Nuclear Data Uncertainty Estimation in DeCART Calculations by Stochastic Sampling Method

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1. Introduction

In a nuclear engineering field, new types of nuclear reactors have been constantly introduced and developed to approach more improved safety, efficiency, and sustainability. Especially, from the safety standpoint, it is very important to estimate the margin or the uncertainties of the design for a new type nuclear reactor. In the process of licensing, a regulating body may and should focus on the uncertainty quantification (UQ) of tools or methodologies, which are used in new types of nuclear reactor design.

Korea Atomic Energy Research Institute (KAERI) has developed the neutronic transport code, DeCART [1] (Deterministic Core Analysis based on Ray Tracing), and has utilized it as the tool for a new nuclear reactor core design. For licensing, the two approaches to estimate output uncertainties due to input uncertainties (e.g. nuclear data, tolerance, material composition) have been developed through the various studies [2,3,4,5,6,7]. One is the sensitivity/uncertainty (S/U) analysis method based on the perturbation techniques. Through the DeCART/MUSAD [7] code systems, the S/U analysis method was already applied. The other is the direct stochastic or statistical sampling (S.S.) method based on the random sampling.

The main goal of this study is to establish and validate the S.S. based DeCART UQ code systems with the MIG [8,9] code. For verification and validation (V&V), some benchmark problems will be conducted by the DeCART/MIG UQ code system.

2. Methods and Results

2.1 DeCART/MIG Stochastic Sampling (S.S.) Code System for Uncertainty Quantification Analysis

The up-to-date MIG code (i.e. version 1.7.0) [8] is used to establish the UQ analysis code system based on the DeCART code. It has a capability of performing multiple-correlated sampling to estimate uncertainties of nuclear reactor core design parameters due to nuclear data uncertainties. The Cholesky covariance matrix decomposition module for multiple-correlated random sampling was implemented into the MIG code. Figure 1 shows the flowchart of the DeCART/MIG UQ analysis code system for the S.S. method. First, the MIG program can generate sampled cross section sets according to raw evaluated nuclear covariance data and a MIG input file. The raw covariance data are edited and reformulated by MIG to be used in DeCART transport calculations.

The cross section sampling can be performed by using the individual and compounded covariance matrix. The compounded covariance matrix for scattering cross section can be provided by elastic (MT2) and inelastic (MT4) scattering cross section as shown in Eq. (1).

$$\begin{aligned}&\mathrm{cov}[\sigma_{s,g},\sigma_{s,g'}]\\&=\mathrm{cov}[\sigma_{e,g},\sigma_{e,g'}]+\mathrm{cov}[\sigma_{i,g'},\sigma_{i,g'}]\\&+\mathrm{cov}[\sigma_{e,g},\sigma_{i,g'}]+\mathrm{cov}[\sigma_{e,g'},\sigma_{i,g}]\end{aligned} \quad (1)$$

$$\sigma_{s,g}=\sigma_{e,g}+\sigma_{i,g} \quad (2)$$

where $\sigma_{e,g}$ and $\sigma_{i,g}$ indicate the g-th energy group elastic, and inelastic scattering cross section. In the same manner, the compounded covariance matrix for absorption cross section can be expressed by

$$\begin{aligned}&\mathrm{cov}[\sigma_{a,g},\sigma_{a,g'}]\\&=\mathrm{cov}[\sigma_{\gamma,g},\sigma_{\gamma,g'}]+\mathrm{cov}[\sigma_{f,g},\sigma_{f,g'}]\\&+\mathrm{cov}[\sigma_{2n,g},\sigma_{2n,g'}]+4\,\mathrm{cov}[\sigma_{3n,g},\sigma_{3n,g'}]\\&+\mathrm{cov}[\sigma_{\gamma,g},\sigma_{f,g'}]-\mathrm{cov}[\sigma_{\gamma,g},\sigma_{2n,g'}]\\&-2\,\mathrm{cov}[\sigma_{\gamma,g},\sigma_{3n,g'}]+\mathrm{cov}[\sigma_{f,g},\sigma_{\gamma,g'}]\\&-\mathrm{cov}[\sigma_{f,g},\sigma_{2n,g'}]-2\,\mathrm{cov}[\sigma_{f,g},\sigma_{3n,g'}]\\&-\mathrm{cov}[\sigma_{2n,g},\sigma_{\gamma,g'}]-\mathrm{cov}[\sigma_{2n,g},\sigma_{f,g'}]\\&+2\,\mathrm{cov}[\sigma_{2n,g},\sigma_{3n,g'}]-2\,\mathrm{cov}[\sigma_{3n,g},\sigma_{\gamma,g'}]\\&-2\,\mathrm{cov}[\sigma_{3n,g},\sigma_{f,g'}]+2\,\mathrm{cov}[\sigma_{3n,g},\sigma_{2n,g'}]\end{aligned} \quad (3)$$

