

Estimation of Time-Dependent Kinetics Parameters by Monte Carlo Transient Simulation

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1. Introduction

The estimation of kinetics parameters is essential for establishing the point kinetics model in reactor transient analysis. In the exact form of the point kinetics equation (PKE) [1], the kinetics parameters are functions of time defined as a ratio of integrals of the time-dependent Boltzmann transport equation over space, energy, and angle. To obtain the exact kinetics parameters, however, the time-dependent shape function and adequate adjoint function are required. Therefore, the practical PKE and kinetics parameters have been used with approximations of shape function and adjoint function as the fundamental-mode solutions of the steady-state transport equation and its corresponding adjoint equation.

With the development of efficient and high fidelity methodologies [2-4] on the time-dependent Monte Carlo (MC) simulation, the time behavior of neutron can be obtained within a practical time range. As for the adjoint calculation, Shim [5] developed efficient MC algorithms to estimate adjoint function in the MC fixed source mode calculations, which are applicable to the MC transient simulation as well. The capability of generating the time-dependent shape function and corresponding adjoint function enables the estimation of kinetics parameters in the time-dependent MC simulation, especially in the transient cases.

The purpose of this paper is to develop efficient algorithms for the estimation of the time-dependent kinetics parameters by MC transient simulation. A modified adjoint calculation algorithm is implemented to McCARD [6] transient analysis module [7] and verified in infinite homogeneous two-group problems with both steady-state and transient conditions.

2. Methodology

2.1. Physical meaning of the adjoint in transient calculation

Starting from the adjoint equation of the outgoing collision density, the Neumann series solution of the adjoint function with arbitrary detector cross section is derived by Shim [5] as

$$\Phi_{\text{det}}^{\dagger} = \sum_{j=0}^{\infty} \Phi_{\text{det},j}^{\dagger} \quad (1)$$

where $\Phi_{\text{det},j}^{\dagger}$ is the adjoint response from the j -th collision. In terms of the kernel, it can be written as

$$\begin{aligned} \Phi_{\text{det},j}^{\dagger} &= (\mathbf{K}^{\dagger})^j \hat{\Sigma}_{\text{det}} \\ &= \int d\mathbf{r}' \int d\mathbf{r}_j \int dE_j \int d\Omega_j \frac{\Sigma_{\text{det}}(\mathbf{r}', E_j, t)}{\Sigma_t(\mathbf{r}', E_j, t)} \tilde{T}(\mathbf{r}_j \rightarrow \mathbf{r}' | E_j, \Omega_j, t) \\ &\quad \cdot \int d\mathbf{r}_{j-1} \int dE_{j-1} \int d\Omega_{j-1} C(E_{j-1}, \Omega_{j-1} | \mathbf{r}_j, t) \tilde{T}(\mathbf{r}_{j-1} \rightarrow \mathbf{r}_j | E_{j-1}, \Omega_{j-1}, t) \\ &\quad \cdots \int d\mathbf{r}_1 \int dE_1 \int d\Omega_1 C(E_1, \Omega_1 | \mathbf{r}_2, t) \tilde{T}(\mathbf{r}_1 \rightarrow \mathbf{r}_2 | E_1, \Omega_1, t) \\ &\quad \cdot C(E, \Omega \rightarrow E_1, \Omega_1 | \mathbf{r}_1, t) \tilde{T}(\mathbf{r} \rightarrow \mathbf{r}_1 | E, \Omega, t) \end{aligned} \quad (2)$$

where the \mathbf{K}^{\dagger} and $\hat{\Sigma}_{\text{det}}$ are the adjoint transport kernel and detector response term defined as equations below.

$$\mathbf{K}^{\dagger} = \int d\mathbf{r}' \int dE' \int d\Omega' \tilde{T}(\mathbf{r} \rightarrow \mathbf{r}' | E, \Omega, t) C(E, \Omega \rightarrow E', \Omega' | \mathbf{r}', t) \quad (3)$$

$$\hat{\Sigma}_{\text{det}} \equiv \int d\mathbf{r}' \tilde{T}(\mathbf{r} \rightarrow \mathbf{r}' | E, \Omega, t) \frac{\Sigma_{\text{det}}(\mathbf{r}', E, t)}{\Sigma_t(\mathbf{r}', E, t)} \quad (4)$$

