

Monte Carlo calculation method for reactor period utilizing differential operator
sampling technique

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Abstract

The inverse reactor period (α) is a fundamental mode eigenvalue of the α -mode nonlinear Boltzmann eigenvalue equation that considers delayed neutron contributions. Thus far, several Monte Carlo methods, including α - k , weight balancing, and transition rate matrix methods, have been developed to calculate α . This study presents a new Monte Carlo method for predicting α by using the derivatives of the k -eigenvalue with respect to α . Formulae are derived to calculate the first and second derivatives using the differential operator sampling method. The key feature of the new proposed method is its ability to estimate the uncertainty of the predicted α by considering the uncertainty of the k -eigenvalue and its derivatives with respect to α .

Keywords: Monte Carlo; reactor period; differential operator sampling; delayed neutron

I. INTRODUCTION

The reactor analysis is typically validated by comparing the calculation results for a physical observable with the corresponding measurement results. The reactor period is one of the measured values used to validate the reactor analysis. The measurable inverse reactor period α is a relatively small value that ranges approximately between -0.0124 s^{-1} and 0.2 s^{-1} . The lower limit is the inverse lifetime of ^{87}Br and the upper limit corresponds to the inverse reactor period that triggers the scram signal.¹ The inverse reactor period α is an eigenvalue of the system of the linear equations that are composed of the neutron Boltzmann transport equation and delayed neutron precursor concentration equations. However, the inverse reactor period α is customarily obtained by solving the nonlinear Boltzmann transport equation that considers delayed neutron contributions.² The Monte Carlo method for solving this equation requires significant computational resources to obtain a small value of α with high reliability.

Several Monte Carlo techniques have been developed to calculate α by solving the α -mode Boltzmann transport equation.³ One such method is the “weight-balancing” method, originally proposed by Nauchi et al.^{4,5}, which was revisited by Josey and Brown.⁶ Another method commonly used is the method typically known as the α - k (or k - α) method.² The third method used for calculating α is the transition rate matrix method (TRMM).⁷⁻¹⁰ TRMM, similar to the fission matrix method for k -eigenvalues, is another approach utilized in calculating α .¹¹ The fission matrix method requires a spatial discretization, whereas TRMM for α -eigenvalues requires a discretization of space, direction, and energy, thereby entailing a significant memory footprint for less biased results. This study proposes a new approach to calculate the inverse reactor period α .

In the α - k method, α is iteratively searched during the course of the power iteration such that the k -eigenvalue of the nonlinear neutron transport equation becomes equal to unity. On the other hand, the new approach proposed in this study finds α that makes k -eigenvalue equal to unity using the derivative of k with respect to α .

This paper is organized as follows. In Sec. II, the fundamental theory of the α -mode Boltzmann transport equation and conventional Monte Carlo algorithms for calculating α are revisited. In Sec. III, a new Monte Carlo algorithm using the differential operator sampling (DOS) method is presented. In Sec. IV, the numerical results with the proposed method are

presented and compared with the α - k method, and the concluding remarks are presented in Sec. V.

II. CONVENTIONAL MONTE CARLO ALGORITHMS FOR REACTOR PERIOD

The α -mode eigenvalue equation to be solved for calculating an inverse reactor period α is^{2a}

$$\frac{\alpha}{v} \phi_\alpha(\mathbf{r}, \mathbf{v}) + \mathbf{L} \phi_\alpha(\mathbf{r}, \mathbf{v}) = \frac{1}{k(\alpha)} \left(\mathbf{F}_p \phi_\alpha(\mathbf{r}, \mathbf{v}) + \sum_i \frac{\lambda_i}{\lambda_i + \alpha} \mathbf{F}_{d,i} \phi_\alpha(\mathbf{r}, \mathbf{v}) \right), \quad (1)$$

where $\mathbf{v}$ is the velocity vector of neutron, $\mathbf{r}$ is the position vector, λ_i is the decay constant of the precursor family i , and $\phi_\alpha(\mathbf{r}, \mathbf{v})$ is the fundamental mode eigenfunction of the following equation:

$$\mathbf{L} \phi_\alpha(\mathbf{r}, \mathbf{v}) = \boldsymbol{\Omega} \cdot \nabla \phi_\alpha(\mathbf{r}, \mathbf{v}) + \Sigma_t \phi_\alpha(\mathbf{r}, \mathbf{v}) - \int \Sigma_s(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) \phi_\alpha(\mathbf{r}, \mathbf{v}') d\mathbf{v}', \quad (2)$$

$$\mathbf{F}_p \phi_\alpha(\mathbf{r}, \mathbf{v}) = \chi_p(\mathbf{r}, v) \int v_p(v') \Sigma_f(\mathbf{r}, v') \phi_\alpha(\mathbf{r}, v') dv', \quad (3)$$

$$\mathbf{F}_{d,i} \phi_\alpha(\mathbf{r}, \mathbf{v}) = \chi_{d,i}(\mathbf{r}, v) \int v_{d,i}(v') \Sigma_f(\mathbf{r}, v') \phi_\alpha(\mathbf{r}, v') dv', \quad (4)$$

where $\boldsymbol{\Omega}$ is the angular direction vector, Σ_t is the total cross section, Σ_s is the scattering cross section, v is the scalar velocity of neutron, $k(\alpha)$ is the eigenvalue^b, χ_p is the fission spectrum of prompt neutrons, and $\chi_{d,i}$ is the fission spectrum of delayed neutrons from the precursor family i . v_p and $v_{d,i}$ are the average number of prompt and delayed neutrons of the precursor family i per fission, respectively. Throughout this study, it is assumed that the parameters $\chi_{d,i}$, $v_{d,i}$, and λ_i are not isotope dependent and are represented for a single isotope. Eqs. (1)–(4) can be rewritten as follows:

$$\frac{\alpha}{v} \phi_\alpha(\mathbf{r}, \mathbf{v}) + \mathbf{L} \phi_\alpha(\mathbf{r}, \mathbf{v}) = \frac{1}{k(\alpha)} \chi_\alpha(\mathbf{r}, v) \int v_\alpha(v') \Sigma_f(\mathbf{r}, v') \phi_\alpha(\mathbf{r}, v') dv', \quad (5)$$

^a If α in this equation is equal to the inverse reactor period of the system, $k(\alpha)$ is exactly equal to unity. Thus, $k(\alpha)$ does not appear explicitly in the regular α -mode eigenvalue equation.

