Annals of Nuclear Energy 121 (2018) 68–76

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

# Sensitivity and uncertainty analysis of nuclear reactor reactivity coefficients by Monte Carlo second-order perturbation method

Seung Yeol Yoo, Hyung Jin Shim *

*Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea*

ARTICLE INFO

*Article history:*
Received 5 March 2018
Received in revised form 17 June 2018
Accepted 27 June 2018

*Keywords:*
Sensitivity and uncertainty
Second-order perturbation
Reactivity coefficient
Monte Carlo
McCARD

ABSTRACT

The uncertainty quantification of the reactivity coefficients such as the fuel temperature coefficient (FTC) and the moderator density coefficient (MDC) is crucial for the nuclear reactor safety margin evaluation. This paper proposes a continuous-energy MC second-order perturbation (MC2P) method as a new way to estimate efficiently the sensitivity of reactivity coefficients to nuclear cross section data. The proposed MC2P method takes into account the second-order effects of the fission operator and the fission source distribution. The effectiveness of the MC2P method implemented in a Seoul National University MC code, McCARD, is demonstrated in a Godiva $^{235}$U density coefficient problem via comparison of its results with direct subtraction MC calculation. It is shown that the new method can predict the cross section sensitivities of the reactivity coefficient more accurately even with much smaller number of MC history simulations than the direct subtraction MC method. It is also shown that the proposed method is applicable for quantifying the uncertainties of the MDC of a LWR pin cell problem and the FTC of a CANDU 6 lattice cell problem due to the uncertainties of the nuclear cross section input data represented by nuclear cross section covariance data.



## 1. Introduction

Reactivity coefficients such as the fuel temperature coefficient (FTC) and the moderator density coefficient (MDC) of a nuclear reactor are one of important reactor physics design parameters indispensable to assess its safety and assure its safe operation. Therefore, an accurate estimation of the reactivity coefficients is crucial to clarify the safety issue of those reactors whose reactivity coefficients are estimated in the proximity to zero, as observed in the FTC of the equilibrium core of CANDU 6 (Schaubel, 2008; Kim et al., 2016). For the accurate estimation of the reactivity coefficients, a direct subtraction (Kim et al., 2016) or the perturbation method (Greenspan, 1976; Williams, 1986) can be applied in the Monte Carlo (MC) neutron transport calculations with continuous-energy cross section libraries and a detailed geometry model. With increasing computing power, the MC direct subtraction method which calculates the reactivity coefficient by subtracting reactivities obtained at a nominal state and a perturbed state due to a small change of a nuclear design parameter has been successfully applied for the CANDU 6 FTC estimation using an extremely large number of neutron histories. The advanced MC perturbation methods were demonstrated to estimate the density coefficients (Rief, 1984; Nagaya and Mori, 2005; Shim and Kim, 2011; Kiedrowski and Brown, 2013) and the FTC (Shim and Kim, 2014) with great efficiency.

In addition to the accurate estimation of the reactivity coefficients, their uncertainty quantification is an important subject for their confidence interval and the safety margin evaluations. There are two main approaches to quantify the uncertainty of a nuclear performance parameter – the stochastic sampling method and the sensitivity and uncertainty analysis method (Cacuci, 2003) – besides recent advances in the uncertainty quantification methodology such as the efficient subspace method (Abdel-Khalik et al., 2008) and the polynomial chaos expansion method (Perkó et al., 2014). The uncertainty of the sodium void reactivity due to the nuclear data uncertainties has been calculated (Rochman et al., 2011) by a stochastic sampling approach in which many MC runs are performed with varying a set of randomized nuclear data. For an efficient uncertainty quantification, the sensitivity and uncertainty analysis has been widely adopted based on the first-order perturbation theory. In the early stage of the generalized perturbation theory development, the sensitivity function for reactivity worth ratios has been expressed (Greenspan, 1982) in a form of the bilinear functional ratio. Williams (Williams, 2007) presented a formulation to express the sensitivity of an eigenvalue difference

* Corresponding author.
*E-mail address:* shimhj@snu.ac.kr (H.J. Shim).

https://doi.org/10.1016/j.anucene.2018.06.047
0306-4549/

to a cross section using eigenvalue sensitivities at the two different states of a nuclear system, which are obtained by the MC perturbation techniques from two independent MC runs. This method (referred to as Williams' method hereafter) was applied to evaluate the uncertainty of the CANDU coolant void reactivity due to the nuclear data uncertainties. Williams' method is effective for large perturbation problems such as uncertainty quantifications of the coolant void reactivity and the control rod worth but may require a large amount of neutron history simulations to estimate accurately sensitivities of the reactivity coefficients such as the FTC.

