Modeling of Effective Delayed Neutron Fraction in the Monte Carlo iMC code for Flowing Fuel Reactors

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1. Introduction

The molten salt reactor (MSR), employing liquid salt as fuel, is investigated as one of the advanced reactor concepts. Considering the liquid form of the fuel, exceptional features stem. Some molten salt reactors circulate the fuel salt for online treatment, requiring additional considerations in transient analysis. The unique behavior and its numerical approach are studied and implemented in Monte Carlo code iMC [1].

Point kinetic approximation is one of the methods for time-dependent reactor analysis. The method assumes neutron flux can be expressed as a separation of variables. In the method, dependence on delayed neutrons is evaluated in the form of the inhour equation, composed of kinetic parameters such as effective delayed neutron fractions. These parameters are tallied by employing the adjoint flux as a weighting function. Although direct evaluation of the adjoint flux is challenging in Monte Carlo transport calculations, an introduction of a concept called iterated fission probability enables the estimation of adjoint-weighted kinetic parameters.

iMC is a continuous energy Monte Carlo neutron transport and reactor analysis code developed in KAIST [2]. In this paper, both neutron treatments in the molten salt reactor and iterated fission probabilities are implemented in the iMC and simulate the exceptional behavior of the molten salt reactor.

2. Method

2.1. Precursor treatment in the MSR

In a typical Monte Carlo neutron transport calculation, delayed neutrons are assumed to be produced and decay out where the fission reaction occurred. However, in the molten salt reactor, the fuel moves and circulates. Recalling that the precursors require some time to be decayed, the delayed neutron emission site is distant from the precursor production site due to fuel movement.

Concerning circulations of the fuel in the molten salt reactors, precursors may escape the active core before delayed neutron emission. Some precursors may produce delayed neutrons before re-entering the active core. These delayed neutrons have no impact on the reactor performance. Hence, the precursors are excluded from the calculation.

Other precursors re-enter the active core and emit delayed neutrons in the active core. In the Monte Carlo transport, the production locations of the delayed neutrons are adjusted utilizing the number of circulations before delayed neutron emission.

The aforementioned destinies of the precursor are expressed in the numerical formula [1]. Before treatment, several assumptions are made. First, the velocity profile in the active core is constant and solely axial. Another assumption is that the radial position of the recirculated precursor is uniformly dispersed.

When the precursor is produced, let the precursor decay constant be λ. Then, decay probability after time t can be expressed as Eq. (1).

$$P(t) = \lambda\, exp[-\lambda t], \qquad (1)$$

From the probability, the cumulative probability density function of the decay $\mathrm{F(t)}$ can be described as Eq. (2).

$$F(t) = 1 - exp[-\lambda t], \qquad (2)$$

From the cumulative probability density function, the unbiased neutron emission time of the precursor can be sampled with a uniform random number $\gamma \in [0,1]$

$$F(t_{emit}) = \gamma = 1 - exp[-\lambda t] \rightarrow t_{emit} = \frac{ln(1-\gamma)}{\lambda} \qquad (3)$$

Accordingly, when the decay constant of a newly produced precursor is determined, its emission time can be sampled with a uniform random number γ.

Based on the sampled emission time, the site of emission of the delayed neutron is adjusted. Suppose that the precursor is produced in an axial position z. Time required the precursor to reach the top of the reactor, $\mathrm{t_{top}}$ is calculated as Eq. (4).

$$t_{top} = \frac{(z_{top} - z)}{v_{flow}}, \qquad (4)$$

where $\mathrm{z_{top}}$ is an axial position of the top of the active core. If the sampled emission time $\mathrm{t_{emit}}$ is shorter than $\mathrm{t_{top}}$, the precursor simply moves upward by $\mathrm{v_{flow}} \times t_{emit}$. Eq. (5) shows how the axial position of the delayed neutron is adjusted.

$$z \leftarrow z + v_{flow} \times t_{emit} \qquad (5)$$

Once the delayed neutron is emitted after reaching the top of the active core, the emission may occur inside or

outside the active core. Suppose that time between fuel escaping and reentering the active core be T_{re}. Then, total circulating time T can be calculated as Eq. (6).

$$T = T_{re} + \frac{z_{top} - z_{bottom}}{v_{flow}}, \quad (6)$$

where z_{bottom} is an axial position of the bottom of the active core. The number of circulations before delayed neutron emission can be evaluated with the T and t_{emit}.

$$N_{circ} = \left[\frac{t_{emit} - t_{top}}{T}\right] \quad (7)$$

where the bracket indicates the largest integer smaller than the target. After N_{circ} recirculations, the remaining time before delayed neutron emission can be written as Eq. (8).

$$(t_{emit} - t_{top}) - N_{circ} \times T \quad (8)$$

If the remaining time is lower than T_{re}, the delayed neutron is emitted before reentering the active core. Therefore, if $(t_{emit} - t_{top}) - N_{circ} \times T < T_{re}$, then the delayed neutron is excluded from the calculation. Otherwise, the delayed neutron reenters the active core and obtains a new position. Its axial position z can be obtained from Eq. (9).

$$z = z_{bottom} + v_{flow}\left(t_{emit} - t_{top} - N_{circ}T - T_{re}\right), \quad (9)$$

and its radial position is randomly sampled due to the aforementioned assumptions.