$$\begin{aligned} T(\mathbf{r} \rightarrow \mathbf{r}' | E, \Omega, t) &= \frac{\Sigma_t(\mathbf{r}', E, t')}{|\mathbf{r}' - \mathbf{r}|^2} \\ &\quad \exp \left[- \int_0^{|\mathbf{r}' - \mathbf{r}|} \Sigma_t \left(\mathbf{r}' - s \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|}, E, t' - \frac{s}{v} \right) ds \right] \delta \left(\Omega \cdot \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|} - 1 \right) \end{aligned} \quad (5)$$

$$\begin{aligned} C(E, \Omega \rightarrow E', \Omega' | \mathbf{r}', t) &= \frac{\Sigma_s(E, \Omega \rightarrow E', \Omega' | \mathbf{r}', t')}{\Sigma_t(\mathbf{r}', E, t')} \\ &\quad + \frac{\nu(\mathbf{r}', E, t') \Sigma_f(\mathbf{r}', E, t')}{\Sigma_t(\mathbf{r}', E, t')} \frac{\chi(\mathbf{r}', E', t')}{4\pi} \end{aligned} \quad (6)$$

$$\begin{aligned} \tilde{T}(\mathbf{r} \rightarrow \mathbf{r}' | E, \Omega, t) &\equiv \frac{\Sigma_t(\mathbf{r}', E, t)}{|\mathbf{r}' - \mathbf{r}|^2} \\ &\quad \exp \left[- \int_0^{|\mathbf{r}' - \mathbf{r}|} \Sigma_t \left(\mathbf{r}' - s \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|}, E, t \right) ds \right] \delta \left(\Omega \cdot \frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|} - 1 \right) \end{aligned} \quad (7)$$

In the above equations, T and C represent the conventional free flight kernel and collision kernel with time-variable terms added. Since the expected importance or adjoint response of a neutron depends on the fixed phase space $(\mathbf{r}, E, \Omega, t)$ when the neutron is introduced, the free flight kernel in the adjoint transport kernel is redefined as equation (7) with fixed time t . The time-dependent cross sections are defined as

$$\Sigma_r(\mathbf{r}, E, t) = \sum_l N^l(\mathbf{r}, t) \sigma_r^l(\mathbf{r}, E) \quad (8)$$

$$\Sigma_s(E', \Omega' \rightarrow E, \Omega | \mathbf{r}, t) = \sum_l N^l(\mathbf{r}, t) \sigma_s^l(E', \Omega' \rightarrow E, \Omega | \mathbf{r}) \quad (9)$$

$$\nu(\mathbf{r}, E, t) = \frac{\sum_l \nu^l(\mathbf{r}, E) N^l(\mathbf{r}, t) \sigma_f^l(\mathbf{r}, E)}{\sum_l N^l(\mathbf{r}, t) \sigma_f^l(\mathbf{r}, E)} \quad (10)$$

$$\begin{aligned} \chi(\mathbf{r}, E, t) &= \frac{\sum_l \chi'_l(\mathbf{r}, E) \int dE' \int d\Omega' v^l(\mathbf{r}, E') N^l(\mathbf{r}, t) \sigma_f^l(\mathbf{r}, E') \Phi(\mathbf{r}, E', \Omega', t)}{\sum_l \int dE' \int d\Omega' v^l(\mathbf{r}, E') N^l(\mathbf{r}, t) \sigma_f^l(\mathbf{r}, E') \Phi(\mathbf{r}, E', \Omega', t)} \end{aligned} \quad (11)$$

where subscript r and l denote reaction type and isotope index. From equation (1) and (2), the adjoint response, $\Phi_{\text{det}}^\dagger(\mathbf{r}, E, \Omega, t)$, can be interpreted as the sum of expected detector signals induced by a neutron at phase space $(\mathbf{r}, E, \Omega, t)$.

