Application of Differential Operator Sampling to Depletion Equation

Yong Hee Choi,* Jin Young Cho*
**Korea Atomic Energy Research Institute, 111, Daedeok-daero 989 beon-gil, Yuseong-gu, Daejeon, 34057, Korea*
Corresponding author: yhchoi@kaeri.re.kr

1. Introduction

Kinetic Monte Carlo (KMC) is a computer simulation method based on Monte Carlo sampling intended to simulate the time evolution of a statistical process. The KMC method is used in many simulations such as adsorption dynamics or atomistic simulation of irradiation damage process. The main advantage of the KMC used in the depletion equation is that it enables us to solve continuous energy depletion equations if required. Additionally, it is simple to implement, as opposed to the deterministic method as numerical methods, such as the matrix exponential and predictor-corrector methods are not necessary.

Despite this potential the KMC method has a severe limitation that parametric studies are too expensive or almost impossible. One of the ways to overcome such difficulties is the Monte Carlo perturbation techniques. Shim [1][2] fully developed the mathematical formulation of KMC and derived the stochastic sampling algorithm based on differential operator method. Another approach [3] was also developed based on the correlated sampling method and its applicability to the depletion equation was verified.

The differential operator method [4] is one of the Monte Carlo perturbation techniques based on the derivative of the random walk process using the product rule. The derivatives are accumulated and used to estimate sensitivities during the simulations.

In this work, the applicability of differential operator sampling to one group depletion equation is examined for the calculation of the sensitivity of a cross section on the nuclide number densities. In fact, the formulation given herein is exactly the same as that of Shim's work, but it is necessary to repeat it here because it will help easily explain the algorithm of the differential operator sampling (DOS) method. The numerical results are provided to determine whether they are in good agreement with the results of the deterministic solution.

2. Methods and Results

2.1 Derivation of KMC Algorithm

According to Fichthron and Weinberg [5], the probability density function of the solution vector $\vec{X}$ for the Poisson process must satisfy the following balance equation:

$$\frac{\partial P\left(\vec{X},t\right)}{\partial t}+k\left(\vec{X}\right)P\left(\vec{X},t\right)=S\left(\vec{X},t\right) \quad , \qquad (1)$$

where

$P(\vec{X},t)$: PDF for state $\vec{X}$ at time t,

$k\left(\vec{X}\right)$: Total transition rate for state $\vec{X}$,

$S\left(\vec{X},t\right)=\int_{\Gamma_{\vec{X}'}} d\vec{X}'\cdot k\left(\vec{X}'\to\vec{X}\right)\cdot P\left(\vec{X}',t\right)$,

$\Gamma_{\vec{X}'}$: Sample space for $\vec{X}'$.

By applying an integrating factor, Eq. (1) can be written as

$$P\left(\vec{X},t\right)=e^{-k(\vec{X})t}P(\vec{X},0)+\int_0^t e^{-k(\vec{X})(t-t')}S\left(\vec{X},t'\right)dt' . \quad (2)$$

Let us define the transition probability density function for $\vec{X}$ at time t as follows:

$$\Psi\left(\vec{X},t\right)=k\left(\vec{X}\right)P\left(\vec{X},t\right). \qquad (3)$$

By multiplying $k(\vec{X})$ on both sides of Eq. (2), we obtain

$$\Psi\left(\vec{X},t\right)=k(\vec{X})e^{-k(\vec{X})t}P(\vec{X},0)+\int_0^t k(\vec{X})e^{-k(\vec{X})(t-t')}S(\vec{X},t')dt' \quad . \qquad (4)$$

Now let us introduce the time flight kernel and first transition kernel as follows:

$$T\left(t'\to t\mid\vec{X}\right)=k\left(\vec{X}\right)e^{-k(X)(t-t')}, \qquad (5)$$

$$\hat{Q}\left(\vec{X},t\right)=T\left(0\to t\mid\vec{X}\right)P\left(\vec{X},0\right). \qquad (6)$$

Then, Eq. (4) can be rewritten as

$$\Psi\left(\vec{X},t\right)=\hat{Q}\left(\vec{X},t\right)+\int_0^t T\left(t'\to t\mid\vec{X}\right)S\left(\vec{X},t'\right)dt' . \quad (7)$$