^b This is a fictitious eigenvalue that is introduced to iteratively search for the true inverse reactor period α .

where

$$v_\alpha(v) = v_p(v) + \sum_i \frac{v_{d,i}(v)\lambda_i}{\lambda_i + \alpha}, \quad (6)$$

$$\chi_\alpha(\mathbf{r}, v) = \chi_p(\mathbf{r}, v) \frac{f_p}{f_\alpha} + \sum_i \chi_{d,i}(\mathbf{r}, v) \frac{f_{d,i}}{f_\alpha} \frac{\lambda_i}{\lambda_i + \alpha}, \quad (7)$$

where

$$f_p = \int v_p(v') \Sigma_f(\mathbf{r}, v') \phi_\alpha(\mathbf{r}, v') d\mathbf{v}', \quad (8)$$

$$f_{d,i} = \int v_{d,i}(v') \Sigma_f(\mathbf{r}, v') \phi_\alpha(\mathbf{r}, v') d\mathbf{v}', \quad (9)$$

$$f_\alpha = \int v_\alpha(v') \Sigma_f(\mathbf{r}, v') \phi_\alpha(\mathbf{r}, v') d\mathbf{v}'. \quad (10)$$

$\chi_\alpha(\mathbf{r}, v)$ in Eq. (7) can be approximated with high accuracy owing to $v_p \gg \sum_i v_{d,i}$ as follows:

$$\chi_\alpha(\mathbf{r}, v) \approx \chi_p(\mathbf{r}, v) \left(1 - \sum_i \frac{\beta_i \lambda_i}{\lambda_i + \alpha} \right) + \sum_i \chi_{d,i}(\mathbf{r}, v) \frac{\beta_i \lambda_i}{\lambda_i + \alpha}, \quad (11)$$

where β_i is the delayed neutron fraction of the precursor family i . This approximation is useful for simplifying the formulae of the differential operator sampling method presented in the next section. This approximation is not strictly required. However, without this approximation, the derivative of the fission spectrum with respect to α becomes excessively involved, particularly beyond the second derivative.

$k(\alpha)$ is equal to unity when α is equal to the true inverse reactor period of the multiplying system. Several Monte Carlo algorithms have been proposed to determine the value of α , which corresponds to the inverse reactor period where $k(\alpha)$ equals unity. One method is the “weight-balancing” method proposed by Nauchi et al.^{4,5} This method calculates each term in Eq. (1) during the course of the power iteration, yielding a polynomial of α of 7 or 9 degree for 6 or 8 delayed neutron precursor families, respectively. At the end of each power iteration, the inverse reactor period is obtained by determining the maximum root of the polynomial. As described in Ref. 5, the weight-balancing method entails larger statistical uncertainty compared to other methods, such as the α - k method.

The α - k method solves Eq. (1) in the same manner as the k -eigenvalue problem. At the beginning of each cycle, the α value to be used for that cycle is established. α/v in the first term on the left-hand side of Eq. (1) is treated as an additional total cross section in the algorithm

of Ref. 2. In another method used in Refs. 10, 12–14, this term is addressed by continuously adjusting the particle weight as it traverses the distance s :

$$w' = w \cdot \exp\left(-\frac{\alpha}{v}s\right), \quad (12)$$

where w and w' are the particle weights before and after the flight distance s , respectively. At the end of the cycle, $k(\alpha)$ is calculated in the same manner as the k -eigenvalue. For example, when using the collision estimator, $k(\alpha)$ is obtained as follows:

$$k(\alpha) = \frac{1}{N} \sum_k v_\alpha(v_k) \frac{\Sigma_{f,k}}{\Sigma_{t,k}} w_k, \quad (13)$$

where k denotes the k th collision and the summation is performed for all collisions within the cycle. N is the number of fission sources per cycle. $v_\alpha(v_k)$ is the effective v value for a neutron with velocity v_k :

$$v_\alpha(v_k) = v(v_k) \left((1 - \beta) + \sum_i \frac{\beta_i \lambda_i}{\lambda_i + \alpha} \right), \quad (14)$$

where β_i is the delayed neutron fraction of the precursor family i , $\beta = \sum_i \beta_i$, $v(v_k)$ is the number of fission neutrons (delayed plus prompt neutrons). The number of fission neutrons n at a fission source site used for the next cycle calculation is determined at each collision site as follows:

$$n = \left\lfloor v_\alpha(v_k) \frac{\Sigma_{f,k}}{\Sigma_{t,k}} w_k + \xi \right\rfloor, \quad (15)$$

where ξ is a uniform pseudorandom number in the range (0,1). In the next cycle, fission neutrons are emitted from the fission source site determined in the previous cycle. The neutron spectrum is determined according to the effective fission neutron spectrum $\chi_\alpha(\mathbf{r}, v)$ in Eq. (11).

The α value used for the next cycle is adjusted so that $k(\alpha)$ approaches unity as discussed in Ref. 2,

$$\alpha_{m+1} = \alpha_m k(\alpha_m), \quad (16)$$

where m denotes the number of cycles. The active cycle starts when $|k(\alpha_m) - 1|$ decreases

below a desired criterion. The power iteration should be repeated until $|\overline{k(\alpha_m)} - 1| \pm \sigma$ falls within a desired range, where $\overline{k(\alpha_m)}$ and σ are the arithmetic mean and standard deviation of $k(\alpha_m)$ during the active cycles, respectively. The final result of the reactor period $\overline{\alpha_m}$ is simply given by the arithmetic mean of α_m during the active cycles.

Although the standard deviation of $\overline{\alpha_m}$ is also calculated using α_m in each cycle, it is underestimated owing to the intercycle correlation of α_m . α_m determined using Eq. (16) inherits the deviation in the previous cycle. As previously stated, the range of α value treated in this study is approximately between $-\min\{\lambda_i\}$ (-0.0124 s^{-1}) and 0.2 s^{-1} . Thus, the inverse reactor period is a significantly small value compared with the prompt neutron decay constant α_p in a subcritical system, signifying that the relative statistical uncertainty of α is larger. The confidence interval of $\overline{\alpha_m}$ is equally important as the mean value $\overline{\alpha_m}$ itself. Therefore, a robust technique for reliably estimating the statistical uncertainty of α should be developed.

