

Sensitivity analysis of prompt neutron decay constant using perturbation theoryTomohiro Endo^{a*}, Akio Yamamoto^a^a *Graduate School of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan;***Abstract**

Experimental results of prompt neutron decay constant α is useful information to validate numerical results of ω -eigenvalue for spatial and energetic fundamental mode. In order to accomplish the data assimilation technique using α , it is desirable to establish an efficient numerical calculation method for sensitivity coefficient analysis of α . For this purpose, the numerical calculation method using the first-order perturbation theory is investigated. A specific theoretical formula is derived to evaluate the sensitivity coefficient of α to nuclear data. The derived rigorous formula utilizes forward and adjoint eigenfunctions which consist of neutron flux and delayed neutron precursor densities. Using the prompt approximation, the derived formula can be simplified without the term involving the delayed neutron precursor densities. By calculating α using the multi energy-group neutron transport code for an ICSBEP benchmark problem, the derived formula for sensitivity analysis using the perturbation theory is verified by comparing with the reference results using the direct method. Consequently, the efficient numerical procedures for uncertainty quantification of α can be established by the aid of the sensitivity coefficients based on the perturbation theory.

Keywords; ω -eigenvalue, sensitivity analysis, first-order perturbation theory, adjoint, uncertainty, covariance

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1. Introduction

Results of critical experiments, which are collected in ICSBEP [1], are effectively utilized to validate a neutron transport code. Since the effective neutron multiplication factor k_{eff} is equal to unity in a just critical state, k_{eff} is mainly utilized as one of neutronics parameters in integral experiments to validate k_{eff} -eigenvalue estimated by the neutron transport code. In a near-critical experimental core where the one-point approximation is applicable, the excess reactivity and control rod worth can be measured using the positive period method and the rod drop method [2]. These experimental results can be used to deduce the negative reactivity (or subcriticality) $-\rho = (1 - k_{\text{eff}})/k_{\text{eff}}$ for a shallow subcritical system. In general, as the subcriticality becomes deeper, spatial and energetic contributions due to higher order modes increase. Because of these higher mode effects, direct measurement of k_{eff} has difficulty for such a deep subcritical system.

Instead of k_{eff} , we have been investigating to utilize experimental results, which can be directly measured even in a subcritical system, for validation of a neutron transport code. For example, using the pulsed neutron source method [3] and the reactor noise analysis method [4], the prompt neutron decay constant α can be directly measured for a deep subcritical system [5,6]. As clarified in our previous research [7], experimental results of α are useful information to validate numerical results of ‘ ω -eigenvalue,’ which is a temporal eigenvalue to express exponentially increasing or decreasing of neutron flux. In addition, there are nuclear data-induced correlations among α and other neutronics parameters (e.g. k_{eff} and neutron generation time Λ) [7]. Thus, such a correlation can be utilized for the data assimilation technique (e.g. the bias factor method [8,9] and the cross-section adjustment method [10,11]) using experimental results of α , to reduce bias and uncertainty of predicted neutronics parameters.

For this purpose, it is desirable to establish an efficient numerical calculation method for sensitivity coefficient analysis (SA) of ω -eigenvalue, or prompt neutron decay constant α . In

the case of k_{eff} -eigenvalue, the numerical calculation method based on the first-order perturbation theory (PT) is effectively applied to SA in existing calculation codes, e.g. SCALE6.2/TSUNAMI [12], SAGEP [13], MARBLE2 [14] and CBZ [15]. If PT is applicable to SA, the calculation cost of SA is dramatically reduced, i.e. two eigenvalue-calculations for forward and adjoint eigenfunctions are enough.

It is noted that, in the case of the rigorous ω -eigenvalue equation, the eigenfunctions consist of neutron flux and delayed neutron precursor densities. Thus, a PT-based theoretical formula for SA of α is not straightforward, compared with that for SA of k_{eff} . One of the main purpose of the present study is to derive the specific theoretical formula for α . In addition, another aim is to verify the PT-based sensitivity coefficients of α using the derived formula by comparing with the reference values using the direct method. For this verification, an existing deterministic neutron transport code, PARTISN [16], is utilized to obtain the forward and adjoint eigenfunctions.

The rest of this paper is organized as follows: Section 2 describes the numerical theory for SA of α using PT. Section 3 explains calculation procedures for the verification using PARTISN, and shows numerical results of sensitivity coefficients and nuclear data-induced uncertainty of α . Finally, concluding remarks are presented in Section 4.

2. Theory

2.1. ω -eigenvalue equation

Let us discuss on the basis of the multi energy-group neutron transport equation with 6 delayed neutron precursor-group. By assuming that time variations of the g th energy-group angular neutron flux ψ_g and the i th delayed neutron precursor density C_i are proportional to $\exp(\omega t)$, the ω -eigenvalue equations for ψ_g and C_i are described as follows [17,18]:

$$\mathbf{B}_p \psi_g(\vec{r}, \vec{\Omega}) + \sum_{i=1}^6 \frac{\chi_{i,g}}{4\pi} \lambda_i C_i(\vec{r}) = \frac{\omega}{v_g} \psi_g(\vec{r}, \vec{\Omega}), \quad (1)$$

$$\sum_{g'=1}^{NG} a_i v_d \Sigma_{f,g'} \int_{4\pi} \psi_{g'}(\vec{r}, \vec{\Omega}') d\Omega' - \lambda_i C_i(\vec{r}) = \omega C_i(\vec{r}), \quad (2)$$

$$\mathbf{B}_p \equiv -\mathbf{A} + \mathbf{F}_p, \quad (3)$$

$$\mathbf{A} \equiv \vec{\Omega} \nabla + \Sigma_{t,g} - \sum_{g'=1}^{NG} \sum_{l=0}^{NL} \frac{2l+1}{4\pi} \Sigma_{s,l,g' \rightarrow g} \sum_{m=-l}^l R_{lm}(\vec{\Omega}) \int_{4\pi} d\Omega' R_{lm}(\vec{\Omega}'), \quad (4)$$

$$\mathbf{F}_p \equiv \frac{\chi_{p,g}}{4\pi} \sum_{g'=1}^{NG} \nu_p \Sigma_{f,g'} \int_{4\pi} d\Omega', \quad (5)$$

where \mathbf{A} , \mathbf{F}_p , and \mathbf{B}_p are net neutron loss, prompt neutron production, and prompt Boltzmann operator, respectively; $\Sigma_{t,g}$, $\Sigma_{f,g}$, and $\Sigma_{s,l,g' \rightarrow g}$ are macroscopic total, fission, and l th order scattering cross-sections, respectively; v_g is neutron velocity; ν_p and ν_d are prompt and delayed neutrons per fission; $\chi_{p,g}$ are $\chi_{i,g}$ are prompt and the i th group delayed fission spectrum; a_i and λ_i are the i th group relative delayed neutron yield and decay constant; $R_{lm}(\vec{\Omega})$ is the spherical harmonic function which satisfies the orthogonality condition of $\int_{4\pi} R_{lm}(\vec{\Omega}') R_{l'm'}(\vec{\Omega}') d\Omega' = \frac{4\pi}{2l+1} \delta_{ll'} \delta_{mm'}$; NG and NL are the total number of neutron energy groups and the maximum order of Legendre expansion for scattering cross-section, respectively.