Objectives of this paper are to develop an alternative MC method to estimate the sensitivity of the reactivity coefficient to cross section from a single MC run by applying second-order eigenvalue perturbation techniques (Rief, 1984; Nagaya and Mori, 2011) and to apply the developed method for the uncertainty quantification of the reactivity coefficient. Rief (1984) developed earlier the second-order differential operator sampling (DOS) method by taking into account second-order derivatives of the transport kernels and Morillon (1998) extended it to an arbitrary order perturbation estimation. Recently Nagaya and Mori (2011) devised a fission source perturbation (FSP) algorithm to calculate higher-order terms of the perturbed source effect (PSE) which can be incorporated with the conventional DOS method to improve the accuracy of MC perturbation estimations. In Section 2, the new sensitivity calculation algorithm for the reactivity coefficient is derived by extending the existing second-order DOS (Rief, 1984) and FSP (Nagaya and Mori, 2011) methods into eigenvalue sensitivities to two different variables. The proposed MC second-order perturbation (MC2P) method is implemented in the Seoul National university Monte Carlo (MC) code, McCARD (Shim et al., 2012) and tested in a two-group homogeneous infinite medium problem by comparing MC2P results with analytic solutions. Its calculation efficiency is examined for the density coefficient of Godiva (Blair et al., 2006) by comparing with the Williams' method. The proposed method is also applied to quantify the uncertainties of the MDC of a LWR pin cell problem and the FTC of a CANDU 6 lattice cell model (Yoo et al., 2015) due to the nuclear covariance data.

## 2. Second-Order perturbation method for reactivity coefficient sensitivity estimation

### 2.1. Sensitivity of reactivity coefficient

The MC reactor design calculations are based on the reactor eigenvalue equation expressed in the operator notation by

$$S = \frac{1}{k}\mathbf{H}S, \tag{1}$$

where $S$ is the fission source distribution and $k$ is the multiplication factor. $\mathbf{H}$ is fission operator with $\mathbf{H}S$ in Eq. (1) meaning

$$\mathbf{H}S = \int d\mathbf{P}' H(\mathbf{P}' \to \mathbf{P}) S(\mathbf{P}'), \tag{2}$$

where $\mathbf{P}$ and $\mathbf{P}'$ denote state vectors of a neutron in the six-dimensional phase space, $(\mathbf{r}, E, \mathbf{\Omega})$ and $(\mathbf{r}', E', \mathbf{\Omega}')$, respectively. $H(\mathbf{P}' \to \mathbf{P})$ means the number of first-generation fission neutrons born per unit phase space volume about $\mathbf{P}$, due to a parent neutron born at $\mathbf{P}'$, which can be explicitly expressed in terms of transport kernels as (Shim and Kim, 2011)

$$H(\mathbf{P}' \to \mathbf{P})S(\mathbf{P}') = \sum_{p=0}^{\infty} \int dE'' \int d\mathbf{\Omega}'' C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) \cdot \int d\mathbf{r}_0 K_{s,p}(\mathbf{r}_0, E', \mathbf{\Omega}' \to \mathbf{r}, E'', \mathbf{\Omega}'') T(E', \mathbf{\Omega}'; \mathbf{r}' \to \mathbf{r}_0) S(\mathbf{P}'), \tag{3}$$

where the fission collision kernel, $C_f$, is defined by

$$C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) = \frac{\chi(E'' \to E)}{4\pi} \cdot \frac{\nu(E'')\Sigma_f(\mathbf{r}, E'')}{\Sigma_t(\mathbf{r}, E'')}. \tag{4}$$