III. NEW MONTE CARLO ALGORITHM WITH DOS METHOD

III.A. Estimation of Reactor Period and its Uncertainty

A different algorithm for determining the inverse period α that makes $k(\alpha)$ equal to unity is presented in this section. It is assumed that $k(\alpha)$ has already been computed for $\alpha = \alpha_0$ and, that the value of $k(\alpha_0)$ is close to unity. The method for estimating a reasonable α_0 is discussed in Sec. IV. $\Delta k(\Delta\alpha)$ is the change of $k(\alpha)$ caused by $\Delta\alpha$, a small change of α from α_0 . It is expressed by the Taylor series expansion as follows:

$$\Delta k(\Delta\alpha) \approx k_{\alpha}^{(1)} \Delta\alpha + \frac{1}{2!} k_{\alpha}^{(2)} (\Delta\alpha)^2 + \dots, \quad (17)$$

where

$$k_{\alpha}^{(1)} = \left. \frac{\partial k(\alpha)}{\partial \alpha} \right|_{\alpha=\alpha_0}, \quad (18)$$

$$k_{\alpha}^{(2)} = \left. \frac{\partial^2 k(\alpha)}{\partial \alpha^2} \right|_{\alpha=\alpha_0}. \quad (19)$$

If $\Delta k(\Delta\alpha)$ is approximated with sufficient accuracy up to the second-order term, $\Delta\alpha$ that makes $k(\alpha)$ equal to unity (i.e., $\Delta k(\Delta\alpha) = k(\alpha_0) - 1$) is predicted by the root of the quadratic equation as follows:

$$\Delta\alpha = \frac{-k_{\alpha}^{(1)} - \sqrt{\left(k_{\alpha}^{(1)}\right)^2 - 2k_{\alpha}^{(2)}(k(\alpha_0) - 1)}}{k_{\alpha}^{(2)}}. \quad (20)$$

Using $\Delta\alpha$ in Eq. (20), the inverse period that makes $k(\alpha)$ equal to unity is estimated as follows:

$$\alpha' = \alpha_0 + \Delta\alpha. \quad (21)$$

If the second-order accuracy is deemed unsatisfactory, it is possible to extend this method to achieve accuracy higher than the second order. The uncertainty of $\Delta\alpha$ in Eq. (20) is dominated by $(k(\alpha_0) - 1)$, as discussed in the next section. The standard deviation of $\Delta\alpha$ caused by the uncertainty of $k(\alpha_0)$ is given by the error propagation rule for Eq. (20):

$$\sigma(\Delta\alpha) = \frac{\sigma(k(\alpha_0))}{\sqrt{\left(k_{\alpha}^{(1)}\right)^2 - 2k_{\alpha}^{(2)}(k(\alpha_0) - 1)}}, \quad (22)$$

where $\sigma(x)$ is the standard deviation of x .

The standard deviation $\sigma(k(\alpha_0))$ is calculated by ordinary statistical processing using $k(\alpha_0)$ values in the active cycles. However, the standard deviation from ordinary statistical processing (denoted as “apparent” standard deviation) is underestimated relative to its “real” value owing to the intercycle correlation of k -eigenvalue. The “real” standard deviation should be used for $\sigma(k(\alpha_0))$ in Eq. (22). Several methods have been proposed to estimate the real standard deviation.^{15–17} However, this is beyond the scope of the present study. In the numerical examples shown below, the “apparent” standard deviation is tentatively used for estimating $\sigma(\Delta\alpha)$ in Eq. (22).

III.B. First and Second Derivatives of $k(\alpha)$

The first and second derivatives of $k(\alpha)$ with respect to α are obtained using the DOS method.^{18–23} The factors that are influenced by α include fission spectrum, transport kernel, and the number of fission neutrons. In the DOS method, the derivatives of these factors with respect to α are scored during the random walk process. Below, we present the calculation of the derivatives using the DOS method.

III.B.1. Fission Spectrum

At the beginning of a particle history, when it is emitted from the fission source, the neutron

energy is determined according to the effective fission spectrum $\chi_\alpha(\mathbf{r}, \mathbf{v})$ defined by Eq. (11). The first and second derivatives of $k(\alpha)$ with respect to α due to the change of $\chi_\alpha(\mathbf{r}, \mathbf{v})$ are, respectively, given as follows:

$$P_\chi^{(1)} = \frac{1}{\chi_\alpha(\mathbf{r}, \mathbf{v})} \frac{d\chi_\alpha(\mathbf{r}, \mathbf{v})}{d\alpha} = \frac{1}{\chi_\alpha(\mathbf{r}, \mathbf{v})} \left(\chi_p(\mathbf{r}, \mathbf{v}) \sum_i \frac{\beta_i \lambda_i}{(\lambda_i + \alpha)^2} - \sum_i \chi_{d,i}(\mathbf{r}, \mathbf{v}) \frac{\beta_i \lambda_i}{(\lambda_i + \alpha)^2} \right), \quad (23)$$

$$P_\chi^{(2)} = \frac{dP_\chi^{(1)}}{d\alpha} = \frac{1}{\chi_\alpha(\mathbf{r}, \mathbf{v})} \chi_\alpha^{(2)}(\mathbf{r}, \mathbf{v}) - \left(P_\chi^{(1)} \right)^2, \quad (24)$$

where

$$\chi_\alpha^{(2)}(\mathbf{r}, \mathbf{v}) = \frac{d^2 \chi_\alpha(\mathbf{r}, \mathbf{v})}{d\alpha^2} = -2\chi_p(\mathbf{r}, \mathbf{v}) \sum_i \frac{\beta_i \lambda_i}{(\lambda_i + \alpha)^3} + 2 \sum_i \chi_{d,i}(\mathbf{r}, \mathbf{v}) \frac{\beta_i \lambda_i}{(\lambda_i + \alpha)^3}. \quad (25)$$

$P_\chi^{(1)}$ and $P_\chi^{(2)}$, which are the weighting coefficients for DOS, are assigned to the particle from the beginning of the history until the particle history is terminated.