2.2. Iterated Fission Probability

Estimating the adjoint flux has been a challenge for the Monte Carlo transport researchers since it requires additional calculations to solve the adjoint transport equation. However, the introduction of the concept called Iterated Fission Probability (IFP) allowed the calculation of the adjoint flux and adjoint-weighted parameters [3]. Especially, adjoint-weighting can be done without direct calculation of the adjoint flux.

In the iMC, the IFP is employed as done in Serpent 2 Monte Carlo code [4]. Basically, the IFP method transfers information from the ancestor until its asymptotic state. The Serpent's method integrates the roles of ancestor, latent, and asymptotic cycles in a single cycle. Given a latent cycle number L, representing minimum cycles that IFP converges, the particle transfers its previous L cycles' information. This method tallies kinetic parameters with IFP calculated from L cycles later. Adopting the method consumes more memory while offering a reduction in computing time.

3. Numerical Calculation

3.1. Problem description

A simple cylindrical molten salt reactor is modeled to simulate the reactor circulation. Figure 1 shows the structure of the reactor, and its specifications are tabulated in Table I.

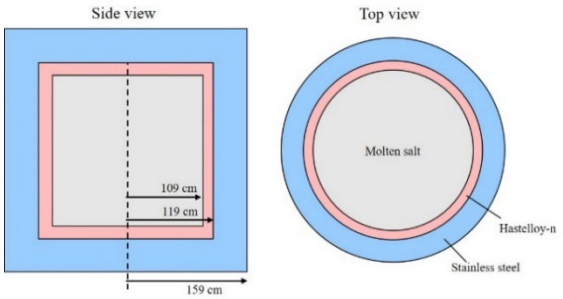


Figure 1. Reactor geometry

Table I. Reactor specification

Molten salt composition	67KCl-33UCl_3
Containment material	Hastelloy-n
Reflector material	Stainless steel

Monte Carlo transport and point kinetic parameter estimations are performed with the iMC code. Every calculation is done with 500,000 histories per cycle, 100 inactive transport cycles, and 500 active transport cycles. The calculation condition results in the standard deviation of k_{eff} being 3.3 pcm. Latent cycle length is determined to be 10 cycles, assuming that the IFP will fully converge before 10 cycles.

To demonstrate treatments for delayed neutrons in circulating fuel, 4 cases of the flow speed (v_{flow}) and 4 cases of the recirculation time (T_{re}) are selected. The flow speed of 50, 100, 150, and 200 cm/s are chosen, and recirculation times of 2, 5, 10, and 1 million seconds are selected.

3.2. Reactivity change

According to the disappearance of precursors, circulation in the molten salt reactor results in a reduction in reactivity. The reactivity reduction due to precursor escape is depicted in Fig. 2. As stated in Fig. 2, reactivity reduction become larger as flow speed increases. As the flow speed increases, more precursors escape and emits neutron outside the core, resulting in lower reactivity. In a similar sense, a larger reduction in reactivity is observed for a longer recirculation time, lowering the probability that escaped precursor re-enters the core.

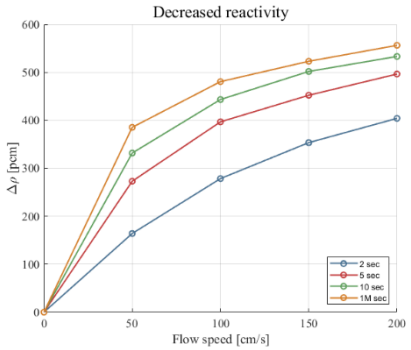
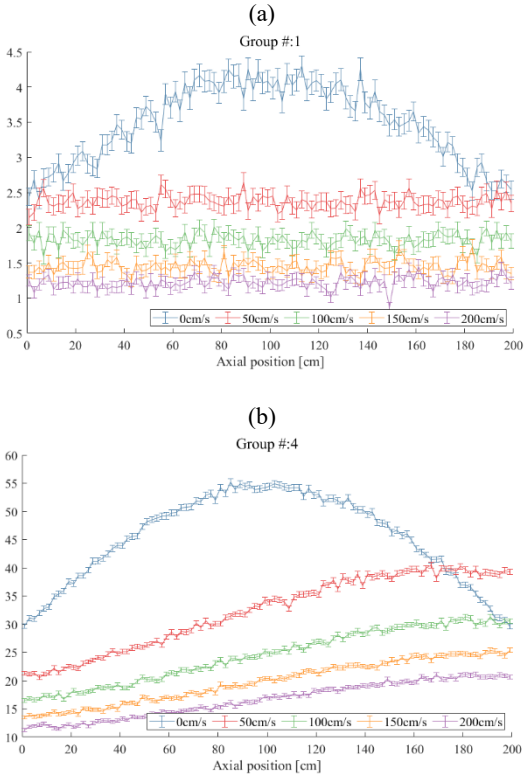


