

Monte Carlo sensitivity analysis method for the effective delayed neutron fraction
with the differential operator sampling method

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Abstract

An exact Monte Carlo method for evaluating the sensitivity coefficients of the effective delayed neutron fraction (β_{eff}) with respect to nuclear data is developed using the differential operator sampling (DOS) method. This development includes combining the two characteristic features of the DOS method: the exact evaluation of β_{eff} and the sensitivity analyses of the k - and α -eigenvalues. Numerical tests are performed to calculate the sensitivity coefficients of β_{eff} with the newly developed Monte Carlo method. The new Monte Carlo method's sensitivities mostly are in accordance with the reference solutions that were obtained by a deterministic discrete ordinates method based on the perturbation theory. In particular, the sensitivities of β_{eff} to the yield and spectrum of delayed neutrons, which are dominant contributors to the uncertainty of β_{eff} , can be predicted precisely by the new method.

Keywords: effective delayed neutron fraction; Monte Carlo; sensitivity analysis; differential operator

1. Introduction

The effective delayed neutron fraction β_{eff} is an important parameter in describing the kinetic behavior of a nuclear reactor. Measured values in a reactor physics experiment (e.g., control rod worth) are usually obtained in units of dollars. Then, the measured values in units of dollars are converted by multiplying them by β_{eff} for comparison with the calculation results.

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Thus, an accurate estimation of β_{eff} is crucially important to ensure the quality of both experiments and calculations. High-accuracy calculation methods of β_{eff} using the continuous energy Monte Carlo method have been developed over the past decade. A calculation capability for obtaining β_{eff} is now installed in many production Monte Carlo codes such as MCNP 6 (Goorley et al., 2013), MVP 2 (Nagaya and Mori, 2011), Serpent 2 (Leppänen et al., 2014), TRIPOLI-4 (Truchet et al., 2015), McCARD (Choi and Shim, 2016; Yoo and Shim, 2018), OpenMC (Peng et al., 2019), MORET 5 (Cochet et al., 2015), and RMC (Qiu et al., 2017). Most of these codes adopt the adjoint-weighted technique by using the iteration fission probability (IFP) (Kiedrowski et al., 2011; Nauchi and Kameyama, 2012; Leppänen et al., 2014). A unique technique that uses the differential operator sampling (DOS) method is adopted in MVP 2 and McCARD.

IFP is also used for sensitivity analyses of the neutron multiplication factor k_{eff} and reaction rate ratios (e.g., the ratio of fission to capture) in production Monte Carlo codes, such as MCNP 6 (Kiedrowski et al., 2011; Kiedrowski and Brown, 2013), TRIPOLI-4 (Terranova et al., 2018), MORET 5 (Jinaphanh et al., 2016), McCARD (Shim and Kim, 2011), and RMC (Qiu et al., 2015; Qiu et al., 2016a; Qiu et al., 2016b). A method that is installed in SCALE code is based on the Contribution theory (Perfetti, 2012; Perfetti and Rearden, 2016). The sensitivity coefficients are useful for quantifying the impact of nuclear data uncertainties in reactor physics applications. The DOS method was applied to obtain the sensitivity coefficients of k_{eff} (Yamamoto, 2018) and of prompt neutron decay constants α (Yamamoto and Sakamoto, 2019a; Yamamoto and Sakamoto, 2019b).

In addition to obtaining an accurate β_{eff} by using the continuous energy Monte Carlo method, quantifying the uncertainty of β_{eff} that is induced by nuclear data uncertainties is also important. Some sensitivity and uncertainty analyses of β_{eff} were performed in a deterministic manner (Hammer, 1979; D'Angelo et al., 1987; D'Angelo, 1990; Zukeran et al., 1999; Kodeli, 2013; Kodeli, 2018). For example, the deterministic approach performed by Kodeli (2013, 2018) estimates the sensitivity coefficients of an approximate β_{eff} that was derived by Bretscher's

“prompt k -ratio method” (Bretscher, 1997).

A Monte Carlo approach that was recently attempted by (Iwamoto et al., 2018a; Iwamoto et al., 2018b; Romojaro et al., 2019) is similar to Kodeli’s deterministic approach. The sensitivity coefficients estimated for β_{eff} are defined by Chiba’s “modified k -ratio method” (Chiba, 2009) as well as Bretscher’s “prompt k -ratio method”. In (Romojaro et al., 2019), only Bretscher’s method was adopted. One problem of the Monte Carlo approach lies in obtaining the sensitivity coefficients of the approximately estimated β_{eff} . In addition, another problem arises when the deterministic approaches are applied to the Monte Carlo method. The sensitivity coefficient of β_{eff} in (Iwamoto et al., 2018a; Iwamoto et al., 2018b) is defined by the small difference between the two sensitivity coefficients of k -eigenvalues. Both the sensitivity coefficients are obtained by a Monte Carlo sensitivity analysis tool such as KSEN option of MCNP6 (Goorley et al., 2016), and thus they necessarily entail statistical uncertainties. The problem with this approach is that the statistical uncertainties of the sensitivity coefficients of β_{eff} become larger as β_{eff} is obtained with less approximation.

Additional previous studies on the sensitivity analysis method of β_{eff} were performed by (Aufiero et al., 2015) and (Burke and Kiedrowski, 2018). The method in (Aufiero et al., 2015) adopted the collision history-based approach to calculate the sensitivities to nuclear data. The study by Burke and Kiedrowski (2018) calculated the sensitivities to system dimensions.

This paper attempts to establish a Monte Carlo algorithm that exactly defines a sensitivity coefficient of β_{eff} to nuclear data parameters by introducing the DOS method. This paper adopts the exact calculation method of β_{eff} through the differential operator sampling method (Nagaya and Mori, 2011). The DOS method (Rief, 1984; Raskach, 2009; Yoo and Shim, 2018) estimates the first or higher-order differential coefficient of a quantity that is scored during the course of the random walk in a Monte Carlo calculation. Thus, the DOS method is an optimal approach for calculating the sensitivity coefficients, i.e., the first derivatives. In the following sections, the DOS method that exactly calculates β_{eff} is revisited (Nagaya and Mori, 2011). Then, a Monte Carlo algorithm for an exact sensitivity coefficient of β_{eff} is presented. The performance of the new

method is tested through simple numerical tests where the sensitivities to various kinds of nuclear data are obtained, and the applicability of the method is evaluated.

