Alpha Eigenvalue Estimation from Dynamic Monte Carlo Calculation for Subcritical Systems

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1. Introduction

The prompt neutron decay constant (referred to as α) is a directly-measurable parameter in reactor physics experiments such as the pulsed neutron method, the reactor noise method, and the exponential method. Calculation of the α by Monte Carlo method is usually performed by neutron transport calculations with a fixed neutron source. From the simulations of the pulsed neutron source (PNS) method or the exponential experimental method [1, 2], the α can be estimated. The α can alternatively be calculated by the α-k iteration algorithm [2] and α iteration algorithm [3], which has already been implemented in the Seoul National University MC code, Monte Carlo Code for Advanced Reactor Design and Analysis (McCARD) code [4].

The dynamic Monte Carlo (DMC) method has been used in the TART code for the α eigenvalue calculations. A unique method has been equipped to measure the α in time-stepwise Monte Carlo simulations. For off-critical systems, the neutron population is allowed to change exponentially over a period of time. The neutron population is uniformly combed to return it to the neutron population started with at the beginning of time boundary [5, 6].

In this study, the conventional dynamic Monte Carlo method has been implemented in the McCARD. There is an exponential change of neutron population at the end of each time boundary for off-critical systems. In order to control this exponential change at the end of each time boundary, a conventional time cut-off controlling population strategy is included in the DMC module implemented in the McCARD.

The main purpose of this paper is to estimate the α eigenvalue from the DMC calculations for subcritical systems. The effectiveness of the results is examined for two-group infinite homogeneous problems with varying the *k*-value by comparisons with analytical solutions. The applicability of the DMC module is also evaluated for an experimental benchmark of the thorium-loaded accelerator-driven system [7] at Kyoto University Critical Assembly (KUCA) by comparisons of α's calculated by the DMC simulations with those from the measurements, the MC α iteration algorithm and the MC PNS simulations.

2. Methodology

An integral form of the time-dependent Boltzmann transport equation for the collision density ψ(P), where P denotes the state vector of a neutron in the seven-dimensional phase space (three in space, two in direction, and one each in energy and time) $(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$ can be written as;

$$\psi(\bar{\mathbf{P}}) = \tilde{S}(\bar{\mathbf{P}}) + \int d\bar{\mathbf{P}}' K(\bar{\mathbf{P}}' \to \bar{\mathbf{P}}) \psi(\bar{\mathbf{P}}') \quad (1a)$$

where;

$$\psi(\bar{\mathbf{P}}) = \tilde{S}(\bar{\mathbf{P}}) + \int d\bar{\mathbf{P}}' K(\bar{\mathbf{P}}' \to \bar{\mathbf{P}}) \psi(\bar{\mathbf{P}}') \quad (1b)$$

= Collision Density

$$K(\bar{\mathbf{P}}' \to \bar{\mathbf{P}}) = C\left(\bar{\mathbf{r}}', t'; E', \hat{\mathbf{\Omega}}' \to E, \hat{\mathbf{\Omega}}\right) T\left(E, \hat{\mathbf{\Omega}}, t; \bar{\mathbf{r}}' \to \bar{\mathbf{r}}\right) \quad (1c)$$

= Transport Kernel

$$C\left(\bar{\mathbf{r}}', t'; E', \hat{\mathbf{\Omega}}' \to E, \hat{\mathbf{\Omega}}\right) = \sum_r \frac{\Sigma_r\left(\bar{\mathbf{P}}'\right)}{\Sigma_t\left(\bar{\mathbf{P}}'\right)} \nu_r f_r\left(E', \hat{\mathbf{\Omega}}' \to E, \hat{\mathbf{\Omega}}\right) \quad (1d)$$