III.B.2. Transport Kernel

The DOS method estimates the differential coefficients with respect to α each time a particle moves along a flight path or collides. The transport kernel for a particle that flies a distance s is given by²⁴:

$$T(s) = \Sigma_t \cdot \exp(-\Sigma_t s) \exp\left(-\frac{\alpha}{v} s\right). \quad (26)$$

As the particle weight changes continuously, as defined by Eq. (12), the last factor $\exp(\alpha s/v)$ is multiplied in Eq. (26). The first-order weighting coefficient of the kernel $T(s)$ for the j th flight path with respect to α is

$$P_{T,j}^{(1)} = \frac{1}{T(s)} \cdot \frac{\partial T(s)}{\partial \alpha} = -\frac{s_j}{v_j}. \quad (27)$$

$P_{T,j}^{(1)}$ is accumulated successively for each flight until the end of the particle history. The second-order weighting coefficient of the transport kernel is 0. For the range of α in this study, $P_{T,j}^{(1)}$ is negligibly small compared to other weighting coefficients, which is discussed in Sec.

IV.

III.B.3. Number of Fission Neutrons

When the particle undergoes the k th collision of the particle history at a point where fission reaction can occur, the change of the number of fission neutrons $\nu_\alpha(\mathbf{v})$ with respect to α is

taken into account. The first- and second-order weighting coefficients of $v_\alpha(v)$ are calculated at every collision point as follows:

$$P_{v,k}^{(1)} = \frac{1}{v_\alpha(v)} \frac{dv_\alpha(v)}{d\alpha} = -\frac{v(v)}{v_\alpha(v)} \sum_i \frac{\beta_i \lambda_i}{(\lambda_i + \alpha)^2}, \quad (28)$$

$$P_{v,k}^{(2)} = \frac{dP_{v,k}^{(1)}}{d\alpha} = \frac{1}{v_\alpha(v)} v_\alpha^{(2)}(v) - \left(P_{v,k}^{(1)}\right)^2, \quad (29)$$

where

$$v_\alpha^{(2)}(v) = \frac{d^2 v_\alpha(v)}{d\alpha^2} = 2v(v) \sum_i \frac{\beta_i \lambda_i}{(\lambda_i + \alpha)^3}. \quad (30)$$

III.B.4. First and Second derivatives of $k(\alpha)$

At the end of the m th particle history, the first and second derivatives of $k(\alpha)$ with respect to α are, respectively, calculated as follows:

$$k_{\alpha,m}^{(1)} = \frac{dk(\alpha)}{d\alpha} = \sum_k v_\alpha(v_k) \frac{\Sigma_{f,k}}{\Sigma_{t,k}} w_k W_{(1),k}, \quad (31)$$

$$k_{\alpha,m}^{(2)} = \frac{d^2 k(\alpha)}{d\alpha^2} = \sum_k v_\alpha(v_k) \frac{\Sigma_{f,k}}{\Sigma_{t,k}} w_k W_{(2),k}, \quad (32)$$

where k denotes the k th collision within the m th history, w_k is the particle weight at the k th collision, and summation is performed for every collision until the end of the m th history. $W_{(1),k}$ and $W_{(2),k}$ are, respectively, the weighting coefficients of the first and second derivatives of $k(\alpha)$ at the k th collision. They are calculated as follows:

$$W_{(1),k} = P_\chi^{(1)} + P_{v,k}^{(1)} - \sum_j \frac{s_j}{v_j}, \quad (33)$$

$$W_{(2),k} = P_\chi^{(2)} + P_{v,k}^{(2)}, \quad (34)$$

where $\sum_j s_j/v_j$ in Eq. (33) is the sum of s/v in the j th flight path up to the k th collision. When a particle history is terminated by Russian roulette or escapes from the external boundary, a new particle is emitted from the fission source. This procedure is repeated until the fission sources in the cycle are exhausted. $k_\alpha^{(1)}$ and $k_\alpha^{(2)}$ of a cycle are, respectively, obtained as follows:

$$k_\alpha^{(1)} = \frac{1}{M} \sum_{m=1}^M k_{\alpha,m}^{(1)}, \quad (35)$$

$$k_{\alpha}^{(2)} = \frac{1}{M} \sum_{m=1}^M k_{\alpha,m}^{(2)}, \quad (36)$$

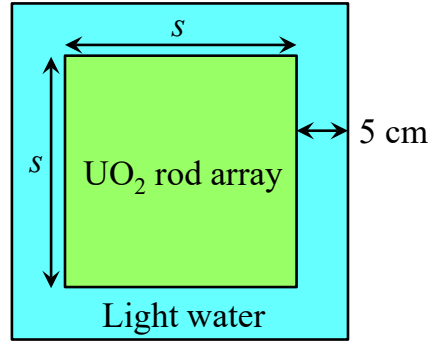
where M denotes the number of fission sources in the cycle. The final results of $k_{\alpha}^{(1)}$ and $k_{\alpha}^{(2)}$ are obtained by averaging them over the active cycles after discarding the inactive cycles before convergence.

A change in α induces perturbations in the fission source distribution. The source perturbation effect is not considered in Eqs. (35) and (36). Consideration of the source perturbation effect is indispensable for correctly estimating the derivatives. A method for implementing the source perturbation effect in the DOS method is presented in Refs. 21, 25–28. The method for the source perturbation effect was adopted in this study. Owing to the complexity of the source perturbation effect, this is not presented herein even though the method for the source perturbation effect was indeed utilized in this study. Readers can refer to Refs. 21, 25, 26 for details on this subject.

IV. NUMERICAL TESTS

IV.A. Overview of Test Problems

This section presents numerical tests used in the proposed method for inverse reactor period calculations. The geometry of the test problems was composed of a two-dimensional homogenized UO₂ fuel rod array surrounded by a light-water reflector with a thickness of 5 cm, as shown in Fig. 1. The calculations were performed using three energy group constants. The group constants and kinetic parameters were prepared using the standard reactor analysis code (SRAC).²⁹ Tables I and II list the group constants for the homogenized fuel rod array and light water, respectively. The scattering was assumed to be isotropic. Tables III and IV present the spectra of the prompt and delayed neutrons and their kinetic parameters, respectively. The nuclear data used for SRAC were based on the nuclear data library JENDL-4.³⁰ The side length s of the fuel rod array in Fig. 1 was varied to adjust the reactor period; $s = 22.872, 22.982, 23.008, 23.050, \text{ and } 23.164 \text{ cm}$.



$$s = 22.872 \sim 23.164 \text{ cm}$$

Fig. 1 Geometry of test problem (not to scale).