2. Review of the exact Monte Carlo method for β_{eff}

Before proceeding to the newly developed sensitivity analysis method, the exact Monte Carlo method that obtains the β_{eff} with the DOS method (Nagaya and Mori, 2011) is briefly reviewed. For simplicity, the delayed neutron family with only one nuclide is assumed to induce the fission reactions.

According to (Chiba, 2009), the exact β_{eff} is given by the following:

$$\beta_{eff} = \lim_{a \rightarrow 0} \frac{1}{k(0)} \frac{k(a) - k(0)}{a} = \frac{1}{k(0)} \left. \frac{dk(a)}{da} \right|_{a=0}, \quad (1)$$

where $k(a)$ is an eigenvalue of the following neutron transport equation for a perturbed system:

$$L\phi(\mathbf{r}, \boldsymbol{\Omega}, E; a) = \frac{1}{k(a)} F\phi(\mathbf{r}, \boldsymbol{\Omega}, E; a). \quad (2)$$

In this perturbed system, the parameter a is the fractional change of the number of delayed neutrons. The operators in Eq. (2) are written as follows:

$$L\phi(\mathbf{r}, \boldsymbol{\Omega}, E; a) = \boldsymbol{\Omega} \cdot \nabla \phi(\mathbf{r}, \boldsymbol{\Omega}, E; a) + \Sigma_t(\mathbf{r}, E)\phi(\mathbf{r}, \boldsymbol{\Omega}, E; a) - \int_{4\pi} d\boldsymbol{\Omega}' \int dE' \Sigma_s(\mathbf{r}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E)\phi(\mathbf{r}, \boldsymbol{\Omega}', E'; a), \quad (3)$$

and:

$$F\phi(\mathbf{r}, \boldsymbol{\Omega}, E; a) = \frac{\chi_p(E)}{4\pi} \int_{4\pi} d\boldsymbol{\Omega}' \int dE' \nu_p(E') \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, \boldsymbol{\Omega}', E'; a) + (1 + a) \frac{\chi_d(E)}{4\pi} \int_{4\pi} d\boldsymbol{\Omega}' \int dE' \nu_d(E') \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, \boldsymbol{\Omega}', E'; a), \quad (4)$$

where Σ_t = the macroscopic total cross-section, Σ_s = the macroscopic scattering cross-section, Σ_f = the macroscopic fission cross-section, χ_p = the prompt neutron spectrum, χ_d = the delayed neutron spectrum, ν_p = the prompt neutron yield, ν_d = the delayed neutron yield, ϕ = the neutron flux, and $\boldsymbol{\Omega}$ = the neutron direction. Differentiating Eq. (4) with respect to a and setting $a = 0$ yields the following:

$$\left. \frac{d}{da} \mathbf{F} \phi(\mathbf{r}, \boldsymbol{\Omega}, E; a) \right|_{a=0} = \frac{\chi_d(E)}{4\pi} \int_{4\pi} d\boldsymbol{\Omega}' \int dE' \nu_d(E') \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, \boldsymbol{\Omega}', E'; 0). \quad (5)$$

Eq. (5) stands for the neutrons emitted by the delayed fission. The DOS method for the β_{eff} calculation is performed during the ordinary k -eigenvalue calculation. The Monte Carlo algorithm of the DOS method for the i th history in the m th cycle is as follows:

(Step 1): When starting a fission source particle for the i th history, determine whether the fission neutron is a prompt or delayed neutron. A pseudo random number ξ between 0 and 1 is generated. If ξ is less than the delayed neutron fraction β , the neutron is a delayed neutron. Otherwise, the neutron is a prompt neutron. The energy of the fission neutron is determined according to $\chi_d(E)$ or $\chi_p(E)$.

(Step 2): A weighting coefficient is assigned to the fission neutron as follows:

$$W_{f,i,m} = 1, \text{ if the neutron is a delayed neutron,} \quad (6)$$

$$W_{f,i,m} = 0, \text{ if the neutron is a prompt neutron.} \quad (7)$$

(Step 3): A random walk process is performed in the same manner as ordinary k -eigenvalue calculations.

(Step 4): At each collision site, the following quantity is scored and is accumulated until the end of the i th history:

$$S_{NP,i,m} = \sum_j \frac{(\nu_{p,j} + \nu_{d,j}) \Sigma_{f,j}}{\Sigma_{t,j}} w_j W_{f,i,m}, \quad (8)$$

where w_j is the particle weight at the j th collision and the summation is carried out over all collisions during the i th history.

(Step 5): At the end of each cycle, the first derivative of $k(a)$ with respect to a is obtained as follows:

$$\left. \frac{dk_{NP}(a)}{da} \right|_{a=0} = \frac{1}{M} \sum_{i=1}^M S_{NP,i,m}, \quad (9)$$

where M is the number of histories in each cycle. Eq. (9) corresponds to an adjoint weighted estimate of the delayed neutron fraction although the perturbed source effect caused by the change of a is not included in it. The subscript NP indicates that Eq. (9) does not include the effect of the fission source distribution that is perturbed by the change of a .

The perturbed source effect due to the change of a can also be calculated by following the procedure presented in (Nagaya and Mori, 2005; Yamamoto, 2018). The perturbed source effect is calculated as follows.

Suppose that the l th fission neutron in the m th cycle is generated at a collision point in the i th particle history. Then, the following quantity is scored at the collision point as follows:

$$w_{l,m,n}^f = W_{f,i,m}, \quad \text{for } n = 1, \quad (10)$$

$$w_{l,m,n}^f = W_{f,i,m} + W_{PS,i,m,n-1}, \text{ for } N \geq n \geq 2, \quad (11)$$

where $W_{f,i,m}$ is the weighting coefficient defined in Eq. (6) or Eq. (7). The subscript n indicates the number of iterations for the perturbed source effect because the perturbed source effect must be calculated by an iteration procedure. $W_{PS,i,m,n}$, which is defined in Eq. (12) below, represents the perturbed source effect in the weighting coefficient, and it is inherited from the previous $(m-1)$ th cycle. N is the maximum iteration number, and this number is chosen so that the perturbed source effect fully converges. In each cycle, $w_{l,m,n}^f$ is stored for $N \geq n \geq 1$ and $L \geq l \geq 1$, where L is the total number of fission neutrons generated in each cycle.