= Collision Kernel

$$T\left(E, \hat{\mathbf{\Omega}}, t; \bar{\mathbf{r}}' \to \bar{\mathbf{r}}\right) = \frac{\Sigma_t\left(\bar{\mathbf{r}}, E\right)}{|\bar{\mathbf{r}} - \bar{\mathbf{r}}'|} \exp\left[-\int_0^{|\bar{\mathbf{r}} - \bar{\mathbf{r}}'|} \Sigma_t\left(\bar{\mathbf{r}} - s\frac{\bar{\mathbf{r}} - \bar{\mathbf{r}}'}{|\bar{\mathbf{r}} - \bar{\mathbf{r}}'|}, E\right) ds\right] \delta\left(\hat{\mathbf{\Omega}} . \frac{\bar{\mathbf{r}} - \bar{\mathbf{r}}'}{|\bar{\mathbf{r}} - \bar{\mathbf{r}}'|} - 1\right)$$

= Transition Kernel (1e)

$$\tilde{S}(\bar{\mathbf{P}}) = \int d\bar{\mathbf{P}} S\left(\bar{\mathbf{r}}'', E, \hat{\mathbf{\Omega}}, t\right) T\left(E, \hat{\mathbf{\Omega}}, t; \bar{\mathbf{r}}'' \to \bar{\mathbf{r}}\right) \quad (1f)$$

= First Collision Source Density

Where, v_r is average number of neutrons produced from reaction type *r*, f_r is probability that a collision of type *r* by a neutron direction $\hat{\mathbf{\Omega}}'$ and energy E' will produce a neutron in direction interval $d\hat{\mathbf{\Omega}}$ about $\hat{\mathbf{\Omega}}$ with energy *dE* about *E* and *S* is source distribution.

After reviewing Neumann series solution, the neutron density tally at the end of m^{th} time step can be calculated as;

$$N_m\left(\mathbf{r}, t\right) = \frac{1}{n_m}\left(f_{m-1} \sum_{i=1}^{n_m} \sum_j w_{i,j} q_{i,j}\right) \quad (2)$$

where, f_{m-1} is a scale factor introduced at the end of $(m-1)^{th}$ time step, $w_{i,j}$ is weight of neutron after the j^{th} collision of neutron *i* and $q_{i,j}$ is response of neutron density tally for the j^{th} collision of neutron *i* [8].

The prompt neutron decay constant α_m at the end of each m^{th} time boundary is estimated by the mathematical expression given in Eq. 3;

$$\alpha_m = \frac{\ln\left(N(t_m)/N(t_{m-1})\right)}{\Delta t_m}; \quad \Delta t_m = t_m - t_{m-1} \qquad (3)$$

