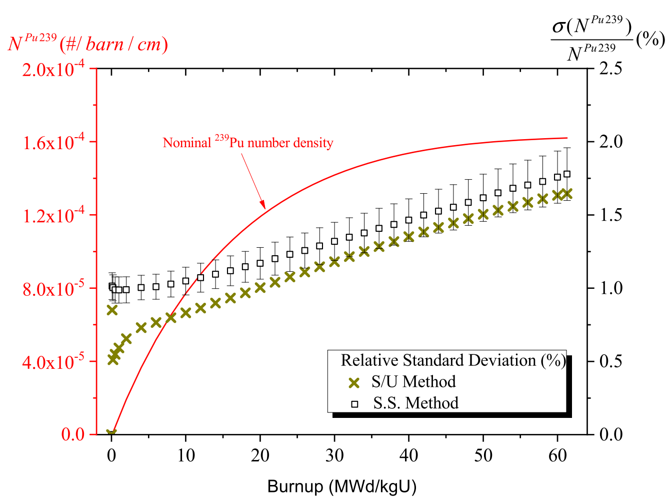

Fig. 14. Uncertainty propagation of ^{239}Pu number density for UAM Exercise I-1b Benchmark Problem with SCALE6 44 group covariance data.

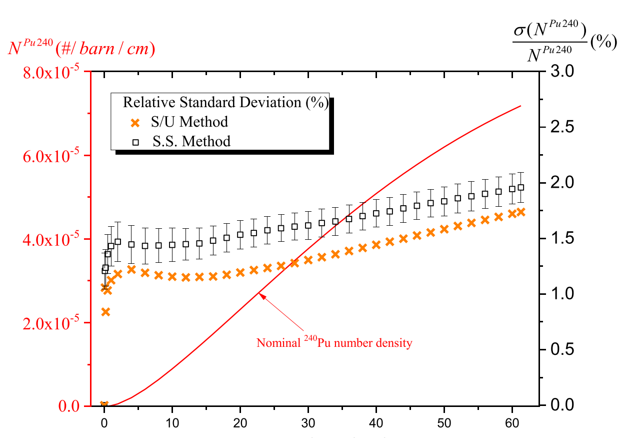

Fig. 15. Uncertainty propagation of ^{240}Pu number density for UAM Exercise I-1b Benchmark Problem with SCALE6 44 group covariance data.

McCARD/MIG S.S. calculations, verify the applicability and the capabilities of the McCARD/MIG S.S. UQ code system for simulations of a PWR core in normal operation.

The UAM benchmark sets include the Exercise I-1b depletion benchmark problem as an extension to Exercise I-1. The subject of the Exercise I-1b problem is to evaluate the uncertainty propagation in the depletion calculation due to uncertainties of input parameters such as nuclear cross section covariance data and number densities. The outputs requested from the Exercise I-1b benchmark are the uncertainties of neutronic parameters such as k_{eff}, nuclide number densities, and reaction rates for a typical fuel rod from the TMI-1 PWR, 15x15 assembly with 4.85 w/o enrichment, as shown in Table 8. The final burnup is 61.28 GWd/MTU with specific power of 33.58 kW/kgU. In a previous study [21], an uncertainty propagation analysis for the UAM Exercise I-1b benchmark was already performed using the McCARD code with the SNU S/U formulation.

The MC burnup uncertainty propagation analyses were conducted by using the SCALE6 covariance based 44 group sampled cross section sets. All McCARD depletion calculations were performed on 200 active cycles with 10,000 histories per cycle. The uncertainties of the requested outputs were estimated by one-hundred McCARD runs from each sampled cross section sets. In all the McCARD depletion calculations, the 95% confidence intervals of the uncertainties of the requested outputs were calculated by 10 repetitions of one-hundred McCARD runs with different sampled cross section sets. Fig. 9 compares the uncertainties of k_{inf} by the McCARD/MIG S.S. and the McCARD S/U calculations with ten actinide covariance data. It is noted that the uncertainties of k_{inf} from the 100 McCARD S.S. runs agree within one standard deviation with the McCARD S/U results. The McCARD S.S. results give a smaller difference in the uncertainties of k_{inf} than 41 pcm. Figs. 10 and 11 compare the uncertainties of ^{235}U and ^{238}U one-group capture microscopic reaction rates by the McCARD/MIG S.S. and the McCARD S/U calculations for burnup analyses. It is observed that there are no considerable differences in the one-group absorption cross sections between the two methods.

Figs. 12–15 present the uncertainties of the number densities of ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu over burnup. It is observed that the uncertainties estimated by the McCARD stand-alone S/U calculations are quite comparable to those by the McCARD/MIG S.S. calculations. As shown in Figs. 11–14, the uncertainties of the number densities by the S.S. method are slightly larger than those by the S/U method. In these depletion calculations, we assumed that ten actinides (i.e. ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, and ^{244}Cm) have uncertainties on their nuclear reaction cross sections. The SNU S/U formulation only considers the internal correlation between only ten actinides, but the S.S. method can handle those between all isotopes including the ten actinides under the assumption. Accordingly, that leads to additional uncertainties from the other isotopes excluding the ten actinides. Therefore, it is inferred that the uncertainties by the S.S. method are slightly larger than those by the S/U method.