At the end of the m th cycle, $w_{l,m,n}^f$ in Eq. (10) or Eq. (11) is normalized as follows:

$$W_{PS,l,m+1,n+1} = w_{l,m,n}^f - \frac{1}{L} \sum_{l=1}^L w_{l,m,n}^f, \quad \text{for } L \geq l \geq 1 \text{ and } N-1 \geq n \geq 1. \quad (12)$$

This normalization process keeps the sample size constant in each cycle. $W_{PS,l,m+1,n+1}$ obtained from Eq. (12) is used in Eq. (11) for the next cycle calculation. The perturbed source effect of the first derivative of $k(a)$ of the i th history in the m th cycle is obtained by the following:

$$S_{PS,i,m} = \sum_j \frac{(v_{p,j} + v_{d,j})\Sigma_{f,j}}{\Sigma_{t,j}} w_j W_{PS,i,m,N}, \quad (13)$$

where the summation for j is carried out at each collision until the end of the i th history. At the end of each cycle, the perturbed source effect of the first derivative of $k(a)$ is obtained as follows:

$$\left. \frac{dk_{PS}(a)}{da} \right|_{a=0} = \frac{1}{M} \sum_{i=1}^M S_{PS,i,m}. \quad (14)$$

The β_{eff} in which the perturbed source effect is included is obtained for the m th cycle:

$$\beta_{eff,m} = \frac{1}{k(0)} \frac{dk(a)}{da} \Big|_{a=0} = \beta_{eff,NP,m} + \beta_{eff,PS,m}, \quad (15)$$

where:

$$\beta_{eff,NP,m} = \frac{1}{k(0)} \frac{dk_{NP}(a)}{da} \Big|_{a=0}, \quad (16)$$

$$\beta_{eff,PS,m} = \frac{1}{k(0)} \frac{dk_{PS}(a)}{da} \Big|_{a=0}. \quad (17)$$

$k(0)$ in Eq. (16) or Eq. (17) is the k -eigenvalue for $a = 0$.

3. Sensitivity analysis methods of β_{eff}

Based on the DOS method for calculating β_{eff} shown in Sec. 2, a new method for determining the sensitivity coefficient of β_{eff} with respect to nuclear data is presented in this section. The algorithm for the sensitivity analysis is different depending on the type of nuclear data. The Monte Carlo algorithms are presented for the nuclear reaction cross-sections such as capture, fission, and scattering (Sec. 3.1), the prompt and delayed neutron yields (Sec. 3.2), and the prompt and delayed neutron spectra (Sec. 3.3).

3.1 Capture, fission, scattering cross-sections

The algorithm for the sensitivity of the reaction cross-section is very similar to the DOS method for the sensitivity coefficients of the k -eigenvalue. The method for the k -eigenvalue is published in (Yamamoto, 2018). The new algorithm in this paper can be derived by following the method in (Yamamoto, 2018).

The first derivative of β_{eff} with respect to a nuclear data x is given by differentiating Eq. (1) as follows:

$$\frac{d\beta_{eff}}{dx} = \frac{d}{dx} \left(\frac{1}{k(0)} \frac{dk(a)}{da} \Big|_{a=0} \right) = \frac{1}{k(0)} \frac{dk'_a}{dx} - \frac{k'_a}{k(0)^2} \frac{dk(0)}{dx}, \quad (18)$$

where:

$$k'_a = \frac{dk(a)}{da} \Big|_{a=0}. \quad (19)$$

Using $k'_a = k(0)\beta_{eff}$, Eq. (18) is rewritten as follows:

$$\frac{d\beta_{eff}}{dx} = \frac{1}{k(0)} \frac{dk'_a}{dx} - \frac{\beta_{eff}}{k(0)} \frac{dk(0)}{dx}. \quad (20)$$

The derivative of $k(0)$ with respect to x , $dk(0)/dx$, in Eq. (18) is identical to the sensitivity of

k_{eff} , and the method in (Yamamoto, 2018) is available for calculating $dk(0)/dx$.

The derivative of k'_a with respect to x , dk'_a/dx , for the i th history in the m th cycle is calculated as follows. Steps 1, 2, and 3 are omitted because these are the same as those in Sec. 2. We start with step 4.

(Step 4): At the j th collision site, the following quantity is scored as follows:

$$s_{NP,i,j,m} = \frac{(v_{p,j} + v_{d,j})\Sigma_{f,j}}{\Sigma_{t,j}} w_j W_{f,i,m} W_{p,j,m}, \quad (21)$$

where w_j is the particle weight at the j th collision; $W_{f,i,m}$ is given by Eq. (6) or Eq. (7). $W_{p,j,m}$ is a differential coefficient of the transport and collision kernels with respect to perturbed nuclear data x , which is given by (Yamamoto, 2019b) as follows:

$$W_{p,j,m} = \frac{1}{(v_p + v_d)\Sigma_{f,i}} \frac{\partial}{\partial x} (v_p + v_d)\Sigma_{f,i} + \sum_{l=1}^{j-1} \frac{1}{\Sigma_{s,l}} \frac{\partial}{\partial x} \Sigma_{s,l} - \sum_k s_k \frac{\partial}{\partial x} \Sigma_{t,k}. \quad (22)$$

$W_{p,j,m}$ is specifically written for $x = \Sigma_c$, Σ_s , and Σ_f as follows:

$$W_{p,j,m} = \begin{cases} -\sum_k s_k, & x = \Sigma_c, \\ \sum_{l=1}^{j-1} \frac{1}{\Sigma_{s,l}} - \sum_k s_k, & x = \Sigma_s, \\ \frac{1}{\Sigma_{f,j}} - \sum_k s_k, & x = \Sigma_f, \end{cases} \quad (23) \quad (24) \quad (25)$$

where Σ_c is a macroscopic capture cross-section; s_k is the flight distance of the k th flight within the region where a perturbed cross-section exists; the summation for k is carried out for all flights until the j th collision; l in Eqs. (23) and (24) stands for the l th collision.

The perturbed source effect due to the change of the cross-section must be calculated as described in Sec. 2. The perturbed source effect can be obtained by following the same procedure as in Sec. 2, except that $W_{f,i,m}$ in Eqs. (10) and (11) is substituted by $W_{f,i,m} W_{p,j,m}$. At the j th collision site, the following quantity is scored for the perturbed source effect:

$$s_{PS,i,j,m} = \frac{(v_{p,j} + v_{d,j})\Sigma_{f,j}}{\Sigma_{t,j}} w_j W_{PS,i,m,N}, \quad (26)$$

where $W_{PS,i,m,N}$ is obtained in the same manner as in Eq. (12). At the end of the history, the sensitivity coefficient with respect to a cross-section x for the i th particle history is calculated as

follows:

$$S_{i,x,m} = \sum_j S_{NP,i,j,m} + \sum_j S_{PS,i,j,m} . \quad (27)$$

The cycle average of dk'_a/dx is given by the following:

$$\frac{dk'_a}{dx} = \frac{1}{M} \sum_{i=1}^M S_{i,x,m} , \quad (28)$$

where M is the number of the histories in each cycle. All quantities in Eq. (18) or Eq. (20) that are needed for $d\beta_{eff}/dx$ are obtained as previously demonstrated.