From Equation (2), C_i can also be expressed by:

$$C_i(\vec{r}) = \frac{1}{\omega + \lambda_i} \sum_{g'=1}^{NG} a_i v_d \Sigma_{f,g'} \int_{4\pi} \psi_{g'}(\vec{r}, \vec{\Omega}') d\Omega'. \quad (6)$$

By substituting Equation (6) into Equation (1), the ω -eigenvalue equation can be rewritten as a nonlinear eigenvalue problem where the eigenfunction can be expressed by only ψ_g :

$$\left(\mathbf{B}_p + \sum_{i=1}^6 \frac{\lambda_i}{\omega + \lambda_i} \mathbf{F}_i \right) \psi_g(\vec{r}, \vec{\Omega}) = \frac{\omega}{v_g} \psi_g(\vec{r}, \vec{\Omega}), \quad (7)$$

$$\mathbf{F}_i \equiv \frac{\chi_{i,g}}{4\pi} \sum_{g'=1}^{NG} a_i v_d \Sigma_{f,g'} \int_{4\pi} d\Omega'. \quad (8)$$

By transposing operators in Equations (1) and (2), the corresponding adjoint ω -eigenvalue equations can be derived as follows [17]:

$$\mathbf{B}_p^\dagger \psi_g^\dagger(\vec{r}, \vec{\Omega}) + \sum_{i=1}^6 a_i \nu_d \Sigma_{f,g} C_i^\dagger(\vec{r}) = \frac{\omega}{v_g} \psi_g^\dagger(\vec{r}, \vec{\Omega}), \quad (9)$$

$$\lambda_i \sum_{g'=1}^{NG} \int_{4\pi} \frac{\chi_{i,g'}}{4\pi} \psi_{g'}^\dagger(\vec{r}, \vec{\Omega}') d\Omega' - \lambda_i C_i^\dagger(\vec{r}) = \omega C_i^\dagger(\vec{r}), \quad (10)$$

$$\mathbf{B}_p^\dagger \equiv -\mathbf{A}^\dagger + \mathbf{F}_p^\dagger, \quad (11)$$

$$\mathbf{A}^\dagger \equiv -\vec{\Omega} \nabla + \Sigma_{t,g} - \sum_{g'=1}^{NG} \sum_{l=0}^{NL} \frac{2l+1}{4\pi} \Sigma_{s,l,g \rightarrow g'} \sum_{m=-l}^l R_{lm}(\vec{\Omega}) \int_{4\pi} d\Omega' R_{lm}(\vec{\Omega}'), \quad (12)$$

$$\mathbf{F}_p^\dagger \equiv \nu_p \Sigma_{f,g} \sum_{g'=1}^{NG} \int_{4\pi} d\Omega' \frac{\chi_{p,g'}}{4\pi}, \quad (13)$$

where the superscript \dagger represents ‘adjoint;’ and the adjoint functions of $\psi_g^\dagger(\vec{r}, \vec{\Omega})$ and $C_i^\dagger(\vec{r})$ indicate importance functions at the spatial position \vec{r} due to one neutron of the g th energy-group with the flight direction $\vec{\Omega}$ and due to one delayed neutron precursor of the i th group, respectively. Equations (9) and (10) physically mean balance equations for generation and loss of importance functions. For example, in Equations (9) and (10), $\sum_{i=1}^6 a_i \nu_d \Sigma_{f,g} C_i^\dagger(\vec{r})$ and $\lambda_i \sum_{g'=1}^{NG} \int_{4\pi} \frac{\chi_{i,g'}}{4\pi} \psi_{g'}^\dagger(\vec{r}, \vec{\Omega}') d\Omega'$ correspond to the generation of precursor- and neutron-importance functions due to the delayed fission reaction by one neutron and due to the decay of one precursor, respectively; $\mathbf{A}^\dagger \psi_g^\dagger(\vec{r}, \vec{\Omega})$ and $\lambda_i C_i^\dagger(\vec{r})$ are related to the loss of neutron- and precursor-importance functions due to the neutron leakage or absorption and due to the decay of precursor, respectively; and the balances of importance functions are maintained by the terms involving ω such as $\frac{\omega}{v_g} \psi_g^\dagger(\vec{r}, \vec{\Omega})$ and $\omega C_i^\dagger(\vec{r})$.

In the same way as Equation (6), C_i^\dagger can also be transformed from Equation (10) to the following expression:

$$C_i^\dagger(\vec{r}) = \frac{\lambda_i}{\omega + \lambda_i} \sum_{g'=1}^{NG} \int_{4\pi} \frac{\chi_{i,g'}}{4\pi} \psi_{g'}^\dagger(\vec{r}, \vec{\Omega}') d\Omega'. \quad (14)$$

By substituting Equation (14) into Equation (9), the non-linear adjoint equation can be obtained as:

$$\left(\mathbf{B}_p^\dagger + \sum_{i=1}^6 \frac{\lambda_i}{\omega + \lambda_i} \mathbf{F}_i^\dagger \right) \psi_g^\dagger(\vec{r}, \vec{\Omega}) = \frac{\omega}{v_g} \psi_g^\dagger(\vec{r}, \vec{\Omega}), \quad (15)$$

$$\mathbf{F}_i^\dagger \equiv a_i v_d \Sigma_{f,g} \sum_{g'=1}^{NG} \int_{4\pi} d\Omega' \frac{\chi_{i,g'}}{4\pi}. \quad (16)$$

2.2. Sensitivity coefficient analysis of ω by the first-order perturbation theory

Let us consider perturbation due to an infinitesimal change of nuclear data. Then, perturbed equations of Equations (1) and (2) are obtained as follows:

$$\begin{aligned} (\mathbf{B}_p + \delta\mathbf{B}_p)(\psi_g + \delta\psi_g) + \sum_{i=1}^6 \frac{\chi_{i,g} + \delta\chi_{i,g}}{4\pi} (\lambda_i + \delta\lambda_i)(C_i + \delta C_i) \\ = \frac{\omega + \delta\omega}{v_g + \delta v_g} (\psi_g + \delta\psi_g), \end{aligned} \quad (17)$$

$$\begin{aligned} \sum_{g'=1}^{NG} (a_i + \delta a_i)(v_d \Sigma_{f,g'} + \delta(v_d \Sigma_{f,g'})) \int_{4\pi} (\psi_{g'} + \delta\psi_{g'}) d\Omega' - (\lambda_i + \delta\lambda_i)(C_i + \delta C_i) \\ = (\omega + \delta\omega)(C_i + \delta C_i). \end{aligned} \quad (18)$$