Table I Three group constants of UO₂ rod array

	1st group	2nd group	3rd group
$\Sigma_t \text{ (cm}^{-1}\text{)}$	0.298289	0.833341	1.63895
$\Sigma_c \text{ (cm}^{-1}\text{)}$	3.74414×10^{-4}	9.77075×10^{-3}	0.0301365
$\Sigma_f \text{ (cm}^{-1}\text{)}$	3.01089×10^{-3}	2.12425×10^{-3}	0.0560435
ν	2.438	2.438	2.438
χ_p	0.878198	0.121802	0.0
$\Sigma_{sg \rightarrow g} \text{ (cm}^{-1}\text{)}$	0.221061	0.777643	1.55277
$\Sigma_{sg \rightarrow g+1} \text{ (cm}^{-1}\text{)}$	0.0738427	0.043803	0.0

Table II Three group constants of light water

	1st group	2nd group	3rd group
$\Sigma_t \text{ (cm}^{-1}\text{)}$	0.332073	1.12647	2.78124
$\Sigma_c \text{ (cm}^{-1}\text{)}$	3.0500×10^{-4}	3.6990×10^{-4}	0.018250
$\Sigma_{sg \rightarrow g} \text{ (cm}^{-1}\text{)}$	0.227126	1.02814	2.76278
$\Sigma_{sg \rightarrow g+1} \text{ (cm}^{-1}\text{)}$	0.104642	0.0979597	0.0

Table III Neutron velocity and prompt and delayed neutron spectra

	1st group	2nd group	3rd group
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$v(cm/s)$	1.66743×10^9	1.73734×10^7	2.78124×10^5
χ_p	0.878198	0.121802	0.0
$\chi_{d,1}$	0.302845	0.697155	0.0
$\chi_{d,2}$	0.390439	0.609561	0.0
$\chi_{d,3}$	0.374032	0.625968	0.0
$\chi_{d,4}$	0.457453	0.542547	0.0
$\chi_{d,5}$	0.396728	0.603272	0.0
$\chi_{d,6}$	0.411100	0.588900	0.0

Table IV Delayed neutron fractions and decay constants

Family	β_i	$\lambda_i(s^{-1})$
1	2.158803×10^{-4}	1.2485124×10^{-2}
2	1.466645×10^{-3}	3.0661454×10^{-2}
3	1.359992×10^{-3}	1.139355×10^{-1}
4	2.771604×10^{-3}	3.074786×10^{-1}
5	9.151014×10^{-4}	1.188787
6	3.247986×10^{-4}	3.176650

In Table V, the approximate effective fission spectrum χ_α defined in Eq. (11) for $\alpha = 0.16782 \text{ s}^{-1}$ was compared with the exact spectrum defined in Eq. (7). The approximate and exact effective fission spectra show agreement up to five decimal places, and the fission spectrum defined in Eq. (11) accurately approximates the exact spectrum.

Table V Exact and approximate effective fission spectrum χ_α for $\alpha = 0.16782 \text{ s}^{-1}$

	Approximate (Eq. (11))	Exact (Eq. (7))
1st group	0.876517	0.876511
2nd group	0.123483	0.123489

IV.B. Validation of DOS

The first and second derivatives calculated with the DOS method were validated by comparison with a deterministic method using the discrete ordinates transport code

DANTSYS.³¹ The deterministic calculations were performed for $s = 23.164$ cm, with the constants shown in Tables I–IV and S_n order 16. Using the deterministic method, $k(\alpha)$'s were calculated for several α values around 0.16782 s^{-1} . $k(\alpha)$ vs. α was plotted and fitted using a cubic polynomial function, as illustrated in Fig. 2. The first, second, and third derivatives of $k(\alpha)$ at $\alpha = 0.16782 \text{ s}^{-1}$ were obtained using the cubic polynomial function.

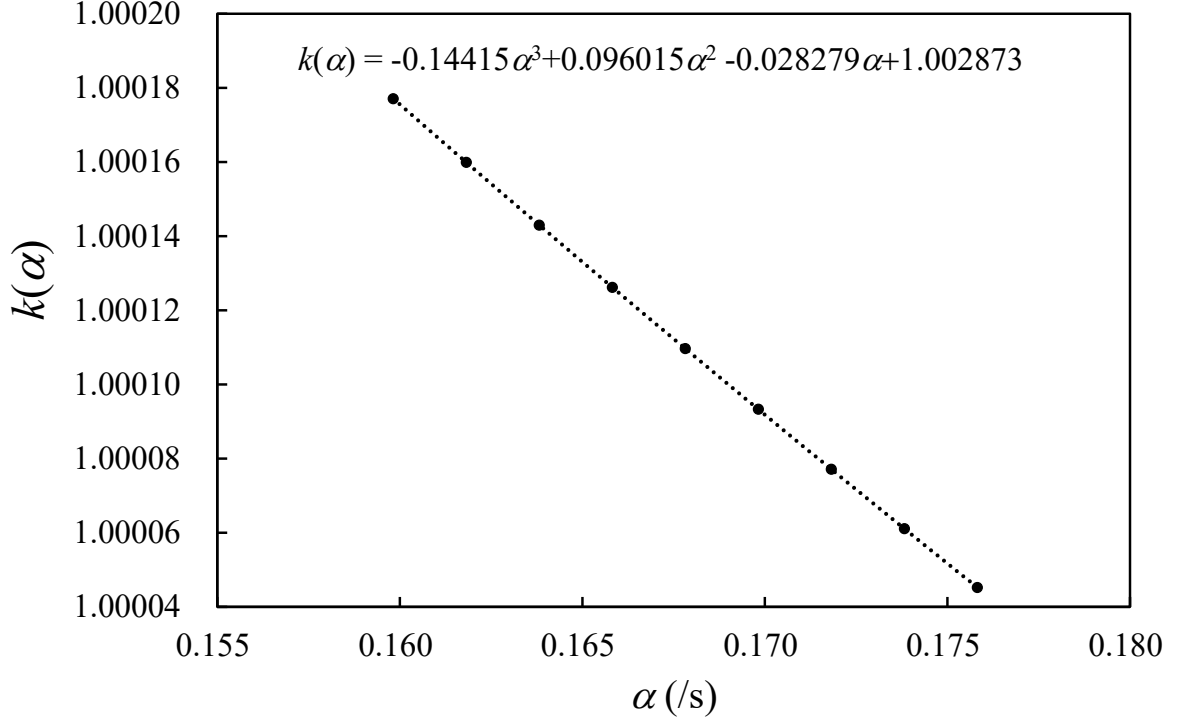


Fig. 2 $k(\alpha)$ vs. α using deterministic method and fitted function.