Figure 2. Reactivity reduction by flow speed and recirculation time compared to reference calculation.

3.3. Axial distribution of precursors

In this section, axial distributions of precursors are evaluated. The distributions are obtained by dividing the core into 100 regions axially. Figure 3 describes axial precursor distribution of precursor for 1st, 4th, and 6th precursor group with recirculation time of 2 seconds, respectively. The distribution of 1st group with the longest half-life is strongly affected by recirculation, flattening the distribution. Moreover, faster flow implies a shorter time remaining in the core, diminishing the amplitude of the distributions. On the other hand, for 6th group with the shortest half-life is not affected by recirculation. Therefore, as flow speed increases, the precursor distribution becomes top-skewed. In the 4th group precursor distribution, both escape and recirculation of the precursor are shown.



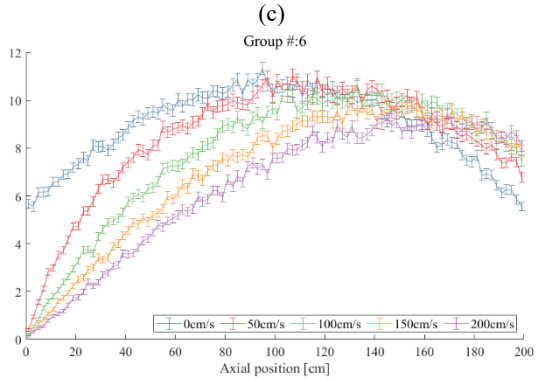


Figure 3. Axial distribution of recirculation time 2 seconds, (a) 1st precursor group, (b) 4th precursor group, (c) 6th precursor group

In the case of a recirculation time of 1 million seconds, the recirculation impact is almost excluded. Figure 4 depicts the axial precursor distribution of 1st delayed neutron group for a recirculation time of 1 million seconds. Compared to Figure 3-(a), the precursor distribution is curtailed in Fig. 4, because of negligible recirculation impact. Instead, a small escalation in the upper region is observed due to the early decay.

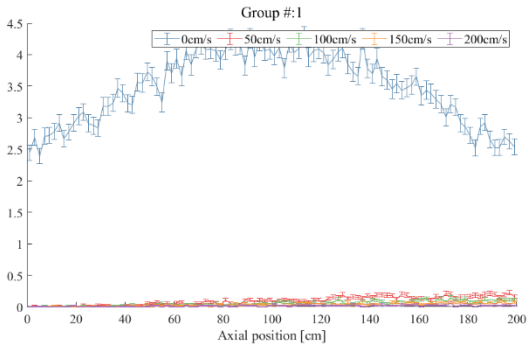
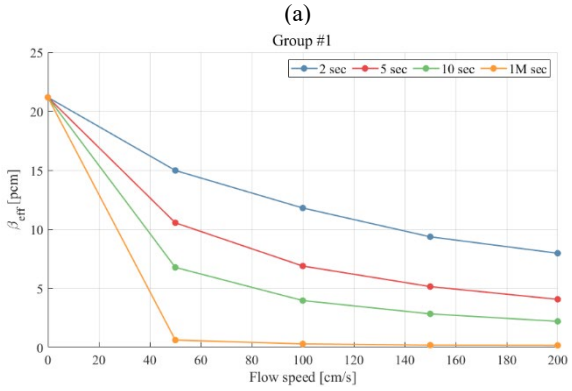


Figure 4. Axial distribution of 1st precursor group of recirculation time of 1 million seconds.

3.4. Effective delayed neutron fraction

Effective delayed neutron fraction, β_{eff} for each group and flow conditions are estimated using both forward-weighting and adjoint-weighting based on IFP.



