Predictor-Corrector Quasi-Static Monte Carlo Method for Molten Salt Reactor Transient Analysis

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1. Introduction

The Molten Salt Reactor (MSR) is one of the Gen-IV reactor concepts, utilizing a liquid molten salt fuel. The MSR concept offers significant potential benefits in safety, sustainability, and economic performance.

One of the critical challenges stemming from the liquid fuel is the delayed neutron precursors (DNPs) migration. In the MSRs, these precursors are transported with the fuel flow, circulating through the reactor core. When DNPs decay outside the active core region, the emitted delayed neutrons have a negligible impact on the fission chain. This reduces the effective delayed neutron fraction, thus affects the reactor response in accidental situation. The DNP migration makes high-fidelity transient analysis essential for an accurate safety assessment and design of the MSR system.

Monte Carlo method is widely regarded as the most accurate approach for neutron transport simulation as it minimizes approximations used for deterministic codes. The MSR is analyzed with the Monte Carlo method, by directly tracking DNP position [1] or solving the convection equation with externally solvers [2,3]. However, these approaches are limited to the steady-state, while high-fidelity transient analysis is demanding for accurate accident simulation.

iMC code is a continuous-energy Monte Carlo neutron transport code developed at KAIST. The iMC code features capabilities for advanced reactors, including modeling circulating fuel for MSRs and its multiphysics analysis. Moreover, transient analysis of the MSR is being developed based on both Predictor-Corrector Quasi-Static Monte Carlo (PCQS-MC) and Dynamic Monte Carlo (DMC) [4].

This work focuses on the implementation and application of the PCQS-MC method within the iMC framework for the transient analysis of MSRs. The study will describe the theoretical basis of the MSR-specialized PCQS-MC, and perform a null transient analysis for DTU TMSR benchmark to demonstrate the stability and performance of the modified PCQS-MC for MSR analysis.

2. Methods and Results

2.1 MSR Steady-State Monte Carlo Analysis

Steady-state Monte Carlo neutron transport solves the following neutron transport equation (NTE), an eigenvalue problem:

$$(L + T - S)\phi = \frac{1}{k}F\phi, \tag{1}$$

where *L*, *T*, and *S* are operators defined as below:

$$L\phi = \vec{\Omega}\cdot\nabla\phi,$$
$$T\phi = \Sigma_t\phi,$$
$$S\phi = \int\int \Sigma_s(\vec{r},\vec{\Omega}'\to\vec{\Omega},E'\to E)\phi(\vec{r},\vec{\Omega}',E')dE'd\vec{\Omega}'. \tag{2}$$

Regarding the fission operator $F\phi$, the fission contribution can be classified into prompt and delayed fission neutrons. The prompt fission contribution $F_p\phi$ can be expressed as:

$$F_p\phi = \frac{\chi_p}{4\pi}\int\int \nu\Sigma_f(\vec{r},\vec{\Omega}',E')\phi(\vec{r},\vec{\Omega}',E')dE'd\vec{\Omega}', \tag{3}$$

while delayed fission neutron is emitted from its precursor decay. Therefore, the delayed neutron contribution can be written as below:

$$F_d\phi = \sum_{g=1}^{G}\frac{\chi_{dg}(E)}{4\pi}\lambda_g C_g(\vec{r}). \tag{4}$$

where g, λ_g, and C_g are delayed neutron precursor group, decay constant and concentration, respectively. *G* is the number of delayed neutron precursor (DNP) group, typically 6 or 8 for conventional nuclear data libraries.

DNP concentration C_g is produced from the fission reaction and lost via decay. In addition, fuel convection needs to be considered for MSRs. Balance of the DNP is then expressed with Eq. (5).

$$\frac{\partial C_g}{\partial t} + \vec{U}\cdot\nabla C_g = -\lambda_g C_g + \beta_g F\phi \tag{5}$$

For static fuel, steady-state solution for C_g is analytically obtainable. However, the equation is not analytically solvable with fuel flow. The iMC code directly tracks the DNP position by sampling DNP lifetime based on their decay constant. The DNP will then emit the delayed neutrons further from their production site. For the delayed neutrons emitted out of the active core, their contribution is neglected, resulting decreased reactivity and effective delayed neutron fraction.

2.2 Predictor-Corrector Quasi-Static Monte Carlo

While the steady-state analysis solves for eigenvalue of the reactor, the time-dependent analysis aims to estimate the temporal change of the neutron flux and corresponding quantities, such as reactor power. Governing equation for the time-dependent analysis is:

$$\frac{1}{v}\frac{\partial\phi}{\partial t} + (L + T - S)\phi = F_p\phi + \sum_g \lambda_g C_g . \quad (6)$$

Two Monte Carlo methods are mainly used to solve the time-dependent NTE: dynamic Monte Carlo (DMC) and Predictor-Corrector Quasi-Static Monte Carlo (PCQS-MC) [5,6]. Unlike DMC, which directly solves the NTE, PCQS-MC solves the time-dependent Monte Carlo by modifying the neutron transport equation.