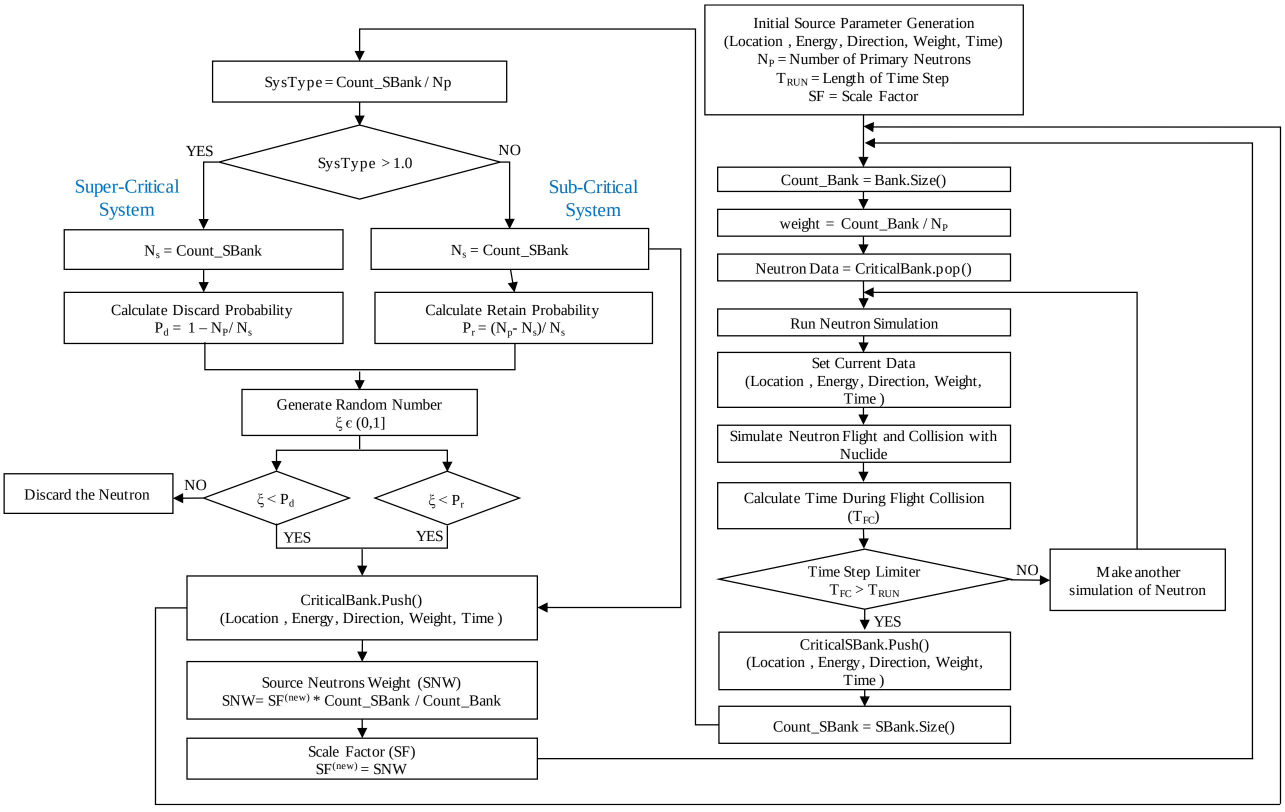


Figure 1: Generalized algorithm for controlling neutron population in dynamic Monte Carlo (DMC) simulations.

3. Numerical Results and Analysis

3.1 Two-Group Infinite Homogeneous Problem

Two-group infinite homogeneous medium problems are used to investigate the effectiveness of DMC module implemented in the McCARD. Table 1 represents the two-group cross sections varying the prompt subcriticality k_p with the differential scattering cross section of the fast group Σ_{s12}.

Table 1: Cross sections for the two-group infinite homogeneous problem [3].

Cross Section	First group (g=1)	Second group (g=2)
Σ_{tg}	0.5	0.5
Σ_{fg}	0.025	0.175
ν_{pg}	2.0	2.0
Σ_{sgg}	0.10	0.20
$\Sigma_{sg'g}$ $(g\neq g')$	Variable	0.00
χ_{pg}	1.0	0.0
$1/\upsilon_g$ [sec/cm]	2.28626×10^{-10}	1.29329×10^{-6}

Table 2 shows the variation of differential scattering cross section along with the values of k_p. Table 3 shows the comparisons of the results for the α eigenvalues using DMC simulations for 10,000 neutron histories and 1500 time steps with 50 inactive time steps with those from the reference, the α iteration algorithm [3] and the α-k iteration method applying the pseudo absorption adjustment [10] with analytical solutions. The time bin size for the DMC simulations is set to 1.0 μsec for each prompt criticality. It is observed that the results are within 95% confidence intervals. Figure 2 shows the convergence of the α eigenvalue using the DMC simulations for different k_p values.

Table 2: Prompt criticality k_p with the varying differential scattering cross section of the first group [3].

Σ_{s12}	k_p
0.265714	0.9
0.197143	0.7
0.128571	0.5
0.060000	0.3
0.008571	0.15

Table 3: Comparisons of α estimates for the two-group infinite homogeneous problem.

k_p	Ref. α	α-k iteration with $\eta = 0$ (SD)	α-k iteration with $\eta = 2$ (SD)	α iteration (SD)	α using DMC (SD)
0.90	26507.1	26500.1 (12.8)	26545.6 (14.8)	26524.4 (14.0)	26511.2 (49.3)
0.70	79523.4	79574.6 (33.8)	79455.7 (38.7)	79522.6 (18.0)	79532.2 (80.4)
0.50	132544.0	132518.0 (70.8)	132431.0 (94.4)	132539.0 (20.9)	132501.0 (94.1)
0.30	185568.0	Fail	Fail	185554.0 (26.6)	185542.0 (120.4)
0.15	225338.0	Fail	Fail	225328.0 (31.3)	225227.0 (147.2)

