

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

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Abstract –This paper proposes the Monte Carlo (MC) second-order perturbation methodology to estimate the uncertainty for the reactivity worth and presents the uncertainty for Coolant Void Reactivity (CVR) of the CANDU fuel lattice cell problem. The Eigenvalue Perturbation Based Method (EPBM) which utilizes the first-order perturbation technique is presented as well. They are applied to predict the cross-section sensitivity of the reactivity change due to the density perturbation. The prediction accuracy of estimated sensitivities is evaluated by comparing with the ones estimated by direct subtraction method. The results show both EPBM and second-order perturbation method agree well with the reference. With those sensitivities, the uncertainty analysis is performed for the CANDU fuel lattice cell problem with the 44-energy group ENDF/B-VII.1 covariance data.

I. INTRODUCTION

In safety analyses of nuclear reactors, it is important to estimate accurate reactivity coefficients. Especially, the coolant void reactivity (CVR) of a CANDU reactor is an important safety parameter since it has a large positive value, which means that the reactor gets positive reactivity feedback as a change of a coolant density with amount of boiling. The CANDU CVR can be accurately calculated by the Monte Carlo (MC) transport analysis using continuous-energy cross section libraries and detailed system geometry models. However, its uncertainty need be carefully estimated for the safety margin evaluation and it is known that uncertainties of nuclear design parameters are mainly due to those of nuclear data dominated by experimental results [1].

The sensitivity and uncertainty (S/U) analysis based on the first-order perturbation theory has been widely utilized for the uncertainty quantification of nuclear design parameters. Uncertainty of the CANDU CVR due to the nuclear data uncertainties has been analyzed by M. L. Williams [2]. In his eigenvalue perturbation based method (EPBM), sensitivities of the reactivity coefficient to cross sections are expressed with first-order sensitivities of eigenvalues for two different states of the nuclear system. It needs two independent MC eigenvalue calculation of each state.

Unlike the EPBM, this study presents an alternative MC method which can predict the sensitivities of the reactivity coefficient to cross sections with a single MC eigenvalue calculation by the MC second-order perturbation method. This MC second-order perturbation method and the EPBM have been implemented in the Seoul National university MC code, McCARD [3] and applied to the CVR of a standard CANDU lattice problem for the S/U analysis.

II. METHODOLOGIES

1. Eigenvalue Perturbation Based Method

From a definition of static reactivity ρ of a nuclear system,

$$\rho = 1 - (1/k), \quad (1)$$

a reactivity change from a nominal state to a perturbed one can be expressed as

$$\Delta\rho = \left(1 - \frac{1}{k_p}\right) - \left(1 - \frac{1}{k}\right) = \frac{1}{k} - \frac{1}{k_p}, \quad (2)$$

where k is the multiplication factor and the subscript p denotes the perturbed system.

In order to derive the EPBM formulation for the MC perturbation calculations, one can start from the eigenvalue equation with the fission source density (FSD), S and the fission operator, \mathbf{H} , written as

$$S = \frac{1}{k} \mathbf{H}S. \quad (3)$$

By taking inner products both sides of Eq. (3) with an arbitrary non-zero weight function, ω , one can obtain

$$k = \frac{\langle \omega, \mathbf{H}S \rangle}{\langle \omega, S \rangle}, \quad (4)$$

Substitutions of Eq. (4) into k 's for the unperturbed and perturbed systems in Eq. (2) yields

$$\Delta\rho = \frac{\langle \omega, S \rangle}{\langle \omega, \mathbf{H}S \rangle} - \frac{\langle \omega, S_p \rangle}{\langle \omega, \mathbf{H}_p S_p \rangle}, \quad (5)$$

A differentiation of $\Delta\rho$ with respect to a cross section, x , gives

$$\frac{\partial(\Delta\rho)}{\partial x} = \frac{\partial}{\partial x} \left[\frac{\langle \omega, S \rangle}{\langle \omega, \mathbf{H}S \rangle} \right] - \frac{\partial}{\partial x} \left[\frac{\langle \omega, S_p \rangle}{\langle \omega, \mathbf{H}_p S_p \rangle} \right]. \quad (6)$$

