Stochastic Sampling Based DeCART2D/MASTER Uncertainty Quantification Analysis with ENDF/B-VII.1 Covariance Data for Hanbit Unit 3 Cycles 1

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*Keywords : Uncertainty Quantification, DeCART2D/MASTER, Hanbit Unit 3, ENDF/B-VII.1

1. Introduction

Currently, both deterministic and Monte Carlo (MC) method-based codes are widely and commonly used for various nuclear design and analysis. To ensure margins of the safe design parameters in a nuclear core system design, uncertainty quantification (UQ) analysis is essential. In the fields of nuclear engineering, there are two approaches to quantifying uncertainty from these parameters. Best Estimate Plus Uncertainty (BEPU) and conservative methods are two approaches used for evaluating the accuracy and safety of designs and analyses.

Especially, the most significant source of uncertainty in nuclear core design and analyses is the nuclear reaction cross-sections. The uncertainties of the nuclear reaction cross-sections can be provided from the covariance data (e.g., MF31 and MF33) in evaluated nuclear data libraries.

Recently, Park developed the multi-correlated nuclear cross-section sampling code MIG [1, 2] for the stochastic sampling method (S.S. method) and established the McCARD/MIG [3] and DeCART/MIG [4] UQ analysis code system. Meanwhile, the Korea Atomic Energy Research Institute (KAERI) has developed its own DeCART2D/MASTER [5,6] two-step nuclear core design code system.

In this study, the main goal of this study was to establish the DeCART2D/MASTER/MIG UQ analysis code system and apply it to UQ analyses of the commercial Hanbit Unit 3 [7] core design parameters due to the uncertainties of ENDF/B-VII.1 [8] nuclear reaction cross-section.

2. Stochastic Sampling Method and Tools

This section presents a DeCART2D/MASTER/MIG code system with stochastic sampling of cross-sections and the methodology of sampling.

2.1 DeCART2D/MASTER/MIG UQ Analysis Code system

Figure 1 shows the flow chart of the MIG nuclear cross-section UQ analysis code in the DeCART2D/MASTER two-step procedure. Firstly, by

using covariance matrix and MIG inputs, MIG 1.7 generates sampled cross-section sets. And then, using sampled cross-section sets, DeCART2D generates FGC (Few Group Constants) from each sampled cross input and cross-section set. With the generated FGC file, MASTER4.0 is used for whole core analysis. Accordingly, nuclear core design parameters (e.g., critical boron concentration and power peaking factors) analysis can be generated as the number of the sampled cross-section sets from MIG 1.7. In this study, 47 group cross-sections and their covariance data from ENDF/B-VII.1 evaluated data library were used.



Fig. 1. Flow chart of the DeCART2D/MASTER/MIG UQ analysis code system

Neutron cross-sections and neutron spectrum of 235 U and 238 U were perturbed and sampled as the SAMPXS files, as shown in Fig. 1. The types of selected nuclear data for UQ analysis are elastic scattering (MT=2), inelastic scattering (MT=4), capture (MT=102) and fission (MT=18) cross-sections by neutron, ν and χ (fission spectrum). For UQ analysis of core design parameters, Total perturbated calculation was conducted 200 times. And the others were conducted 100 times of repeated DeCART2D/MASTER/MIG calculations.

2.2 Cross-section sampling method

In the cross-section sets sampling, the correlation between cross-sections for each reaction energy group and type should be properly considered. This process is called multiple correlated sampling. In this study, the Cholesky covariance matrix decomposition method was used for the multiple correlated sampling. Eq. (1) shows the equation for the Cholesky covariance matrix decomposition method.

$$\mathbb{C} = \mathbb{B} \cdot \mathbb{B}^T \tag{1}$$

where \mathbb{B} is a lower triangular matrix that $\mathbb{B} \cdot \mathbb{B}^T$ can be identical with the given covariance matrix \mathbb{C} . Then the Box-Muller method was used for sampling crosssections, using the calculated matrix \mathbb{B} from Eq. (1).

$$X_k = \overline{X} + \mathbb{B} \cdot \mathbb{Z} \tag{2}$$

where \overline{X} presents mean cross-section vector and \mathbb{Z} presents random normal vector. This stochastic sampling procedure for multiple correlated sampling is a well-known and widely used.

