Sensitivity and Uncertainty Analysis for Coolant Void Reactivity in a CANDU Fuel Lattice Cell Model

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1. Introduction

First-order perturbation theory has been widely utilized in the sensitivity and uncertainty (S/U) analysis. The S/U analysis for a difference between the eigenvalues for two different states of a system was proposed by Mark L. Williams [1]. An eigenvalue perturbation-based method (EPBM) utilizes the first-order adjoint-weighted perturbation (AWP) technique to estimate the sensitivity of the eigenvalue difference. Furthermore this method can be easily applied in a S/U analysis code system equipped with the eigenvalue sensitivity calculation capability.

In this study, the EPBM is implemented in the Seoul National university Monte Carlo (MC) code, McCARD [2] which has the uncertainty evaluation capability for the multiplication factors, *k*, by the AWP method [3, 4]. The implementation is verified by comparing sensitivities of the lambda eigenvalue difference—i.e., the difference of the reciprocal of *k*'s—to the microscopic cross sections computed by the EPBM and the direct subtractions for the TMI-1 pin-cell problem [5]. The uncertainty of coolant void reactivity (CVR) in a CANDU fuel lattice model due to the ENDF/B-VII.1 covariance data is calculated by its sensitivities estimated by the EPBM.

2. Methodologies

The reactivity is defined as

$$\rho = \left(1 - \frac{1}{k}\right). \tag{1}$$

A reactivity change, i.e., the lambda eigenvalue difference, can be expressed as a variation of the reactivity of unperturbed and perturbed system.

$$\Delta\rho = \left(1 - \frac{1}{k_\mathrm{p}}\right) - \left(1 - \frac{1}{k}\right) = \frac{1}{k} - \frac{1}{k_\mathrm{p}} = \lambda - \lambda_\mathrm{p}, \tag{2}$$

where k_p corresponds to a variation of the Boltzmann operator such that:

$$\mathbf{M} \to \mathbf{M}_\mathrm{p}\left(= \mathbf{M} + \Delta\mathbf{M}\right). \tag{3}$$

The operator **M** denotes the net loss operator **T** or fission production operator **F**. And $\Delta\rho$ can be shown as

$$\Delta\rho = \frac{\langle \omega, \mathbf{T}\phi \rangle}{\langle \omega, \mathbf{F}\phi \rangle} - \frac{\langle \omega_\mathrm{p}, \mathbf{T}_\mathrm{p}\phi_\mathrm{p} \rangle}{\langle \omega_\mathrm{p}, \mathbf{F}_\mathrm{p}\phi_\mathrm{p} \rangle}, \tag{4}$$

where ω is the arbitrary weighting function. A sensitivity of $\Delta\rho$ to variations of *x* are given as in

$$\frac{\partial(\Delta\rho)}{\partial x} = \frac{\partial}{\partial x}\left[\frac{\langle \omega, \mathbf{T}\phi \rangle}{\langle \omega, \mathbf{F}\phi \rangle}\right] - \frac{\partial}{\partial x}\left[\frac{\langle \omega, \mathbf{T}_\mathrm{p}\phi_\mathrm{p} \rangle}{\langle \omega, \mathbf{F}_\mathrm{p}\phi_\mathrm{p} \rangle}\right]. \tag{5}$$

The first term of RHS in Eq. (5) can be written in

$$\begin{aligned}
\frac{\partial}{\partial x}\left[\frac{\langle \omega, \mathbf{T}\phi \rangle}{\langle \omega, \mathbf{F}\phi \rangle}\right] &= \frac{\left[\left\langle \frac{\partial\omega}{\partial x}, \mathbf{T}\phi \right\rangle + \left\langle \omega, \frac{\partial \mathbf{T}}{\partial x}\phi + \mathbf{T}\frac{\partial\phi}{\partial x} \right\rangle\right]\langle \omega, \mathbf{F}\phi \rangle}{\langle \omega, \mathbf{F}\phi \rangle\langle \omega, \mathbf{F}\phi \rangle} \\
&\quad - \frac{\lambda\langle \omega, \mathbf{F}\phi \rangle\left[\left\langle \frac{\partial\omega}{\partial x}, \mathbf{F}\phi \right\rangle + \left\langle \omega, \frac{\partial \mathbf{F}}{\partial x}\phi + \mathbf{F}\frac{\partial\phi}{\partial x} \right\rangle\right]}{\langle \omega, \mathbf{F}\phi \rangle\langle \omega, \mathbf{F}\phi \rangle} \\
&= \frac{\left[\left\langle \omega, \frac{\partial \mathbf{T}}{\partial x}\phi - \lambda\frac{\partial \mathbf{F}}{\partial x}\phi \right\rangle + \left\langle \omega, \mathbf{T}\frac{\partial\phi}{\partial x} - \lambda\mathbf{F}\frac{\partial\phi}{\partial x} \right\rangle\right]}{\langle \omega, \mathbf{F}\phi \rangle} \\
&= \frac{\left\langle \omega, \frac{\partial \mathbf{T}}{\partial x}\phi - \lambda\frac{\partial \mathbf{F}}{\partial x}\phi \right\rangle + \left\langle \omega, \mathbf{T}\frac{\partial\phi}{\partial x} - \lambda\mathbf{F}\frac{\partial\phi}{\partial x} \right\rangle}{\langle \omega, \mathbf{F}\phi \rangle}.
\end{aligned} \tag{6}$$