The first term on the right hand side (RHS) of Eq. (6) can be written as

$$\begin{aligned} & \frac{\partial}{\partial x} \left[\frac{\langle \omega, S \rangle}{\langle \omega, \mathbf{H}S \rangle} \right] \\ &= \frac{\left[\left(\left\langle \frac{\partial \omega}{\partial x}, S \right\rangle + \left\langle \omega, \frac{\partial S}{\partial x} \right\rangle \right) \langle \omega, \mathbf{H}S \rangle - \langle \omega, S \rangle \left(\left\langle \frac{\partial \omega}{\partial x}, \mathbf{H}S \right\rangle + \left\langle \omega, \frac{\partial(\mathbf{H}S)}{\partial x} \right\rangle \right) \right]}{\langle \omega, \mathbf{H}S \rangle^2}. \end{aligned} \quad (8)$$

Using $S = k^{-1}\mathbf{H}S$ of Eq. (3), Eq. (8) can be expressed as

$$\begin{aligned} & \frac{\partial}{\partial x} \left[\frac{\langle \omega, S \rangle}{\langle \omega, \mathbf{H}S \rangle} \right] \\ &= k^{-2} \cdot \frac{\left\langle \omega, -\frac{\partial \mathbf{H}}{\partial x} S \right\rangle + k \left\langle \omega, (\mathbf{I} - k^{-1}\mathbf{H}) \frac{\partial S}{\partial x} \right\rangle}{\langle \omega, S \rangle}, \end{aligned} \quad (9)$$

where \mathbf{I} is the identity operator. By letting ω be the k -adjoint, ϕ^\dagger to make the second term on the RHS of Eq. (9) vanish as

$$\left\langle \phi^\dagger, (\mathbf{I} - k^{-1}\mathbf{H}) \frac{\partial S}{\partial x} \right\rangle = \left\langle \frac{\partial S}{\partial x}, (\mathbf{I} - k^{-1}\mathbf{H}^\dagger) \phi \right\rangle = 0, \quad (10)$$

one can obtain

$$\frac{\partial}{\partial x} \left[\frac{\langle \omega, S \rangle}{\langle \omega, \mathbf{H}S \rangle} \right] = k^{-2} \frac{\left\langle \phi^\dagger, -\frac{\partial \mathbf{H}}{\partial x} S \right\rangle}{\langle \phi^\dagger, S \rangle}. \quad (11)$$

Then insertions of Eq. (11) into the second term on the RHS of Eq. (6) for the perturbed system as well as the first term for the nominal state gives

$$\frac{\partial(\Delta\rho)}{\partial x} = k_p^{-2} \frac{\left\langle \phi_p^\dagger, \frac{\partial \mathbf{H}_p}{\partial x} S_p \right\rangle}{\langle \phi_p^\dagger, S_p \rangle} - k^{-2} \frac{\left\langle \phi^\dagger, \frac{\partial \mathbf{H}}{\partial x} S \right\rangle}{\langle \phi^\dagger, S \rangle}. \quad (12)$$

Let x be α -type reaction cross-section of nuclide i in energy group g , $x_{\alpha,g}^i$, and the perturbed system be a system of which coolant is voided. Then Eq. (12) can be used to

estimate the sensitivity of the CANDU CVR to $x_{\alpha,g}^i$. Note that the two terms of the RHS of Eq. (12) can be estimated in two independent MC eigenvalue calculations by the first-order adjoint weighted perturbation (AWP) method [4] or the first-order differential operator sampling augmented with the fission source perturbation method (hereafter, DOS/FSP method) [5].