$$\sigma_{a,g}=\sigma_{\gamma,g}+\sigma_{f,g}-\sigma_{2n,g}-2\sigma_{3n,g} \quad (4)$$

where $\sigma_{\gamma,g}$, $\sigma_{f,g}$, $\sigma_{2n,g}$, $\sigma_{3n,g}$, are the g-th energy group (n,g), fission, (n,2n), (n,3n) reaction cross section, respectively. After the processing of MIG, the DeCART neutronic calculations are performed for each sampled cross section set. Finally, the statistical analyses are performed on the DeCART results to determine the uncertainties of the target design parameters due to the cross section uncertainties.

2.2 Implementation of S/U Module Based on Direct Subtraction Method (S/U-DS)

Equation (5) shows a S/U analysis equation for uncertainty quantification of output parameter *Q* due to uncertain input parameters (i.e., $x_{k'}$ and $x_{k''}$). It involves

a first-order Taylor series expansion about the uncertain input parameters. Accordingly, S/U analysis equations have sensitivity coefficients and covariance data. In the S/U analysis, the sensitivity coefficients ($\partial\overline{Q}/\partial x_{k'}$ and $\partial\overline{Q}/\partial x_{k''}$) are generally calculated by the perturbation technique for quick calculation. Meanwhile, as the alternative way, the direct subtraction calculations can be adopted to obtain the sensitivity coefficients.

$$\sigma^2[Q] = \lim_{N\to\infty}\frac{1}{N-1}\left(Q_k-\overline{Q}\right)^2$$
$$\cong \lim_{N\to\infty}\frac{1}{N-1}\left(\sum_{k'}\sum_{k''}\left(x_{k'}-\overline{x_{k'}}\right)\left(x_{k''}-\overline{x_{k''}}\right)\cdot\frac{\partial\overline{Q}}{\partial x_{k'}}\cdot\frac{\partial\overline{Q}}{\partial x_{k''}}\right) \quad (5)$$

For the application of the direct subtraction calculations, the sensitivity coefficients can be approximated as

$$\frac{\partial\overline{Q}}{\partial x_{k'}} = \frac{\partial\overline{Q}\left(x_{k'}+\sigma(x_{k'})\right)-\partial\overline{Q}\left(x_{k'}\right)}{\sigma(x_{k'})} \quad (6)$$

The perturbed term ($\partial\overline{Q}\left(x_{k'}+\sigma(x_{k'})\right)$) and reference term ($\partial\overline{Q}\left(x_{k'}\right)$) about $x_{k'}$ can be calculated by two direct DeCART calculations. The S/U analysis based on the direct subtraction (S/U-DS) needs the calculations of the numerous input parameter values. Nevertheless, the best benefit of this method is that one can obtain accurate S/U analysis solutions and it can be used as reference. The S/U-DS analysis modules are implemented into the DeCART/MIG code system.

2.3 Validation and Verification for DeCART/MIG Code System

To validate the newly-established DeCART/MIG code system for UQ analysis, the pressurized water reactor (PWR) based TMI-1 hot full power (HFP) pin problem is first considered. The TMI-1 HFP pin problem is one of the UQ analysis problems included in the uncertainty analysis in modelling (UAM) [10] workshop benchmark. Table I shows the configuration of UAM TMI-1 HFP pin problem.

Table I: Configuration of UAM TMI-1 HFP pin problem

Parameter	Value
Pin pitch	1.4427 cm
Fuel Pellet Radius	0.46955 cm
Cladding Inner Radius	0.4791 cm
Cladding Outer Radius	0.5464 cm
Fuel/Cladding/Moderator Material	UO_2/Zircaloy-4/H_2O
Fuel Enrichment	4.85 w/o
Fuel/Cladding/Moderator Temperature	900.0/600.0/562.0

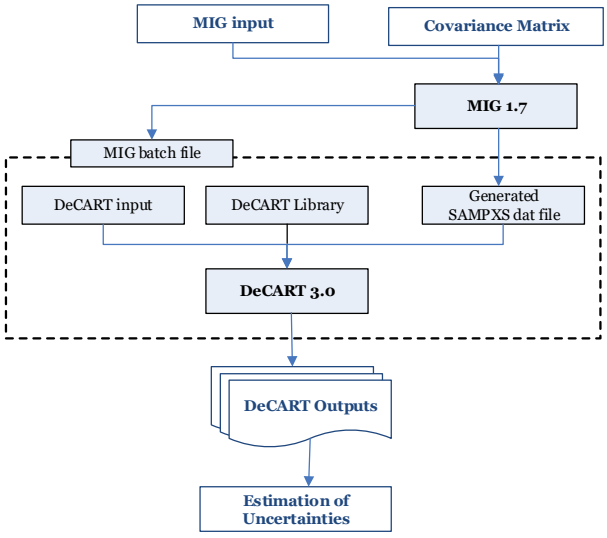

Fig. 1. Flowchart of DeCART/MIG uncertainty quantification analysis code system.