2.2. MC algorithm for the estimation of kinetics parameters in transient simulation

From the exact forms of PKE, the adjoint weighted kinetics parameters, $\beta(t)$ and $\Lambda(t)$, are expressed as

$$\beta(t) \equiv \sum_i \beta_i(t) = \sum_i \frac{\langle \Phi_{\text{det}}^\dagger, \mathbf{F}_{di} \psi \rangle}{\langle \Phi_{\text{det}}^\dagger, \mathbf{F} \psi \rangle} \quad (12)$$

$$\Lambda(t) \equiv \frac{\langle \Phi_{\text{det}}^\dagger, \psi / v \rangle}{\langle \Phi_{\text{det}}^\dagger, \mathbf{F} \psi \rangle} \quad (13)$$

where ψ is the time-dependent shape function and the bracket $\langle \rangle$ means the inner product of the components over (\mathbf{r}, E, Ω) . The Neumann series solution of the collision density equation gives the fission operator term in the bracket as

$$\begin{aligned} \langle \mathbf{F} \psi \rangle &= \sum_{j=0}^{\infty} \int d\mathbf{r} \int dE \int d\Omega \int d\mathbf{r}_j \frac{v(\mathbf{r}, E, t) \Sigma_f(\mathbf{r}, E, t)}{\Sigma_t(\mathbf{r}, E, t)} T(\mathbf{r}_j \rightarrow \mathbf{r} | E, \Omega, t) \\ &\cdot \int d\mathbf{r}_{j-1} \int dE_{j-1} \int d\Omega_{j-1} C(E_{j-1}, \Omega_{j-1} | \mathbf{r}_j, t_j) T(\mathbf{r}_{j-1} \rightarrow \mathbf{r}_j | E_{j-1}, \Omega_{j-1}, t_j) \\ &\cdots \int d\mathbf{r}_1 \int dE_1 \int d\Omega_1 C(E_1, \Omega_1 | \mathbf{r}_2, t_2) T(\mathbf{r}_1 \rightarrow \mathbf{r}_2 | E_1, \Omega_1, t_2) \\ &\cdot C(E', \Omega' \rightarrow E_1, \Omega_1 | \mathbf{r}_1, t_1) T(\mathbf{r}' \rightarrow \mathbf{r}_1 | E', \Omega', t') s_t(\mathbf{r}', E', \Omega', t') \end{aligned} \quad (14)$$

where s_t denotes the time source density in transient simulation which consists of the survival neutron source from the previous time step and the delayed neutron source. By combining the Neumann series solutions of the collision density equation with that of the adjoint response, equation (1), the time-dependent kinetics parameters can be calculated.

Without any approximations, this can be exactly done by producing additional particles at each fission event and simulating them to obtain the adjoint response tally. However, this so-called Contribution method [8] is quite burdensome which may take hundreds of times depending on the system, especially if applied to the transient cases. So we utilize a more efficient MC algorithm developed by Shim [5] with an assumption to apply it for transient simulation. We assume the effect of system changes for the adjoint response within each time step is considerably small that the adjoint response obtained by fixing the system to the starting time of each time step would be accurate enough. Although this method costs extra particles for the estimation of kinetics parameters, this can be done as the fixed source mode calculation without making additional particles during a transient simulation. Then the adjoint weighted terms in equation (12) and (13) at each time step are calculated as

$$\langle \Phi_{\text{det}}^\dagger, \mathbf{F} \psi \rangle \cong \frac{1}{N} \sum_{n=1}^N \sum_{n'} \sum_{j \in D_{fa}^{(n, n')}} J^{(n, n')} w_{j+1}^{(n, n')} \left(\frac{1}{w_{j+1}^{(n, n')}} \sum_{\substack{j'=j+1 \\ j' \notin \{D_c^{(n, n')}\} | n'' < n'}}^{J_L^{(n, n')} j} \left(w_{j'}^{(n, n')} \frac{\Sigma_{\text{det}}^{(n, n')} j'}{\Sigma_t^{(n, n')} j'} \right) \right) \quad (15)$$

$$= \frac{1}{N} \sum_{n=1}^N \sum_{n'} \sum_{\substack{j=1 \\ j \notin \{D_c^{(n, n')}\} | n'' < n'}} \left(m_{f, L}^{(n, n')} w_j^{(n, n')} \frac{\Sigma_{\text{det}}^{(n, n')} j}{\Sigma_t^{(n, n')} j} \right)$$

$$\langle \Phi_{\text{det}}^\dagger, \sum_i \mathbf{F}_{di} \psi \rangle \cong \frac{1}{N} \sum_{n=1}^N \sum_{n'} \sum_{j \in D_{fa}^{(n, n')}} J^{(n, n')} w_{j+1}^{(n, n')} \left(\frac{1}{w_{j+1}^{(n, n')}} \sum_{\substack{j'=j+1 \\ j' \notin \{D_c^{(n, n')}\} | n'' < n'}}^{J_L^{(n, n')} j} \left(w_{j'}^{(n, n')} \frac{\Sigma_{\text{det}}^{(n, n')} j'}{\Sigma_t^{(n, n')} j'} \right) \right) \quad (16)$$