3.2 ν_d and ν_p

The algorithm for calculating the sensitivity coefficient with respect to the prompt and delayed neutron yields is shown in this section. The sensitivity coefficient that we need to calculate is as follows:

$$\frac{d\beta_{eff}}{dv_x} = \frac{1}{k(0)} \frac{dk'_a}{dv_x} - \frac{\beta_{eff}}{k(0)} \frac{dk(0)}{dv_x} , \quad (29)$$

where $x = p$ or d . First, the method for calculating $dk(0)/dv_x$ is discussed. The covariance of nuclear data that is used for sensitivity and uncertainty analyses is provided in multigroup form.

Thus, the formulation in this paper is presented in multigroup form.

The delayed neutron fraction is rigorously defined as follows:

$$\beta_g = \frac{\nu_{d,g}}{\nu_{d,g} + \nu_{p,g}} , \quad (30)$$

where g denotes the energy group of a neutron that induced the fission reaction. The fission neutron spectrum for the g th energy group is given by the following:

$$\chi_{t,g} = (1 - \beta_g) \chi_{p,g} + \beta_g \chi_{d,g} . \quad (31)$$

Thus, the perturbation of $\nu_{d,g}$ or $\nu_{p,g}$ causes the change of the fission neutron spectrum through the change of β_g . The change of the fission neutron spectrum is taken into account as follows.

When starting a fission source particle for the i th history in the m th cycle, the weighting coefficient is assigned to the particle as follows:

$$W_{s,i,m} = \frac{1}{\chi_{t,g}} \frac{d\chi_{t,g}}{dv_{d,g}} = \frac{1}{\chi_{t,g}} \frac{1 - \beta_g}{\nu_{d,g} + \nu_{p,g}} (-\chi_{p,g} + \chi_{d,g}) , \quad \text{for } x = d, \quad (32)$$

and:

$$W_{s,i,m} = \frac{1}{\chi_{t,g}} \frac{d\chi_{t,g}}{dv_{p,g}} = \frac{1}{\chi_{t,g}} \frac{\beta_g}{v_{d,g} + v_{p,g}} (\chi_{p,g} - \chi_{d,g}), \quad \text{for } x = p. \quad (33)$$

Because the energy group g in Eqs. (32) and (33) denotes the energy group of a neutron that induced the fission reaction as mentioned previously instead of the energy group of the fission source particle, the energy group that induced the fission reaction has to be stored for each fission neutron. This information is usually unnecessary in the conventional Monte Carlo calculations. However, the sensitivity calculations to $v_{d,g}$ or $v_{p,g}$ exceptionally require the energy group of the parent neutron to be inherited to the next cycle.

Expression $dk(0)/dv_x$ for the i th particle history in the m th cycle is calculated by following the steps below.

(Step 1): This step is the same as Step 1 in Sec. 2.

(Step 2): According to the energy group of the neutron that produced the starting particle, a weighting coefficient $W_{s,i,m}$ is assigned to the particle using Eq. (32) or Eq. (33).

(Step 3): A random walk process is performed in the same manner as ordinary k -eigenvalue calculations.

(Step 4): At the j th collision site, the following quantity is scored:

$$s_{NP,i,j,m} = \frac{(v_{p,j} + v_{d,j})\Sigma_{f,j}}{\Sigma_{t,j}} w_j (W_{s,i,m} + W_{p,j,m}), \quad (34)$$

where:

$$W_{p,j,m} = \frac{1}{(v_{d,g} + v_{p,g})\Sigma_{f,g}} \frac{d}{dv_{x,g}} (v_{d,g} + v_{p,g})\Sigma_{f,g} = \frac{1}{v_{d,g} + v_{p,g}}. \quad (35)$$

Notably, the energy group g in Eq. (35) is not of the colliding particle but is instead of the neutron that produced the starting particle. The remaining procedures are the same as those in Sec. 3.1, including the calculation for the perturbed source effect.

Next, we calculate dk'_a/dv_x in Eq. (29). The procedures for calculating k'_a are presented in Sec. 2. In step 1 in Sec. 2, whether the starting fission particle is a delayed or prompt neutron is determined according to β_g . The perturbation of $v_{d,g}$ or $v_{p,g}$ changes β_g as seen in Eq. (30). Thus, the weighting coefficient assigned to the starting particle is given by the following:

$$W_{s,i,m} = \frac{1}{\beta_g} \frac{d\beta_g}{dv_{d,g}} = \frac{1}{\beta_g} \frac{1 - \beta_g}{v_{d,g} + v_{p,g}}, \quad \text{for } x = d, \quad (36)$$

and:

$$W_{s,i,m} = \frac{1}{\beta_g} \frac{d\beta_g}{dv_{p,g}} = -\frac{1}{v_{d,g} + v_{p,g}}, \quad \text{for } x = p. \quad (37)$$

Next, dk'_a/dv_x for the i th particle history is calculated by the following steps. Steps 1 and 2 are the same as those in Sec. 2. We start with step 3.

(Step 3): According to the energy group of the neutron that produced the starting particle, a weighting coefficient $W_{s,i,m}$ is assigned to the particle using Eq. (36) or Eq. (37).

(Step 4): A random walk process is performed in the same manner as ordinary k -eigenvalue calculations.

(Step 5) At the j th collision site, the following quantity is scored:

$$s_{NP,i,j,m} = \frac{(v_{p,j} + v_{d,j})\Sigma_{f,j}}{\Sigma_{t,j}} w_j W_{f,i} (W_{s,i,m} + W_{p,j,m}), \quad (38)$$

where $W_{p,j,m}$ is defined by Eq. (22) as follows:

$$W_{p,j,m} = \frac{1}{(v_{d,g} + v_{p,g})\Sigma_{f,g}} \frac{d}{dv_{x,g}} (v_{d,g} + v_{p,g})\Sigma_{f,g} = \frac{1}{v_{d,g} + v_{p,g}}, \quad (39)$$

and $W_{f,i}$ is defined by Eq. (6) or Eq. (7). The remaining procedures are the same as in the previous sections.