In the same way, the second term of RHS in Eq. (5) can be written

$$\begin{aligned}
&\frac{\partial}{\partial x}\left[\frac{\langle \omega, \mathbf{T}_\mathrm{p}\phi_\mathrm{p} \rangle}{\langle \omega, \mathbf{F}_\mathrm{p}\phi_\mathrm{p} \rangle}\right] \\
&= \frac{\left\langle \omega_\mathrm{p}, \frac{\partial \mathbf{T}_\mathrm{p}}{\partial x}\phi_\mathrm{p} - \lambda_\mathrm{p}\frac{\partial \mathbf{F}_\mathrm{p}}{\partial x}\phi_\mathrm{p} \right\rangle + \left\langle \omega_\mathrm{p}, \mathbf{T}_\mathrm{p}\frac{\partial\phi_\mathrm{p}}{\partial x} - \lambda_\mathrm{p}\mathbf{F}_\mathrm{p}\frac{\partial\phi_\mathrm{p}}{\partial x} \right\rangle}{\langle \omega_\mathrm{p}, \mathbf{F}_\mathrm{p}\phi_\mathrm{p} \rangle}.
\end{aligned} \tag{7}$$

Let ω be the lambda mode adjoint function, ϕ^*, then Eq. (4) becomes

$$\frac{\partial(\Delta\rho)}{\partial x} = \frac{\left\langle \phi^*, \frac{\partial \mathbf{T}}{\partial x}\phi - \lambda\frac{\partial \mathbf{F}}{\partial x}\phi \right\rangle}{\langle \phi^*, \mathbf{F}\phi \rangle} - \frac{\left\langle \phi_\mathrm{p}^*, \frac{\partial \mathbf{T}_\mathrm{p}}{\partial x}\phi_\mathrm{p} - \lambda_\mathrm{p}\frac{\partial \mathbf{F}_\mathrm{p}}{\partial x}\phi_\mathrm{p} \right\rangle}{\langle \phi_\mathrm{p}^*, \mathbf{F}_\mathrm{p}\phi_\mathrm{p} \rangle}. \tag{8}$$

Eq. (8) can be used to get the sensitivity. However, in the MC perturbation formulation, Eq. (8) can be rewritten as

$$\frac{\partial(\Delta\rho)}{\partial x}=\frac{\left\langle \phi_{\mathrm{p}}^{*},\lambda_{\mathrm{p}}^{2}\frac{\partial \mathbf{H}_{\mathrm{p}}}{\partial x}S_{\mathrm{p}}\right\rangle}{\left\langle \phi_{\mathrm{p}}^{*},S_{\mathrm{p}}\right\rangle}-\frac{\left\langle \phi^{*},\lambda^{2}\frac{\partial \mathbf{H}}{\partial x}S\right\rangle}{\left\langle \phi^{*},S\right\rangle}, \quad (9)$$

where S and **H** are the fission source density and fission operator, respectively [3]. They are defined as

$$S\equiv\lambda\mathbf{F}\phi, \quad (10)$$

$$\mathbf{H}=\mathbf{F}\mathbf{T}^{-1}. \quad (11)$$

Once the sensitivity is known, the uncertainty can be estimated with the covariance data. It is defined as

$$\sigma[\Delta\rho]=\sqrt{\sum_{i,\alpha,g}\sum_{i',\alpha',g'}\mathrm{cov}\left[x_{\alpha,g}^{i},x_{\alpha',g'}^{i'}\right]\left[\frac{\partial(\Delta\rho)}{\partial x_{\alpha,g}^{i}}\right]\left[\frac{\partial(\Delta\rho)}{\partial x_{\alpha',g'}^{i'}}\right]}. \quad (12)$$

where x_{α}^{i} denotes α type reaction cross section of i isotope and g denotes an energy group. Furthermore the standard deviation (SD) is defined as

$$\sigma_{\alpha\alpha'}^{ii'}[\Delta\rho]=\sqrt{\sum_{g}\sum_{g'}\mathrm{cov}\left[x_{\alpha,g}^{i},x_{\alpha',g'}^{i'}\right]\left[\frac{\partial(\Delta\rho)}{\partial x_{\alpha,g}^{i}}\right]\left[\frac{\partial(\Delta\rho)}{\partial x_{\alpha',g'}^{i'}}\right]}. \quad (13)$$

3. Results

3.1 Verification of the EPBM implemented in McCARD

A verification of the EPBM module in McCARD is performed by comparing sensitivity coefficients estimated by the EPBM module with the ones estimated by the direct subtraction method. The TMI-1 fuel pin cell problem is utilized for the verification. The sensitivity coefficient is described as

$$S_{\rho,\alpha}^{i}=\frac{\partial(\Delta_{\mathrm{D}}\rho)/\Delta_{\mathrm{D}}\rho}{\partial x_{\alpha}^{i}/x_{\alpha}^{i}}. \quad (14)$$

$\Delta_{\mathrm{D}}\rho$ denotes the reactivity response to two different states of TMI-1 fuel pin cell problem that are nominal state and the state which has the coolant density increased to 110% of the normal density. MC calculations are performed for 50 inactive and 5,000 active cycles on 100,000 histories per cycle while the MC calculation for the direct subtraction method with 10,000,000 histories per cycle and 1,000 active cycles are performed.