By neglecting higher order infinitesimals (e.g. $\delta\mathbf{B}_p \delta\psi_g$) in Equations (17) and (18), and substituting Equations (1) and (2) into them, the following perturbation formulae can be derived:

$$\delta\mathbf{B}_p \psi_g + \mathbf{B}_p \delta\psi_g + \sum_{i=1}^6 \left(\delta \left(\frac{\chi_{i,g}}{4\pi} \lambda_i \right) C_i + \frac{\chi_{i,g}}{4\pi} \lambda_i \delta C_i \right) \approx \frac{\delta\omega}{v_g} \psi_g + \frac{\omega}{v_g} \delta\psi_g - \frac{\omega \delta v_g}{v_g^2} \psi_g, \quad (19)$$

$$\sum_{g'=1}^{NG} \int_{4\pi} (\delta(a_i v_d \Sigma_{f,g'}) \psi_{g'} + a_i v_d \Sigma_{f,g'} \delta\psi_{g'}) d\Omega' - \delta\lambda_i C_i - \lambda_i \delta C_i \approx \delta\omega C_i + \omega \delta C_i. \quad (20)$$

By multiplying both sides of Equation (19) by ψ_g^\dagger and integrating over all phase space, the following equation is obtained:

$$\begin{aligned} & \langle \psi_g^\dagger \delta \mathbf{B}_p \psi_g \rangle + \langle \psi_g^\dagger \mathbf{B}_p \delta \psi_g \rangle + \langle \psi_g^\dagger \delta \left(\frac{\chi_{i,g}}{4\pi} \lambda_i \right) C_i \rangle + \langle \psi_g^\dagger \frac{\chi_{i,g}}{4\pi} \lambda_i \delta C_i \rangle \\ & \approx \delta \omega \left\langle \frac{\psi_g^\dagger \psi_g}{v_g} \right\rangle + \omega \left\langle \frac{\psi_g^\dagger \delta \psi_g}{v_g} \right\rangle - \omega \left\langle \psi_g^\dagger \frac{\delta v_g}{v_g^2} \psi_g \right\rangle, \end{aligned} \quad (21)$$

where the bracket $\langle \rangle$ represents integral over all phase space, i.e. the spatial integration over the whole volume, the directional integration over the whole solid angle, and the summation over all energy- and precursor-groups. In order to eliminate terms relating perturbation of $\delta \psi_g$ and δC_i in Equation (21), adjoint equations of Equations (9) and (10) are utilized as shown below. Firstly, by multiplying both sides of Equation (9) by the perturbation of flux $\delta \psi_g$, integrating over all phase space, and using the following relationship of adjoint operator $\langle \delta \psi_g \mathbf{B}_p^\dagger \psi_g^\dagger \rangle = \langle \psi_g^\dagger \mathbf{B}_p \delta \psi_g \rangle$, the following equation is obtained:

$$\langle \psi_g^\dagger \mathbf{B}_p \delta \psi_g \rangle + \langle C_i^\dagger a_i v_d \Sigma_{f,g} \delta \psi_g \rangle = \omega \left\langle \frac{\psi_g^\dagger \delta \psi_g}{v_g} \right\rangle. \quad (22)$$

By substituting Equation (22) into Equation (21), $\langle \psi_g^\dagger \mathbf{B}_p \delta \psi_g \rangle$ and $\left\langle \frac{\psi_g^\dagger \delta \psi_g}{v_g} \right\rangle$ can be eliminated as follows:

$$\begin{aligned} & \langle \psi_g^\dagger \delta \mathbf{B}_p \psi_g \rangle + \langle \psi_g^\dagger \delta \left(\frac{\chi_{i,g}}{4\pi} \lambda_i \right) C_i \rangle + \langle \psi_g^\dagger \frac{\chi_{i,g}}{4\pi} \lambda_i \delta C_i \rangle - \langle C_i^\dagger a_i v_d \Sigma_{f,g} \delta \psi_g \rangle \\ & \approx \delta \omega \left\langle \frac{\psi_g^\dagger \psi_g}{v_g} \right\rangle - \omega \left\langle \psi_g^\dagger \frac{\delta v_g}{v_g^2} \psi_g \right\rangle. \end{aligned} \quad (23)$$

Secondly, by multiplying both sides of Equation (20) by the adjoint function C_i^\dagger and integrating over all phase space, the following equation is obtained:

$$\begin{aligned} & \langle C_i^\dagger \delta (a_i v_d \Sigma_{f,g}) \psi_g \rangle + \langle C_i^\dagger a_i v_d \Sigma_{f,g} \delta \psi_g \rangle - \langle C_i^\dagger \delta \lambda_i C_i \rangle - \langle C_i^\dagger \lambda_i \delta C_i \rangle \\ & \approx \delta \omega \langle C_i^\dagger C_i \rangle + \omega \langle C_i^\dagger \delta C_i \rangle. \end{aligned} \quad (24)$$

By adding Equations (23) and (24), $\langle C_i^\dagger a_i v_d \Sigma_{f,g} \delta \psi_g \rangle$ can be eliminated as follows:

$$\begin{aligned}
& \langle \psi_g^\dagger \delta \mathbf{B}_p \psi_g \rangle + \langle \psi_g^\dagger \delta \left(\frac{\chi_{i,g}}{4\pi} \lambda_i \right) C_i \rangle + \langle \psi_g^\dagger \frac{\chi_{i,g}}{4\pi} \lambda_i \delta C_i \rangle + \langle C_i^\dagger \delta (a_i v_d \Sigma_{f,g}) \psi_g \rangle \\
& \quad - \langle C_i^\dagger \delta \lambda_i C_i \rangle - \langle C_i^\dagger \lambda_i \delta C_i \rangle \\
& \approx \delta \omega \left(\left\langle \frac{\psi_g^\dagger \psi_g}{v_g} \right\rangle + \langle C_i^\dagger C_i \rangle \right) + \omega \left(\langle C_i^\dagger \delta C_i \rangle - \langle \psi_g^\dagger \frac{\delta v_g}{v_g^2} \psi_g \rangle \right).
\end{aligned} \tag{25}$$

Thirdly, by multiplying both sides of Equation (10) by perturbation δC_i and integrating over all phase space, the following formula is obtained:

$$\langle \psi_g^\dagger \frac{\chi_{i,g}}{4\pi} \lambda_i \delta C_i \rangle - \langle C_i^\dagger \lambda_i \delta C_i \rangle = \omega \langle C_i^\dagger \delta C_i \rangle. \tag{26}$$

By substituting Equation (26) into Equation (25), the terms relating to the perturbation δC_i can be eliminated as follows:

$$\begin{aligned}
& \langle \psi_g^\dagger \delta \mathbf{B}_p \psi_g \rangle + \langle \psi_g^\dagger \delta \left(\frac{\chi_{i,g}}{4\pi} \lambda_i \right) C_i \rangle + \langle C_i^\dagger \delta (a_i v_d \Sigma_{f,g}) \psi_g \rangle - \langle C_i^\dagger \delta \lambda_i C_i \rangle \\
& \approx \delta \omega \left(\left\langle \frac{\psi_g^\dagger \psi_g}{v_g} \right\rangle + \langle C_i^\dagger C_i \rangle \right) - \omega \langle \psi_g^\dagger \frac{\delta v_g}{v_g^2} \psi_g \rangle.
\end{aligned} \tag{27}$$