3.3 χ_d and χ_p

The algorithm for calculating the sensitivity coefficient of the prompt or delayed neutron spectrum is shown in this section. Note that the sensitivity coefficient with respect to the fission spectrum that is derived in this paper is an unconstrained one (Nagaya et al., 2009). The sensitivity coefficient with respect to the prompt or delayed neutron spectrum is as follows:

$$\frac{d\beta_{eff}}{d\chi_x} = \frac{1}{k(0)} \frac{dk'_a}{d\chi_x} - \frac{\beta_{eff}}{k(0)} \frac{dk(0)}{d\chi_x}, \quad (40)$$

where $x = p$ or d . However, $dk'_a/d\chi_x = 0$ for $x = p$ because k'_a is calculated for delayed neutrons only and the prompt neutron spectrum does not influence k'_a at all. Thus, Eq. (40) is rewritten for $x = p$ as follows:

$$\frac{d\beta_{eff}}{d\chi_p} = -\frac{\beta_{eff}}{k(0)} \frac{dk(0)}{d\chi_p}. \quad (41)$$

If $x = d$, $dk'_a/d\chi_d$ is identical to $dk(0)/d\chi_d$. This is because both derivatives represent the k -eigenvalue sensitivities with respect to the delayed neutron spectrum when a delayed neutron is

emitted from the fission source site. Thus, Eq. (40) is rewritten as follows:

$$\frac{d\beta_{eff}}{d\chi_d} = \frac{1}{k(0)} \frac{dk(0)}{d\chi_d} (1 - \beta_{eff}). \quad (42)$$

$dk(0)/d\chi_x$ in Eq. (41) or Eq. (42) is calculated by the following steps.

(Step 1): This step is the same as step 1 in Sec. 2.

(Step 2): A weighting coefficient is assigned to a fission neutron that is emitted from a fission source site as follows:

$$W_{f,i,m} = \frac{1}{\chi_{d,g}} \frac{d\chi_{d,g}}{d\chi_{d,g}} = \frac{1}{\chi_{d,g}}, \quad \text{if the neutron is a delayed neutron and } x = d, \quad (43)$$

$$W_{f,i,m} = \frac{1}{\chi_{p,g}} \frac{d\chi_{p,g}}{d\chi_{p,g}} = \frac{1}{\chi_{p,g}}, \quad \text{if the neutron is a prompt neutron and } x = p. \quad (44)$$

(Step 3): A random walk process is performed in the same manner as ordinary k -eigenvalue calculations.

(Step 4): At the j th collision site, the following quantity is scored and this score is accumulated until the end of the history:

$$S_{NP,i,j,m} = \frac{(\nu_{p,j} + \nu_{d,j})\Sigma_{f,j}}{\Sigma_{t,j}} w_j W_{f,i,m}. \quad (45)$$

The remaining procedures are the same as in the previous sections.

4. Numerical tests for sensitivity coefficients of β_{eff}

4.1 Uranium fuel thermal system

The Monte Carlo algorithm for calculating the sensitivity coefficients of β_{eff} that is described in Sec. 3 is tested in this section. The first test problem deals with a thermal system that is composed of a homogenized light-water moderated UO_2 fuel rod array surrounded by a light-water reflector layer. The geometry of the test problem is shown in Fig. 1. The geometry is a two-dimensional rectangular shape. Table 1 shows the three-energy group constants for the two materials. The group constants are prepared with a standard reactor analysis code (SRAC) (Okumura et al., 2007). Throughout this paper, the scatterings are assumed to be isotropic. The sensitivity coefficients are calculated with respect to the macroscopic cross-sections (capture, fission, scattering cross sections), ν_p , ν_d , χ_d , and χ_p . The Monte Carlo calculations are

performed with an in-house research-purpose program developed by the authors, which is only available for the purpose of performing this study.

[Fig. 1][Table 1]

The reference calculations for the sensitivity coefficients are performed with the discrete ordinates transport code DANTSYS (Alcouffe et al., 1995) using the same group constants in Table 1. The three-energy group forward and adjoint fluxes of the k -eigenvalue mode are calculated with the angular quadrature order 8. Using the fluxes, β_{eff} is calculated according to the conventional definition of β_{eff} using a postprocessing program developed by the authors as follows:

$$\beta_{eff} = \frac{B}{F}, \quad (46)$$

$$B = \langle \sum_g \phi_g^* \chi_{d,g} \sum_{g'} \nu_{dg'} \Sigma_{fg'} \phi_{g'} \rangle, \quad (47)$$

$$F = \langle \sum_g \phi_g^* \left(\chi_{p,g} \sum_{g'} \nu_{pg'} \Sigma_{fg'} \phi_{g'} + \chi_{d,g} \sum_{g'} \nu_{dg'} \Sigma_{fg'} \phi_{g'} \right) \rangle, \quad (48)$$

where $\langle \rangle$ denotes the volume integration for the whole region; ϕ_g^* is the adjoint flux of the g th group; ϕ_g is the forward flux of the g th group. In Table 2, k_{eff} and β_{eff} calculated by the Monte Carlo method are compared with the deterministic method. The results of both methods precisely agree with each other. The Monte Carlo calculation uses 10,000 cycles, 80,000 particles per cycle, and 20 inactive cycles. The number of iterations for the perturbed source effect throughout this paper is 10, including the calculations for the sensitivity coefficients. This number of iterations is large enough to obtain the converged solutions for the perturbed source effect.

[Table 2]

No exact method for obtaining the sensitivity coefficients of β_{eff} has been developed thus far, except for χ_d and χ_p . Thus, the reference solutions of the sensitivity coefficients of β_{eff} with respect to nuclear data are approximately obtained according to the method by (Iwamoto et al., 2018a):

$$S_{x,a}^{\beta_{eff}} \simeq \frac{k(a)}{k(0)} \frac{1}{\beta_{eff}} (S_{x,a}^k - S_{x,0}^k) \frac{1}{a}, \quad (49)$$

where $S_{x,a}^k$ is the sensitivity coefficient of k_{eff} with respect to x when the delayed fissions are

increased by a as shown in Eq. (4). $S_{x,a}^k$ and $S_{x,0}^k$ are calculated using the forward and adjoint fluxes based on the conventional perturbation theory. A postprocessing program for DANTSYS developed by the authors is used for the sensitivity calculations (Yamamoto, 2018). The exact sensitivity coefficient is obtained by the limit of Eq. (49) when a approaches 0. After calculating $S_{x,a}^{\beta_{eff}}$ at $a = 0.5$ and 1.0 , the reference solutions are obtained by linearly extrapolating $S_{x,a}^{\beta_{eff}}$ to $a = 0.0$.