2. MC Second-Order Perturbation Method

Let a difference of eigenvalue k due to a change of a dependent parameter, x , be $\Delta_x k$. Then, a variation of $\Delta_x k$ induced by a change of another parameter y , denoted by $\Delta_y \Delta_x k$, can be expressed with k 's at four states as

$$\begin{aligned} \Delta_y \Delta_x k &= \Delta_y [k(x + \Delta x, y) - k(x, y)] \\ &= [k(x + \Delta x, y + \Delta y) - k(x + \Delta x, y)] \\ &\quad - [k(x, y + \Delta y) - k(x, y)]. \end{aligned} \quad (13)$$

By applying the Taylor series expansion to the second order, eigenvalues for the perturbed three states $-k(x + \Delta x, y)$, $k(x, y + \Delta y)$, and $k(x + \Delta x, y + \Delta y)$ - can be written as

$$k(x + \Delta x, y) = k + \frac{\partial k}{\partial x} \Delta x + \frac{1}{2} \frac{\partial^2 k}{\partial x^2} (\Delta x)^2, \quad (14)$$

$$k(x, y + \Delta y) = k + \frac{\partial k}{\partial y} \Delta y + \frac{1}{2} \frac{\partial^2 k}{\partial y^2} (\Delta y)^2, \quad (15)$$

$$\begin{aligned} k(x + \Delta x, y + \Delta y) &= k + \frac{\partial k}{\partial x} \Delta x + \frac{\partial k}{\partial y} \Delta y + \frac{1}{2} \frac{\partial^2 k}{\partial x^2} (\Delta x)^2 \\ &\quad + \frac{1}{2} \frac{\partial^2 k}{\partial y^2} (\Delta y)^2 + \frac{\partial^2 k}{\partial x \partial y} (\Delta x \Delta y). \end{aligned} \quad (16)$$

Insertions of Eqs. (14), (15), and (16) into Eq. (13) gives

$$\Delta_y \Delta_x k = \frac{\partial^2 k}{\partial x \partial y} (\Delta x \Delta y). \quad (17)$$

Using Eq. (4), the second derivative of k with respect to x and y , $\partial^2 k / \partial x \partial y$, can be written as

$$\frac{\partial^2 k}{\partial y \partial x} = \frac{\partial}{\partial y} \frac{\partial}{\partial x} \left[\frac{\langle \omega, \mathbf{HS} \rangle}{\langle \omega, S \rangle} \right] = \frac{\partial}{\partial y} \left\{ \frac{\left[\left\langle \frac{\partial \omega}{\partial x}, \mathbf{HS} \right\rangle + \left\langle \omega, \frac{\partial(\mathbf{HS})}{\partial x} \right\rangle \right]}{\langle \omega, S \rangle} - \frac{\langle \omega, \mathbf{HS} \rangle \left[\left\langle \frac{\partial \omega}{\partial x}, S \right\rangle + \left\langle \omega, \frac{\partial S}{\partial x} \right\rangle \right]}{\langle \omega, S \rangle^2} \right\}. \quad (18)$$

Using $\mathbf{HS}=kS$, terms involving the partial derivative of ω in the RHS of Eq. (18) are eliminated and it becomes

$$\frac{\partial^2 k}{\partial y \partial x} = \frac{\partial}{\partial y} \left[\frac{\left\langle \omega, \frac{\partial(\mathbf{HS})}{\partial x} - k \frac{\partial S}{\partial x} \right\rangle}{\langle \omega, S \rangle} \right]. \quad (19)$$

By applying the derivative with respect to y for the terms in the rectangular bracket, Eq. (19) can be written as

$$\frac{\partial^2 k}{\partial y \partial x} = \frac{\left[\left\langle \frac{\partial \omega}{\partial y}, \frac{\partial(\mathbf{HS})}{\partial x} - k \frac{\partial S}{\partial x} \right\rangle + \left\langle \omega, \frac{\partial}{\partial y} \left(\frac{\partial(\mathbf{HS})}{\partial x} - k \frac{\partial S}{\partial x} \right) \right\rangle \right]}{\langle \omega, S \rangle} - \frac{\left\langle \omega, \frac{\partial(\mathbf{HS})}{\partial x} - k \frac{\partial S}{\partial x} \right\rangle \left[\left\langle \frac{\partial \omega}{\partial y}, S \right\rangle + \left\langle \omega, \frac{\partial S}{\partial y} \right\rangle \right]}{\langle \omega, S \rangle^2}. \quad (20)$$

