Molten Salt Reactor Simulation Capability Using MPACT

Benjamin Collins, Cole Gentry, Shane Stimpson

Oak Ridge National Laboratory, 1 Bethel Valley Rd., PO Box 2008 MS-6172, Oak Ridge, TN 37831
collinsbs@ornl.gov, gentryca@ornl.gov, stimpsonsg@ornl.gov

Abstract – *The recent interest in molten salt reactor technology by the nuclear industry has sparked significant interest in developing modeling and simulation tools for molten salt reactors. The MPACT whole core transport solver has been adapted to address several unique features of molten salt reactors. This paper discusses implementation of a depletion methodology which simulates the mixing of fuel throughout the core, the continuous removal of fission products, and the continuous addition of new fuel into the system. It also presents the methodology used to treat the transport of delayed neutron precursors. These new methods are demonstrated using models based on Transatomic Power Corporation's molten salt reactor design.*

I. INTRODUCTION

The US Department of Energy (DOE) and industry have shown significant interest in advanced reactors, as evidenced by 1.3 billion dollars in private investment in companies aiming to develop advanced reactor concepts [1]. More than seven of these advanced reactor concepts use molten salt reactor (MSR) technology. In response to the interest in MSR technology, Oak Ridge National Laboratory (ORNL) is developing MSR simulation, extending capabilities in VERA [2] to model this high profile reactor concept. In addition, ORNL is also developing similar capabilities into SCALE for 2D lattice codes [3].

The extension of MPACT's deterministic neutron transport capability for VERA has been adapted to address liquid fuel MSRs. This work focuses on modifications to depletion algorithms to account for isotopic mixing, continuous feed, and continuous removal. Additionally, a new model is added to account for drift of precursors as the liquid fuel flows upward in the reactor. Finally, initial simulations are performed for two different reactor types.

II. SIMULATION METHODOLOGY

The 3D pin-resolved reactor transport code MPACT has been under development by ORNL and the University of Michigan. The methods in MPACT are documented in literature [4,5,6], and a brief outline is presented here to discuss the 3D solution mechanism using the 2D/1D method.

The 2D/1D method is used to solve the neutron flux distribution throughout the core. This is accomplished by using the 2D method of characteristics (MOC) in the radial planes to capture the heterogeneity in the radial direction with high accuracy. Each pin cell is explicitly modeled, and even sub-pin detail can be captured. In the axial direction, a low-order transport solution is obtained through NEM-P3 on a pin-cell homogenized basis. The axial and radial solutions are linked through the use of transverse leakage terms, ensuring neutron balance in every pin cell at convergence. A coarse mesh finite difference (CMFD) [7] solver is used to accelerate the convergence of the radial and axial solvers. More detail on the 2D/1D methodology used in MPACT can be found in Collins 2014 [6]. In this work, MPACT uses a 252 energy group cross section library based on ENDF/B VII.1 data with subgroup parameters to capture self-shielding effects.

1. Liquid Fuel Depletion

The existing depletion capability implemented in MPACT [8] uses ORIGEN [9] to deplete fixed fuel with multiple radial rings in each axial plane. Since the liquid fuel of MSRs is not fixed and is instead a flowing mixing system, the MPACT depletion capability must be updated to handle the fluid nature of MSR fuel. For steady-state analysis, which is the initial focus of this work, the mixing fluid depletion model can be simplified. The fluid will circulate throughout the reactor core at a rate of several cycles each hour. Since steady-state analysis can address time steps on the order of weeks or even months, it can be assumed that the fuel is well mixed. This assumption allows for depletion of the primary loop as a single lumped depletion region in which the integrated reaction rates of the entire fuel salt are applied uniformly over the entire salt volume. This applies not only to the fuel volume within the reactor region, but also to the volume residing outside the core in a negligible flux environment.

When performing a typical depletion simulation, MPACT calculates the isotopic reaction rates for absorption and fission for each depletion region using the local shielding-corrected cross sections and the local multigroup fluxes solved for during the transport calculation. MPACT then passes these isotopic reaction rates to ORIGEN—along with the initial nuclide vector and the time step—to perform the depletion calculation. To achieve the desired salt-integrated reaction rate behavior for the well-mixed salt assumption, the local shielding corrected cross sections and multigroup fluxes are averaged over the entire salt:

$$\bar{\sigma}_{i,g} = \frac{\sum_j \sigma_{i,j,g} \phi_{j,g} V_j}{\sum_j \phi_{j,g} V_j}, \quad (1)$$

$$\bar{\phi}_g = \frac{\sum_j \phi_{j,g} V_j}{TSV}, \quad (2)$$

where i denotes the isotopic cross section index, j is the in-core depletion region index, g is the energy group, σ is the depletion region microscopic cross section, ϕ is the depletion region flux, V is the depletion region volume, and TSV is the total salt volume specified in the model input. These salt-averaged cross sections and fluxes are then used in place of the original region cross sections and fluxes to invoke uniform reaction rates for all fuel regions while preserving the integrated reaction rates of the entire salt volume. The TSV variable is used to capture the effect of some portion of the salt volume residing outside the reactor region, where a zero flux condition is assumed. This type of implementation is the least intrusive modification to the current coding structure for the depletion subroutines and has a negligible impact on computation times.