The sensitivity coefficients with respect to $\chi_{d,g}$ and $\chi_{p,g}$ can be exactly obtained by differentiating Eq. (46), because the changes in these parameters do not change any other nuclear data. The sensitivity coefficients with respect to $\chi_{d,g}$ and $\chi_{p,g}$ are, respectively, given by the following:

$$S_{\chi_{d,g}}^{\beta_{eff}} = \frac{\chi_{d,g}}{\beta_{eff}} \frac{\partial \beta_{eff}}{\partial \chi_{d,g}} = \frac{\chi_{d,g}}{\beta_{eff}} \frac{B_{\chi_{d,g}}(F - B)}{F^2}, \quad (50)$$

$$S_{\chi_{p,g}}^{\beta_{eff}} = \frac{\chi_{p,g}}{\beta_{eff}} \frac{\partial \beta_{eff}}{\partial \chi_{p,g}} = -\frac{\chi_{p,g}}{\beta_{eff}} \frac{F_{\chi_{p,g}} B}{F^2}, \quad (51)$$

where:

$$B_{\chi_{d,g}} = \frac{\partial B}{\partial \chi_{d,g}} = \langle \phi_g^* \sum_{g'} \nu_{dg'} \Sigma_{fg'} \phi_{g'} \rangle, \quad (52)$$

$$F_{\chi_{p,g}} = \frac{\partial F}{\partial \chi_{p,g}} = \langle \phi_g^* \sum_{g'} \nu_{pg'} \Sigma_{fg'} \phi_{g'} \rangle. \quad (53)$$

The sensitivity coefficients calculated by the deterministic method and the new Monte Carlo method are compared in Table 3 (capture), Table 4 (fission), Table 5 (scattering), Table 6 (delayed neutron yield), Table 7 (prompt neutron yield), Table 8 (delayed neutron spectrum), and Table 9 (prompt neutron spectrum). The results of the Monte Carlo calculations include the perturbed source effect. The sensitivity coefficient with respect to the scattering cross-section in the third group is inconsequential and is omitted in Table 4.

[Table 3][Table 4][Table 5][Table 6][Table 7][Table 8][Table 9]

The sensitivity coefficients to the cross-sections (capture, fission, and scattering) calculated by the new Monte Carlo method mostly agree with the reference results within the two standard

deviations, but some of them differ from the reference results by up to 5%. The large differences especially occur in the 2nd group where the large statistical uncertainties are involved. The large statistical uncertainties are caused by the small difference between the two terms on the right-hand side of Eq. (20), which are subtracted from each other. For example, $S_x^{\beta_{eff}}$ for the 2nd group capture cross-section is $-7.74 \times 10^{-3} \pm 1.4 \times 10^{-4}$, which is obtained by subtracting -0.13235 ± 0.00011 from -0.14009 ± 0.00009 . Considering that the statistical uncertainties are involved in the Monte Carlo method and that the reference results are not necessarily exact, the proposed Monte Carlo method yields reasonable results.

The sensitivity coefficients to the nuclear data (ν_d , ν_p , χ_d , and χ_p) calculated with the proposed Monte Carlo method agree with the reference results within a difference of 1%. For the fission spectra, the results of the Monte Carlo method almost exactly agree with the reference results.

4.2 Plutonium fuel fast system

The next test problem deals with a two-dimensional light-water reflected plutonium metal system. The configuration is shown in Fig. 2. Table 10 shows the three-energy group constants for the two materials. In Table 11, k_{eff} and β_{eff} calculated with the Monte Carlo method are compared with the deterministic method. The agreement of k_{eff} between both methods is not as strong as in the previous test problem, which is probably because the ray effect in the deterministic discrete ordinates method is more important in this fast metal system.

[Table 10][Table 11]

The sensitivity coefficients calculated with the deterministic method and the new Monte Carlo method are compared in Table 12 (capture), Table 13 (fission), Table 14 (scattering), Table 15 (delayed neutron yield), Table 16 (prompt neutron yield), Table 17 (delayed neutron spectrum), and Table 18 (prompt neutron spectrum). While the results of the two methods mostly agree within 1% of each other, some show a significant disagreement of ~6% beyond the three standard deviations. No specific reason can be stated presently for why this disagreement occasionally occurs for some cross-sections. The noticeable disagreement in the results of the scattering

cross-sections are commonly observed in both the test problems. However, the derivative of β_{eff} with respect to a scattering cross-section is generally small because it is calculated by taking the difference of two similar terms as seen in Eq. (24). The same result occurs for the scattering cross-sections in the collision history-based approach (Aufiero et al., 2015). Although some disagreement with the reference results is found in the proposed Monte Carlo method, the method generally produces accurate sensitivity estimates.

According to (Iwamoto et al., 2018a), the most dominant effect on the uncertainty of β_{eff} is caused by the delayed neutron fraction ν_d . Although the effect of the delayed neutron spectrum χ_d was unfortunately not evaluated in (Iwamoto et al., 2018a) due to a lack of covariance data, the effect is expected to be substantial. The newly developed method produces precise results for ν_d and χ_d , which are major contributors to the uncertainties of β_{eff} , as shown in Tables 6, 8, 15, and 17. Thus, the proposed method can be a potential tool for use in sensitivity analyses for nuclear data parameters that are important in terms of the accuracy of β_{eff} .

5. Conclusions

A previously developed Monte Carlo method for the sensitivity analysis of β_{eff} experienced difficulties in obtaining less approximate sensitivity coefficients while reducing statistical uncertainties. This paper proposes a new Monte Carlo method that can calculate the exact sensitivity coefficients of β_{eff} . For this purpose, the differential operator sampling (DOS) technique is adopted. The DOS method is one of the Monte Carlo techniques that can yield an exact β_{eff} . Additionally, the DOS method can be applied in calculating the sensitivity coefficients of the k - and α -eigenvalues with respect to nuclear data parameters. In this paper, both capabilities of the DOS method are combined to calculate the exact sensitivity coefficients of β_{eff} . The newly developed Monte Carlo method is tested through comparing the results of the new method with results from a deterministic method based on the perturbation theory using a discrete ordinates transport code. The sensitivity coefficients calculated with the new Monte Carlo method are in accordance in most cases with the coefficients calculated by the deterministic

method. The new method's sensitivity coefficients show a noticeable disagreement beyond the statistical uncertainties, especially for small sensitivities such as the scattering cross-sections. However, the sensitivities to the delayed neutron spectrum χ_d and the delayed neutron yield ν_d , which have direct and dominant effects on β_{eff} , are precisely predicted with the new method. Future developments will include the implementation of the new proposed method into a production continuous energy Monte Carlo code and an uncertainty quantification of β_{eff} using the code and the covariance data of a cross-section library.