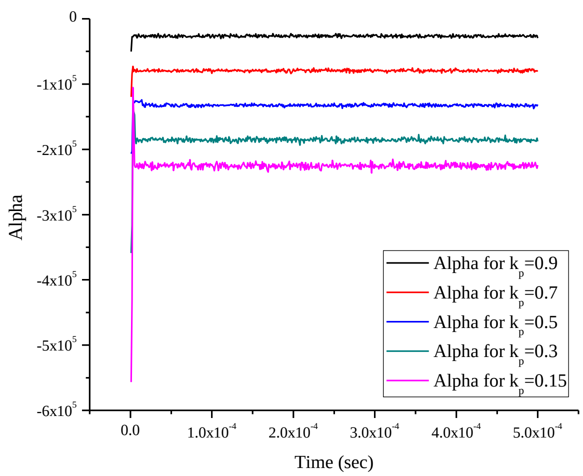


Figure 2: Convergence of alpha using DMC simulations for different k_p vlues.

3.2 Application to Th-ADS Experimental Benchmarks

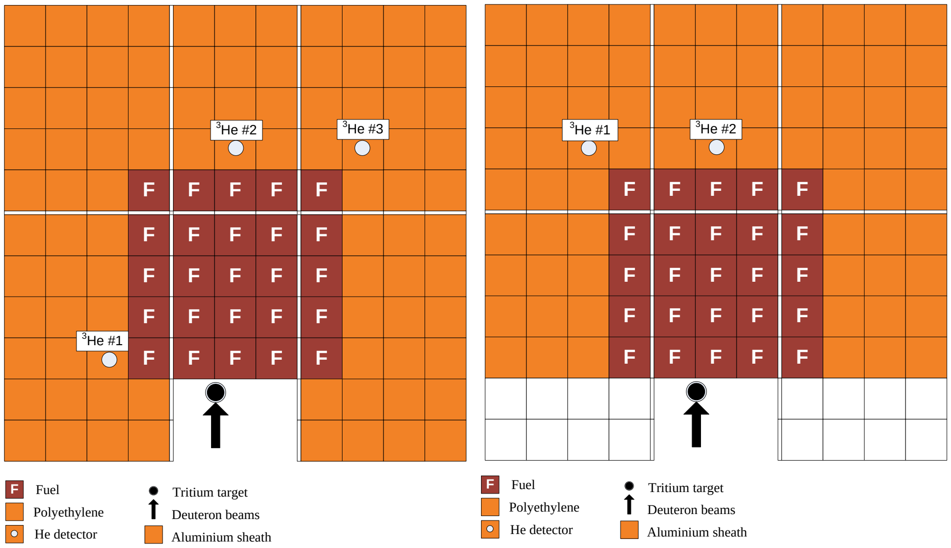
The DMC algorithm is applied to calculate the α eigenvalue for the experimental benchmarks performed on the thorium-loaded accelerator-driven system (Th-ADS). The solid-moderated and solid-reflected type A core of KUCA facility is used to perform Th-ADS experiments. Seven core configurations are combined with the accelerator, generating the 14 MeV pulsed neutrons by D-T (deuteron-tritium) reactions or a synchrotron type proton accelerator. The highly enriched uranium (HEU), thorium (Th), and natural uranium (NU) fuel was loaded together with the reflectors, including polyethylene (PE), graphite (Gr), and beryllium (Be) [7].

Figure 3(a) represents a core configuration for Th-PE, Th-Gr, Th-Be, Th-HEU-PE, and NU-PE cores with 3 He detectors and Figure 3(b) shows a core configuration for Th-HEU-5PE and Th-HEU-Gr-PE cores with 2 He detectors having accelerator generating 14 MeV pulsed neutrons. The effective multiplication factors, k_{eff}'s, of all the cores are shown in the Table 4.

Table 4: k_{eff}'s of the seven core configurations.