From Equation (27), the perturbation $\delta \omega$ can be expressed by:

$$\begin{aligned}
& \delta \omega \\
& \approx \frac{\langle \psi_g^\dagger \left(\delta \mathbf{B}_p + \omega \frac{\delta v_g}{v_g^2} \right) \psi_g \rangle + \langle \psi_g^\dagger \delta \left(\frac{\chi_{i,g}}{4\pi} \lambda_i \right) C_i \rangle + \langle C_i^\dagger \delta (a_i v_d \Sigma_{f,g}) \psi_g \rangle - \langle C_i^\dagger \delta \lambda_i C_i \rangle}{\left\langle \frac{\psi_g^\dagger \psi_g}{v_g} \right\rangle + \langle C_i^\dagger C_i \rangle}.
\end{aligned} \tag{28}$$

Finally, on the basis of the first-order perturbation theory, the relative sensitivity coefficient of ω with respect to arbitrary nuclear data σ can be estimated using the adjoint functions of ψ_g^\dagger and C_i^\dagger as follows:

$$\begin{aligned}
& \frac{\sigma}{\omega} \frac{\partial \omega}{\partial \sigma} \\
& \approx \frac{\sigma}{\omega} \frac{\langle \psi_g^\dagger \left(\frac{\partial \mathbf{B}_p}{\partial \sigma} + \frac{\omega}{v_g^2} \frac{\partial v_g}{\partial \sigma} \right) \psi_g \rangle + \langle \psi_g^\dagger \frac{\partial \left(\frac{\chi_{i,g}}{4\pi} \lambda_i \right)}{\partial \sigma} C_i \rangle + \langle C_i^\dagger \frac{\partial (a_i v_d \Sigma_{f,g})}{\partial \sigma} \psi_g \rangle - \langle C_i^\dagger \frac{\partial \lambda_i}{\partial \sigma} C_i \rangle}{\left\langle \frac{\psi_g^\dagger \psi_g}{v_g} \right\rangle + \langle C_i^\dagger C_i \rangle}.
\end{aligned} \tag{29}$$

As shown in Equation (29), the forward and adjoint eigenfunctions of delayed neutron precursor densities, C_i and C_i^\dagger , are necessary when delayed neutron contributions are considered in the PT-based SA of ω .

2.3. Sensitivity coefficient analysis of α using prompt approximation

In this subsection, let us focus on the numerical analysis of prompt neutron decay constant α , which corresponds to the most negative ω -eigenvalue for spatial and energetic fundamental mode $\omega_{0,7}$. Note that the value of α means an exponential decay constant of neutron flux, or $\psi_g \propto \exp(-\alpha t)$, thus α corresponds to the absolute value of $\omega_{0,7}$ in this paper, *i.e.* $\alpha \equiv -\omega_{0,7}$. In Equations (7) and (15), conditions of $\mathbf{F}_p \gg \left| \sum_{i=1}^6 \frac{\lambda_i}{\omega_{0,7} + \lambda_i} \mathbf{F}_i \right|$ and $\mathbf{F}_p^\dagger \gg \left| \sum_{i=1}^6 \frac{\lambda_i}{\omega_{0,7} + \lambda_i} \mathbf{F}_i^\dagger \right|$ are generally satisfied, because $\left| \frac{a_i \lambda_i v_d / v_p}{\omega_{0,7} + \lambda_i} \right| \ll 1$. For example, $\left| \frac{a_6 \lambda_6 v_d / v_p}{\omega_{0,7} + \lambda_6} \right| \approx 10^{-5}$ when $a_6 = 0.066$, $\lambda_6 = 2.85$ (1/s), $v_d / v_p = 0.007$, and $\alpha = -\omega_{0,7} = 100$ (1/s) for a thermal fission system of ^{235}U . Thus, the forward and adjoint ω -eigenvalue equations of Equations (7) and (15) can be reasonably approximated as the ‘prompt ω -eigenvalue equations’ to evaluate α :

$$\mathbf{B}_p \psi_{p,g}(\vec{r}, \vec{\Omega}) = \frac{\omega_p}{v_g} \psi_{p,g}(\vec{r}, \vec{\Omega}), \quad (30)$$

$$\mathbf{B}_p^\dagger \psi_{p,g}^\dagger(\vec{r}, \vec{\Omega}) = \frac{\omega_p}{v_g} \psi_{p,g}^\dagger(\vec{r}, \vec{\Omega}), \quad (31)$$

where the subscript p in $\psi_{p,g}$, $\psi_{p,g}^\dagger$ and ω_p indicates the prompt approximation. Using the prompt approximation, the prompt neutron decay constant can be reasonably evaluated by an existing neutron transport code (e.g. PARTISN) as reported in the previous study [7].

Here, the corresponding delayed neutron precursor densities $C_{p,i}$ and $C_{p,i}^\dagger$ can be estimated by Equations (6) and (14), if necessary:

$$C_{p,i}(\vec{r}) \approx \frac{1}{\omega_p + \lambda_i} \sum_{g'=1}^{NG} a_i v_d \Sigma_{f,g'} \int_{4\pi} \psi_{p,g'}(\vec{r}, \vec{\Omega}') d\Omega', \quad (32)$$

$$C_{p,i}^+(\vec{r}) \approx \frac{\lambda_i}{\omega_p + \lambda_i} \sum_{g'=1}^{NG} \int_{4\pi} \frac{\chi_{i,g'}}{4\pi} \psi_{p,g'}^+(\vec{r}, \vec{\Omega}') d\Omega'. \quad (33)$$

Note that, in the prompt approximation where $|\omega_p| \gg \lambda_i$, Equations (32) and (33) clarify that magnitudes of $C_{p,i}$ and $C_{p,i}^+$ are negligibly small. Thus, in the SA of ω_p , the relative sensitivity coefficient by Equation (29) can be approximated without $C_{p,i}$ and $C_{p,i}^+$:

$$\frac{\sigma}{\omega_p} \frac{\partial \omega_p}{\partial \sigma} \approx \frac{\sigma}{\omega_p} \frac{\langle \psi_{p,g}^+ \left(\frac{\partial \mathbf{B}_p}{\partial \sigma} + \frac{\omega_p}{v_g^2} \frac{\partial v_g}{\partial \sigma} \right) \psi_{p,g} \rangle}{\langle \frac{\psi_{p,g}^+ \psi_{p,g}}{v_g} \rangle}. \quad (34)$$

The numerical methodology of Equation (34) is almost the same in the case of k_{eff} [12]. In our previous study using the multi-group diffusion calculation [19], the applicability of the prompt approximation of Equation (34) was verified by comparing the rigorous sensitivity coefficient using Equation (29).

