Verification of Sensitivity and Uncertainty Analysis Code with the GODIVA and VHTR fuel

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1. Introduction

Korea Atomic Energy Research Institute has designed a UO2 fueled 200 MWth prismatic very high temperature reactor (PMR200) and DeCART/CAPP [1] code systems with two-step procedure have been established for the core analysis. However, it is necessary to analyze the sensitivity and uncertainty analysis for the nuclear design and safety analysis of the new core and the code validation. For this reason, we are developing a sensitivity and uncertainty analysis for DeCART), which has the specific functions of producing the sensitivity coefficients and uncertainty quantification to the system multiplication factor (k_{eff}) using the covariance data and the group constants.

In this paper, the methodology of the sensitivity and uncertainty analysis code was described and the calculation results on the GODIVA benchmark and the PMR200 pin cell problem were compared with the results by TSUNAMI of SCALE 6.1 [2] and McCARD [3].

2. Methods and Results

The main uncertainty to affect k_{eff} in the core analysis is caused by the uncertainty of the nuclear data. From the sandwich rule [4], this uncertainty can be calculated using the sensitivity of k_{eff} due to the perturbation of the cross section data and the covariance data inside the evaluated nuclear data.

In the next section, the method for producing the sensitivity of k_{eff} and its uncertainty based on the classical perturbation theory is presented and then the calculation results for the verification of the S&U analysis code are summarized.

2.1 Sensitivity Analysis

From the first order perturbation theory, one can readily obtain the sensitivity of k_{eff} as Eq.(1).

$$S = \frac{\delta k}{\delta \Sigma_x} \frac{\Sigma_x}{k} = -\frac{\Sigma_x}{k} \frac{\langle \phi^* \left(\frac{\delta A}{\delta \Sigma_x} - \frac{1}{\delta B} \frac{\delta B}{k \delta \Sigma_x}\right) \phi \rangle}{\langle \phi^* \frac{B}{k^2} \phi \rangle}$$
(1)

Thus, the sensitivity coefficients for reaction x, isotope i, energy group g, and region z can be represented as

$$S_{xgz}^{i} = \frac{T_{1xgz}^{i} + T_{2xgz}^{i} + T_{3xgz}^{i}}{D}$$
(2)

If the Pn method form is used in the sensitivity coefficients, the each coefficients of Eq.(2) could be as followings.

$$D = \frac{1}{4\pi k} \sum_{z} V_{z} \sum_{i} \sum_{g} \left(\bar{\nu}_{g}^{i} \Sigma_{fg}^{i} \phi_{g} \right) \sum_{g'} \left(\chi_{g'}^{i} \phi_{g'}^{*} \right) \quad (3)$$

$$T_{1xg}^{i} = -\Sigma_{xg}^{i} V_{z} \sum_{l} \sum_{m} \frac{2l+1}{4\pi} \phi_{glm} \phi_{glm}^{*}$$
(4)

$$\Gamma_{2g}^{l} = \frac{1}{4\pi k} V_{z} \overline{v}_{g}^{l} \Sigma_{fg}^{l} \phi_{g} \Sigma_{g'} \left(\chi_{g'}^{l} \phi_{g'}^{*} \right)$$
(5)

$$T_{3xgz}^{i} = V_{z} \sum_{g'} \sum_{l} \frac{2i+1}{4\pi} \sum_{sgg'}^{ll} \sum_{m} \phi_{glm} \phi_{g'lm}^{*}$$
(6)

Here, l is the Legendre order and m is flux moments corresponding to l.

Therefore, the sensitivity coefficients for the individual cross section are summarized as followings.

i. (n,
$$\gamma$$
), (n, α), (n,p)
 $S_{xg}^{i} = \frac{T_{1xg}^{i}}{D}$
(7)
ii. (n,f)

$$S_{fg}^{i} = \frac{T_{1fg}^{i} + T_{2fg}^{i}}{D}$$
(8)

iii. **v**, **x**

$$S_{xg}^i = \frac{T_{2xg}^i}{D} \tag{9}$$

iv. (n,n), (n,n'), (n,2n),(n,3n)

$$S_{sg}^{i} = \frac{T_{isg}^{i} + T_{isg}^{i}}{D}$$
(10)

2.2 Uncertainty Quantification

The uncertainty of the core response caused by the nuclear data can be obtained using the sandwich rule as the followings.

$$\sigma^{2}(k_{xy}^{ij}) = S_{\alpha_{x}^{i}} Cov(\alpha_{x}^{i}, \alpha_{y}^{j}) S_{\alpha_{y}^{j}}^{T}$$
(11)

Here, $C_{\alpha_x^i \alpha_y^j}$ is relative covariance matrix for *x*, *y* reaction pair of *i*, *j* nuclide and $S_{\alpha_x^i}$ sensitivity coefficient vector for *x* reaction of *i* nuclide.

2.3 Procedures of MUSAD

First, the covariance data is obtained from ENDF/B-VII.1 using ERRORR(J) of NJOY. Once DeCART performs the forward and adjoint calculations and makes the input parameters for the uncertainty analysis code including the forward and adjoint flux and the cross sections, etc. Then, MUSAD can produce the sensitivity coefficients and the uncertainty of k_{eff} by the method described in the previous section. However, the adjoint flux production of DeCART is function in development at present. Thus, the forward and adjoint flux were obtained from KENO-VI of SCALE and the individual multi-group cross sections were produced by McCARD for this verification calculation. Fig. 1 shows the procedures of the sensitivity and uncertainty analysis using MUSAD.



