

## Application of Kinetic Monte Carlo Method to Point Kinetic Equations Coupled with Simplified T/H Feedback Model

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### 1. Introduction

A simple program based on a stochastic method is developed for solving the reactor point kinetic equations(PKEs) coupled with a simplified T/H feedback model. Most of the existing programs solving the PKEs utilizes the deterministic methods such as Runge-Kutta method[1] or CRAM[2], etc. In this paper, we introduce stochastic algorithm based on the kinetic Monte Carlo(KMC) method. The main advantage of the KMC lies in that it is simple and easy to implement. But, the longer running time and stochastic errors are inevitably involved.

In the subsequent chapters, we present a brief description about the methodology employed in the code and the numerical results for a test problem is provided. The calculated results are compared with the ones obtained using the deterministic method.

### 2. Method of solution

The PKEs is a 0-D model which gives a transient behavior of the nuclear power reactor. The feedback mechanism oriented from the fuel and coolant temperatures variations makes the equations nonlinear. The basic PKEs take the following form when we assume six groups of delayed neutron precursors:

$$\frac{dn}{dt} = \frac{\rho - \beta}{\Lambda} n + \sum_{i=1}^6 \lambda_i C_i, \quad (1)$$

$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n - \lambda_i C_i. \quad (2)$$

And the simplified feedback mechanism[3] coming from the fuel and coolant temperatures can be written as:

$$\rho = \rho_0 + \alpha_T^c (T_c - T_{c,ref}) + \alpha_T^f (T_f - T_{f,ref}), \quad (3)$$

$$m_F c_{pF} \frac{dT_F}{dt} = a_F n - h(T_F - T_C), \quad (4)$$

$$m_C c_{pC} \frac{dT_C}{dt} = h(T_F - T_C) - 2W_C c_{pC} (T_C - T_{cin}), \quad (5)$$

where  $T_{c,ref}$  and  $T_{f,ref}$  are the reference temperatures of coolant and fuel for reactivity changes,  $\alpha_T^F$  and  $\alpha_T^C$  are the reactivity temperature coefficients,  $m_F$  and  $m_C$  are the mass of fuel and coolant in the core,  $C_{pF}$  and  $C_{pC}$  are specific heat of fuel and coolant,  $h$  is the heat transfer coefficient between fuel and coolant,  $W_C$  is the coolant

mass flow rate and  $T_{cin}$  are the coolant inlet temperatures,  $a_F$  is the power conversion factor for neutron density.

The above equations can be rewritten in the matrix-vector form in the following way:

$$\frac{d}{dt} \vec{X} = \mathbf{A} \vec{X} + \vec{b}, \quad (6)$$

where  $\vec{X}$  is the state vector defined as

$$X = (n, C_i, T_f, T_m), i = 1, \dots, 6, \quad (7)$$

and  $\mathbf{A}$  and  $\vec{b}$  are the corresponding coefficient matrix and vector.

In KMC, the state vector  $\vec{X}$  is regarded as a random variable. And it assumes that the state of the system follows the Poisson process. Then we can construct the balance equation for the probability density function for  $\vec{X}$  at time  $t$ . Thanks to Shim's work[4], we can find a mathematical formula of the KMC algorithm using the Neumann series solution of the balance equation. Based on the mathematical solution, the KMC algorithm for solving PKEs is given in the following way:

- 1) Set the time  $t = 0$  and prepare for an initial state  $\vec{X}(t = 0)$ .
- 2) Make the list of all kinds of events which can happen in the current state  $i$  and calculate their transition rates  $k(\vec{X}_i \rightarrow \vec{X}_j)$ .
- 3) Calculate the total transition rate by accumulating all transition rates,  $k_i = \sum_j k(\vec{X}_i \rightarrow \vec{X}_j)$ .
- 4) Update the current time  $t_j = t_i + \Delta t_{ij}$ , where  $\Delta t_{ij} = -\log \xi / k_i$  and  $\xi$  is a uniform random number  $\xi \in (0,1]$ .
- 5) Select an event randomly from the event list using its transition rates. Carry out the selected event and find the next state.
- 6) Return to step 2 until the simulation time is over.

For applying the KMC algorithm to the PKEs, every term consisting of the coefficient matrix  $\mathbf{A}$  and  $\vec{b}$  can be thought as an independent event. Then all transition rates at the time  $t$  in the state  $i$  can be evaluated using  $\mathbf{A} \vec{X}_i + \vec{b}$ .

### 3. Numerical results

We introduce a test problem provided in the reference book[3] to test the code. The following parameters are used in the calculation.