As can be suggested from the derivation of Equation (34), it is expected that sensitivity coefficients of ω_p to delayed neutron parameters are negligibly small. To roughly estimate a relative sensitivity coefficient to a delayed neutron parameter, the approximated values of $C_{p,i}$ and $C_{p,i}^+$ are useful, e.g. the relative sensitivity coefficients to relative delayed neutron yield a_i and decay constant λ_i can be estimated by Equations (35)-(37), respectively:

$$\left(\frac{a_i}{\omega_p} \frac{\partial \omega_p}{\partial a_i} \right)_{\text{constrained}} = \frac{a_i}{\omega_p} \frac{\partial \omega_p}{\partial a_i} - a_i \sum_{i'=1}^6 \frac{a_{i'}}{\omega_p} \frac{\partial \omega_p}{\partial a_{i'}}, \quad (35)$$

$$\frac{a_{i'}}{\omega_p} \frac{\partial \omega_p}{\partial a_{i'}} \approx \frac{a_{i'}}{\omega_p} \frac{\langle C_{p,i}^+ \delta_{ii'} v_d \Sigma_{f,g} \psi_{p,g} \rangle}{\langle \frac{\psi_{p,g}^+ \psi_{p,g}}{v_g} \rangle + \langle C_{p,i}^+ C_{p,i} \rangle}, \quad (36)$$

$$\frac{\lambda_{i'}}{\omega_p} \frac{\partial \omega_p}{\partial \lambda_{i'}} \approx \frac{\lambda_{i'}}{\omega_p} \frac{\langle \psi_{p,g}^+ \frac{\chi_{i,g}}{4\pi} \delta_{ii'} C_{p,i} \rangle - \langle C_{p,i}^+ \delta_{ii'} C_{p,i} \rangle}{\langle \frac{\psi_{p,g}^+ \psi_{p,g}}{v_g} \rangle + \langle C_{p,i}^+ C_{p,i} \rangle}. \quad (37)$$

Note that the sensitivity coefficients to a_i satisfy the constrained condition in the same way as the fission spectrum [20], since the total sum of a_i is normalized to unity.

3. Numerical calculations

3.1. Calculation procedures

In order to verify SA of α using the first-order perturbation theory, we numerically solved one of the ICSBEP benchmark problems, HEU-SOL-THERM-012, which is a thermal system (98% of fissions caused by neutrons below 0.625eV) as reported in the reference [21]. The experimental core is a highly enriched uranium oxyfluoride solution (93.2 wt% ^{235}U) in a $\sim 27.9\text{cm}$ inner radius sphere with a 0.2cm aluminum spherical shell. The sphere was surrounded by an effectively infinite water reflector (15.0cm thickness). Because the experimental core can be modeled by the one-dimensional spherical geometry, the calculation time can be saved to obtain the reference sensitivity coefficient using the direct method. Thus, HEU-SOL-THERM-012 was used in this verification.

Firstly, SCALE6.2.2/TSUNAMI-1D [12] was utilized to prepare 252 energy-group microscopic cross-section data based on ENDF/B-VII.1 [22] and to carry out SA of k_{eff} . As a result of TSUNAMI-1D shown in Table 1, it was confirmed that implicit effects of k_{eff} -sensitivity coefficients, which is associated with changes in resonance-shielded multigroup cross sections [23, 24], are relatively small in the case of HEU-SOL-THERM-012. Thus, we approximately neglected the implicit effects in the evaluation of α -sensitivity coefficients. Using the PALEALE module for an AMPX master formatted binary file (ft42f001) which was produced through the TSUNAMI-1D run, the microscopic effective cross-section data for all nuclides were obtained. After that, using these microscopic effective cross-section data with their nuclide number densities, the 252 energy-group macroscopic cross-section data were prepared for the subsequent PARTISN calculation.

Secondary, conventional forward and adjoint k_{eff} -eigenvalue calculations were carried out by PARTISN. The spatial mesh sizes Δr were approximately 0.1 cm. The order of angular quadrature is S_{64} , and P_5 scattering cross-sections were considered. The numerical results of

PARTISN were follows: $k_{\text{eff}} = 0.99944$, effective delayed neutron fraction $\beta_{\text{eff}} = 725$ (pcm), neutron generation time $\Lambda = 80.73$ (μsec), and the prompt neutron decay constant based on the one-point approximation $\frac{\beta_{\text{eff}} - \rho}{\Lambda} = 96.76$ (1/sec), respectively. Note that β_{eff} and Λ were evaluated by an in-house tool using the forward and adjoint PARTISN k_{eff} -flux moment files (rmflux and amflux). In addition, SA of k_{eff} was also carried out using the in-house tool with these flux files, followed by uncertainty quantification (UQ) using the 252 group SCALE covariance library (scale.rev08.252groupcov7.1) [12]. The PARTISN result of k_{eff} -uncertainty was 0.8114 ($\% \delta k/k$), which is almost the same value as the TSUNAMI-1D result 0.8113 ($\% \delta k/k$), as shown in Table 1. Consequently, the basic numerical procedures for SA and UQ were verified.

<Table 1>

After verification of SA and UQ for k_{eff} , forward and adjoint ω_p -eigenvalue calculation was carried out by PARTISN with the alpha search mode to obtain the prompt neutron decay constant α . Convergence criteria for inner and outer iterations were 10^{-10} to reduce numerical errors as much as possible. Using the in-house tool with forward and adjoint PARTISN ω_p -flux moment files, SA of α to 252 group microscopic data was carried out on the basis of Equation (34). For comparison, sensitivity coefficients of α to a_i and λ_i were estimated only for ^{235}U by Equations (35)-(37), in order to check whether these sensitivity coefficients to a_i and λ_i are negligibly small.

Finally, in order to verify the PT-based sensitivity coefficients of α , the sensitivity coefficients of α were also estimated using the direct method to obtain their reference values. Namely, each of 252 group microscopic nuclear data was directly perturbed to estimate the

reference sensitivity coefficients $\left(\frac{\sigma}{\omega_p} \frac{\partial \omega_p}{\partial \sigma} \right)_{\text{ref}}$ using the second-order central difference:

$$\left(\frac{\sigma}{\omega_p} \frac{\partial \omega_p}{\partial \sigma}\right)_{\text{ref}} \approx \frac{1}{2h} \frac{\omega_{p,\sigma(1+h)} - \omega_{p,\sigma(1-h)}}{\omega_{p,\sigma}}, \quad (38)$$

where $h = \frac{\delta\sigma}{\sigma}$ is relative perturbation from the unperturbed nuclear data σ ; $\omega_{p,\sigma}$ is unperturbed ω_p -eigenvalue; $\omega_{p,\sigma(1\pm h)}$ is perturbed ω_p -eigenvalue due to perturbation of $\sigma(1 \pm h)$, respectively. It is noted that, if the sensitivity coefficient $\frac{\sigma}{\omega_p} \frac{\partial \omega_p}{\partial \sigma}$ and the relative perturbation h are too small, number of significant digits for the difference between $\omega_{p,\sigma(1+h)}$ and $\omega_{p,\sigma(1-h)}$ is not sufficient in the estimation by Equation (38). Thus, h in Equation (38) was empirically determined for each of nuclear data as follows:

$$h = \min\left(\frac{0.01}{\left(\frac{\sigma}{\omega_p} \frac{\partial \omega_p}{\partial \sigma}\right)_{\text{PT}}}, 0.25\right), \quad (39)$$

where $\left(\frac{\sigma}{\omega_p} \frac{\partial \omega_p}{\partial \sigma}\right)_{\text{PT}}$ is the relative sensitivity coefficient which is guessed by PT. Note that the

direct method requires a lot of computational times for S_N calculations, thus the reference sensitivity coefficients are estimated only for the following nuclear data:

^{235}U : fission cross-section $\sigma_{f,g}$, prompt fission spectrum $\chi_{p,g}$, (n,2n) cross-section $\sigma_{(n,2n),g}$;
 ^1H : (n, γ) cross-section $\sigma_{(n,\gamma),g}$, elastic scattering cross-section $\sigma_{\text{ela},g}$; and
neutron velocity v_g .