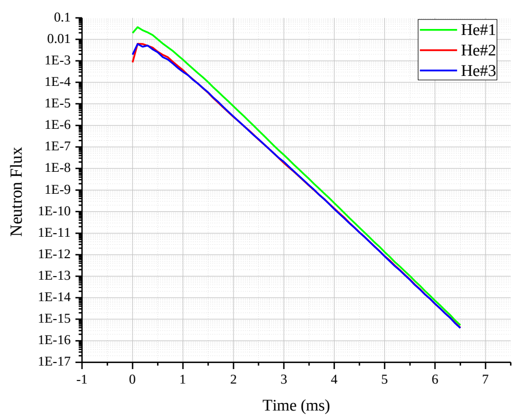
Core	k_{eff}
Th-PE	0.00613
Th-Gr	0.00952
Th-Be	0.00765
Th-HEU-PE	0.58754
NU-PE	0.50867
Th-HEU-5PE	0.85121
Th-HEU-Gr-PE	0.35473

The McCARD calculations along with the DMC module are performed with continuous-energy cross section libraries produced from the ENDF/B-VII.0 for all the cores. The results for the α eigenvalues using DMC simulations for 10,000 neutron histories and 250 time steps with 50 inactive time steps are shown in the Table 5. The time bin size for the DMC simulations is set to 0.1 msec for each core. From the comparisons with the measurements, the MC PNS simulations and the MC α iteration show that the α eigenvalue measured by the DMC method are quite comparable and it is observed that the results are within 95% confidence intervals. Figure 4(a) and Figure 4(b) show the neutron flux distribution with time for Th-Gr and Th-HEU-5PE cores respectively. Figure 5(a) and Figure 5(b) represent the convergence of the α from DMC simulations for Th-Gr and Th-HEU-5PE cores respectively.

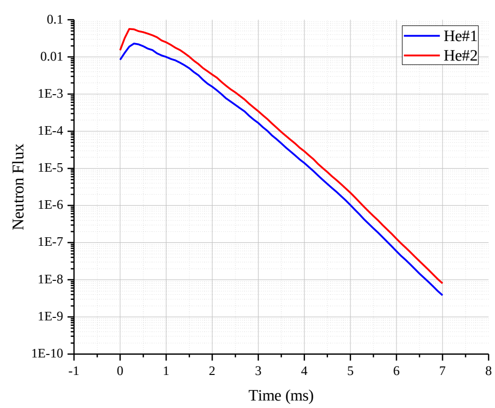


(a). Th-PE, Th-Gr, Th-Be, Th-HEU-PE, and NU-PE (b). Th-HEU-5PE and Th-HEU-Gr-PE

Figure 3: Core configurations with 14 MeV pulsed neutrons for Th-ADS experimental benchmarks.

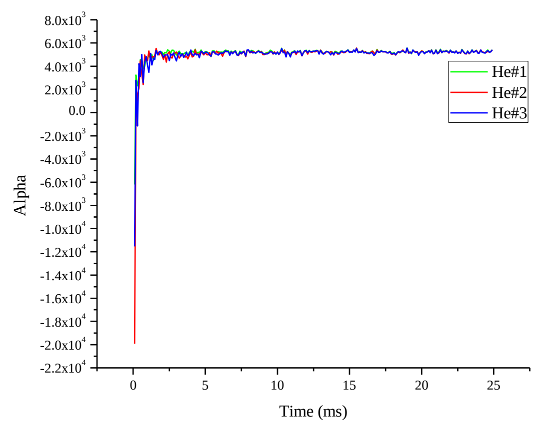


(a) Th-Gr Core

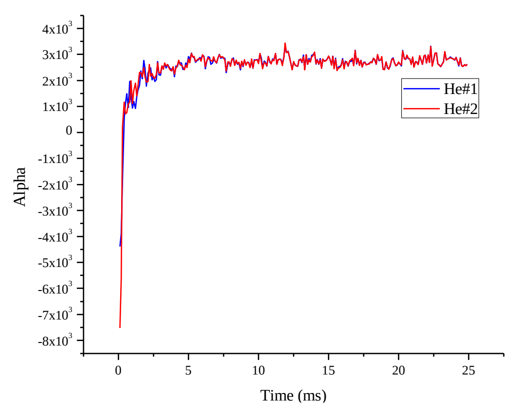


(b) Th-HEU-5PE Core

Figure 4: DMC neutron flux for the Th-ADS benchmark problems.