Fig. 1. Procedures for the sensitivity and uncertainty analysis using MUSAD.

2.4 Calculation Results

For the verification of this code, the results of the code on GODIVA with fast spectrum and PMR200 pin cell with thermal spectrum were compared to them of two codes, TSUNAMI and McCARD. In the calculations, TSUNAMI used the covariance data of SCALE 44 group built in SCALE 6.1 and McCARD used the covariance data of ENDF/B-VII.1 with 239 group structure which is the same structure of the fine group in TSUNAMI and the covariance data of SCALE 44 group. This 239 group structure was also used in the analysis using MUSAD.

Table I shows the comparisons of the uncertainty of keff induced by the perturbed cross sections of U235 and U238. Except v and elastic scattering, three codes produced similar results because ENDF/B-VII.1 and SCALE data contain the same covaraince data for U235 and U238. On the contrary, the v value of SCALE covaraince data originates from JENDL-3.1. Also, the discrepancy of the uncertainty by the elastic scattering between MUSAD and the others may be related to differences in using scattering moment. MUSAD uses only 0th order scattering matrix due to difficulty of obtaining the scattering matrix for the first or higher order scattering moment.

The uncertainty calculation results on PMR200 pin cell problem are shown in Table II. It presented the similar trend as like GODIVA problem. Howerver, the difference of the uncertainty by the elastic scattering might be attributed to the fact that the results of TSUNAMI and MUSAD just considered the explicit effect by the unshielded cross sections.

Table I:	GODIVA	Problem
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Nuclide	Cov. XS	McC	ARD	TSUNAMI	MUSAD
		σ _{xx} (k) (%)	σ_{xx} (k) (%)	σ_{xx} (k) (%)
XS. data		ENDF/B-VII.0		ENDF/B-VII.0	
Cov. Data		ENDF/B-VII.1	SCALE	SCALE	ENDF/B-VII.1
		238G	44G	44G	238G
U235	ν, ν	0.544	0.148	0.148	0.549
	(n,γ), (n,γ)	0.863	0.840	0.816	0.840
	(n,γ), (n,n)	0.244	0.256	0.354	0.313
	(n,f), (n,f)	0.268	0.268	0.273	0.277
	(n,f), (n,n)	0.053	0.057	0.081	0.086
	(n,n), (n,n)	0.306	0.304	0.345	0.745
	(n,n), (n,n')	0.418	0.516	0.625	0.680
	(n,n'), (n,n')	0.702	0.664	0.685	0.711
U238	ν, ν	0.010	0.010	0.011	0.011
	(n,γ), (n,γ)	0.001	0.002	0.002	0.001
	(n,f), (n,f)	0.003	0.003	0.003	0.003
	(n,n), (n,n)	0.032	0.034	0.036	0.102
	(n,n), (n,n')	0.060	0.062	0.071	0.095
	(n,n'), (n,n')	0.121	0.114	0.088	0.091
Total		1.195	0.972	1.055	1.335

Table II: PMR200 Pin Cell Problem

Nuclide	Cov XS	McCA	ARD	TSUNAMI	MUSAD			
	COV. AS	σ_{xx} (k)) (%)	σ_{xx} (k) (%)	σ_{xx} (k) (%)			
XS. data		ENDF/B-VII.0		ENDF/B-VII.0				
Corr. Doto		ENDF/B-VII.1	SCALE	SCALE	ENDF/B-VII.1			
Cov. Data		238G	44G	44G	238G			
U235	ν, ν	0.646	0.285	0.285	0.646			
	$(n,\gamma), (n,\gamma)$	0.215	0.223	0.222	0.213			
	(n,γ), (n,f)	0.075	0.078	0.107	0.076			
	(n,γ), (n,n)	0.007	0.010	0.003	0.002			
	(n,f), (n,f)	0.067	0.067	0.069	0.070			
	(n,f), (n,n)	0.002	0.004	0.001	0.001			
	(n,n), (n,n)	0.001	0.001	0.000	0.000			
	(n,n'), (n,n')	0.001	0.001	0.000	0.000			
	ν, ν	0.006	0.006	0.006	0.006			
	(n,γ), (n,γ)	0.293	0.262	0.326	0.376			
	(n,γ), (n,n)	0.026	0.031	0.032	0.016			
U238	(n,f), (n,f)	0.001	0.001	0.001	0.001			
	(n,n), (n,n)	0.091	0.085	0.010	0.008			
	(n,n), (n,n')	0.009	0.005	0.000	0.000			
	(n,n'), (n,n')	0.041	0.029	0.001	0.001			
Total		0.759	0.476	0.524	0.784			

3. Conclusions

In this paper, the methodology for the sensitivity and uncertainty analysis code, MUSAD, was described and the verification calculations on the GODIVA benchmark and the PMR200 pin cell problem were carried out. As a result, they are in a good agreement when compared with the results by TSUNAMI and McCARD. From this study, it is expected that MUSAD code can produce accurate results, if the cross sections and the core parameter for the S&U analysis could be completely obtained from DeCART.

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