Cross Section Sensitivity and Uncertainty Analysis Using Monte Carlo Forward Calculation

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1. Introduction

Estimation of uncertainties in k_{eff} and power density calculations is important in nuclear design and safety analyses, code validation, data evaluation, etc. There are two main sources of uncertainties; the cross section data and the modeling. If one eliminates the modeling uncertainty by using a detailed geometrical input and precise material data, the cross section data present the most significant source of the uncertainties.

The prediction uncertainty of a nuclear parameter can be estimated in terms of its sensitivities to cross sections [1]. The objectives of this paper are to realize a sensitivity and uncertainty (S/U) analysis module in McCARD (Monte Carlo Code for Advanced Reactor Design and analysis) [2] and to examine its performance in comparison with other codes: TSUNAMI [3] and SUSD3D [4]. This work will provide a useful basis of continuous energy Monte Carlo (MC) calculations aimed at conducting the S/U analysis.

2. Uncertainty Quantification

2.1 Propagated Uncertainty

A nuclear parameter Q can be viewed as a function of various input parameters such as system geometry, material composition, cross section data, etc. Then Q can be expressed as

$$Q \equiv Q(\cdots, \underbrace{\cdots, x^i_{r,g}, \cdots}_{x^i_{r,g}(i\in I,\, r\in\Gamma, g\in G)}, \cdots) . \qquad (1)$$

$x^i_{r,g}$ is the g-th group microscopic cross-section of reaction type r of isotope i. I, Γ, and G represents the total number of isotopes, reaction types, and energy groups, respectively.

Because of the data uncertainties, there can be an infinitely different set of cross section inputs to Q. This may result in different Q's as many as the number of input sets. Let's designate the k-th cross section input set which may be sampled from the cross section distribution by $\left(x^i_{r,g}\right)_k$ (k=1,2, …). The value of Q from this set can be expressed as

$$Q_k \equiv Q(\cdots, \underbrace{\cdots, \left(x^i_{r,g}\right)_k, \cdots}_{\left(x^i_{r,g}\right)_k(i\in I,\, r\in\Gamma, g\in G)}, \cdots) . \qquad (2)$$

The mean of Q, $\overline{Q}$, and its variance about $\overline{Q}$, $\sigma^2\left[Q\right]$, can then be given by

$$\overline{Q} = \lim_{N\to\infty} \frac{1}{N}\sum_k^N Q_k \quad . \qquad (3)$$

$$\sigma^2\left[Q\right] = \lim_{N\to\infty} \frac{1}{N-1}\sum_k^N \left(Q_k - \overline{Q}\right)^2 . \qquad (4)$$

Let's assume that $\overline{Q}$ is determined by

$$\overline{Q} \equiv Q(\cdots, \underbrace{\cdots, \overline{x^i_{r,g}}, \cdots}_{\overline{x^i_{r,g}}(i\in I,\, r\in\Gamma, g\in G)}, \cdots) \qquad (5)$$

with $\overline{x^i_{r,g}}$ denoting the mean of the cross section which is defined in the same way as $\overline{Q}$ in Eq. (3). The Taylor series expansion of Eq. (2) to the first order of the cross section variations about their mean values, $\left(Q_k - \overline{Q}\right)$ in Eq. (4) leads to

$$Q_k - \overline{Q} \cong \sum_{i,r,g}\left(\left(x^i_{r,g}\right)_k - \overline{x^i_{r,g}}\right)\left(\frac{\partial Q}{\partial x^i_{r,g}}\right). \qquad (6)$$

The substitution of Eq. (6) into Eq. (4) results in

$$\sigma^2\left[Q\right] \cong \lim_{N\to\infty}\frac{1}{N-1}\sum_k^N \left\{ \sum_{i,r,g}\sum_{i',r',g'}\left(\left(x^i_{r,g}\right)_k - \overline{x^i_{r,g}}\right)\left(\left(x^{i'}_{r',g'}\right)_k - \overline{x^{i'}_{r',g'}}\right)\left(\frac{\partial Q}{\partial x^i_{r,g}}\right)\left(\frac{\partial Q}{\partial x^{i'}_{r',g'}}\right)\right\} \qquad (7)$$