2.3 Uncertainty quantification

Through DeCART2D/MASTER/MIG UQ analyses, hundreds of repeated calculations can be conducted to get nuclear core design parameters and its uncertainty due to the uncertainties of nuclear data. The mean value and uncertainty of the core design parameter u from cross-section perturbation of isotope i and its reaction type j are defined by

$$\overline{u_{i,j}} = \frac{1}{N} \sum_{k=1}^{N} u_{i,j,k}$$
(3)

$$\sigma_{u_{i,j}}^2 = \frac{1}{N-1} \sum_{k=1}^{N} (u_{i,j,k} - \overline{u_{i,j}})^2$$
(4)

where k indicates k-th perturbation set which was used to calculate the core design parameter.

3. Uncertainty analysis of core design parameters

3.1 Specification of Hanbit Unit 3

In this study, Hanbit Unit 3 cycle 1 was selected as the target system for UQ analysis of core design parameters. Hanbit Unit 3 is a commercial 2815 MWth PWR nuclear reactor located in the Republic of Korea. The core of Hanbit Unit 3 is composed of 177 fuel assemblies (FAs), which consists of 16 x 16 array of 236 fuel rods. In Cycle 1, 8 FA types (i.e., A0, B0, B1, B2, C0, C1, D0, D1, and D2 FA) are loaded in the core. The enrichments of the UO_2 fuels in the FAs ranged from 1.30 w/o to 3.36 w/o. In calculation with MASTER, the core was axially analyzed in 26 nodes from bottom to top.

3.2 Uncertainty quantification of CBC

Table 1 shows over all uncertainty in critical boron concentration (CBC) from nuclear data of U-235 and U-238. In the paper, the reaction types were referred to as U5XX or U8XX. U5XX means the result from a perturbed 'XX' nuclear data of ²³⁵U. The XX portion can be replaced with XI for fission spectrum, N for ν , E for elastic scattering, I for inelastic scattering, F for fission reaction, G for capture reaction, and others. Lastly, 'Total' refers to the case that all data are perturbed simultaneously.

Fable 1. Uncertainties in CBC of Hanbit Unit 3 cycle 1 due to uncertainties for each nuclear reaction cross-section

		BOC 0 EFPD		MOC	EC	C
Isotope	Reaction type			188 EFPD	370 EFPD	
		HZP	HFP	HFP	HZP	HFP
U-235	χ	19.831	21.793	13.992	9.742	10.605
	ν	45.082	44.836	32.612	23.030	23.477
	(n,n)	0.033	0.015	0.015	0.015	0.010
	(n,n')	0.015	0.016	0.011	0.012	0.011
	(n,f)	10.221	9.536	4.854	2.446	2.061
	(n,γ)	11.463	11.475	9.888	8.308	8.632
U-238	χ	3.516	3.899	4.579	4.010	4.603
	ν	6.248	12.458	9.495	6.597	7.406
	(n,n)	2.431	3.506	4.170	3.844	4.795
	(n,n')	2.370	3.294	3.894	3.593	4.433
	(n,f)	2.412	2.412	2.595	2.291	2.459
	(n,γ)	15.991	16.899	12.439	7.921	9.854
Total	Total	51.233	51.617	37.391	26.979	28.330



