Depletion of molten salt reactor with online salt conditioning in the Monte Carlo iMC code

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1. Introduction

The molten salt reactor (MSR), which is often regarded as one of the Gen IV advanced reactor systems, utilizes liquid fuel in the form of salt. The use of liquid fuel incurs incorporation of original concepts that are hardly found in contemporary reactors including the off-gas system, helium bubbling system, and online feeding.

The bubbling system injects sparse helium bubbles at the bottom of the reactor which rise to the top and then escape from the reactor. During the rise of the bubbles, the insoluble fission products are captured alongside and are removed from the reactor system as the bubbles egress the active core. The removed materials are majorly noble metals including Se, Tc. Furthermore, the noble gas also floats by itself and escapes the system as well. One could envision that the removal of these fission products, especially highly absorbing fission products, could enhance reactor performance. Another system that influences reactor performance is online feeding, which includes various feeding strategies such as continuous refueling.

Accommodation of such aforementioned systems is crucial for analyzing the MSR reactor, especially for depletion calculation which depends on the material concentration change at the previous steps.

In this paper, the implementation of such systems to Monte Carlo (MC) transport simulation code iMC is considered. Nuclide removal and fuel feeding are realized by modifying the burnup matrix which is used during depletion calculation. The mathematical expression of conditioning and actual application in the code will be discussed, along with the analysis result of a simple molten salt reactor model.

2. Methods

2.1 Nuclide removal

During reactor lifetime, fission products are produced and some long-lived products are accumulated by the fission reaction. The fission products may noticeably discourage reactor performances if they have relatively high absorbing cross-sections. Thus, extracting them from the reactor ensures reactor performance enhancement.

In the molten salt reactor, insoluble fission products can be removed from the reactor by an off-gas system. By injecting sparse helium bubbles from the bottom of the reactor, they will rise to the top of the reactor then eventually escape from the reactor. During the rise of the bubbles, noble metals can be attached to the surface of the bubbles and carried out of the reactor. In addition, the noble gas will egress from the liquid fuel and be removed from the reactor. Due to the absorption cross-section of the removed nuclides, the overall performance of the reactor is expected to be improved. Therefore, considering the nuclide removal is essential in burnup calculation for precise simulation.

Simulating fuel depletion is done by applying a burnup matrix, offering the rate of change of each nuclide due to neutron interaction and decay. Implementing both removal and feeding are done by modifying such matrix. Removal of the nuclide is proportional to the concentration of removed nuclides. Therefore, nuclide removal can be implemented by adopting fictitious decay constants [2]. These decay constants can be obtained from removal efficiency and circulation time

The concentration changes of nuclides due to decay can be obtained from exponentials of decay constants. Concentration after time t is defined as

$$\mathrm{N(t) = N(0)\exp[-\lambda t]}, \tag{1}$$

where λ is decay constant, N is a concentration of the nuclide.

The concentration of removed nuclide after time t, N(t), is utilized to express the extent of removal via fictitious decay constants. When the removal procedure is applied, various parameters can affect the removal rate. Hence, for the presented study, such considerations are all integrated into efficiency, which corresponds to a fraction of removed nuclides after the removal procedure. Then, using the definition, concentration after circulation time T, N(T) can be written as Eq. (2) when time-dependent concentration without removal procedure, $\mathrm{N_0(T)}$ is given.

$$\mathrm{N(T) = N_0(T)(1-R)} \tag{2}$$

Regarding decay, $\mathrm{N_0(t)}$ can be defined as Eq. (3).

$$\mathrm{N_0(t) = N_0(0)\exp[-\lambda_0 t]} \tag{3}$$

where λ_0 is the decay constant of the material.

When fictitious decay constant is applied, its concentration after procedure period T can be induced from Eqs. (1)-(3), as Eq. (4). The fictitious decay constant can be defined with removal efficiency R and procedure period T.

$$\frac{N(T)}{N_0(0)} = \exp[-\lambda T] = (1-R)\exp[-\lambda_0 t] \\ \rightarrow \lambda_{fic} = \lambda - \lambda_0 = -\frac{\ln(1-R)}{T} \quad (4)$$

In iMC, prior to depletion calculation, fictitious decay constants are calculated based on the input file. The input includes removed materials' atomic numbers, their removal efficiency R, and circulation time T. Only atomic numbers are required in this case, since only physical characteristics of the material affect the off-gas system which is majorly determined by atomic number. During depletion calculation, the fictitious decay constants are added to the burnup matrix. Other steps are identical to typical depletion calculation.