In the same way to obtain Eq. (19) from Eq. (18), Eq. (20) can be written as

$$\frac{\partial^2 k}{\partial y \partial x} = \frac{\left[\left\langle \frac{\partial \omega}{\partial y}, \frac{\partial k}{\partial x} S \right\rangle + \left\langle \omega, \frac{\partial}{\partial y} \left(\frac{\partial(\mathbf{HS})}{\partial x} - k \frac{\partial S}{\partial x} \right) \right\rangle - k \frac{\partial^2 S}{\partial y \partial x} \right]}{\langle \omega, S \rangle} - \frac{\left\langle \omega, \frac{\partial k}{\partial x} S \right\rangle \left[\left\langle \frac{\partial \omega}{\partial y}, S \right\rangle + \left\langle \omega, \frac{\partial S}{\partial y} \right\rangle \right]}{\langle \omega, S \rangle^2} \quad (21)$$

$$= \frac{1}{\langle \omega, S \rangle} \left[\left\langle \omega, \frac{\partial^2 \mathbf{H}}{\partial y \partial x} S + (\mathbf{H} - k) \frac{\partial^2 S}{\partial y \partial x} \right\rangle + \left\langle \omega, \left(\frac{\partial \mathbf{H}}{\partial x} - \frac{\partial k}{\partial x} \right) \frac{\partial S}{\partial y} \right\rangle + \left\langle \omega, \left(\frac{\partial \mathbf{H}}{\partial y} - \frac{\partial k}{\partial y} \right) \frac{\partial S}{\partial x} \right\rangle \right].$$

The ω function may be used to simplify Eq. (21) as the usage of k -adjoint as ω vanishes the source derivative term in Eq. (10). However, in this study, we apply the MC first- and second-order source perturbation techniques [6] for direct estimations of source derivatives such as $\partial^2 S / \partial y \partial x$, $\partial S / \partial x$, and $\partial S / \partial y$ in Eq. (21) with setting ω to unity as

$$\frac{\partial^2 k}{\partial y \partial x} = \left\langle \frac{\partial^2 \mathbf{H}}{\partial y \partial x} S + \mathbf{H} \frac{\partial^2 S}{\partial y \partial x} + \frac{\partial \mathbf{H}}{\partial x} \frac{\partial S}{\partial y} + \frac{\partial \mathbf{H}}{\partial y} \frac{\partial S}{\partial x} \right\rangle. \quad (22)$$

Note that $\partial^2 \mathbf{H} / \partial y \partial x$, $\partial \mathbf{H} / \partial x$, and $\partial \mathbf{H} / \partial y$ can be calculated by the conventional differential operator sampling method. By differentiating Eq. (1) with respect to the coolant density, D^{coolant} and multiplying the coolant density change of $\Delta D^{\text{coolant}}$, the CVR, $\Delta_D \rho$ can be expressed as

$$\Delta_D \rho = k^{-2} \frac{\partial k}{\partial D^{\text{coolant}}} \Delta D^{\text{coolant}}. \quad (23)$$

By differentiating Eq. (23) with respect to $x_{\alpha,g}^i$, the sensitivity of the CVR to $x_{\alpha,g}^i$ is obtained as

$$\frac{\partial(\Delta_D \rho)}{\sigma x_{\alpha,g}^i} = k^{-2} \frac{\partial^2 k}{\partial x_{\alpha,g}^i \partial D^{\text{coolant}}} (\Delta D^{\text{coolant}}) - 2k^{-3} \frac{\partial k}{\partial x_{\alpha,g}^i} \cdot \frac{\partial k}{\partial D^{\text{coolant}}} (\Delta D^{\text{coolant}}). \quad (24)$$

By letting x and y be D^{coolant} and $x_{\alpha,g}^i$, respectively, in Eq. (22), $\partial^2 k / \partial x_{\alpha,g}^i \partial D^{\text{coolant}}$ in Eq. (24) can be calculated by Eq.

(22). Note that $\partial k/\partial x_{\alpha,g}^i$ and $\partial k/\partial D^{\text{coolant}}$ can be estimated by the first-order AWP method or DOS/FSP method.