$$= \frac{1}{N} \sum_{n=1}^N \sum_{n'} \sum_{\substack{j=1 \\ j \notin \{D_c^{(n, n')}\} | n'' < n'}} \left(m_{d, L}^{(n, n')} w_j^{(n, n')} \frac{\Sigma_{\text{det}}^{(n, n')} j}{\Sigma_t^{(n, n')} j} \right)$$

$$\langle \Phi_{\text{det}}^\dagger, \frac{\psi}{v} \rangle \cong \frac{1}{N} \sum_{n=1}^N \sum_{n'} \sum_{j=1}^{J^{(n, n')}} w_{j+1}^{(n, n')} \frac{\Delta J_j^{(n, n')}}{v_j^{(n, n')}} \left(\frac{1}{w_{j+1}^{(n, n')}} \sum_{\substack{j'=j+1 \\ j' \notin \{D_c^{(n, n')}\} | n'' < n'}}^{J_L^{(n, n')} j} \left(w_{j'}^{(n, n')} \frac{\Sigma_{\text{det}}^{(n, n')} j'}{\Sigma_t^{(n, n')} j'} \right) \right) \quad (17)$$

$$= \frac{1}{N} \sum_{n=1}^N \sum_{n'} \sum_{\substack{j=1 \\ j \notin \{D_c^{(n, n')}\} | n'' < n'}} \left(m_{t, L}^{(n, n')} w_j^{(n, n')} \frac{\Sigma_{\text{det}}^{(n, n')} j}{\Sigma_t^{(n, n')} j} \right)$$

In the equations, n and n' are a neutron source and its branch index of multiplicative reactions such as (n,fis), (n,2n), and (n,3n) within a time step. So, (n,n') means the n' th branch of the n th neutron source, and N is the total number of neutron sources. $D_f^{(n,n')}$, $D_{fd}^{(n,n')}$, and $D_c^{(n,n')}$ are the collection of fission, delayed fission, and collision indices respectively. $J(n,n')$ indicates the last collision index within a time step. In the transient simulation, tracking a neutron and its branches to the end is inefficient or impossible. Therefore, as in the k -adjoint calculation, the adjoint convergence interval (L) is introduced to set a limit on the adjoint tracking. $J_L(n,n')$ term in the equations indicates the last collision index within the forward interval L from the j th collision.

Then the equations (15) to (17) mean adding up the adjoint responses when the corresponding events such as fission, delayed fission and collision happen. By defining $m_{f,L}^{(n,n')j}$ and $m_{d,L}^{(n,n')j}$ as the number of fissions and delayed fissions occurred before the j th collision within L , one can estimate equation (15) and (16) through the forward MC transient simulation. In a similar way, with the use of the cumulated flight time before the j th collision within L , $m_{t,L}^{(n,n')j}$, equation (17) is calculated in the forward simulation.

3. Application Results

3.1. Infinite homogeneous two-group steady-state problem

The suggested MC algorithm for kinetics parameter estimation is implemented to McCARD transient analysis module. For the verification, kinetics parameters are estimated in infinite homogeneous two-group problems. The two-group cross sections are given in Table 1 varying the differential scattering cross section. In this study, $\Sigma_{s,21}$ are set to make the infinite multiplication factor from 0.6 to 1.002 and $\nu\Sigma_{fg}$ is used for detector cross sections. McCARD calculation is done with 1,000,000 histories for 1 second in the subcritical cases, and with 10,000 histories for 0.01 second in the supercritical case. The initial neutron source is set to the fast energy group for all problems. To investigate the convergence of kinetics parameters according to the adjoint convergence interval, simulations are conducted varying the value L .

Figure 1 is the comparison results of the estimated Λ with its reference value in k_{inf} of 0.6 and 0.98 cases. The estimates converge to the reference value as L increases, and it requires a larger L to get converged value in 0.98 case where the neutron chain is relatively longer. Table 2 is the comparison results of kinetics

parameters in various cases, and it shows a good agreement within 95% confidence intervals.