For all UQ analysis in this study, the DeCART ENDF/B-VII.1 based cross section library and the 100 cross section sample sets for ^{235}U and ^{238}U were prepared. The sampling was conducted on the 47-group cross sections and the corresponding 47-group covariance matrix in multi-group representation. The explicit resonance self-shielding was not considered for sampling. Especially, the sampled elastic and inelastic scattering cross section sets were provided by the individual covariance matrix, not the compounded one. In the sampled cross section sets, *ν*, capture, (n,2n), (n,3n), fission, elastic and inelastic scattering reaction cross sections, and fission spectrum are considered.

Table II: Uncertainties in k_{inf} for UAM TMI-1 pin problem

Nuclide	Cov. Data*	*Uncertainties in k (%)*		
		MUSAD	MIG	
		S/U	S/U-DS	S.S.
^{235}U	*ν*	0.604	0.604	0.606±0.072
	(n,γ)	0.210	0.213	0.208±0.017
	(n,f)	0.077	0.077	0.072±0.007
	(n,n)	-	0.001	0.001±0.001
	(n,n')	-	0.001	0.001±0.001
	χ	-	0.156	0.152±0.009
^{238}U	*ν*	0.071	0.072	0.070±0.005
	(n,γ)	0.382	0.390	0.392±0.030
	(n,f)	0.015	0.015	0.015±0.001
	(n,n)	-	0.056	0.052±0.004
	(n,n')	-	0.055	0.049±0.007
	χ	-	0.028	0.028±0.003
Total (w/o χ)		0.759	0.765	0.762±0.072
Total		0.771	0.775	0.781±0.091

* Covariance data for each reaction type (e.g., ν = MT451, (n,γ) = MT102, (n,fis) = MT18, (n,n) = MT2, (n,n') = MT4).

Table II and Figure 2 present the uncertainties in k_{inf} for the TMI-1 HFP pin problem for each reaction. In the DeCART/MIG results, the total k_{inf} uncertainty due to cross section uncertainties excluding fission spectrum is about 1068 pcm (0.76%). The largest contributions for each isotope are ^{235}U ν (849 pcm, 0.61%) and ^{238}U (n,γ) cross section (550 pcm, 0.39%). It is worthwhile to note that there are significant contributions from the ^{235}U and ^{238}U fission spectrum uncertainties. The MUSAD [7] and S/U-DS MIG results are provided for comparison. Overall, the uncertainties in k_{inf} by the DeCART S.S. and the others are in good agreement with considering their statistical uncertainties. It is confirmed that the DeCART/MIG UQ analysis code systems works well.

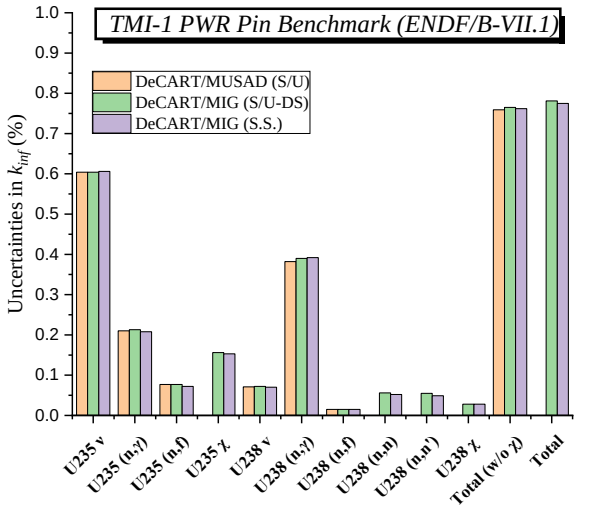

Fig. 2. Comparison between the uncertainties in k_{inf} by the S.S. and S/U method for UAM TMI-1 HFP pin problem

2.4 Nuclear Data Uncertainty for BEAVRS Benchmark

BEAVRS benchmark [11] provides a highly-detailed PWR specification with two-cycles of measured operation data such as control rod bank worth (CRBW), isothermal temperature coefficient (ITC), fuel assembly(FA)-wise detector signals, and critical boron concentrations with two-cycles burnup. The UQ analyses for the BEAVRS benchmark were conducted by the DeCART/MIG cross section random sampling code system with ENDF/B-VII.1 covariance data. We used 100 cross section samples for the S.S. calculations. The same multi-group cross section library and cross section sample sets as the ones that used in the UAM benchmark are utilized for the BEAVRS benchmark.