Monte Carlo calculations were performed for $\alpha = 0.16782 \text{ s}^{-1}$ with 250,000 particles per cycle, 200,000 active, and 30 inactive cycles, which provided $k(\alpha)$, $k^{(1)}(\alpha)$, and $k^{(2)}(\alpha)$. In this study, the number of iterations for the fission source perturbation was 10. The first and second derivatives of the deterministic and DOS methods are listed in Table VI. The results obtained from the DOS method concur with those obtained from the deterministic method, thereby confirming the validity of the DOS method for calculating the derivatives of $k(\alpha)$.

Table VI First, second, and third derivatives of $k(\alpha)$ at $\alpha = 0.16782 \text{ s}^{-1}$

	DOS	Deterministic
$k^{(1)}(\alpha)$	-0.008267 $(0.000002)^*$	-0.008232
$k^{(2)}(\alpha)$	0.04655	0.04688

	(0.00012)	
$k^{(3)}(\alpha)$	—	-0.8649

*Values in parentheses represent one standard deviation of mean value.

The Monte Carlo result of $k(\alpha)$ is 1.0000351 ± 0.0000028 for $\alpha = 0.16782 \text{ s}^{-1}$. $\Delta\alpha$ that makes $k(\alpha)$ equal to unity, which is predicted by Eq. (20), is $\sim 0.0043 \text{ s}^{-1}$. The first, second, and third-order terms of the Taylor expansion of $\Delta k(\alpha)$ caused by $\Delta\alpha = 0.0043 \text{ s}^{-1}$ are -3.54 , 0.0434 , and -0.00115 pcm , respectively. Thus, the second-order approximation is accurate if $\Delta k(\alpha)$ is sufficiently small. In this example, the relative uncertainty of $(k(\alpha_0) - 1)$ in Eq. (22) (i.e., $\sigma(k(\alpha_0) - 1)/(k(\alpha_0) - 1)$) is ~ 0.1 , which is significantly larger than the relative uncertainties of $k^{(1)}(\alpha)$ and $k^{(2)}(\alpha)$. Neglecting the uncertainties of $k^{(1)}(\alpha)$ and $k^{(2)}(\alpha)$ is justified when the uncertainty of $\Delta\alpha$ is estimated using Eq. (22). It is sufficient to consider only the uncertainty of $(k(\alpha_0) - 1)$ in Eq. (22).

As stated in Sec. III.B.2, the contribution of the transport kernel was significantly less than 1% of the first derivative of $k(\alpha)$.

IV.C. Examples of Inverse Reactor Period Calculation with Inhour Equation

The inverse reactor periods were calculated using the proposed method for the reactor shown in Fig. 1. First, $k(0)$ was calculated by setting $\alpha = 0$ in Eq. (1). The Monte Carlo calculation was performed using 250,000 particles per cycle, 60,000 active cycles, and 30 inactive cycles. The reactivity of the reactor ρ is given by $1 - 1/k(0)$. Then, the inverse reactor period α that corresponds to the reactivity ρ was obtained from the root-finding method for the inhour equation:

$$\rho = 1 - \frac{1}{k(0)} = \frac{\alpha l}{\alpha l + 1} + \frac{1}{\alpha l + 1} \sum_{i=1}^6 \frac{\alpha \beta_{eff,i}}{\alpha + \lambda_i}, \quad (37)$$

where l is the neutron life time, $\beta_{eff,i}$ is the effective delayed neutron fraction of family i . l and $\beta_{eff,i}$ were calculated with the deterministic code DANTSYS. This inverse reactor period is a rough estimate for comparison with the other methods. The reactivity and inverse reactor period α obtained from the inhour equation are listed in Table VII.

Table VII Reactivity and inverse reactor period α with inhour equation

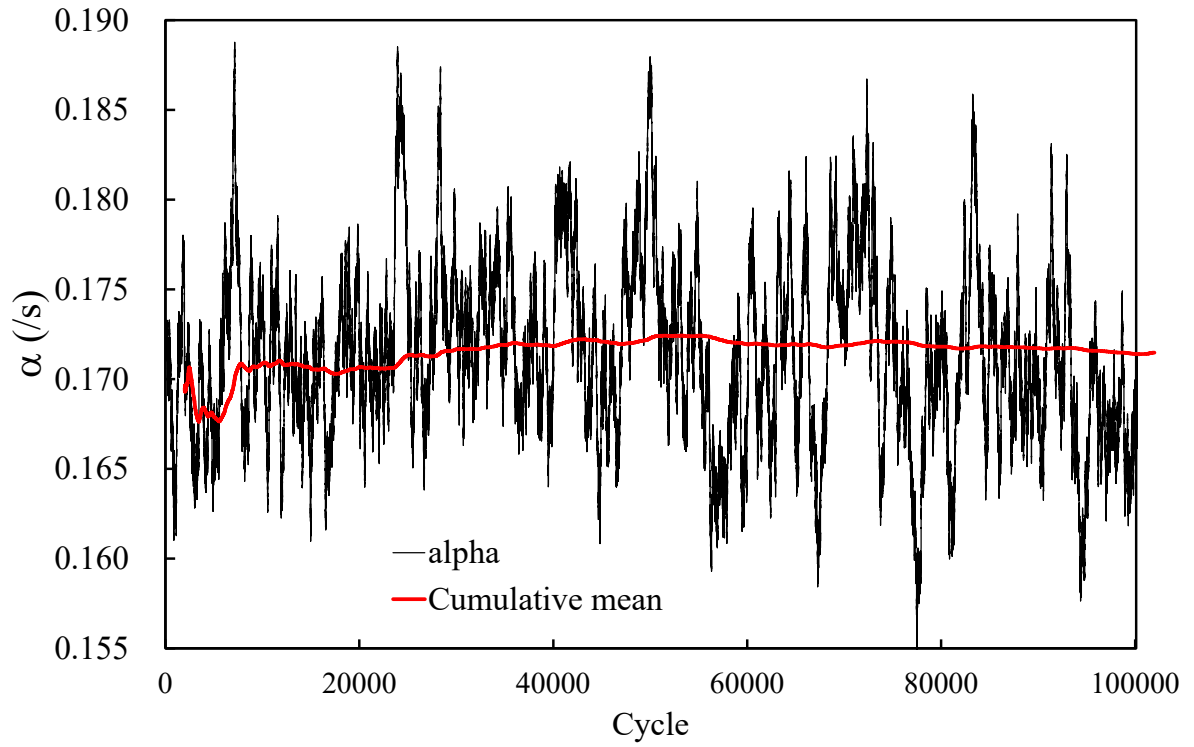
Case	Side length s (cm)	$k(0)$	ρ (pcm)	α (s^{-1})
1	23.164	1.0036715 (0.0000052)*	365.8 (0.5)	0.17348 (0.00065)
2	23.050	1.0017690 (0.0000063)	176.6 (0.6)	0.03769 (0.00023)
3	23.008	1.0010709 (0.0000059)	107.0 (0.6)	0.01721 (0.00014)
4	22.982	1.0006308 (0.0000055)	63.0 (0.5)	0.00854 (0.00009)
5	22.872	0.9987786 (0.0000058)	-122.3 (0.6)	-0.00818 (0.00007)