The PCQS-MC method provide solution for each timestep. Each time step comprises two steps: predictor and corrector steps. First, the predictor step solves the transient fixed-source problem (TFSP). The NTE is modified with three major approximations: implicit Euler method, linear variation of fission source, and exponential transformation [5]. Then the fixed source problem can be re-defined for time t_s, which treats previous contribution at time t_{s-1} as an external source.

$$\begin{aligned}&(L + T_{PCQS} - S)\phi_s \\ &= \frac{e^{\gamma_s\Delta t}}{v\Delta t}\phi_{s-1} + \sum_{g=1}^{G} f_{1g}\lambda_g C_{gs-1} + \sum_{g=1}^{G} f_{2g}\beta_g F\phi_{s-1} \\ &\quad + \sum_{g=1}^{G} f_{3g}\beta_g F\phi_s + (1-\beta)F\phi_s \quad (7)\end{aligned}$$

where

$$\begin{aligned}T_{PCQS} &= T + (v\Delta t)^{-1} + \frac{\gamma}{v} \\ \gamma &= \frac{1}{\Delta t} ln\left(\frac{\int\int\int \phi_{s-1} d\vec{r} d\vec{\Omega} dE}{\int\int\int \phi_{s-2} d\vec{r} d\vec{\Omega} dE}\right) \\ f_{1g} &= exp(-\lambda_g\Delta t) \\ f_{2g} &= \frac{1}{\lambda_g\Delta t}\left(1 - (1 - \lambda_g\Delta t)f_{1g}\right) \\ f_{3g} &= 1 - f_{1g} - f_{2g} \quad (8)\end{aligned}$$

After solving the predictor step, point kinetics (PK) method is solved and adjusts the predictor solution. The point kinetics approach is based on factorization of the angular neutron flux ϕ into shape and amplitude functions:

$$\phi(\vec{r},\vec{\Omega},E,t) = n(t)\varphi(\vec{r},\vec{\Omega},E,t) \quad (9)$$

The amplitude and shape functions satisfies the condition. The integration over the space, energy, and angle is expressed with the bracket.

$$\langle W, \frac{1}{v}\phi\rangle = \langle W, \frac{1}{v}\phi_0\rangle \quad (10)$$

where W is a weighting function. In this study, the weighting function is fixed to unity for simplicity.

The time-dependent NTE is re-visited and integrated over space, energy, and angle, with weighting faction W is applied.

$$\begin{aligned}&\frac{\partial}{\partial t}\langle W, \frac{1}{v}\phi\rangle + \langle W, (L + T - S)\phi\rangle \\ &= \langle W, F_p\phi\rangle + \sum_{g=1}^{G}\langle W, \lambda_g C_g\rangle . \quad (11)\end{aligned}$$

By applying the shape function, the integrated NTE can be expressed with amplitudes:

$$\frac{\partial n}{\partial t} = \frac{\rho - \beta}{\Lambda} n + \sum_{g=1}^{G} \lambda_g c_g \ , \quad (12)$$

where

$$\begin{aligned}\rho(t) &= 1 - k^{-1}, k(t) = \frac{\langle W, F\varphi\rangle}{\langle W, (L + T - S)\varphi\rangle} \\ \beta(t) &= \frac{\langle W, \beta F\varphi\rangle}{\langle W, F\varphi\rangle} \Lambda(t) = \frac{\langle W, \frac{1}{v}\varphi\rangle}{\langle W, F\varphi\rangle} c_g(t) = \frac{\langle W, C_g\rangle}{\langle W, F\varphi\rangle}. \quad (13)\end{aligned}$$

The quantities are tallied during the predictor step. Similarly, the DNP balance equation can be expressed with amplitude n and c_g.

$$\frac{\partial c_g}{\partial t} = -\lambda_g c_g + \frac{\beta_g}{\Lambda} n \quad (14)$$

The PK equation system is solved from t_{s-1} to t_s. The neutron flux and corresponding tallies, such as power distribution, is adjusted with n.

2.3 Application to MSR

To apply the PCQS-MC to MSR transient, the method needs to be modified to handle DNP properly. For predictor step, linear variation of the fission source is assumed to estimate evolution of DNP concentration. The fission term is now expressed with linear variation of two fission source, but with at different location $\vec{r}_{s-1}$ and $\vec{r}_s$.

$$\begin{aligned}F\phi(\vec{r}(t),\vec{\Omega},E,t) &= \frac{t_s - t}{\Delta t} F\phi(\vec{r}_{s-1},\vec{\Omega},E,t_{s-1}) \\ &+ \frac{t - t_{s-1}}{\Delta t} F\phi(\vec{r}_s,\vec{\Omega},E,t_s) . \quad (15)\end{aligned}$$

The change transforms the f_{2g} term's position into previous timestep's, but keeping position for current timestep. Also, DNP migration is considered in f_{1g} term.