(a) Th-Gr Core



(b) Th-HEU-5PE Core

Figure 5: Convergence of alpha using DMC simulations for the Th-ADS benchmark problems.

Table 5: Comparison of the α eigenvalues for the Th-ADS experimental benchmarks.

CORE	Measurement with 14 MeV neutrons (SD)			MC PNS Simulation (SD)	MC α iteration (SD)	α using DMC (SD) [Rel. Diff. (%)]			Mean α Rel. Diff. [%] (w/PNS Sim.) [w/α iteration]
	^{3}HE #1	^{3}HE #2	^{3}HE #3			^{3}HE #1	^{3}HE #2	^{3}HE #3	
TH-PE	6642 (11)	6224 (27)	5751 (25)	5245.4 (4.9)	5243.3 (1.3)	5240.9 (4.7) [21.1]	5196.1 (4.8) [16.5]	5177.0 (4.8) [10.0]	5204.6 (0.8) [0.7]
TH-GR	6451 (12)	5945 (15)	5701 (17)	5310.1 (7.7)	5239.7 (1.3)	5233.5 (3.3) [18.9]	5193.2 (3.6) [12.6]	5190.0 (4.1) [9.0]	5205.5 (2.0) [0.7]
TH-BE	6515 (8)	6111 (17)	5746 (20)	5224.2 (7.2)	5240.1 (1.4)	5223.6 (5.2) [19.8]	5148.3 (5.5) [15.8]	5186.4 (5.1) [9.7]	5198.1 (0.5) [0.8]
TH-HEU-PE	5692 (11)	5275 (7)	5231 (9)	5025.6 (6.3)	5131.2 (2.8)	5051.3 (5.1) [11.3]	5027.7 (5.4) [4.7]	5015.8 (5.8) [4.1]	5031.6 (0.1) [1.9]
NU-PE	5748 (11)	6592 (15)	5010 (11)	4995.1 (6.4)	5163.8 (3.5)	5106.3 (6.7) [11.2]	5065.8 (6.0) [23.2]	5053.7 (5.5) [0.9]	5075.3 (1.6) [1.7]
TH-HEU-5PE	3110 (11)	3104 (10)	--	2977.1 (1.4)	2954.1 (1.2)	2745.6 (4.3) [11.7]	2745.1 (5.1) [11.6]	--	2745.3 (7.8) [7.1]
TH-HEU-GR-PE	4980 (40)	4939 (50)	--	4761.0 (2.9)	4766.7 (10.2)	4772.8 (6.6) [5.2]	4779.5 (6.1) [5.2]	--	4776.1 (0.3) [0.2]

4. Conclusions

In this paper, the conventional combing method to control the neutron population for off-critical systems is implemented. Instead of considering the cycles, the simulation is divided in time intervals. At the end of each time interval, neutron population control is applied on the banked neutrons. Randomly selected neutrons are discarded, until the size of neutron population matches the initial neutron histories at the beginning of time simulation.

The prompt neutron decay constant α is estimated from DMC algorithm for subcritical systems. The effectiveness of the results is examined for two-group infinite homogeneous problems with varying the *k*-value. From the comparisons with the analytical solutions, it is observed that the results are quite comparable with each other for each *k*-value. The applicability of the DMC module is also evaluated for an experimental benchmark of the thorium-loaded accelerator-driven system. From the comparison of α's calculated by the DMC simulations with those from measurements, MC α-iteration algorithm and MC PNS simulations, it is seen that the α results are quite comparable with each other for the cases where the experiments provide reliable estimates.

5. Future Work

The next step will be the development of DMC method to solve the coupled Boltzmann and kinetic equations with exact geometry and continuous energy, using only Monte Carlo techniques for reactor kinetics calculations [9].

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