The source term on the RHS of Eq. (1) can be rewritten as

$$S\left(\vec{X},t\right)=\int_{\Gamma_{\vec{X}'}} d\vec{X}'\cdot\frac{k\left(\vec{X}'\to\vec{X}\right)}{k(\vec{X}')}\cdot k(\vec{X}')P\left(\vec{X}',t\right) \\ =\int_{\Gamma_{\vec{X}'}} d\vec{X}'\cdot C\left(\vec{X}'\to\vec{X}\right)\cdot\Psi\left(\vec{X}',t\right) \quad (8)$$

where

$$C\left(\vec{X}'\to\vec{X}\right)=\frac{k\left(\vec{X}'\to\vec{X}\right)}{k\left(\vec{X}'\right)} \quad . \quad (9)$$

From Eqs. (7) and (8), we obtain

$$\Psi\left(\vec{X},t\right)=\hat{Q}\left(\vec{X},t\right)+ \\ \int_0^t\int_{\Gamma_{\vec{X}'}} K\left(\vec{X}',t'\to\vec{X},t\right)\Psi\left(\vec{X}',t'\right)d\vec{X}'dt' \quad , \quad (10)$$

where

$$K\left(\vec{X}',t'\to\vec{X},t\right)=T\left(t'\to t\mid\vec{X}\right)C\left(\vec{X}'\to\vec{X}\right) \quad . \quad (11)$$

Eq. (10) is the integral equation for the transition probability density function. The solution of Eq. (10) can be expressed by the Neumann series solution:

$$\Psi\left(\vec{X},t\right)=\sum_{j=0}^{\infty}\psi_j\left(\vec{X},t\right) \quad , \quad (12)$$

where

$$\psi_j\left(\vec{X},t\right)=\int_0^t dt_0\int_{\Gamma_{\vec{X}_0}} d\vec{X}_0 \\ K_j\left(\vec{X}_0,t_0\to\vec{X},t\right)\hat{Q}\left(\vec{X}_0,t_0\right) \quad , \quad (13)$$

and

$$K_0\left(\vec{X}_0,t_0\to\vec{X},t\right)=\delta\left(\vec{X}_0-\vec{X}\right)\delta\left(t_0-t\right), \\ K_1\left(\vec{X}_0,t_0\to\vec{X},t\right)=K\left(\vec{X}_0,t_0\to\vec{X},t\right), \\ \cdots$$

$$K_j\left(\vec{X}_0,t_0\to\vec{X},t\right)= \\ \int_{t_{j-2}}^t dt_{j-1}\int_{\Gamma_{\vec{X}_{j-1}}} d\vec{X}_{j-1}\cdots\int_{t_0}^t dt_1\int_{\Gamma_{\vec{X}_1}} d\vec{X}_1 \\ K\left(\vec{X}_{j-1},t_{j-1}\to\vec{X},t\right)\cdots K\left(\vec{X}_0,t_0\to\vec{X}_1,t_1\right) \quad .$$

Eq. (13) shows that the mathematical form of the transition probability consists of the products and summation of $K\left(\vec{X}',t'\to\vec{X},t\right)$ which is made up of two probability functions $T\left(t'\to t\mid\vec{X}\right)$ and $C\left(\vec{X}'\to\vec{X}\right)$. Eq. (13) indicates that the transition probability for $\vec{X}$ at time t can be computed by summing all the contributions obtained by sequential samplings of random variable $\vec{X}$ and t through the kernel functions. Based on Eq. (13), the overall sampling algorithm of KMC can be derived for $\vec{X}$ and t.

2.2 Derivation of DOS Algorithm

In the KMC simulations, a system parameter to be analyzed, R, can be expressed as

$$R=\int_0^{\infty}\int_{\Gamma_{\vec{X}}}\Psi\left(\vec{X},t\right)r\left(\vec{X},t\right)d\vec{X}dt \quad , \quad (14)$$

where $r\left(\vec{X},t\right)$ is the response function of the system that we want to analyze.

In Eq. (10), $\hat{Q}$ represents the transition probability that the current state is the same with the initial condition. In most of the depletion process, this is not the case. So we set $\hat{Q}$ by zero. Then, from Eqs. (10), (12) and (14), the system parameter at the j-th transition step is written as

$$R_j=\int_{t'}^{\infty}\int_{\Gamma_{\vec{X}}}\int_0^{t=\infty}\int_{\Gamma_{\vec{X}'}} K\left(\vec{X}',t'\to\vec{X},t\right)\psi_{j-1}\left(\vec{X}',t'\right) \\ r_j\left(\vec{X},t\right)d\vec{X}'dt'd\vec{X}dt \quad . \quad (15)$$