Then by the error propagation rule, the uncertainty of the CVR can be calculated by

$$\sigma^2 [\Delta_D \rho] = \sum_{i,\alpha,g} \sum_{i',\alpha',g'} \text{cov}[x_{\alpha,g}^i, x_{\alpha',g'}^{i'}] \left[\frac{\partial(\Delta_D \rho)}{\partial x_{\alpha,g}^i} \right] \left[\frac{\partial(\Delta_D \rho)}{\partial x_{\alpha',g'}^{i'}} \right] \quad (25)$$

where $\text{cov}[x_{\alpha,g}^i, x_{\alpha',g'}^{i'}]$ denotes the covariance between $x_{\alpha,g}^i$ and $x_{\alpha',g'}^{i'}$.

III. NUMERICAL RESULTS

1. Verification for the sensitivity coefficient

Verifications of the EPBM and DOS/FSP modules in McCARD are performed by comparing $\Delta_x \Delta_D k$ and sensitivity coefficients estimated by the EPBM and the second-order DOS/FSP modules with the ones estimated by the direct subtraction method. The Godiva and TMI pin cell problems are utilized for the verification. The $\Delta_x \Delta_D k$ and sensitivity coefficient are described respectively as

$$\Delta_x \Delta_D k = \frac{\partial^2 k}{\partial x_{\alpha}^i \partial D} \times \Delta x_{\alpha}^i \times \Delta D, \quad (26)$$

$$S_{\rho,\alpha}^i = \frac{\partial(\Delta_D \rho)/\Delta_D \rho}{\partial x_{\alpha}^i/x_{\alpha}^i}. \quad (27)$$

$\Delta_x \Delta_D k$ denotes the effect on k from the perturbation of density change of 5% and ^{235}U cross section change of 1% for Godiva problem. $\Delta_D \rho$ denotes the reactivity response to two different states of the problem that are nominal state and the state which has the density increased to 110% of the TMI-1 design density. The MC eigenvalue calculations are performed on 1,000 active cycles with 10,000,000 histories per cycle for the direct subtraction calculation, 100 active cycles with 500,000 histories per cycle for EPBM method, and 100 active cycles with 100,000 particles per cycle.

A. Godiva problem

Table I shows $\Delta_x \Delta_D k$ values estimated by EPBM, the second-order DOS/FSP, and the direct subtraction methods. It is shown with a unit of PCM. RSD in the table stands for the relative standard deviation with a unit of percent. The first column shows the isotope and its reaction type whose cross section value increase to 101% and the density increase to 105% of their original values. The second

column shows $\Delta_x \Delta_D k$ obtained from the direct subtraction method. The direct subtraction has done from four independent MC runs. The third column shows $\Delta_x \Delta_D k$ from the EPBM. The values are obtained from two independent MC runs. The fourth column shows $\Delta_x \Delta_D k$ from the second-order DOS/FSP method. In this case MC calculation is needed only once. The results show that the $\Delta_x \Delta_D k$ values estimated by EPBM and the second-order perturbation method are consistent with each other and have good agreement with the one from the direct subtraction method. Furthermore they show the effect on $\Delta_x \Delta_D k$ from the variation of nu value is the most dominant.

Table I: Comparison of $\Delta_x \Delta_D k$ for the Godiva problem

Reaction Type	$\Delta_x \Delta_D k$ (PCM)		
	Dir. Sub. ¹⁾ (RSD, %)	EPBM (RSD, %)	2 nd -order DOS/FSP (RSD, %)
$\nu, 1\%$	41 (28)	40 (1)	40 (1)
$(n,\gamma), 1\%$	-2 (32)	-4 (3)	-3 (2)
$(n,\text{fis}), 1\%$	9 (16)	11 (4)	11 (3)
$(n,n'), 1\%$	3 (38)	4 (5)	4 (19)

1) Dir. Sub.: Direct Subtraction Method

B. TMI-1 pin cell problem

Table II shows the sensitivity coefficient estimated by EPBM, the second-order DOS/FSP, and the direct subtraction method. The sensitivity coefficients for the reactivity worth, $\Delta_D \rho$ are estimated by the cross section change of 1% of each reaction type and isotope individually. The table configuration is same as Table I. It presents that the sensitivity coefficients estimated by the EPBM and the second-order DOS/FSP method show good agreement with the direct subtraction method. The results show nu value is the most sensitive to the reactivity worth, $\Delta_D \rho$.