2.2 Fuel feed

During the operation of the reactor, i.e., fission reaction occurs, fissionable materials are depleted, which directly determines the lifetime of the reactor. To increase the reactor lifetime, fresh fuel can be fed into the reactor. Since the addition of fissionable material will noticeably affect reactor performance, considering fuel feeding is imperative for reactor simulation under such circumstances.

In this research, continuous refueling has been postulated [3], which indicates continuous refueling of fresh fuel to balance the number of fission materials consumed by fission. Whereupon, the fresh fuel feed rate becomes identical to the fission rate with continuous refueling:

$$\Delta\left(\frac{dN_i}{dt}\right) = +r_i R_{fission}, \quad (5)$$

where Δ refers to increment of rate of change, $R_{fission}$ is fission rate, and r_i is an atomic ratio of nuclide i compared to the total amount of fissionable materials in the feed. The fraction r_i needs to be compared to the total amount of fissionable materials since the scheme aims to refill fissionable materials according to the fission rate. Hence, continuous refueling applies fictitious cross-section to transform fissionable material into fresh fuel materials. An increase in the feed material concentration can be written as below, which hinges upon neutron flux and fictitious cross-section

$$\Delta\left(\frac{dN_i}{dt}\right) = \sum_{j=fiss.} r_i \sigma_{j,f} \phi N_j, \quad (6)$$

where j is fissionable nuclides, $\sigma_{j,f}$ is microscopic fission cross section of nuclide j and ϕ is neutron flux.

3. Validation

A simple molten salt reactor model is proposed to test nuclide removal and feed. The configuration of the reactor is illustrated in Fig. 1, and its specification is enumerated in table I.

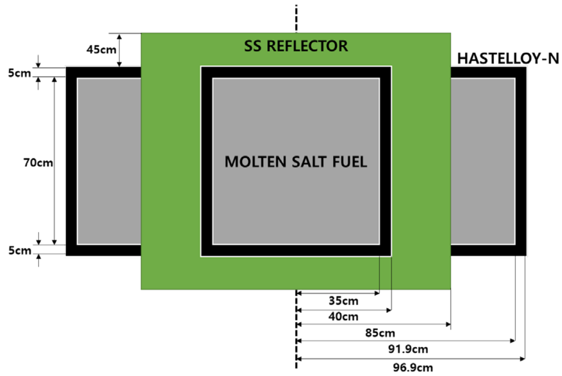

Figure 1. Reactor geometry

Table I. Reactor specification

Molten salt composition	67KCl-33TRUCl
Containment material	Hastelloy-n
Reflector material	Stainless steel
Nominal power	100MWth

Monte Carlo transport simulation is done with the iMC code developed in KAIST [4]. The calculation was done with 20,000 histories per cycle, 100 inactive cycles, and 200 active cycles, resulting in a standard deviation of about 30 pcm. The reactor is depleted for 20 years and the depletion step varies from few days to years. Chebyshev Rational Approximation Method (CRAM) is used as a matrix exponential solver.

Nuclide removal is applied to noble metals and noble gases. Target noble metals include 10 elements such as Se, Mo, Tc. The method also removes noble gas including Xe and Kr. Both noble metal and gas are removed periodically with circulation time T = 10 seconds, while their removal efficiency differs and compared. Fuel feed is done with continuous refueling of fresh fuel with composition as same as initial fuel of the reactor, 67KCl-33TRUCl.

Validity testing has been conducted for implementing both nuclide removal and continuous refueling strategies respectively. Changes in both effective multiplication factor (k-eff) and nuclide concentration will be measured and compared with the conventional depletion calculation result where removal nor feeding schemes are applied.

Nuclide removal is simulated with different removal efficiency with the same removal periods. The test cases are given in Table II. Noticeable change in nuclide concentration and following additional reactivity is observed due to removal of absorbing nuclides. Furthermore, validity of the nuclide removal is tested by comparing material concentration with estimated value based on deterministic calculation.

Continuous feeding is tested for its impact on reactor performance. The refueling scheme solely compensates for fuel loss due to fission reaction, not considering material buildup due to decay or neutron capture in this scope. The impact may be significant for some types of fuel.