Table 1. Two-group cross section data

Cross-section	First group (g=1)	Second group (g=2)	
Σ_{fg}	0.5	1.3	
Σ_{fd}	0.001	0.090	
ν_g	2.4	2.4	
Σ_{sgg}	0.48	1.09	
$\Sigma_{sgg} (g \neq g')$	Variable	0.0019	
χ_{pg}	1.0	0.0	
χ_{dg}	0.5	0.5	
$1/\nu_g$ [s/cm]	2.28626×10^{-10}	1.29329×10^{-6}	
β_{ig}	$i=1$	0.003	
	$i=2$	0.003	
λ_i [1/s]	$i=1$	0.16504	
	$i=2$	1.44726	

Table 2. Comparison results of kinetics parameters for infinite homogenous steady-state problems

k_{inf}	Kinetics parameter	Analytic solution	McCARD (RSD[%])	Relative error [%]
0.6	Λ	8.26688×10^{-6}	8.26832×10^{-6} (0.15)	0.02
	β_{eff}	8.16340×10^{-3}	8.20670×10^{-3} (1.25)	0.53
0.7	Λ	7.34565×10^{-6}	7.35283×10^{-6} (0.12)	0.10
	β_{eff}	7.43094×10^{-3}	7.47752×10^{-3} (1.14)	0.63
0.8	Λ	6.59940×10^{-6}	6.60594×10^{-6} (0.11)	0.10
	β_{eff}	6.88160×10^{-3}	6.90917×10^{-3} (1.06)	0.40
0.9	Λ	5.98623×10^{-6}	5.99692×10^{-6} (0.09)	0.18
	β_{eff}	6.45432×10^{-3}	6.46293×10^{-3} (1.01)	0.13
0.98	Λ	5.57037×10^{-6}	5.57156×10^{-6} (0.08)	0.02
	β_{eff}	6.17530×10^{-3}	6.22503×10^{-3} (0.89)	0.81
1.0	Λ	5.47921×10^{-6}	5.47952×10^{-6} (0.02)	0.01
	β_{eff}	6.11520×10^{-3}	6.09597×10^{-3} (0.22)	0.31
1.002	Λ	5.46531×10^{-6}	5.46295×10^{-6} (0.04)	0.04
	β_{eff}	6.10607×10^{-3}	6.08095×10^{-3} (0.44)	0.41

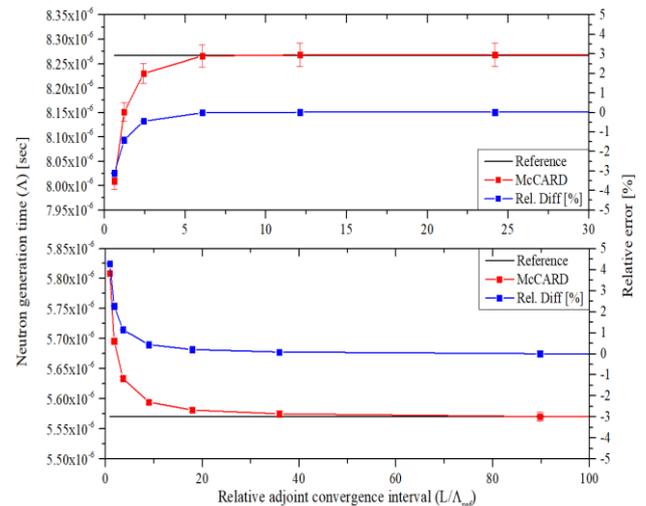


Figure 1. Comparison results of the estimated Λ regarding L (upper: 0.6 case, lower: 0.98 case)

3.2. Infinite homogeneous two-group transient problem

For the transient problem, a simple transient scenario is postulated by mixing the two material used in the steady-state problems. The two materials with k_{inf} of 1.0 (A) and 0.6 (B) are selected and mixed linearly from pure A material to pure B material until 5ms. For the next 5ms, the mixture is changed vice versa. McCARD transient calculation is done with 1,000,000 histories and the initial neutron source is set to fast energy group given at $t=0$. The kinetics parameters are estimated at