Fig. 2. Uncertainties in CBC due to the uncertainties of the 235 U cross-section



Fig. 3. Uncertainties in CBC due to the uncertainties of the 238 U cross-section

Figures 2 and 3 present the uncertainties in CBC by nuclear data uncertainties of ²³⁵U and ²³⁸U nuclear reaction cross-section during hot full power operation, respectively. In Fig. 2, it is observed that the most significant impact for the uncertainties in CBC is ν of ²³⁵U (U5N), which is directly related to criticality. Following the ν value of ²³⁵U, the uncertainties of fission spectrum, χ , of ²³⁵U affected the large uncertainties in CBC. Results of CBC showed normality in all types of perturbation types. Though at some points in ²³⁵U inelastic scattering, results of CBC distribution showed high kurtosis, which means lost of normality. The high kurtosis is due to very low impact of ²³⁵U inelastic scattering to CBC as uncertainty seen in Figures 2.

In two group (i.e., fast and thermal energy group) whole core calculations with the range of 0.1 eV to 1.0 eV cut-off energy, the χ values of fast and thermal energy group are commonly adjusted to 0.0 and 1.0. It means that even if there is perturbation in χ , there is no direct effect on core design parameters. Accordingly, it is noted that the χ of ²³⁵U (U5XI) is not directly related to criticality, but it contributes to the perturbation of FGC from the shift of neutron spectrum from the perturbation

of χ . Table 2 presents example cases for the differences of FGCs in A0 fuel assembly due to fission spectrum perturbation. Comparing two samples, Case 79 and Case 85, Case 85 had a relatively hardened neutron spectrum before group condensation. After group condensation into two groups, Case 85 showed decreasing in 1st group fission, capture, and down scattering cross-sections. On the other hand, in the softened case, Case 79, showed increasing in group constants. Accordingly, a fission spectrum perturbation leads to the change in reactivity.

Table 2. Examples of FGC change [%] in A0 FA from reference case due to χ perturbation of ²³⁵U

Reaction type	Group	Change of FGC due to Perturbation [%]		
••		Case 79	Case 85	
210-	1	2.1510	-2.0549	
VOf	2	0.0099	-0.0077	
σ	1	2.7784	-2.6247	
υγ	2	0.0116	-0.0071	
$\sigma_{s \ 1 \to 2}$		2.7615	-2.6131	
k _{inf}		-0.8175	0.7642	

Table 3 shows cycle lengths and their uncertainties due to nuclear reaction cross-section uncertainties. The mean cycle length was about 364 days. The ν of ²³⁵U (U5N) contributed most of the uncertainties in cycle length, which was 7.379 EFPD. Then, χ of ²³⁵U (U5XI) and (n, γ) of ²³⁸U (U8G) followed next, with values of uncertainty 3.343 and 3.085 EFPD.

Table 3. Cycle lengths and their uncertainties due to crosssection uncertainties for Hanbit Unit 3 Cycle 1

Casa	Cycle length	Uncertainty	
Case	[EFPD]	[1σ, EFPD]	
U5XI	364.667	3.343	
U5N	364.282	7.379	
U5E	364.384	0.003	
U5I	364.385	0.003	
U5F	364.618	0.656	
U5G	364.730	2.410	
U8XI	364.536	1.425	
U8N	364.479	2.327	
U8E	364.364	1.492	
U8I	364.537	1.370	
U8F	364.455	0.763	
U8G	364.175	3.085	
Total	365.845	8.818	

3.3 Uncertainty quantification of 3D pin peaking factor

Figures 4 and 5 present uncertainties in 3-D pin peaking factor (FQP) with nuclear data perturbation from ²³⁵U and ²³⁸U covariance data during hot full power operation, respectively. Uncertainties in 3D pin peaking factor in hot zero power condition at BOC and EOC were very closed to the uncertainties in hot full power condition. Similar to CBC, ν and χ values (i.e., U5N and U5XI) of ²³⁵U highly contributed to the uncertainties in FQP.