Table II. Test cases and their removal efficiencies

Case #	Noble gas [%]	Noble metal [%]
Reference	0	0
1	90	90
2	50	50
3	90	50
4	90	0

4. Result

4.1 Nuclide removal

Nuclide removal is applied to the molten salt reactor model with circulation time T = 10 seconds. Effective multiplication factor and material-wise comparison are done with different removal efficiencies.

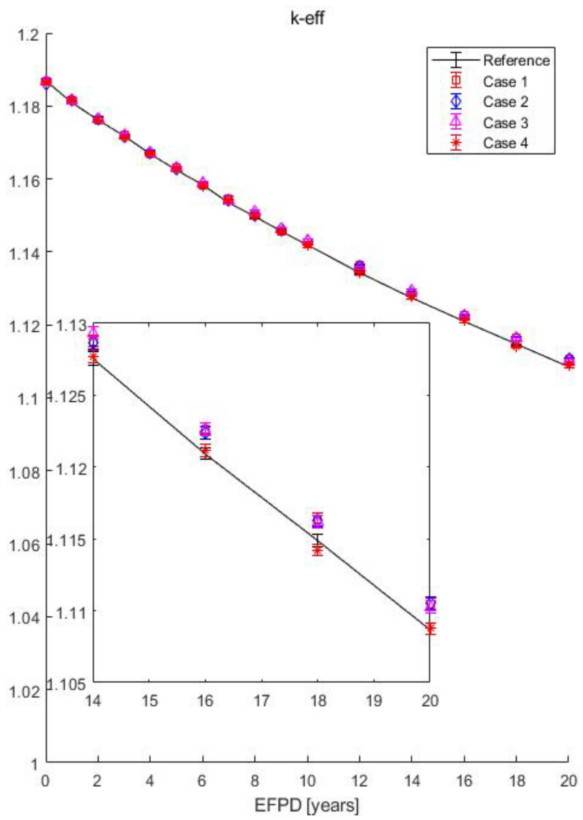

Figure 2. k-eff comparison between reference and removal test cases with different removal efficiencies. Error plotted with 2σ

Figure 2 shows that removing nuclides from the reactor enhances reactor performance as the reactor gets depleted. In terms of reactivity, the difference in the removal efficiency does not have a serious effect since circulation time is negligibly short compared to burnup step, resulting in sufficient removal with lower efficiency. In contrast to the thermal reactors, where Xenon severely discourages the reactivity, noble gas removal merely affects reactor performance due to lower absorption cross-section for fast neutrons. However, removing noble metals affects reactivity considerably by virtue of their relatively high fast neutron absorption cross-section. These impacts can be easily seen when comparing cases (1)-(3) and case (4). While cases (1)-(3) showed definite offset in consequence of sufficient removal of noble metal, when only noble gas removal is done as case (4), reactivity had no meaningful change from the reference.

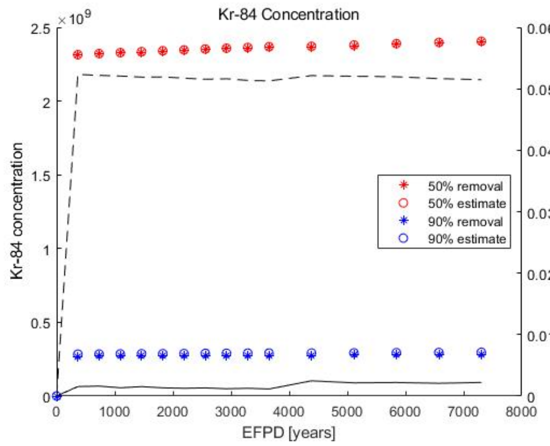

Figure 3. Kr-84 concentration and an estimation as a representative of removed noble gas