Thus, the aforementioned sources are stored for next timestep with their position changed by the fuel flow. Then the modified TFSP is expressed below:

$$\begin{aligned}(L + T_{PCQS} - S)\phi_s\vec{r}(t_s) &= \frac{e^{\gamma_s\Delta t}}{v\Delta t}\phi_{s-1}\left(\vec{r}(t_s)\right) \\ &+ \sum_{g=1}^{G} f_{1g}\lambda_g C_{gs-1}\left(\vec{r}(t_{s-1})\right) \\ &+ \sum_{g=1}^{G} f_{2g}\beta_g F\phi_{s-1}\left(\vec{r}(t_{s-1}), \vec{\Omega}, E\right) \\ &+ \sum_{g=1}^{G} f_{3g}\beta_g F\phi_s\left(\vec{r}(t_s)\right) + (1-\beta)F\phi_s\left(\vec{r}(t_s)\right) \quad (16)\end{aligned}$$

where $\vec{r}(t_s)$ is a position after migration of Δt from $\vec{r}(t_{s-1})$.

In the MSR, DNP balance equation is modified into Eq. (5). The precursor balance equation is again integrated over active core region, with weighting function *W* multiplied.

$$\frac{\partial}{\partial t}\langle W, C_g\rangle + \langle W, \vec{U}\cdot\nabla C_g\rangle = -\lambda\langle W, C_g\rangle + \langle W, \beta_g F\phi\rangle \quad (17)$$

By applying definition from Eq. (13) and divergence theorem to convection term, the integrated DNP balance equation can be re-written as below.

$$\frac{\partial c_g}{\partial t} = -\lambda_g c_g - R_g + \frac{\beta}{\Lambda}n. \quad (18)$$

where R_g can be written as a net loss rate of the DNP from the active core, weighted with *W*. Considering the structure of the active core, the term stands for leakage and re-entrance of the DNP at time t_s.

Since the DNP leakage and re-entrance needs to be considered, ex-core DNP needs to be properly handled. As in steady-state, ex-core DNPs have negligible contribution to the overall fission chain. In the modified PCQS-MC, ex-core precursor's amplitude c_{go} is additionally treated. This rewrites the DNP balance in the active core as below:

$$\frac{\partial c_g}{\partial t} = -\left(\lambda_g + R_{leak}\right)c_g + R_{re-enter}c_{go} + \frac{\beta}{\Lambda}n, \quad (19)$$

and the balance of ex-core DNP can be expressed as:

$$\frac{\partial c_{go}}{\partial t} = -\left(\lambda_g + R_{re-enter}\right)c_{go} + R_{leak}c_g. \quad (20)$$

The rates of DNP leakage and re-entrance are evaluated based on their migration in between timesteps. R_{leak} stands for a fraction of in-core DNPs leaking out within time $t \in [t_{s-1}, t_s]$. In practical sense, snapshot of the leakage rate is nearly impossible to estimate. Therefore, time-integrated DNP leakage is used to evaluate the rate. For the time bin $t \in [t_{s-1}, t_s]$, R_{leak} can be estimated as below. $R_{re-enter}$ can be calculated in a similar way.

$$R_{leak}(t) = \frac{1}{C}\frac{dC}{dt}_{leak} \cong \frac{\Delta C_{leak}}{C\Delta t} \quad (21)$$

When TFSP analysis is completed with tallying the PK parameters, a system of PK equation is constructed. Conventional PK comprises *G + 1* equations, one of Eq. (12) and Eq. (14) for *G* DNP groups. However, due to introduciton of flow rates within in-core and ex-core, *2G + 1* equations is required for the modified PK. The system is composed of one Eq. (12), Eqs. (19) and (20) for each DNP groups.

During the predictor step, time-dependent $k(t)$ and $\beta(t)$ are tallied based on Eq. (13). Suppose that the steady-state is critical, then corresponding $k(t)$ is expected to be larger than unity as 'snapshot' at certain timestep cannot reflect reduction in reactivity and effective delayed neutron fraction. The reduction is also omitted for $\beta(t)$. As point kinetics contains $\rho - \beta$, this will not cause bias during the transient.