Table I: Comparison of the sensitivity coefficients

Reaction Type		$S_{\Delta\rho,\sigma}$	
		EPBM [a]	Dir. Sub. [b]
^{235}U	ν	-0.64 ± 0.10	-0.64 ± 0.07
	(n,γ)	0.29 ± 0.03	0.29 ± 0.07
	(n,fis)	-0.23 ± 0.03	-0.23 ± 0.07
^{238}U	ν	-0.35 ± 0.01	-0.35 ± 0.07
	(n,γ)	0.86 ± 0.02	0.86 ± 0.07
	(n,fis)	-0.19 ± 0.01	-0.19 ± 0.07
	(n,n')	0.07 ± 0.01	0.07 ± 0.07
Total		-0.24 ± 0.10	-0.24 ± 0.07

a) 5,000 active and 50 inactive cycles with 100,000 histories per cycle
b) 1,000 active and 20 inactive cycles with 10,000,000 histories per cycle

Table I shows that the results calculated by the EPBM predicts well the reference solutions estimated by the direct subtraction method. Additionally, the S/U analysis is performed for the ρ_{D} with the 44 energy group ENDF/B-VII.1 covariance data. The ρ_{D} estimated as 0.00906 ± 0.00002.

Table II: Uncertainties and SD of ρ_{D} for the TMI-1 fuel pin problem with the covariance data of ^{235}U and ^{238}U

Covariance Data		SD
^{235}U	ν,ν	0.00007
	$(n,\gamma),(n,\gamma)$	0.00009
	$(n,\gamma),(n,\mathrm{fis})$	0.00001
	$(n,\mathrm{fis}),(n,\mathrm{fis})$	0.00002
^{238}U	ν,ν	0.00004
	$(n,\gamma),(n,\gamma)$	0.00012
	$(n,\mathrm{fis}),(n,\mathrm{fis})$	0.00001
	$(n,n),(n,n)$	0.00001
	$(n,n),(n,n')$	0.00002
	$(n,n'),(n,n')$	0.00012
Total		0.00021

5,000 active and 50 inactive cycles with 100,000 histories per cycle

Table II shows that the contributions of ^{235}U and ^{238}U cross section uncertainties to the SD of ρ_{D} by reaction type and the covariance data. From Table II, it is noted that the uncertainty contributions of gamma reaction of ^{238}U and inelastic reaction of ^{238}U are dominant.

3.2 S/U analysis for the CANDU fuel lattice problem

The uncertainty analysis is performed for CVR of the CANDU fuel lattice problem with the 44 energy group ENDF/B-VII.1 covariance data. The CVR is calculated by subtracting the *k*'s computed for the nominal state and 100% void state with hot full power and zero burnup conditions. The CVR is estimated as 0.01661 ± 0.00004.

Table III: Uncertainty and SD of CVR for the CANDU fuel lattice problem with the covariance data of ^{235}U and ^{238}U

Covariance Data		SD
^{235}U	ν,ν	0.00014

	$(n,\gamma),(n,\gamma)$	0.00003
	$(n,\gamma),(n,\mathrm{fis})$	0.00002
	$(n,\mathrm{fis}),(n,\mathrm{fis})$	0.00004
^{235}U	ν,ν	0.00003
	$(n,\gamma),(n,\gamma)$	0.00019
	$(n,\mathrm{fis}),(n,\mathrm{fis})$	0.00001
	$(n,n),(n,n)$	0.00001
	$(n,n),(n,n')$	0.00001
	$(n,n'),(n,n')$	0.00007
Total		0.00025

5,000 active and 50 inactive cycles with 100,000 histories per cycle

Table III shows that the contributions of ^{235}U and ^{238}U cross section uncertainties to the SD of the CVR by the reaction type and the covariance data. From Table III, it is noted that the uncertainty contributions of nu value of ^{235}U and gamma reaction of ^{238}U are dominant.

4. Conclusion

The EPBM is implemented in McCARD code and verified by showing good agreement with the reference solutions. Then the McCARD S/U analysis have been performed with the EPBM module for the TMI-1 fuel pin cell problem and the CVR in CANDU fuel lattice problem. In the case of CANDU fuel lattice problem, it shows that the CVR has 1.5% relative uncertainty and the uncertainty contributions of nu value of ^{235}U and gamma reaction of ^{238}U are dominant.

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