Table II: Comparison of the sensitivity coefficients

Reaction Type	$S_{\Delta\rho,\sigma}$		
	Dir. Sub (RSD, %)	EPBM (RSD, %)	2 nd -order DOS/FSP (RSD, %)
ν , 1%	-0.64 (11)	-0.64 (16)	-0.51 (14)
^{235}U (n,γ), 1%	0.29 (24)	0.29 (10)	0.27 (16)
(n,fis), 1%	-0.23 (30)	-0.23 (13)	-0.26 (52)

2. S/U analysis for the CANDU fuel lattice cell problem

The sensitivity coefficient for the CVR of the CANDU fuel lattice cell problem is estimated. The sensitivity coefficients for the reactivity worth, $\Delta\rho$ are estimated by the cross section change of 1% of each reaction type and isotope individually. Table III's configuration is same as Table II. The results show that the sensitivity coefficients estimated by two methods are consistent.

Table III: Comparison of the sensitivity coefficients

Reaction Type	$S_{\Delta\rho,\sigma}$	
	EPBM (RSD, %)	2 nd -order DOS/FSP (RSD, %)
ν , 1%	-0.88 (8)	-0.92 (12)
^{235}U (n,γ), 1%	0.07 (9)	0.07 (38)
(n,fis), 1%	-0.52 (8)	-0.58 (26)
ν , 1%	0.14 (7)	0.14 (28)
^{238}U (n,γ), 1%	0.57 (5)	0.63 (17)
(n,fis), 1%	0.06 (15)	0.07 (48)
(n,n'), 1%	0.03 (393)	0.10 (427)

The uncertainty analysis is performed for the CVR of the CANDU fuel lattice cell problem with the 44-energy group ENDF/B-VII.1 covariance data. As it described in Eq. (25), the uncertainty can be obtained by multiplying the covariance to the sensitivity estimated in Table III. The results are shown in Table IV. The sensitivity estimated by EPBM method is utilized for analyzing the uncertainty of CVR in Table IV. The CVR is estimated as 0.01661. It is calculated by subtracting the k 's computed for the nominal

state and 100% void state with hot full power and zero burnup conditions.

Table IV 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. The RSD is the contribution of each reaction type uncertainties to the uncertainty of the CVR and it is estimated by Eq. (28).

$$\text{RSD} = \frac{\sigma_{aa'}^{ii'}}{\Delta\rho} [\Delta\rho] = \frac{1}{\Delta\rho} \sqrt{\sum_g \sum_{g'} \text{cov}[x_{\alpha,g}^i, x_{\alpha',g'}^{i'}]} \left[\frac{\partial(\Delta\rho)}{\partial x_{\alpha,g}^i} \right] \left[\frac{\partial(\Delta\rho)}{\partial x_{\alpha',g'}^{i'}} \right]. \quad (28)$$

From the Table IV, it is noted that the uncertainty contributions of nu value of ^{235}U and gamma reaction of ^{238}U are dominant to the CVR.

Table IV: Uncertainty of CVR for the CANDU fuel lattice problem due to ENDF/B-VII.1 covariance data of ^{235}U and ^{238}U

Covariance Data		RSD, %
^{235}U	ν, ν	0.84
	(n,γ), (n,γ)	0.18
	(n,γ), (n,fis)	0.12
	(n,fis), (n,fis)	0.24
^{238}U	ν, ν	0.18
	(n,γ), (n,γ)	1.14
	(n,fis), (n,fis)	0.06
	(n,n), (n,n)	0.06
	(n,n), (n,n')	0.06
(n,n'), (n,n')	0.42	
Total		1.51

IV. CONCLUSION

The EPBM and the second-order perturbation method are implemented in McCARD code and verified by showing good agreement with the reference solutions. Then McCARD S/U analysis have been performed for the CVR of CANDU fuel lattice problem. The results show that the CVR has 1.51% relative uncertainty and the uncertainty contributions of nu value of ^{235}U and gamma reaction of ^{238}U are dominant.

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