3. Numerical Result

3.1 Problem description

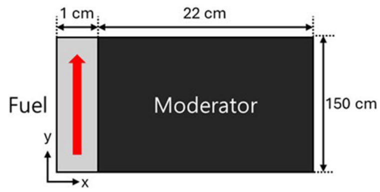

Fig. 1. DTU TMSR benchmark model (not to scale)

The DTU TMSR benchmark model is solved with the modified MSR PCQS-MC scheme [1,7]. This model is widely utilized to verify the performance of high-fidelity codes for time-dependent MSR analysis. The system is composed of a liquid fuel salt channel and a graphite moderator. For the graphite, thermal scattering library S(α, β) is utilized to accurately analyze the graphite-moderated thermal system. The physical properties, including temperature and density distributions, are applied to the iMC calculation mesh-wise. For the null transient, the steady-state distributions of temperature, density, and flow velocity are utilized as the initial condition [1].

For the Monte Carlo analysis, 500,000 histories per cycle and 20 inactive cycles are used to obtain a converged initial state. After the convergence of the fission source, the PCQS-MC calculation is performed with timestep of 0.1 seconds. PCQS-MC step comprises 20 inactive and 100 active cycles per timestep.

The current study focuses on the sole neutronics behavior, so it excludes any thermal feedback during the simulation. For the neutron cross-section library, ENDF/B-VII.1 is utilized. The steady-state eigenvalue of the reactor is calculated, and for the null transient, the reactor is forced to be critical by adjusting the neutron yield with steady-state k_{inf}, 0.99660.

3.2 Null-transient result

Figures 2 and 3 denotes evolution in relative power to the initial state, and dynamic reactivity, respectively. Error bars in Fig. 3 stands for 1-sigma uncertainty, where the value is around 30 pcm.

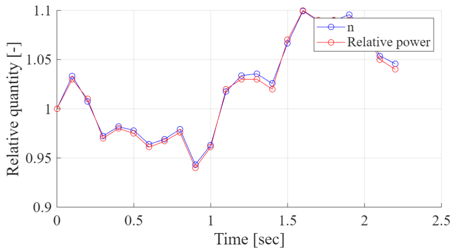

Fig. 2. Relative power evolution during null transient

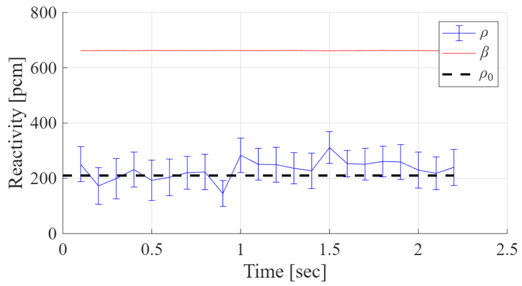

Fig. 3. Dynamic reactivity and delayed neutron fraction

As mentioned in previous seciton, although the steady-state solution is critical, dynamic reactivity is clearly positive due to ex-core DNPs. Nevertheless, the power evolution stays 10 % within steady-state power. According to Eq. (12), $\partial n/\partial t = 0$ can be obtained with:

$$\rho_0 = \beta - \frac{\Lambda}{n}\sum_g \lambda_g c_g \tag{22}$$

where ρ_0 can be estimated to 210 pcm, plotted on Fig. 3.

The transient fixed source problem considers previous timestep's contribution as external sources as in Eq. (11). Fig. 4 shows k-value evaluated from each source. Recalling the definition of v^{-1} term, mostly composed of thermal neutrons, its k-value excels others. In other hand, precursor showed noticeably low k-value, as the distribution is up-skewed, causing more leakage.

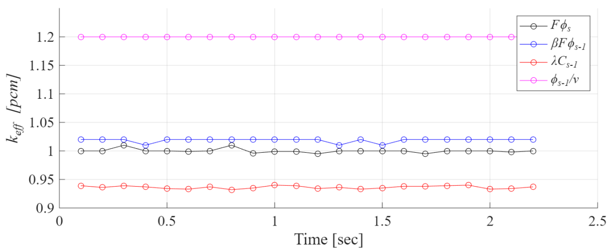

Fig. 4. k-value of various sources in predictor step.

4. Conclusions

This study suggests a time-dependent Monte Carlo method for molten salt reactors by adapting the Predictor-Corrector Quasi-Static Monte Carlo (PCQS-MC) method for flowing fuel systems. The PCQS-MC methodology is specifically modified to account for the transport of delayed neutron precursors (DNPs). Preliminary null transient results using the DTU TMSR benchmark demonstrate that the balance between the neutron and precursor populations is preserved, ensuring that the steady-state solution is maintained throughout the transient. This approach provides a robust tool for accurate safety analysis and design of MSRs.

The work will be extended to complete transient analysis of the MSR by coupling with external programs, including OpenFOAM computational fluid dynamics code. Furthermore, validation and verification will be conducted for various MSR designs and scenarios by comparing with experimental data, deterministic codes, and Dynamic Monte Carlo method.

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