Equation (7) can be rewritten as

$$\sigma^2\left[Q\right] \cong \sum_{i,r,g}\sum_{i',r',g'} \mathrm{cov}\left[x^i_{r,g}, x^{i'}_{r',g'}\right]\left(\frac{\partial Q}{\partial x^i_{r,g}}\right)\left(\frac{\partial Q}{\partial x^{i'}_{r',g'}}\right), \qquad (8)$$

where

$$\mathrm{cov}\left[x^i_{r,g}, x^{i'}_{r',g'}\right] = \lim_{N\to\infty}\frac{1}{N-1}\sum_k^N\left(\left(x^i_{r,g}\right)_k - \overline{x^i_{r,g}}\right)\left(\left(x^{i'}_{r',g'}\right)_k - \overline{x^{i'}_{r',g'}}\right) . \qquad (9)$$

From Eq. (8), the relative variance of Q is obtained by

$$\left(\frac{\sigma[Q]}{\overline{Q}}\right)^2 \cong \sum_{i,r,g}\sum_{i',r',g'} \frac{\text{cov}\left[x_{r,g}^i, x_{r',g'}^{i'}\right]}{\overline{x_{r,g}^i}\cdot\overline{x_{r',g'}^{i'}}} S_Q\left[x_{r,g}^i\right] S_Q\left[x_{r',g'}^{i'}\right], \quad (10)$$

where $S_Q\left[x_{r,g}^i\right]$ is the sensitivity coefficient of Q to $x_{r,g}^i$ defined by

$$S_Q\left[x_{r,g}^i\right] \equiv \frac{\overline{x_{r,g}^i}}{\overline{Q}}\cdot\frac{\partial Q}{\partial x_{r,g}^i}. \quad (11)$$

2.2 Calculation of Sensitivity Coefficient

The derivative, $\partial Q/\partial x_{r,g}^i$, in Eq. (11), can be approximated by

$$\frac{\partial Q}{\partial x_{r,g}^i} \cong \frac{Q\left(\overline{x_{r,g}^i}+\sigma\left[x_{r,g}^i\right]\right)-Q\left(\overline{x_{r,g}^i}\right)}{\sigma\left[x_{r,g}^i\right]} = \frac{\delta Q\left[x_{r,g}^i\right]}{\sigma\left[x_{r,g}^i\right]}; \quad (12)$$

$$\delta Q\left[x_{r,g}^i\right] \equiv Q\left(\overline{x_{r,g}^i}+\sigma\left[x_{r,g}^i\right]\right)-Q\left(\overline{x_{r,g}^i}\right). \quad (13)$$

$\delta Q\left[x_{r,g}^i\right]$ can be estimated in the MC forward calculations by the MC perturbation techniques [5, 6].

3. Numerical Results

The uncertainty of k_{eff} for the GODIVA problem [7] was investigated using the McCARD code and the covariance data of JENDL-3.3. The ERRORJ code [8] was used to produce the 30-group covariance matrices based on the JENDL-3.3.

Table I shows a comparison of the results from other S/U analysis code systems, TSUNAMI and SUSD3D, which were reported in Ref. [9]. From the table, we can see that the uncertainties by the McCARD code agree well with those from other code systems.

3. Conclusions

We augmented the McCARD capability with the cross section S/U analysis module. This work will enable users to conduct a satisfactory S/U analysis using continuous cross-section libraries.

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Table I. Comparison of k_{eff} and uncertainties due to the covariance in U-235 JENDL-3.3 for the GODIVA problem

Code		KENO-V.a	ANISN	McCARD
	Spectrum/ Eigenvalue	KENO-V.a	ANISN	McCARD
	Sensitivity/ Uncertainty	TSUNAMI	SUSD3D	
XS Library		JENDL 3.3		
Energy Group		238	44	Cont.
keff (SD)		1.00322 (0.0002)	1.01108 (NA)	1.00398 (0.0006)
Covariance Data		238 grp	44 grp	30 grp
Unc. due to U-235 (%)	ν, ν	0.15	0.15	0.15
	(n,γ), (n,γ)	0.15	0.17	0.16
	(n,γ), (n,n)	0.07	0.05	0.05
	(n,2n), (n,2n)	0.02	0.01	0.01
	(n,2n), (n,n)	0	0	0.00
	(n,fis.), (n,fis.)	0.17	0.17	0.17
	(n,fis.), (n,n)	-0.05	-0.03	-0.03
	(n,n), (n,n)	0.33	0.32	0.36
	total[a)]	0.43	0.43	0.45

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