Table III shows the uncertainties in CRBW due to ^{235}U and ^{238}U cross section uncertainties. The maximum errors of individual and total CRBWs considering both of the difference between measurements and DeCART and the cross section uncertainties are 11.4% and 2.2%. The design review criteria (DRC) [12] of individual and total CRBW for start-up and operation are 10% and 15%, respectively. Therefore, the DeCART results meets the DRC of CRBW in a typical PWR start-up case. Figure 3 shows the FA-wise power distributions for hot-zero power (HZP) condition. In Fig. 3, first and second line indicates the normalized FA-wise power distribution for measurement and DeCART whereas third and fourth line means the difference between measurement and DeCART and the uncertainties due to ^{235}U and ^{238}U cross section uncertainties. It is observed that the error of the FA-wise power distribution is 5.0% at C11 FA. The DRC of FA-wise power distribution is 10% in a typical PWR start-up case. Considering it, the DeCART result for FA-wise power distribution meets the DRC. Table IV shows the uncertainties in ITCs due to ^{235}U and ^{238}U cross section uncertainties. The maximum error of ITC is 1.99 pcm/^{o}F. It narrowly meets the DRC values (2.0 pcm/^{o}F).

Table III: Uncertainties in control rod bank worth due to ^{235}U and ^{238}U cross section uncertainties

Case	CRBW and its Uncertainties by DeCART/MIG			
	DeCART (pcm)	Diff * (%)	Unc.** (%)	|Diff| +Unc. (%)
ARO	781	0.8	0.7	1.5
D in	1246	-3.6	0.6	4.2
D, C in	1252	-7.0	1.0	8.0
D, C, B in	499	8.9	2.5	11.4
D, C, B, A in	458	0.6	2.1	2.7
Total	4236	-1.6	0.6	2.2

* Diff (%) = (CRBW$_{Measurement}$ − CRBW$_{DeCART}$)/CRBW$_{DeCART}$ x 100,
** Unc.(%) is the relative uncertainties in CRBW due to cross section uncertainties.

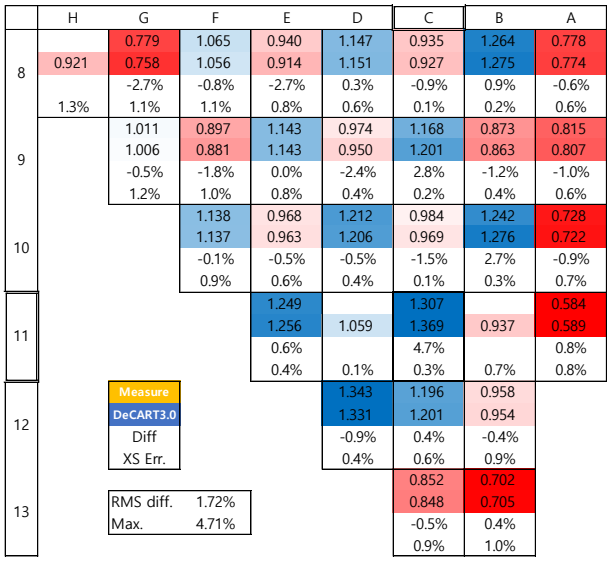

Fig. 3. Uncertainties of assembly-wise power distribution due to ^{235}U and ^{238}U cross section uncertainties

3. Conclusions

The DeCART/MIG cross section random sampling code system was successfully established and verified through the UAM and BEAVRS benchmark problems. To validate the DeCART/MIG cross section random sampling code system, the S/U analysis module based on the direct subtraction were additionally implemented into the MIG code. From the MIG results for the UAM benchmark, the uncertainties in k_{inf} by the DeCART /MIG S.S. calculations agree very well with the S/U perturbation method based DeCART/MUSAD and the S/U direct subtraction based DeCART/MIG results. In the application for the BEAVRS benchmark, the errors of the design parameters (i.e. CRBW, ITC, FA-wise power distribution) are less than the DRC of a typical PWR start-up case.

This newly-developed DeCART/MIG UQ analysis code system by S.S. method can be usefully utilize as uncertainty analysis and margin estimation tools for DeCART code licensing.

Table IV: Uncertainties in isothermal temperature coefficients due to ^{235}U and ^{238}U cross section uncertainties

Case	ITC and its Uncertainties by DeCART/MIG (pcm/^{o}F)			
	Measured	Diff	Unc.*	|Diff| +Unc. **
ARO	-1.75	-1.35	0.20	1.55
D in	-2.75	-1.79	0.20	1.99
D, C in	-8.01	-1.53	0.20	1.73

* 'Unc.' is the uncertainties in ITC due to cross section uncertainties,
** |Diff|+Unc. = ($|ITC_{Measurement} - ITC_{DeCART}|$+Unc.).

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