4. Conclusions

In this study, nuclear cross section S.S. capability was successfully implemented into both the McCARD continuous energy MC code and MIG multiple-correlated cross section sampling code. Through various benchmark calculations for verification and validation of the UQ capability, the McCARD/MIG results are verified to be consistent with the McCARD S/U results and other S.S. results (i.e. XSUSA). An uncertainty quantification analysis for Three Mile Island Unit 1, Peach Bottom Unit 2, and Kozloduy-6 fuel pin problems was conducted to provide the uncertainties of k_{eff}, and microscopic and macroscopic cross sections by McCARD/MIG cross section stochastic sampling calculations. Moreover, the SNU S/U formulations for uncertainty propagation in a MC depletion analysis are validated by comparison with the McCARD/MIG S.S. results for the UAM Exercise I-1b benchmark. The uncertainties of the MC estimates (i.e. k_{inf} and reaction rate) and number densities over burnup by the SNU S/U formulations are in excellent agreement with the McCARD/MIG results. Therefore, it is concluded that the SNU S/U formulation offers the capability to accurately estimate the uncertainty propagation in a MC depletion analysis.

Owing to the versatility of the S.S. capability in the MIG code, the McCARD/MIG UQ analysis code system can be widely and usefully applied to all kinds of MC nuclear core design analyses.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

[1] R.P. Martin, A. Petruzzi, Progress in international best estimate Plus uncertainty analysis methodologies, Nucl. Eng. Des. 374 (2021), 111033.
[2] A. Aures, et al., Reactor simulations with nuclear data uncertainties, Nucl. Eng. Deg. 355 (2019), 110313.
[3] M. Pusa, Incorporating sensitivity and uncertainty analysis to a lattice physics code with application to CASMO-4, Ann. Nucl. Energy 40 (2012) 153–162.
[4] M.L. Williams, et al., A statistical sampling method for uncertainty analysis with SCALE and XSUSA, Nucl. Technol. 183 (2013) 515–526.
[5] A.J. Koning, D. Rochman, Towards sustainable nuclear energy; putting nuclear physics to work, Ann. Nucl. Energy 35 (2008) 2024–2030.
[6] SCALE, A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation Version 6, 2009. ORNL/TM-2005/39.
[7] H.J. Shim, C.H. Kim, Adjoint sensitivity and uncertainty analyses in Monte Carlo forward calculations, J. Nucl. Sci. Technol. 48 (2011) 1453–1461.
[8] H.J. Shim, et al., McCARD: an Monte Carlo code for advanced reactor design and analysis, Nucl. Eng. Tech. 44 (2) (2012) 161–176.
[9] K. Ivanov, et al., Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of LWRs, Volume I: Specification and Support Data for the Neutronics Cases (Phase I)," NEA/NSC/DOC(2012), OECD Nuclear Energy Agency, 2012.
[10] H.J. Park, H.J. Shim, C.H. Kim, Uncertainty propagation in Monte Carlo depletion analysis, Nucl. Sci. Eng. 167 (2011) 196–208.
[11] G.E.P. Box, Mervin E. Muller, A note on the generation of random number deviates, Ann. Math. Statist. 29 (2) (1958) 610–611.
[12] H.J. Park, et al., Generation of few-group diffusion theory constants by Monte Carlo code McCARD, Nucl. Sci. Eng. 172 (2012) 66–77.
[13] H.J. Park, et al., Implementation of cross section random sampling code system for direct sampling method in continuous energy Monte Carlo calculations, Trans. Korean Nucl. Soc. Virtual Meet. (2020). July 9-10, Korea.
[14] R. Macfarlane, et al., The NJOY Nuclear Data Processing System Version," LA-UR-17-20093, Los Alamos National Laboratory, NW, USA, 2016.
[15] International Handbook of Evaluated Criticality Safety Benchmark Experiments," September 2010 Edition, available on DVD-ROM, NEA/NSC/DOC(95) 03.
[16] International Handbook of Evaluated Reactor Physics Benchmark Experiments," March 2010 Edition, available on DVD-ROM, NEA/NSC/DOC(2006)1.
[17] W. Zwermann, et al., Status of XSUSA for sampling based nuclear data uncertainty and sensitivity analysis, EPJ Web Conf. 42 (2013), 03003.
[18] T. Takeda, et al., Estimation of error propagation in Monte-Carlo burnup calculations," J, Nucl. Sci. Technol. 36 (1999) 738.
[19] H.J. Shim, C.H. Kim, Error propagation module implemented in the MC-CARD Monte Carlo code, Trans. Am. Nucl. Soc. 86 (2002) 325.
[20] N. Garcia-Herranz, et al., Propagation of statistical and nuclear data uncertainties in Monte Carlo burnup calculations, Ann. Nucl. Energy 35 (2008) 185.
[21] H.J. Park, et al., Uncertainty propagation analysis for PWR burnup pin-cell benchmark by Monte Carlo code McCARD, Sci. Technol. Nucl. Install. (2012), 616253, (2012).