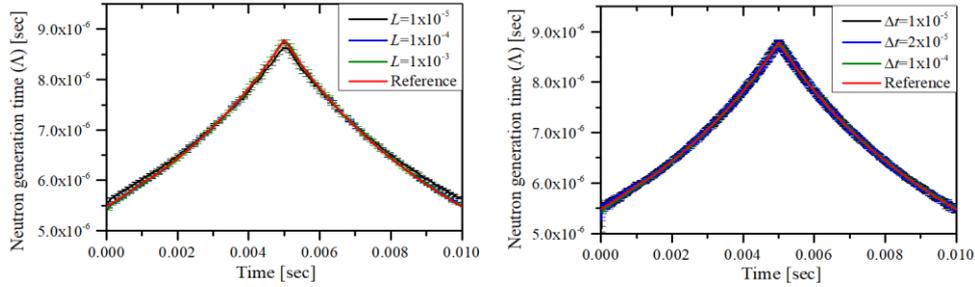


Figure 2. Comparison results of Λ regarding L and Δt in the transient problem

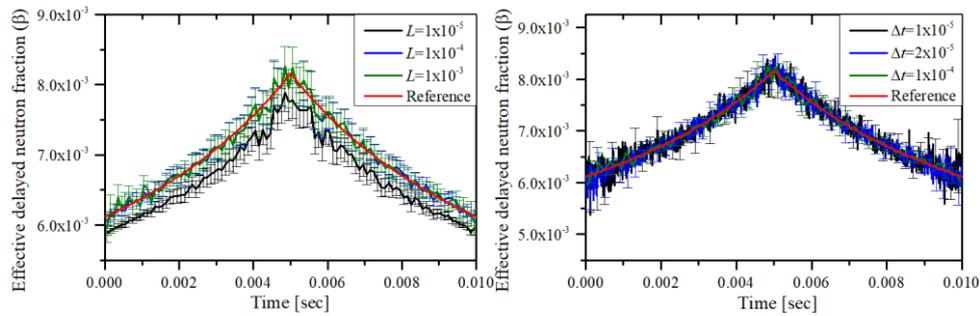


Figure 3. Comparison results of β regarding L and Δt in the transient problem

4. Conclusion

The MC algorithm for estimating the time-dependent adjoint weighted kinetics parameters by MC transient calculation is developed base on the Neumann series solution of the exact shape function and adjoint response. The proposed algorithm is implemented in McCARD transient analysis module. The kinetics parameters are estimated for infinite homogeneous two-group problems including the steady-state and transient cases. McCARD calculation results match well with the analytic solution.

REFERENCES

[1] K. O. Ott and R. J. Neuhold, "Introductory Nuclear Reactor Dynamics," La Grange Park (IL), American Nuclear Society, (1985).
[2] D. E. Cullen et al., "Static and Dynamic Criticality: Are They Different?," UCRL-TR-201506, Lawrence Livermore National Laboratory, (2003).

each time step varying the interval of time step (Δt) and L and compared with the reference solution.

Figures 2 and 3 show the comparison results of the estimated Λ and β . In the figures on left, Δt is fixed to 0.1ms, and L is fixed to 1ms in the right ones. In both cases, the estimated values show a significant difference when it does not reflect sufficiently large L , which is more than 20 times Λ , on the adjoint calculation. But as to the time interval, it shows good agreement with the reference regardless of the size of Δt .

[3] D. Legrady and J. E. Hoogenboom, "Scouting the Feasibility of Monte Carlo Reactor Dynamics Simulations," *Proc. PHYSOR 2008*, Interlaken, Switzerland, Sep 14–19 (2008).
[4] B. L. Sjenitzer and J. E. Hoogenboom, "Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations," *Nucl. Sci. Eng.*, **175**, 94-107 (2013).
[5] H. J. Shim et al., "Estimation of Kinetics Parameters by Monte Carlo Fixed-source Calculations for Point Kinetics Analysis of Accelerator-driven System," *J Nucl. Sci. Technol.*, **57**, 2, 177-186 (2020).
[6] H. J. Shim et al., "McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis," *Nucl. Eng. Technol.*, **44**, 161-176 (2012).
[7] S. H. Jang and H. J. Shim, "Monte Carlo Transient Analysis of C5G7-TD Benchmark 3D Problems Using McCARD," *Proc. ANS Annual Meeting 2020*, Online Virtual Meeting, Jun 8-11 (2020).
[8] M. L. Williams, "The Relations Between Various Contribution Variables Used in Spatial Channel Theory Applied to Reactor Shielding Analysis," *Nucl. Sci. Eng.*, **63**, 220 (1977).