As shown in Figs 4 and 5, there are strong changes of the uncertainties in around 15 EFPDs, 120 EFPDs and 240 EFPDs because of moving of position where 3-D pin peaking appears. The numbers in parentheses refer to the position of pin within an assembly. In the Fig. 6. as an example, the change of FQP position changed from the 11th axial node of (N,11) assembly's (12,2) pin position at 1.3 EFPD to the 11th axial node of (L,13) assembly's (2,5) pin position at 13.4 EFPDs. And then 3-D pin peaking position moved to the 12th axial node of (J,11) assembly's (2,5) pin position at 26.9 EFPDs.

Except χ perturbation case of ²³⁸U, most of perturbation types showed normal distribution in FQP results. But in other perturbation cases, some points with non-normality were found, which is because of the position change of the peaking pin, like the uncertainty in FQP.



Fig. 4. Uncertainties in 3-D Pin Peaking Factor due to the uncertainties of the 235 U cross-section



Fig. 5. Uncertainties in 3-D Pin Peaking Factor due to the uncertainties of the 238 U cross-section



Fig. 6. Change of 3-D peaking pin position changes from 1.3 EFPDs to 13.4 EFPDs and 26.9 EFPDs

3.4 Uncertainty quantification of axial offset (power)

Figures 7 and 8 show uncertainties in Axial Offset (AO) with nuclear data perturbations of ²³⁵U and ²³⁸U cross-sections during hot full power operation, respectively. Uncertainties in axial offset in hot zero power condition at BOC and EOC were also very closed to the uncertainties in hot full power condition. Likewise, the top 3 nuclear data were χ and ν values of ²³⁵U (U5XI and U5N) and (n, γ) cross-section of ²³⁸U (U8G). Both elastic and inelastic scattering reaction of ²³⁵U showed non-normality. After 280EFPD, χ and fission reaction of ²³⁸U also lost normality. All the non-normality of results were due to very high kurtosis, like χ of ²³⁸U in FQP, because of very small impact of perturbed reaction types on uncertainty in axial offset.

Uncertainty in axial offset shrinks around 150 EFPD, as seen in figures 7 and 8, due to average axial offset value approaches zero. However, the other point where average axial offset value approaches zero, around 256 EFPD, does not show drop of uncertainty as 150EFPD. Around 150 EFPD, the axial layer where maximum axial power appeared were identical in 100 repeated calculations. But around 256EFPD, the maximum axial power layers distributed in opposing directions. This resulted in higher uncertainty in axial offset at 256 EFPD.



Fig. 7. Uncertainties in AO due to the uncertainties of the 235 U cross-section



Fig. 8. Uncertainties in AO due to the uncertainties of the 238 U cross-section

4. Conclusion

In this study, the DeCART2D/MASTER/MIG UQ analysis code system was established, and the UQ analysis of nuclear core design parameters for Hanbit Unit 3 Cycle 1 using ENDF/B-VII.1 has been performed using ENDF/B-VII.1 covariance data.

It is noted that the ν and fission spectrum of ²³⁵U and the capture cross-section of ²³⁸U were the three largest contributors to the CBC uncertainties. As the effect on cycle length uncertainties, the biggest uncertainty was about 7.4 EFPDs. The general DRC (design review criteria) values of CBC and reactivity are 50 ppm and 500 pcm [9]. In this study, it is observed that only except the very beginning of the cycle, the uncertainties of the CBCs met DRC. In the uncertainty estimation of the 3-D pin peaking factor (FQP), ν and the fission spectrum of ²³⁵U are the large contributors to the uncertainties, but there is no significant contribution by the capture crosssection of ²³⁸U. Lastly in the AO case, ν and the fission spectrum of ²³⁵U and the capture cross-section of ²³⁸U were the three largest contributors.

In the near future, the uncertainties from various actinide and activation isotopes, including the existing major nuclides (235 U and 238 U), will be considered to analyze the uncertainties of the nuclear core parameters for multiple cycles using the up-to-date covariance data.

Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science and ICT) (No. RS-2024-00422848).

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