Table 1 PKE kinetic parameters for test problem

Group number	$\beta_i$	$\lambda_i$
1	0.000215	0.0124
2	0.001424	0.0305
3	0.001274	0.111
4	0.002568	0.301
5	0.000748	1.14
6	0.000273	3.01
$\beta=0.006502, \Lambda=0.001$		

Table 2 T/H parameters for test problem

Parameter	Unit	Value
$m_F$	$Kg$	40000
$m_C$	$Kg$	7000
$C_{pF}$	$JKg^{-1}K^{-1}$	200
$C_{pC}$	$JKg^{-1}K^{-1}$	4000
$\alpha_F^C$	$K^{-1}$	-0.00001
$\alpha_C^F$	$K^{-1}$	-0.00001
$W_C$	$Kgs^{-1}$	8000
$a_F$	$Jm^3s^{-1}$	$7 \times 10^6$
$h$	$JK^{-1}s^{-1}$	$4 \times 10^6$
$T_{C,ref}$	$K$	600
$T_{F,ref}$	$K$	900

The fuel temperature( $T_F$ ) and coolant temperature( $T_C$ ) are specified as 900K and 600K in the initial condition.

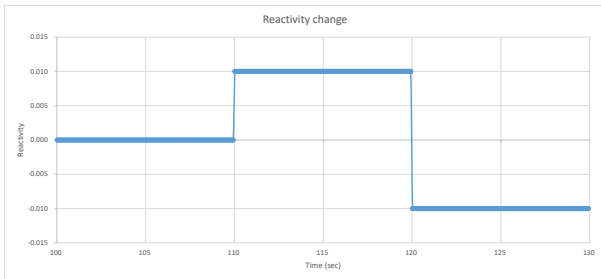


Figure 1 Reactivity insertion of test problem

It is assumed that the stepwise reactivity insertion as much as 0.01 happens at 110 sec during 10 sec and the scram follows for shutdown of the reactor. The KMC simulations are repeated 10 times to evaluate statistical error at each time steps. We use 4<sup>th</sup> order Runge-Kutta method to find the reference solution.

Figs 2 and 3 show the comparison of the results for the neutron density and fuel temperature. It shows the results of KMC simulation always include the reference solution obtained from the deterministic method.

The size of the error bars depends on the scaling factors introduced in the actual implementation in the following way:

$$c \frac{d}{dt} \vec{X} = cA\vec{X} + c\vec{b}, \quad (8)$$

where the multiplication factor  $c$  denotes the scaling factor. In this simulation,  $c$  is specified as 1000. In terms of computing time, KMC shows ~400 secs per a single run for each problem which is ~100 times larger than the 4<sup>th</sup> order Runge-Kutta method.

#### 4. Conclusions

Simulation techniques using KMC can be alternative tool for predicting the transient behavior of the nuclear power reactor. In order to find the feasibility of the KMC method, we solved the simple test problem coupled with T/H feedback model. It shows they have a good agreement with each other.

#### REFERENCES

- [1] H. L. Dodds, Jr., R. M. Westfall, SKINATH – A Computer Program for solving the Reactor Point Kinetics Equations with Simple Thermal-Hydraulic Feedback, ORNL/CSD/TM-210, 1984.
- [2] Farrokh Khoshahval, Morteza Akbari, A New Method for the Solution of the Point Kinetics Equations in the Presence of Newtonian Temperature Feedback, Progress In Nuclear Journal 119, 2020.
- [3] Henryk Anglart, Nuclear Reactor Dynamics and Stability, 2011
- [4] H. J. Shim, Kinetic Monte Carlo Perturbation Analysis for Adsorption Dynamics, Transaction of the Korean Nuclear Society Spring Meeting, Gwangju, Korea, May 30-31, 2013.

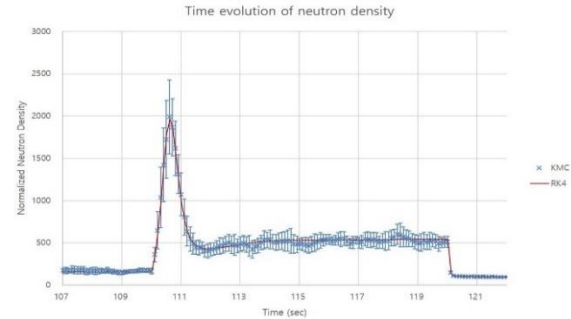


Figure 2 Comparison of time evolution of neutron density for test problem between KMC and 4th order Runge-Kutta

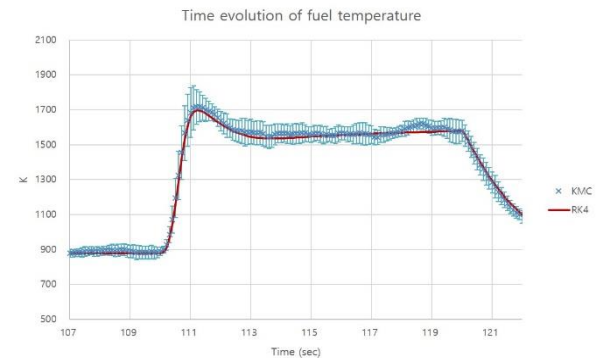


Figure 3 Comparison of time evolution of fuel temperature between KMC and 4th order Runge-Kutta