*Values in parentheses represent one standard deviation of mean value.

IV.D. α - k Method

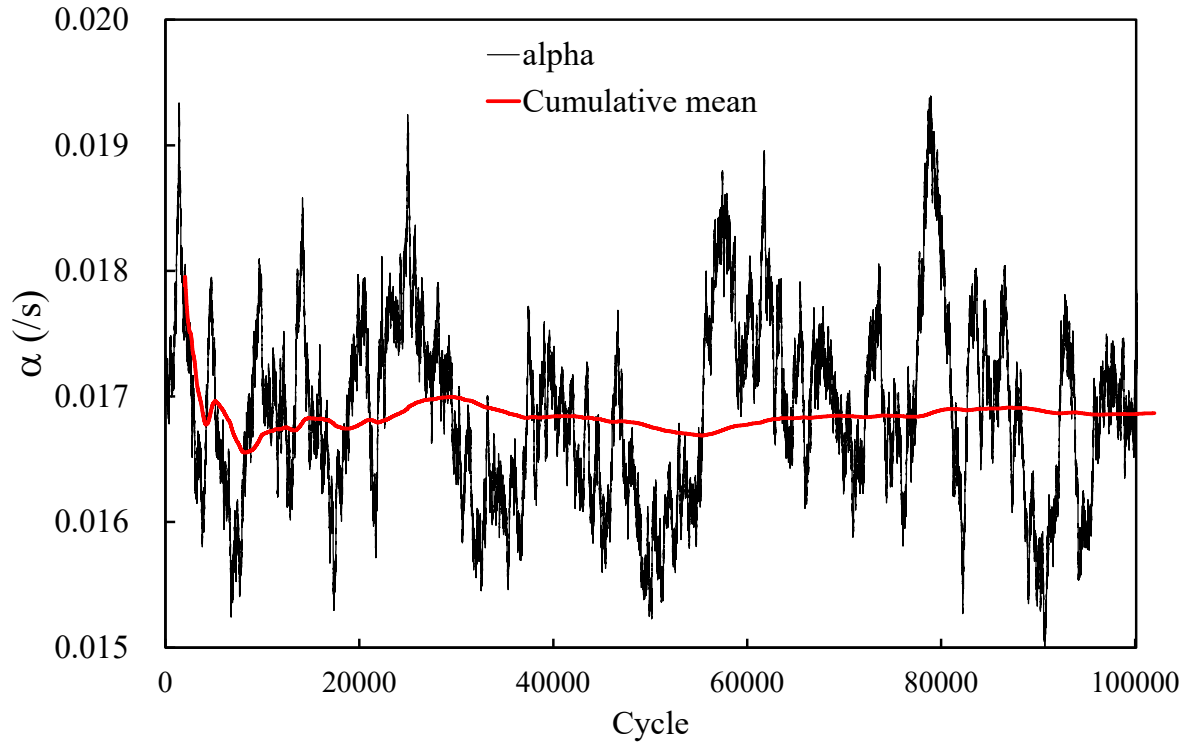
To compare the proposed method with conventional α search methods, calculations were performed using the α - k method. The Monte Carlo calculations were performed using 200,000 particles per cycle, 100,000 active cycles, and 2,000 inactive cycles. In the α - k method, an α value that deviates from the true α value continues to have a lasting impact on subsequent cycles. Therefore, to set an initial α value for active cycles as close to the true value as possible, a larger number of inactive cycles were employed. The plots of α and the cumulative mean of α vs. the cycle are shown in Figs. 3 and 4 for $s = 23.164$ and 23.008 cm, respectively. The mean values and standard deviations of α and $k(\alpha)$ for the five cases are presented in Table VIII.

1



2

3 Fig. 3 α - k method for Case 1 ($s = 23.164$ cm) (black: α of each cycle, red: cumulative
4 mean of α).



5

6 Fig. 4 α - k method for Case 3 ($s = 23.008$ cm) (black: α of each cycle, red: cumulative
7 mean of α).

8

Table VIII Mean values and standard deviations of α and $k(\alpha)$ with the α - k method

Case	Side length s (cm)	$\overline{k(\alpha)}$	$\bar{\alpha}$ (s^{-1})
1	23.164	1.0000013 (0.0000045)*	0.171472 (0.000016)
2	23.050	1.0000006 (0.0000028)	0.0373454 (0.0000042)
3	23.008	0.9999996 (0.0000023)	0.0168680 (0.0000023)
4	22.982	1.0000020 (0.0000028)	0.0085971 (0.0000012)
5	22.872	0.9999989 (0.0000024)	-0.0081627 (0.0000006)

*Values in parentheses represent one standard deviation of mean value.