3.2. Results for relative sensitivity coefficients of α

Using the PARTISN code, the numerical result of prompt neutron decay constant was obtained as $\alpha = -\omega_p = 96.13$ (1/s), which is almost equal to the approximated value $\frac{\beta_{\text{eff}} - \rho}{\Lambda} = 96.76$ (1/s) in the case of critical benchmark problem such as HEU-SOL-THERM-012.

Figure 1 shows numerical results of relative sensitivity coefficients of α using the first-order perturbation theory using Equation (34) (denoted by ‘PT’) and the reference values

(denoted by ‘ref’). Note the positive sign of sensitivity coefficient correspond to an increase in the magnitude of prompt neutron decay constant α due to the positive perturbation of nuclear data $+\delta\sigma$, and vice versa. For example of the negative sensitivity coefficient, if thermal fission cross-section of ^{235}U slightly increases, the positive reactivity perturbation $+\delta\rho$ is added; thus α decreases towards zero because fission chain reaction lasts longer to result in smaller decay constant.

From Figure 1, it is verified that the numerical results obtained by PT agree well with reference values. As can be seen from Figure 1, it is confirmed that the magnitude of sensitivity coefficients of α to neutron velocity v_g is relatively small compared with those of dominant nuclide-reaction-pairs, e.g. $\sigma_{f,g}$ of ^{235}U and $\sigma_{(n,\gamma),g}$ of ^1H .

<Figure 1>

Figure 2 shows the approximated relative sensitivity coefficients of α to a_i and λ_i of ^{235}U using Equations (35)-(37). As compared with Figure 1, the magnitudes of these sensitivity coefficients to a_i and λ_i are the order of 0.002 (%/%) and comparable to that of $\sigma_{(n,2n),g}$ of ^{235}U . Consequently, it is confirmed that the relative sensitivity coefficients of α to a_i and λ_i are negligibly small.

<Figure 2>

3.3. Results for nuclear data-induced uncertainty of α

By utilizing the PT-based sensitivity coefficients with the 252 group SCALE covariance library (scale.rev08.252groupcov7.1), UQ of α was also carried out. Note that covariance data of $\chi_{p,g}$ is not contained in this covariance data. Thus, covariance data of total fission spectrum χ_g was utilized as an alternative covariance data for $\chi_{p,g}$, since χ_g is roughly equal to $\chi_{p,g}$.

Table 2 summarizes contributions to the nuclear data-induced α -uncertainty due to each covariance data among nuclide-reaction-pairs. In Table 2, ‘contribution to α -uncertainty’ is defined by the square root of the absolute value of nuclear data-induced covariance of α , and the negative sign of contribution corresponds to the anti-correlation due to the covariance of α . As can be seen from Tables 1 and 2, the dominant order of contributions to α -uncertainty is almost the same as that to k_{eff} -uncertainty.

The total uncertainty of α is 103.97 (% $\delta\alpha/\alpha$), which means that the absolute standard deviation due to nuclear covariance data is about 100 (1/s). This large uncertainty of α is reasonably explained by the uncertainty propagation with the one-point approximation of $\alpha \approx \frac{\beta_{\text{eff}} - \rho}{\Lambda}$. As discussed in our previous study [7], the magnitude of $\delta\alpha/\alpha$ is well approximated by:

$$\frac{\delta\alpha}{\alpha} \approx \frac{-\delta\rho}{\beta_{\text{eff}} - \rho} \approx \frac{1}{1 - k_{\text{eff}}(1 - \beta_{\text{eff}})} \frac{\delta k_{\text{eff}}}{k_{\text{eff}}}. \quad (40)$$

By substituting $\frac{\delta k_{\text{eff}}}{k_{\text{eff}}} = 0.8114$ (%), $k_{\text{eff}} = 0.99944$, and $\beta_{\text{eff}} = 725$ (pcm) into Equation (40), the value of $\frac{-\delta\rho}{\beta_{\text{eff}} - \rho}$ is evaluated as 103.94 (%) and is nearly equal to the numerical results of α -uncertainty $\delta\alpha/\alpha$ by PT. Consequently, it is confirmed that $\frac{-\delta\rho}{\beta_{\text{eff}} - \rho}$ is the major contribution to nuclear data-induced uncertainty of α . In other words, $\delta\alpha/\alpha$ is roughly equal to the absolute uncertainty of reactivity $\delta\rho$ in dollar units, 112 (\$), since $-\rho = 56$ (pcm) is smaller than β_{eff} in the case of critical benchmark problem.

Finally, using the PT-based relative sensitivity coefficients both for k_{eff} and α with the SCALE covariance library, the nuclear-data induced covariance between k_{eff} and α was evaluated as -84.33 ((% $\delta k/k$)(% $\delta\alpha/\alpha$)). Consequently, it is confirmed that the nuclear-data induced correlation between k_{eff} and α is strongly negative, $\frac{-84.33}{0.8114 \times 103.97} \approx -0.9996$. This fact implies that the numerical predictions of k_{eff} can be improved by the data assimilation technique using measurement value of prompt neutron decay constant α to reduce

the nuclear data-induced uncertainty and bias of k_{eff} . Above-mentioned discussion on the correlation between k_{eff} and α is essentially the same as that for subcritical systems ($0.90 < k_{\text{eff}} < 0.98$) reported in our previous study [7].

<Table 2>

4. Issues in the future study

Although the ω_p -eigenvalue calculation is practically applicable to the evaluation of prompt neutron decay constant α , the fast and stable numerical algorithm for rigorous ω -eigenvalue calculation based on transport theory is one of the interesting research subjects, e.g. verification by the direct method with the rigorous consideration of delayed neutron effect. Such an effective numerical algorithm for rigorous ω -eigenvalue calculation is also useful to evaluate the inverse reactor period [19].

For simplicity, we neglected the implicit effect on SA of α in this study. To more appropriately evaluate the sensitivity coefficient using PT of α in the deterministic codes, it is preferable to treat the implicit effect [23, 24]. To avoid such a cumbersome procedure, the research and development for SA of α using the continuous energy Monte Carlo code is desired. The generalized iterated fission probability method [25] may enable us to achieve SA of α using the Monte Carlo code.

In order to accomplish UQ of α and the evaluation of covariance between α and k_{eff} for the data assimilation using actual subcritical measurement data, further enhancement of minor covariance data is also necessary, e.g. covariance of $\chi_{p,g}$; and correlations between χ_g and $\chi_{p,g}$.