$\nu$ is the mean number of neutrons produced from a fission reaction and $\chi$ is the energy spectrum of the fission neutron. $K_{s,p}$ is the $p$-th scattering kernel defined by

$$\begin{aligned} &K_{s,0}(\mathbf{P}_0 \to \mathbf{P}) = \delta(\mathbf{P}_0 - \mathbf{P}), \\ &K_{s,1}(\mathbf{P}_0 \to \mathbf{P}) = K_s(\mathbf{P}_0 \to \mathbf{P}), \\ &K_{s,p}(\mathbf{P}_0 \to \mathbf{P}) = \int d\mathbf{P}_{p-1} \cdots \int d\mathbf{P}_1 K_s(\mathbf{P}_{p-1} \to \mathbf{P}) \cdots K_s(\mathbf{P}_0 \to \mathbf{P}_1); \\ &p = 2, 3, \ldots, \end{aligned} \tag{5}$$

where $\mathbf{P}_p$ ($p$ = 0,1,...) denote $(\mathbf{r}_p, E_p, \mathbf{\Omega}_p)$. $K_s$ is the transition kernel defined by a product of the scattering collision kernel, $C_s$, and the free flight kernel, $T$, as follows;

$$K_s(\mathbf{P}' \to \mathbf{P}) = T(E, \mathbf{\Omega}; \mathbf{r}' \to \mathbf{r}) \cdot C_s(\mathbf{r}'; E', \mathbf{\Omega}' \to E, \mathbf{\Omega}); \tag{6}$$

$$T(E, \mathbf{\Omega}; \mathbf{r}' \to \mathbf{r}) = \frac{\Sigma_t(\mathbf{r}, E)}{|\mathbf{r} - \mathbf{r}'|^2} \exp\left[ -\int_0^{|\mathbf{r}-\mathbf{r}'|} \Sigma_t\left( \mathbf{r} - s\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}, E \right) ds \right] \times \delta\left( \mathbf{\Omega} \cdot \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} - 1 \right), \tag{7}$$

$$C_s(\mathbf{r}'; E', \mathbf{\Omega}' \to E, \mathbf{\Omega}) = \sum_m \sum_{r \neq fis.} \nu_r^m \frac{\Sigma_r^m(\mathbf{r}', E')}{\Sigma_t(\mathbf{r}', E')} f_r^m(E', \mathbf{\Omega}' \to E, \mathbf{\Omega}). \tag{8}$$

$\nu_r^m$ and $\Sigma_r^m$ are the number of neutrons produced from, and the macroscopic cross section of, $r$-type reaction of isotope $m$, respectively. $f_r^m$ is the transfer probability function with $f_r^m(E', \mathbf{\Omega}' \to E, \mathbf{\Omega}) dE d\mathbf{\Omega}$ denoting the probability that a collision of type $r$ of isotope $m$ by a neutron of direction $\mathbf{\Omega}'$ and energy $E'$ will produce a neutron in direction interval $d\mathbf{\Omega}$ about $\mathbf{\Omega}$ with energy in $dE$ about $E$. Other notations follow standard.

The eigenvalue $k$ in Eq. (1) implies the number of next-generation fission neutrons generated from a source neutron sampled by the current-generation fission source distribution, $S$. With the use of the normalization condition $\int S(\mathbf{P}) d\mathbf{P} = 1$, then, it can be determined by

$$k = \langle \mathbf{H}S \rangle. \tag{9}$$

The angular bracket < > implies the phase space integral (PSI) of the quantity in it over $\mathbf{P}$. Thus $k$ or $\langle \mathbf{H}S \rangle$ represents simply the PSI of Eq. (3) over $\mathbf{P}$.

The multiplication factor $k$ is related to the static reactivity $\rho$ of the nuclear reactor system by

$$\rho = 1 - \frac{1}{k}. \tag{10}$$

Because of this relation, $\rho$ is viewed as a function of both the reactor state variables like fuel or moderator temperature, coolant density, etc. and uncertain model parameters such as nuclear cross section data which are inputted to determine $k$ by Eq. (1). If one denotes uncertain nuclear cross section input parameters by $x$ and the reactor state parameters by $y$, then one may presume the functional relationship of $\rho$ and $k$ with these parameters by $\rho \equiv \rho(x, y)$ and $k \equiv k(x, y)$, respectively. Noting that the reactivity coefficient for the reactor state parameter $y$ is defined as $\partial\rho/\partial y$, one can obtain the following expression for it from Eqs. (9) and (10).

$$\frac{\partial \rho}{\partial y} = \frac{1}{\langle \mathbf{H}S \rangle^2} \frac{\partial \langle \mathbf{H}S \rangle}{\partial y} = \frac{1}{\langle \mathbf{H}S \rangle^2} \left( \left\langle \frac{\partial \mathbf{H}}{\partial y} S \right\rangle + \left\langle \mathbf{H} \frac{\partial S}{\partial y} \right\rangle \right) \tag{11}$$