Note that the response at the j-th transition step can be rewritten by

$$r_j\left(\vec{X},t\right)=\Delta r_j\left(\vec{X}',t'\to\vec{X},t\right)+r_{j-1}\left(\vec{X}',t'\right) \quad , \quad (16)$$

and let us denote R*=R(α+Δα) as the system parameter of the perturbed system for an input parameter α at the j-th transition. Then, from Eqs. (15) and (16), we obtain

$$R_j^*=\int_{t'}^{\infty}\int_{\Gamma_{\vec{X}}}\int_0^{\infty}\int_{\Gamma_{\vec{X}'}} K^*\left(\vec{X}',t'\to\vec{X},t\right)\Delta r_j^* \\ \psi_j^*\left(\vec{X}',t'\right)d\vec{X}'dt'd\vec{X}dt+R_{j-1}^* \quad , \quad (17)$$

where K^* and ψ_j^* are kernels and transition density probability functions for the perturbed system. Then, the change of the response function at the j-th transition step can be obtained from the unperturbed system by using Taylor series expression as follows:

$$R_j^* = \int_{t'}^{\infty}\int_{\Gamma_{\vec{X}}}\int_0^{\infty}\int_{\Gamma_{\vec{X}'}} K\left(\vec{X}',t'\to X,t\right)U_j\Delta r_j \psi_j^*\left(\vec{X}',t'\right)d\vec{X}'dt'd\vec{X}dt + R_{j-1}^* \quad , \quad (18)$$

where

$$U_j = 1+\left\{\frac{1}{K}\frac{\partial K}{\partial\alpha}+\frac{1}{\Delta r_j}\frac{\partial\Delta r_j}{\partial\alpha}\right\}(\Delta\alpha)+\cdots \quad , \quad (19)$$

and K and Δr_j is the kernel function and j-th response change of the unperturbed system. The response functions of the KMC used in depletion equation are the number of isotopes and system time. In either case, there's no way of knowing the derivatives of the response functions with respect to input parameters in advance. So we simply assume

$$\frac{\partial\Delta r_j}{\partial\alpha}=0 \quad . \quad (20)$$

Then we obtain,

$$U_j = 1+\frac{1}{K}\frac{\partial K}{\partial\alpha}(\Delta\alpha)+\frac{1}{2!}\frac{1}{K}\frac{\partial^2 K}{\partial\alpha^2}(\Delta\alpha)^2\cdots \quad . \quad (21)$$

2.3 NUMERICAL RESULTS

The DOS algorithm based on Eq. (18) is applied to one group depletion equation. The one-group ORIGEN library is used in the actual computations. The calculation results are compared with MEDEAC code [6] which is developed in KAERI and based on the Krylov subspace method.

Table I: Initial conditions for the test problem

Isotope	Mol	Isotope	Mol	Isotope	Mol
U-235	5.11E+01	U-238	1.01E+03	Xe-135	1.01E+03

Table I shows the initial conditions of the test problem at a specified region of the core. For simplicity, we assume that there are only 3 types of different nuclides as an initial condition. While the burn proceeds, the flux level is assumed to be constant as 10^{14} /cm^2-sec. To test the perturbation algorithm, we introduce the perturbation of (n,γ) cross section of U-238 by an amount of 40% larger than the original value. (The original value is 8.546e-01 barn.) Then it is expected that the perturbation of (n,γ) cross section of U-238 will cause the change of the time evolutions of some nuclide number densities compared to the unperturbed case.

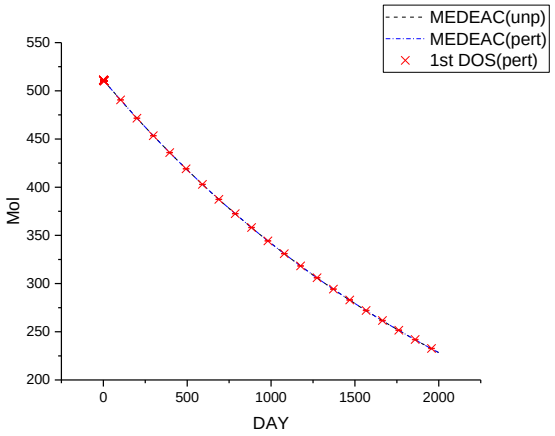

Fig. 1. Comparison of time evolution of numbers of U-235. The result shows the sensitivity of (n,γ) cross section of U-238 to U-235 is negligible. This means that the perturbation of (n,γ) cross section of U-238 has no effect on the U-235 number density in depletion process.