5. Conclusion

In this paper, the specific theoretical formulae for SA of prompt neutron decay constant α using PT was derived. Using the prompt approximation, the derived formula can be simplified without the term involving the delayed neutron precursor densities. By the aid of this approximation, the relative sensitivity coefficients of α to delayed neutron parameters (relative delayed neutron yield a_i and decay constant λ_i) can be roughly estimated without cumbersome calculation based on the more rigorous ω -eigenvalue equation, although these sensitivity coefficients are expected to be the negligibly small impact on the numerical prediction of α .

For verification of PT-based SA, relative sensitivity coefficients of α were evaluated for the one of the ICSBEP benchmark problems (HEU-SOL-THERM-012), using the S_N neutron transport code, PARTISN. As a result, it was verified that the relative sensitivity coefficients of α agree well with reference values by the direct method. Furthermore, nuclear data-induced UQ of α was also carried out using the SCALE covariance library. Thereby, the efficient numerical procedures for UQ of α were established. Namely, by the aid of PT, only two forward and adjoint ω_p -eigenvalue calculations are enough for UQ of α . The results of present study are useful to accomplish SA of α using the existing neutron transport code with the prompt approximation.

Future plans are the uncertainty quantification of α using PT for actual subcritical experiments, and the data assimilation technique using actual measurement values of α to reduce bias and uncertainty of predicted neutronics parameters.

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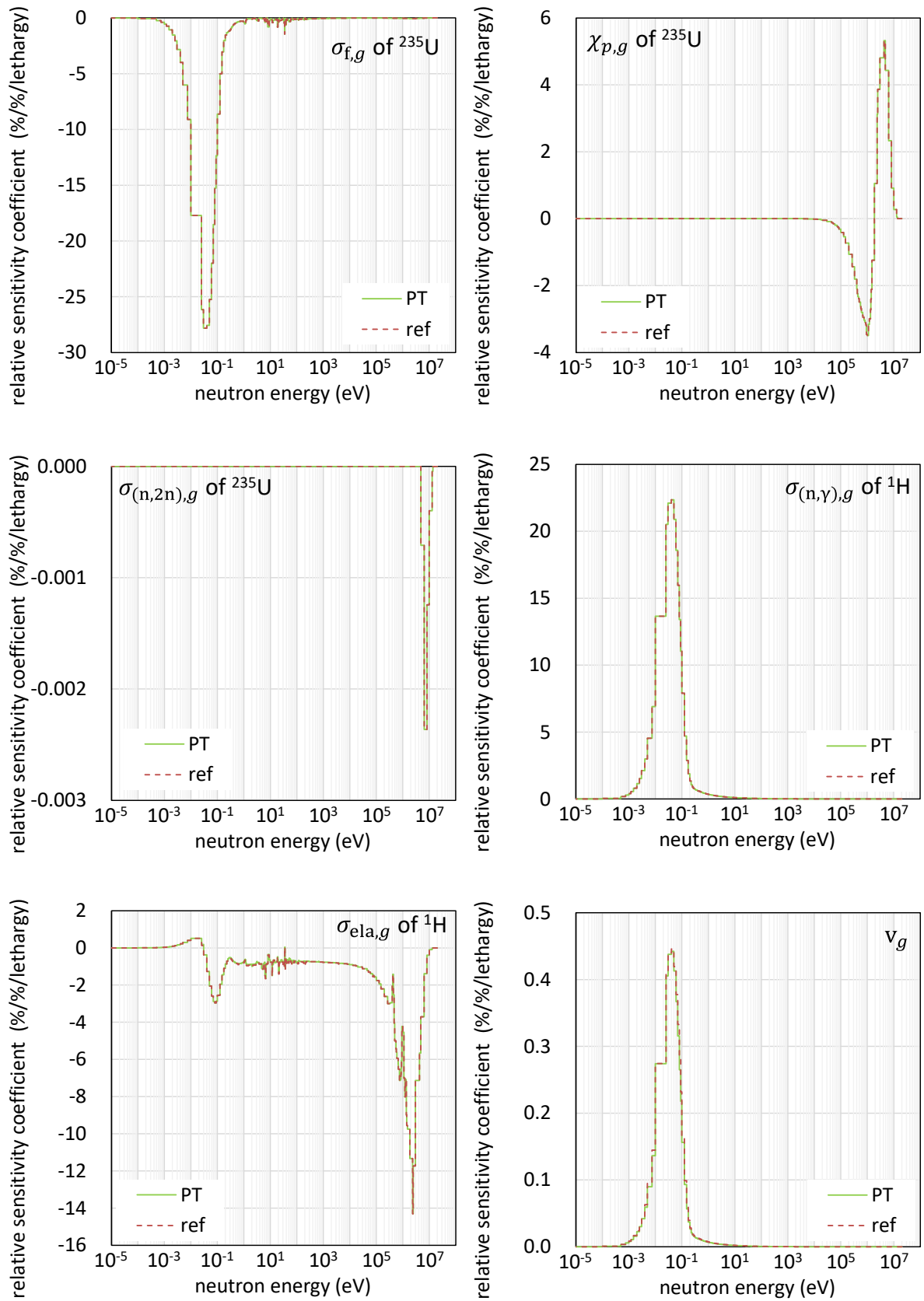


Figure 1. Comparison of relative sensitivity coefficients of α .

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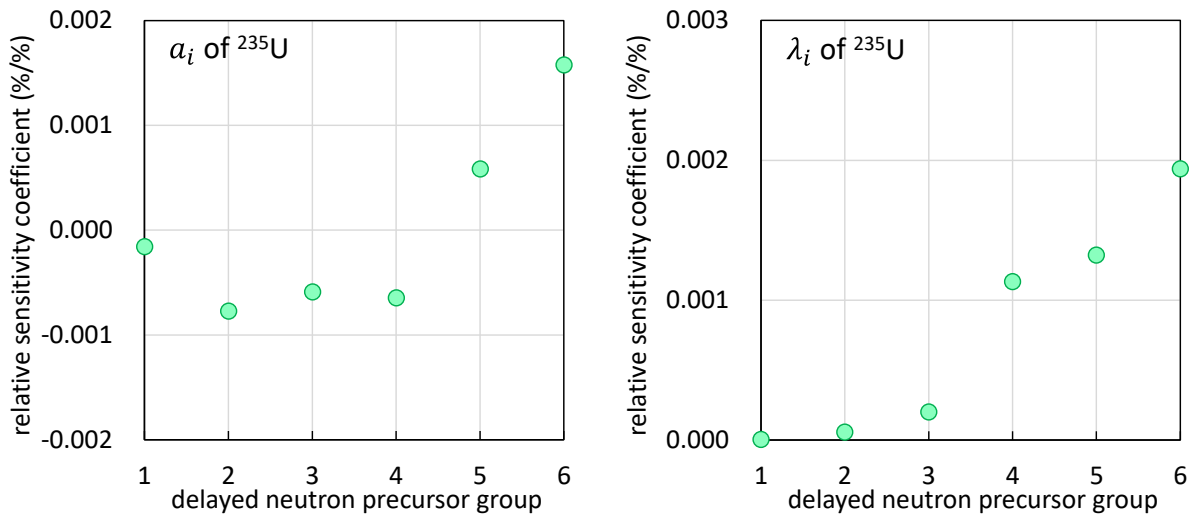


Figure 2. Relative sensitivity coefficients of α to delayed neutron parameters.