The inverse reactor period by the α - k method mostly agrees with the inhour equation in Table VII and the proposed method shown later. $\overline{k(\alpha)}$ converges to unity within one standard deviation. Moreover, one standard deviation of $\bar{\alpha}$ appears considerably underestimated, which may be caused by the intercycle correlation. Thus, one standard deviations of $\bar{\alpha}$ in Table VIII are questionable to be used as the confidence interval.

IV.E. New Proposed Method

In the first step of the new proposed method, an initial inverse reactor period α_0 is chosen. The initial inverse reactor period should be determined such that $|k(\alpha_0) - 1|$ is a reasonable value. If $|k(\alpha_0) - 1|$ is significantly large, the prediction of $\Delta\alpha$ calculated with Eq. (20) is less accurate. In this study, $|k(\alpha_0) - 1|$ was set to a few pcm. For $|k(\alpha_0) - 1|$ to be statistically significant, $\sigma(k(\alpha_0))$ needs to be less than a fraction of pcm.

The new proposed method was performed according to the following steps.

- (1) α_0 was determined using the root-finding method for the inhour equation Eq. (37) such that $|k(\alpha_0) - 1|$ is a few pcm.
- (2) Using α_0 determined in step (1), Monte Carlo calculation was performed to obtain $k(\alpha_0)$, and first and second derivatives of $k(\alpha_0)$ by solving Eq. (1). The power iteration was continued until $|k(\alpha_0) - 1|$ was less than a fraction of pcm.
- (3) Using Eqs. (20) and (21), the inverse reactor period α_0 was updated to α' . Using Eq. (22),

$\sigma(\alpha')$ was obtained.

(4) Using α' obtained in step (3), $k(\alpha')$ was calculated to confirm whether $k(\alpha')$ sufficiently converged to unity. The purpose of this step was to validate the new method, which was not necessarily mandatory.

As in Sec. IV.B, Monte Carlo calculations were performed using 250,000 particles per cycle, 200,000 active cycles, and 30 inactive cycles. The calculation results for the five cases are summarized in Table IX. $|k(\alpha') - 1|$ calculated with the predicted inverse reactor period α' is approximately one tenth of pcm and is less than one standard deviation. Thus, the inverse reactor period α' is considered to provide reasonable predictions using the proposed method.

The inverse reactor periods obtained using the three methods (inhour equation, α - k method, and proposed method) are shown for comparison in Table X. The inverse reactor periods from the three methods concur with each other, except for Case 3. The result of the α - k method in Case 3 may be biased, exemplifying the weakness of the α - k method. This calculation of the α - k method should have been continued further to reach the reasonable result. One standard deviations of the α - k method are significantly smaller than those of the proposed method, despite requiring less particle histories. The underestimated uncertainty of the α - k method is caused by the intercycle correlation.

Table IX Results of proposed method for reactor period calculation

Case	1	2	3	4	5
$\alpha_0(s^{-1})$	0.16782	0.03579	0.01610	0.00798	-0.00805
$ k(\alpha_0) - 1 $ (pcm)	3.51 (0.28)	4.23 (0.27)	4.65 (0.28)	3.51 (0.28)	2.86 (0.24)
$k^{(1)}(\alpha_0)$	-0.008267 (0.000002)*	-0.02848 (0.00001)	-0.04549 (0.00001)	-0.06108 (0.00002)	-0.27158 (0.00009)
$k^{(2)}(\alpha_0)$	0.04655 (0.00012)	0.5271 (0.0017)	1.4055 (0.0045)	2.6080 (0.0034)	76.46 (0.17)
$\alpha'(s^{-1})$	0.17212 (0.00035)	0.03729 (0.00010)	0.01714 (0.00006)	0.00856 (0.00005)	-0.00815 (0.00001)
$ k(\alpha') - 1 $ (pcm)	0.177 (0.245)	0.060 (0.420)	0.040 (0.284)	0.200 (0.284)	0.109 (0.245)

*Values in parentheses represent one standard deviation of mean value.

Table X Comparison of inverse periods by the three methods

Case	$\alpha'(s^{-1})$		
	Inhour equation	α - k method	Present method
1	0.17348 (0.00065)*	0.17147 (0.00002)	0.17212 (0.00035)
2	0.03769 (0.00023)	0.037345 (0.000004)	0.03729 (0.00010)
3	0.01721 (0.00014)	0.016868 (0.000002)	0.01714 (0.00006)
4	0.00854 (0.00009)	0.008597 (0.000001)	0.00856 (0.00005)
5	-0.00818 (0.00007)	-0.008163 (0.000001)	-0.00815 (0.00001)

*Values in parentheses represent one standard deviation of mean value.

V. CONCLUSIONS

This study proposes a new approach of the Monte Carlo method for calculating an inverse reactor period α that can be measured in a reactor experiment. As the inverse reactor period α is a small value compared to the prompt neutron decay constants in subcritical multiplying systems, a unique technique is required to accurately calculate the inverse reactor period using the Monte Carlo method. In this study, α that makes $k(\alpha)$ equal to unity is obtained using the derivative of $k(\alpha)$ with respect to α . The DOS method is used to calculate the first and second derivatives. The formulae for the first and second derivatives used in the DOS algorithm are derived in this study. The derivative of $k(\alpha)$ up to the second-order approximation is accurate if the initial prediction of α is chosen in such a way that $|k(\alpha) - 1|$ is less than a few pcm. The key feature of the present method is that the uncertainty of α can be fairly derived from the derivatives and the uncertainty of $|k(\alpha) - 1|$. The standard deviation of $k(\alpha)$ should be much less than $|k(\alpha) - 1|$, preferably less than a fraction of pcm.

If $k(\alpha)$ is obtained using a commonly employed statistical processing method, it is known that the uncertainty of $|k(\alpha) - 1|$ can be underestimated owing to the intercycle correlation of the fission source distribution. In order to estimate the real standard deviation of $k(\alpha)$, several techniques that have been developed can be applied to the present method to estimate the uncertainty of α .

The DOS method up to the second-order accuracy is already implemented in a general-purpose continuous-energy Monte Carlo code MVP.³² Modifications to the code for the method proposed in this study can be relatively easily achievable.

Disclosure statement

The authors report there are no competing interests to declare.

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