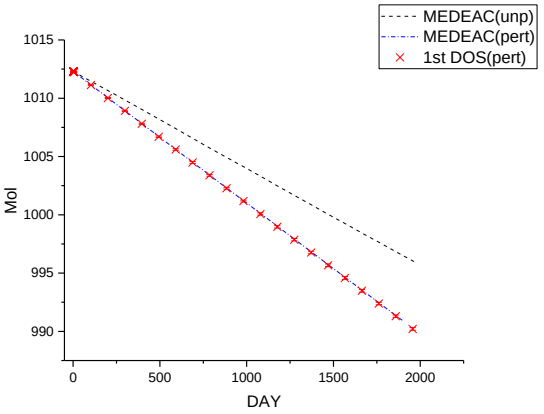

Fig. 2. Comparison of time evolution of numbers of U-238. The result shows the sensitivity of (n,γ) cross section of U-238 to U-238 is almost linear.

Fig. 1 shows the time evolution of U-235 and Fig. 2 shows the time evolution of U-238 for both the perturbed and unperturbed cases. The dashed lines represent the results of MEDEAC and the dots with error bars represent the results of DOS. To estimate the statistical uncertainties, all KMC calculations are repeated 30 times (30 time histories) with different random number seeds. The figures show that the two sets of results are consistent with each other. Note that the error bars are almost invisible because they are so small in this case. From the calculation results, we conclude that the assumption we introduce in Eq. (20) is valid in this case because the amount of the perturbation

of the response function is well predicted through this algorithm.

To test another perturbation case, the (n,γ) cross section of Xe-135 is increased by an amount of 40% larger than the original value. (The original value of cross section is 1.640e+5 barn.) Fig. 3 shows the time evolution of Xe-135 for the unperturbed and perturbed systems. Since the (n,γ) cross section of Xe-135 is much larger than others, the (n,γ) reaction of Xe-135 is dominant at the initial stage of depletion process. It means that the increase of (n,γ) cross section has effects directly on the time evolution of Xe nuclide number densities. Fig. 3 shows that DOS algorithm predicts the same results with that of MEDEAC.

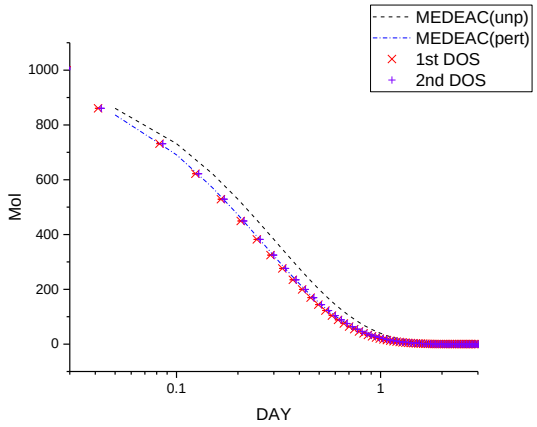

Fig. 3. Comparison of time evolution of numbers of Xe-135 for the case that Xe-135 (n,γ) cross section is perturbed.

3. Conclusions

The DOS method for the depletion equation by using a one-group ORIGEN library has been tested. To show the performance, the numerical results of the test problem were compared with those of the deterministic code MEDEAC. The results show that the change of nuclide number density caused by the cross section perturbation is well predicted by the DOS algorithm in either case where the sensitivity is small or high.

REFERENCES

[1] H. J. Shim, Kinetic Monte Carlo Perturbation Analysis for Adsorption Dynamics, Transactions of the Korean Nuclear Society Autumn Meeting, Gwangju, Korea, May 30-31, 2013.
[2] H. J. Shim, Stochastic Perturbation Algorithm for Kinetic Monte Carlo Simulations, Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA+MC2013), Paris, France, October 27-31, (2013)
[3] Y. H. Choi, Application of Correlated Sampling Algorithm to Depletion Equation, Transactions of the Korean Nuclear Society Autumn Meeting, Gyeongju, Korea, October 30-31, 2017.
[4] H. Rief, Generalized Monte Carlo Perturbation Algorithm for Correlated Sampling And A Second-order Taylor Series Approach, Ann. nucl. Energy, Vol. 11, No. 9, pp. 455-476, 1984.
[5] K. A. Fichthorn and W. H. Weinberg, Theoretical Foundations of Dynamical Monte Carlo Simulations, J. Chem. Phys., 95, 2, 1090, 1991.
[6] J. Y. Cho etc., MEDEAC: Matrix Exponential based isotope DEpletion and Analysis Code, Transactions of the Korean Nuclear Society Autumn Meeting, Gyeongju, Korea, October 26-27, 2017.