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Table 1. Comparison of nuclear-data-induced k_{eff} -uncertainty.

covariance matrix		contribution of uncertainty due to this matrix ($\% \delta k/k$) [†]		
nuclide-reaction	with nuclide-reaction	TSUNAMI-1D with implicit effect	TSUNAMI-1D without implicit effect [‡]	PARTISN
$^{235}\text{U}-\chi$	$^{235}\text{U}-\chi$	0.4920	0.4920	0.4921
$^1\text{H}-\sigma_{(n,\gamma)}$	$^1\text{H}-\sigma_{(n,\gamma)}$	0.4162	0.4162	0.4162
$^{235}\text{U}-\nu$	$^{235}\text{U}-\nu$	0.3835	0.3835	0.3835
$^{235}\text{U}-\sigma_f$	$^{235}\text{U}-\sigma_f$	0.1729	0.1730	0.1730
$^{235}\text{U}-\sigma_{(n,\gamma)}$	$^{235}\text{U}-\sigma_{(n,\gamma)}$	0.1392	0.1392	0.1392
$^{235}\text{U}-\sigma_f$	$^{235}\text{U}-\sigma_{(n,\gamma)}$	0.1384	0.1384	0.1384
$^1\text{H}-\sigma_{\text{ela}}$	$^1\text{H}-\sigma_{\text{ela}}$	0.1309	0.1306	0.1306
$^{16}\text{O}-\sigma_{\text{ela}}$	$^{16}\text{O}-\sigma_{\text{ela}}$	0.1011	0.1019	0.1019
$^{16}\text{O}-\sigma_{(n,n')}$	$^{16}\text{O}-\sigma_{(n,n')}$	0.0056	0.0056	0.0056
$^{27}\text{Al}-\sigma_{\text{ela}}$	$^{27}\text{Al}-\sigma_{\text{ela}}$	0.0038	0.0038	0.0038
$^{16}\text{O}-\sigma_{(n,\alpha)}$	$^{16}\text{O}-\sigma_{(n,\alpha)}$	0.0036	0.0036	0.0036
$^{16}\text{O}-\sigma_{\text{ela}}$	$^{16}\text{O}-\sigma_{(n,n')}$	-0.0027	-0.0027	-0.0027
$^{234}\text{U}-\sigma_{(n,\gamma)}$	$^{234}\text{U}-\sigma_{(n,\gamma)}$	0.0021	0.0021	0.0021
$^{16}\text{O}-\sigma_{(n,\gamma)}$	$^{16}\text{O}-\sigma_{(n,\gamma)}$	0.0019	0.0019	0.0019
$^{235}\text{U}-\sigma_{\text{ela}}$	$^{235}\text{U}-\sigma_f$	-0.0018	-0.0022	-0.0022
$^{27}\text{Al}-\sigma_{(n,n')}$	$^{27}\text{Al}-\sigma_{(n,n')}$	0.0015	0.0015	0.0015
$^{27}\text{Al}-\sigma_{(n,\gamma)}$	$^{27}\text{Al}-\sigma_{(n,\gamma)}$	0.0015	0.0015	0.0015
$^{235}\text{U}-\sigma_{\text{ela}}$	$^{235}\text{U}-\sigma_{(n,\gamma)}$	0.0013	0.0016	0.0016
$^{235}\text{U}-\sigma_{(n,n')}$	$^{235}\text{U}-\sigma_{(n,n')}$	0.0008	0.0008	0.0008
$^{238}\text{U}-\sigma_{(n,\gamma)}$	$^{238}\text{U}-\sigma_{(n,\gamma)}$	0.0007	0.0007	0.0007
$^{19}\text{F}-\sigma_{(n,n')}$	$^{19}\text{F}-\sigma_{(n,n')}$	0.0007	0.0007	0.0007
Total		0.8113	0.8113	0.8114

[†] See page 6-142 in the SCALE6.2.2 manual [12]

[‡] These results were obtained by TSUNAMI-1D with the 'PARM=CENTRM' option

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Table 2. Summary of contributions to the nuclear data-induced α -uncertainty.

covariance matrix		contribution of uncertainty
nuclide-reaction	with nuclide-reaction	due to this matrix ($\% \delta\alpha/\alpha$)
$^{235}\text{U}-\chi_p$	$^{235}\text{U}-\chi_p$	62.72
$^1\text{H}-\sigma_{(n,\gamma)}$	$^1\text{H}-\sigma_{(n,\gamma)}$	53.65
$^{235}\text{U}-\nu_p$	$^{235}\text{U}-\nu_p$	49.28
$^{235}\text{U}-\sigma_f$	$^{235}\text{U}-\sigma_f$	21.94
$^{235}\text{U}-\sigma_{(n,\gamma)}$	$^{235}\text{U}-\sigma_{(n,\gamma)}$	17.93
$^{235}\text{U}-\sigma_f$	$^{235}\text{U}-\sigma_{(n,\gamma)}$	17.69
$^1\text{H}-\sigma_{\text{ela}}$	$^1\text{H}-\sigma_{\text{ela}}$	16.76
$^{16}\text{O}-\sigma_{\text{ela}}$	$^{16}\text{O}-\sigma_{\text{ela}}$	13.06
$^{16}\text{O}-\sigma_{(n,n')}$	$^{16}\text{O}-\sigma_{(n,n')}$	0.72
$^{27}\text{Al}-\sigma_{\text{ela}}$	$^{27}\text{Al}-\sigma_{\text{ela}}$	0.49
$^{16}\text{O}-\sigma_{(n,\alpha)}$	$^{16}\text{O}-\sigma_{(n,\alpha)}$	0.47
$^{16}\text{O}-\sigma_{\text{ela}}$	$^{16}\text{O}-\sigma_{(n,n')}$	-0.35
$^{235}\text{U}-\sigma_{\text{ela}}$	$^{235}\text{U}-\sigma_f$	-0.27
$^{234}\text{U}-\sigma_{(n,\gamma)}$	$^{234}\text{U}-\sigma_{(n,\gamma)}$	0.27
$^{16}\text{O}-\sigma_{(n,\gamma)}$	$^{16}\text{O}-\sigma_{(n,\gamma)}$	0.24
$^{235}\text{U}-\sigma_{\text{ela}}$	$^{235}\text{U}-\sigma_{(n,\gamma)}$	0.20
$^{27}\text{Al}-\sigma_{(n,\gamma)}$	$^{27}\text{Al}-\sigma_{(n,\gamma)}$	0.20
$^{27}\text{Al}-\sigma_{(n,n')}$	$^{27}\text{Al}-\sigma_{(n,n')}$	0.19
$^{235}\text{U}-\sigma_{(n,n')}$	$^{235}\text{U}-\sigma_{(n,n')}$	0.10
$^{238}\text{U}-\sigma_{(n,\gamma)}$	$^{238}\text{U}-\sigma_{(n,\gamma)}$	0.09
$^{19}\text{F}-\sigma_{(n,n')}$	$^{19}\text{F}-\sigma_{(n,n')}$	0.09
Total		103.97

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