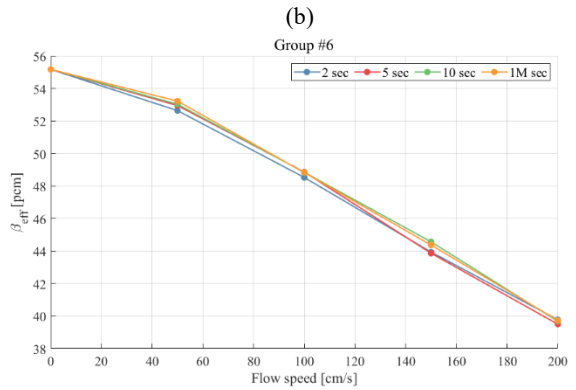


Figure 5. Adjoint-weighted effective delayed neutron fraction, (a) 1st precursor group, (b) 6th precursor group

Figure 5-(a) and (b) indicate adjoint-weighted delayed neutron fraction of precursor groups 1 and 6, respectively. Recirculation time affects significantly the 1st group since the recirculation impact is larger for longer living precursors. Additionally, as flow speed increases, both fractions decrease due to a higher probability of the precursor disappearance.

Table II. Effective delayed neutron fraction in a stationary state

Group	Forward [pcm]	Adjoint [pcm]
1	23.135 ± 0.265	21.563 ± 0.186
2	124.491 ± 0.633	118.605 ± 0.458
3	121.952 ± 0.605	117.494 ± 0.433
4	283.804 ± 0.898	283.013 ± 0.717
5	130.534 ± 0.635	133.624 ± 0.477
6	54.389 ± 0.394	55.909 ± 0.314
Total	738.305 ± 1.502	730.208 ± 1.141

Table II compares forward-weighted and adjoint-weighted effective delayed neutron fractions for each precursor group in stationary fuel. As the comparison shows, noticeable discrepancies exceeding 2σ are observed. Furthermore, the adjoint weighting resulted in lessened uncertainties compared to forward weighting.

However, when the precursor treatment is applied, uncertainty in adjoint-weighted delayed neutron fraction becomes larger. Table III shows a comparison as done in Table II for flow speed of 100 cm/s and recirculation time of 2 seconds. In the forward-weighted delayed neutron fractions, their relative uncertainties are conserved after the precursor treatments. On the other hand, in the adjoint-weighted delayed neutron fractions, its relative and absolute uncertainties exceed the stationary reactor's uncertainties.

Table III. Effective delayed neutron fraction with a flow speed of 100cm/s and recirculation time of 2 seconds

Group	Forward [pcm]	Adjoint [pcm]
1	11.734 ± 0.134	12.011 ± 0.242
2	64.991 ± 0.321	64.715 ± 0.544
3	63.693 ± 0.314	63.076 ± 0.537
4	154.354 ± 0.462	154.027 ± 0.868
5	81.547 ± 0.331	83.974 ± 0.629
6	47.503 ± 0.249	48.184 ± 0.456
Total	423.823 ± 0.766	425.988 ± 1.413

Both in the stationary and moving fuels, some discrepancies are observed. Note that the differences are smaller than in typical PWR due to the hard spectrum in the current fast-spectrum molten salt reactor.

4. Conclusions

In this paper, two essential features in analyzing the molten salt reactor and its delayed neutrons. A numerical approach for precursors in moving flow is studied and implemented in the iMC code. Plus, iterated fission probability is introduced for adjoint-weighted kinetic parameters. For a model molten salt reactor problem, reactivity change, spatial distribution, and effective delayed neutron fractions are investigated. The result concludes that the numerical approach fully considers precursor disappearance and recirculation. Moreover, the effective delayed neutron fraction leads to the importance of adjoint-weighting despite wide usage of forward-weighting in Monte Carlo calculation.

Currently, no other Monte Carlo code handles flowing precursors as done in the iMC code. The research can offer a guideline for Monte Carlo-based molten salt reactor analysis. Further studies will aim to perform a transient analysis of the molten salt reactor based on the adjoint-weighted parameters. In addition, validation by comparing with deterministic transient analysis can be accomplished due to the adjoint-weighting.

ACKNOWLEDGEMENTS

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REFERENCES

[1] H. KIM and Y. KIM, "Monte Carlo Simulation of Liquid Fuel Flow in Molten Salt Reactor in the iMC Code", Transactions of ANS (2021)
[2] H. T. KIM and Y. KIM, "Unstructured Mesh–Based Neutronics and Thermomechanics Coupled Steady-State Analysis on Advanced Three-Dimensional Fuel Elements with Monte Carlo Code iMC," Nuclear Science and Engineering (2021)
[3] Y. NAUCHI and T. KAMEYAMA, "Development of Calculation Technique for Iterated Fission Probability and Reactor Kinetic Parameters Using Continuous-Energy Monte Carlo Method," Journal of Nuclear Science and Technology **47** 11, 977, Informa UK Limited (2010)
[4] J. LEPPÄNEN et al., "Calculation of effective point kinetics parameters in the Serpent 2 Monte Carlo code," Annals of Nuclear Energy **65**, 272 (2014)