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1 List of figures

2 Fig. 1 Geometry of the test problem for sensitivity analyses (UO₂ rod array problem).

3
4 3 Fig. 2 Geometry of the test problem for sensitivity analyses (Pu metal problem).

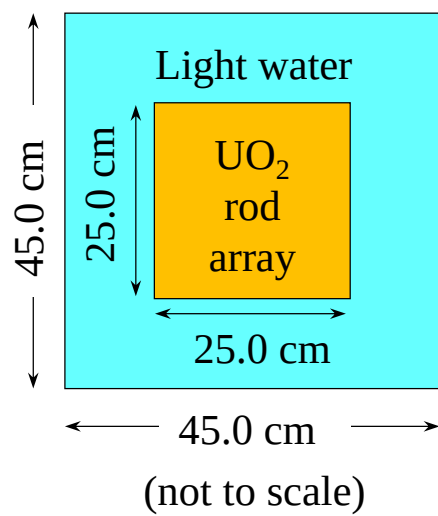


Fig. 1 Geometry of the test problem for sensitivity analyses (UO₂ rod array problem)

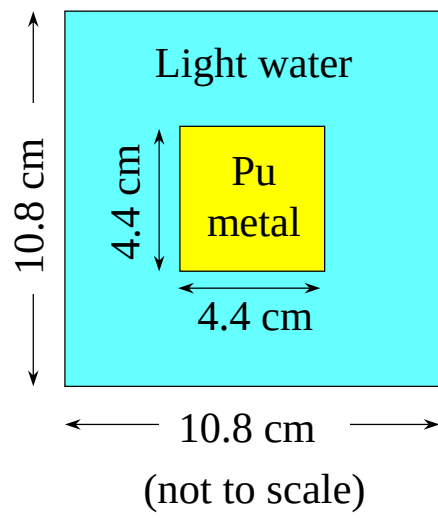


Fig. 2 Geometry of the test problem for sensitivity analyses (Pu metal problem).

Table 1 Three-group constants for UO₂ fuel rod array and light water.

		UO ₂ fuel rod array	Light water
Total cross section (cm ⁻¹)	Σ_{t1}	0.29829	0.33207
	Σ_{t2}	0.83334	1.1265
	Σ_{t3}	1.6389	2.7812
Fission cross section (cm ⁻¹)	Σ_{f1}	0.0030586	—
	Σ_{f2}	0.0021579	—
	Σ_{f3}	0.056928	—
Absorption cross section (cm ⁻¹)	Σ_{a1}	0.003385	0.00030500
	Σ_{a2}	0.011895	0.00036990
	Σ_{a3}	0.086180	0.0182500
Group transfer cross section (cm ⁻¹)	$\Sigma_s^{1 \rightarrow 2}$	0.073843	0.10464
	$\Sigma_s^{1 \rightarrow 3}$	0.0	0.0
	$\Sigma_s^{2 \rightarrow 3}$	0.043803	0.097961
Prompt fission yield	ν_p	2.383095	—
delayed fission yield	ν_d	0.016905	—
Prompt neutron spectrum	$\chi_{p,1}$	0.881487	—
	$\chi_{p,2}$	0.118513	—
	$\chi_{p,3}$	0	—
Delayed neutron spectrum	$\chi_{d,1}$	0.414609	—
	$\chi_{d,2}$	0.585391	—
	$\chi_{d,3}$	0	—

Energy boundaries (10 MeV: 235 keV: 1.27 eV)

Table 2 k_{eff} and β_{eff} for UO₂ fuel rod array.

	k_{eff}	β_{eff} (pcm)
Deterministic method	1.04906	747.58
Monte Carlo method	1.04903	746.93
	(0.000013)*	(0.62)

*The value in the parenthesis is the absolute one standard deviation.

Table 3 $S_x^{\beta_{eff}}$ to the capture cross-section Σ_c for UO₂ fuel rod array.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	1.544×10^{-3}	-8.194×10^{-3}	-9.886×10^{-3}
Monte Carlo method	1.546×10^{-3} (3×10^{-6})*	-7.74×10^{-3} (1.4×10^{-4})	-1.001×10^{-2} (4.2×10^{-4})
MC/Deterministic	1.001	0.9446	1.013

*The value in the parenthesis is the absolute one standard deviation.

Table 4 $S_x^{\beta_{eff}}$ to the fission cross-section Σ_f for UO₂ fuel rod array.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	-1.959×10^{-2}	2.005×10^{-3}	1.141×10^{-2}
Monte Carlo method	-1.973×10^{-2} (8×10^{-5})*	1.726×10^{-3} (7.5×10^{-5})	1.161×10^{-2} (6.0×10^{-4})
MC/Deterministic	1.007	0.9446	1.017

*The value in the parenthesis is the absolute one standard deviation.

Table 5 $S_x^{\beta_{eff}}$ to the scattering cross-section Σ_s for UO₂ fuel rod array.

	1st Gr.	2nd Gr.
Deterministic method	-7.570×10^{-2}	1.679×10^{-2}
Monte Carlo method	-7.884×10^{-2} (6.0×10^{-4})*	1.61×10^{-2} (1.9×10^{-3})
MC/Deterministic	1.041	0.9589

*The value in the parenthesis is the absolute one standard deviation.

Table 6 $S_x^{\beta_{eff}}$ to the delayed neutron yield ν_d for UO₂ fuel rod array.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	6.087×10^{-2}	5.984×10^{-2}	8.718×10^{-1}
Monte Carlo method	6.089×10^{-2} (1.7×10^{-4})*	5.984×10^{-2} (2.3×10^{-4})	8.716×10^{-1} (9×10^{-4})
MC/Deterministic	1.000	1.000	1.000

*The value in the parenthesis is the absolute one standard deviation.