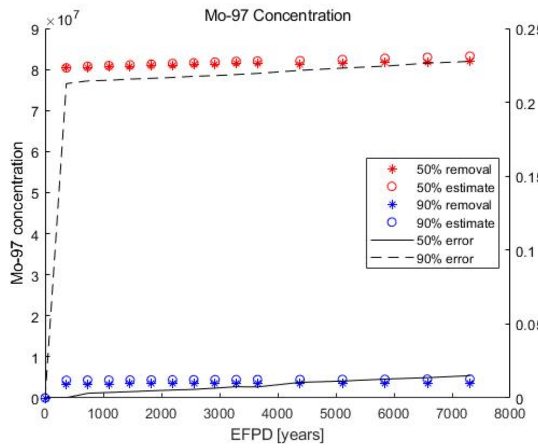

Figure 4. Molybdenum-97 concentration as a representative of removed noble metal

Figures 3 and 4 show comparisons of nuclide concentration to observe change due to nuclide removal. Figure 3 shows the concentration of Kr-84 as a representative of removed noble gas. As a representative of noble metal, Mo-97 concentration is plotted in Fig. 4. Both nuclides' concentrations are compared with estimation based on following procedure. Removal of the target's parent nuclides is considered by recalculating concentration, excluding the target nuclide removal only. Based on the result, deterministic removal is simulated to evaluate a concentration of the removed nuclide. Every result showed agreement with estimations.

4.2 Continuous refueling

A continuous refueling scheme is applied to MSR and approved. The scheme targets to feed fissionable materials with amount identical to fissionable materials loss from a fission reaction.

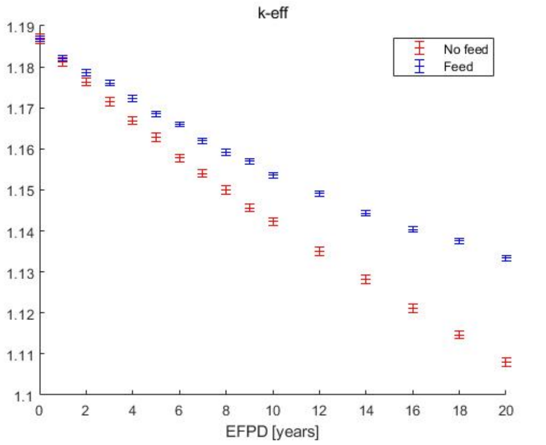

Figure 5. k-eff comparison between reference and continuous refueling. Error plotted with 2σ

As Fig. 5 displays, the effective multiplication factor is conserved in some measure due to the compensation of fissionable materials of the reactor. Reactivity loss is expected to be originated from non-fission loss of fissionable materials and accumulation of fission products.

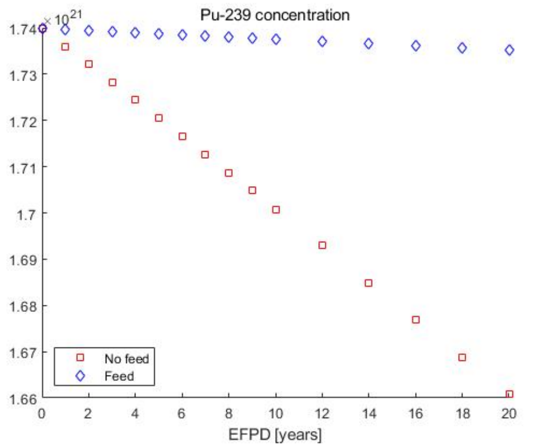

Figure 6. Pu-239 concentration

In addition to the multiplication factor, comparisons on fissionable materials' concentrations are done. Fig. 6 compares Pu-239 concentration. It can be clearly seen that the Pu-239, which is major fissile nuclide of the reactor is virtually conserved due to the continuous refueling scheme.

5. Conclusion

In this study, nuclide removal using the off-gas system and refueling scheme was considered. The systems highly affect reactor performance. Thus, the development of reactor depletion calculation to accommodate such systems is imperative for accurate analyses of the molten salt reactor. Whereupon, numerical expression and implementation in the depletion module for Monte-Carlo code iMC has been conducted accordingly.

Based on fictitious decay constant and cross-section, preliminary depletion calculation was performed for a simple molten salt reactor model comprised of uranium chloride fuel. Both nuclide removal and refueling considerations were applied to the reactor model respectively and a comparison has been made to the conventional depletion calculation.

Removing noble metal and gas species showed clear reactor performance improvement as expected, where the material-wise comparison also agreed with the removal scheme. The adoption of a continuous refueling concept also exhibited a salient increase in the reactor performance, which is characterized by enhanced Pu239 concentration.

The observed result comprehensively attests to the effectiveness of the proposed schemes for considering the unique systems of MSR. Further research will aim to contemplate a more realistic MSR reactor system.

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