Table 7 $S_x^{\beta_{eff}}$ to the prompt neutron yield ν_p for UO₂ fuel rod array.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	-9.512×10^{-2}	-5.613×10^{-2}	-8.397×10^{-1}
Monte Carlo method	-9.503×10^{-2} (1.9×10^{-4}) *	-5.660×10^{-2} (2.1×10^{-4})	-8.413×10^{-1} (8×10^{-4})
MC/Deterministic	0.999	1.008	1.002

*The value in the parenthesis is the absolute one standard deviation.

Table 8 $S_x^{\beta_{eff}}$ to the delayed neutron spectrum χ_d for UO₂ fuel rod array.

	1st Gr.	2nd Gr.
Deterministic method	3.815×10^{-1}	6.111×10^{-1}
Monte Carlo method	3.817×10^{-1} (5×10^{-4}) *	6.113×10^{-1} (6×10^{-4})
MC/Deterministic	1.001	1.000

*The value in the parenthesis is the absolute one standard deviation.

Table 9 $S_x^{\beta_{eff}}$ to the prompt neutron spectrum χ_p for UO₂ fuel rod array.

	1st Gr.	2nd Gr.
Deterministic method	-8.611×10^{-1}	-1.314×10^{-1}
Monte Carlo method	-8.611×10^{-1} (7×10^{-4}) *	-1.313×10^{-1} (1×10^{-4})
MC/Deterministic	1.000	0.999

*The value in the parenthesis is the absolute one standard deviation.

Table 10 Three-group constants for the plutonium metal and the light water

		Plutonium metal	Light water
Total cross section (cm ⁻¹)	Σ_{t1}	0.28573	0.301663
	Σ_{t2}	0.35423	0.686824
	Σ_{t3}	0.62448	1.48258
Fission cross section (cm ⁻¹)	Σ_{f1}	0.072424	—
	Σ_{f2}	0.052973	—
	Σ_{f3}	0.13267	—
Absorption cross section (cm ⁻¹)	Σ_{a1}	0.073056	0.002842
	Σ_{a2}	0.064640	0.00001
	Σ_{a3}	0.022681	0.00225
	$\Sigma_s^{1 \rightarrow 2}$	0.029374	0.18638
Group transfer cross section (cm ⁻¹)	$\Sigma_s^{1 \rightarrow 3}$	0	0
	$\Sigma_s^{2 \rightarrow 3}$	0.00030767	0.11244
Prompt fission yield	ν_p	3.19338	—
Delayed fission yield	ν_d	0.00662	—
Prompt neutron spectrum	$\chi_{p,1}$	0.77409	—
	$\chi_{p,2}$	0.22451	—
	$\chi_{p,3}$	0	—
Delayed neutron spectrum	$\chi_{d,1}$	0.165982	—
	$\chi_{d,2}$	0.834018	—
	$\chi_{d,3}$	0	—

Energy boundaries (10 MeV: 821 keV: 19.3 keV)

Table 11 k_{eff} and β_{eff} for Pu metal.

	k_{eff}	β_{eff} (pcm)
Deterministic method	1.00146	218.37
Monte Carlo method	1.00059	218.33
	(0.000017) *	(0.31)

*The value in the parenthesis is the absolute one standard deviation.

Table 12 $S_x^{\beta_{eff}}$ to the capture cross-section Σ_c for Pu metal.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	1.052×10^{-3}	-2.073×10^{-2}	-4.350×10^{-2}
Monte Carlo method	1.053×10^{-3} (3×10^{-6}) [*]	-2.066×10^{-2} (8×10^{-5})	-4.312×10^{-2} (3.9×10^{-4})
MC/Deterministic	1.001	0.997	0.991

*The value in the parenthesis is the absolute one standard deviation.

Table 13 $S_x^{\beta_{eff}}$ to the fission cross-section Σ_f for Pu metal.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	-3.009×10^{-1}	1.979×10^{-1}	7.296×10^{-2}
Monte Carlo method	-3.009×10^{-1} (7×10^{-4}) [*]	1.976×10^{-2} (8.4×10^{-4})	6.987×10^{-2} (5.4×10^{-4})
MC/Deterministic	1.000	0.998	0.958

*The value in the parenthesis is the absolute one standard deviation.

Table 14 $S_x^{\beta_{eff}}$ to the scattering cross-section Σ_s for Pu metal.

	1st Gr.	2nd Gr.
Deterministic method	-3.117×10^{-2}	2.078×10^{-2}
Monte Carlo method	-2.985×10^{-2} (1.9×10^{-4}) [*]	2.230×10^{-2} (5.7×10^{-4})
MC/Deterministic	0.958	1.073

*The value in the parenthesis is the absolute one standard deviation.

Table 15 $S_x^{\beta_{eff}}$ to the delayed neutron yield ν_d for Pu metal.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	5.255×10^{-1}	2.399×10^{-1}	2.340×10^{-1}
Monte Carlo method	5.277×10^{-1} (1.1×10^{-3}) [*]	2.385×10^{-1} (8×10^{-4})	2.333×10^{-1} (8×10^{-4})
MC/Deterministic	1.004	0.994	0.997

*The value in the parenthesis is the absolute one standard deviation.

Table 16 $S_x^{\beta_{eff}}$ to the prompt neutron yield ν_p for Pu metal.

	1st Gr.	2nd Gr.	3rd Gr.
Deterministic method	-9.544×10^{-1}	5.261×10^{-2}	-9.709×10^{-2}
Monte Carlo method	-9.488×10^{-1} (1.3×10^{-3}) *	5.330×10^{-2} (1.0×10^{-4})	-1.035×10^{-1} (9×10^{-4})
MC/Deterministic	0.994	1.013	1.066

*The value in the parenthesis is the absolute one standard deviation.

Table 17 $S_x^{\beta_{eff}}$ to the delayed neutron spectrum χ_d for Pu metal.

	1st Gr.	2nd Gr.
Deterministic method	1.537×10^{-1}	8.442×10^{-1}
Monte Carlo method	1.541×10^{-1} (8×10^{-4}) *	8.438×10^{-1} (3.3×10^{-3})
MC/Deterministic	1.003	0.999

*The value in the parenthesis is the absolute one standard deviation.

Table 18 $S_x^{\beta_{eff}}$ to the prompt neutron spectrum χ_p for Pu metal.

	1st Gr.	2nd Gr.
Deterministic method	-7.578×10^{-1}	-2.400×10^{-1}
Monte Carlo method	-7.578×10^{-1} (1.1×10^{-3}) *	-2.401×10^{-1} (3×10^{-4})
MC/Deterministic	1.000	1.000

*The value in the parenthesis is the absolute one standard deviation.