Another component that must be considered in the depletion methodology for MSRs is the handling of both continuous feed of fuel material and subsequent removal of fission products. While ORIGEN has the capability to handle both of these mechanisms, the tracking of removed isotopes is not straightforward. Removed isotope tracking is necessary for waste accounting, determining fission gas retention times, and eventual recycling streams. Therefore, MPACT manages the addition and removal of material external to ORIGEN, and it allows for batched material transfer before or after any depletion step, as well as continuous transfers which occur at the end of depletion renormalization substeps. Since MPACT controls the addition and removal mechanisms, it can easily track and report the material transfers that are made.

2. Precursor Drift

Although it can be assumed that the fuel is uniformly mixed during steady state depletion analysis, the drift of precursors to delayed neutron emission cannot be ignored. To account for this effect, the standard 6 precursor groups are used. The standard precursor balance equation is modified to have a convection term of precursor concentration carried by the fluid velocity:

$$\frac{dC_k}{dt} = \beta_k \int \nu \Sigma_f \phi dE - \lambda_k C_k - \vec{\nabla} \cdot \left(C_k \vec{v}\right), \quad (3)$$

where C_k is the k-th precursor group, β is the fission yield of the k-th group, λ is the precursor decay constant, and $\vec{v}$ is the fluid velocity vector. The implementation into MPACT assumes steady-state axial drift, which simplifies equation (3) to:

$$\frac{d\left(C_k v_z\right)}{dz} + \lambda_k C_k = \beta_k \int \nu \Sigma_f \phi dE. \quad (4)$$

The axial velocity is also assumed to be constant based on user input. With this assumption, an analytic solution can be obtained for the precursor concentration across a mesh element with a constant fission source:

$$C_k(z) = C_k(0) e^{-\frac{\lambda_k}{v_z} z} + \frac{\beta_k}{\lambda_k} \Psi \left(1 - e^{-\frac{\lambda_k}{v_z} z}\right), \quad (5)$$

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where Ψ is the total fission source.

The precursor concentration distribution is known if the incoming precursor concentration is known. The average precursor concentration can be calculated by integrating over a mesh cell of height H to obtain

$$\bar{C}_k = \frac{\left(C_k(0) - C_k(H)\right) v_z}{\lambda_k H} + \frac{\beta_k \Psi}{\lambda_k}. \quad (7)$$

With this formulation, the precursor concentration can be determined by starting at the bottom of the core and progressing upward across each axial plane for every flow channel using Eq. (7) to determine the cell average concentration, as well as Eq. (6) to determine the outgoing concentration, which becomes the incoming concentration for the next cell.

The outgoing flow from the top of the core is averaged by flow channel area to obtain the concentration outside of the core. This average concentration is modeled around the remainder of the primary loop represented by L_{ext}. Since it is assumed that there is not a fission source outside the core, Eq. (6) simplifies to:

$$C_{k,core,in} = C_{k,core,out} e^{-\frac{\lambda_k}{v_z} L_{ext}}. \quad (8)$$

The new core inlet concentration is used to resolve the core concentration until the inlet concentration change is small. This process is continued for all six precursors.

Once the concentrations are known for all groups throughout the core, the delayed neutron source can be determined:

$$\Psi_{delayed} = \sum_{k=1}^{6} \lambda_k \overline{C}_k \ . \qquad (9)$$

The fission source term is

$$Q_{fission,g} = (1-\beta)\chi_g \Psi + \chi_{d,g} \sum_{k=1}^{6} \lambda_k \overline{C}_k \ . \qquad (10)$$

MPACT uses CMFD acceleration to converge the eigenvalue of the system. To modify the fission source into a form where there is no inhomogeneous source, the delayed precursor source is modified to be scaled by the fission source from the previous iteration:

$$Q_{fission,g} = \left((1-\beta)\chi_g + \chi_{d,g} \frac{\sum_{k=1}^{6} \lambda_k \overline{C}_k}{\Psi_{old}} \right) \Psi \ . \qquad (11)$$

At convergence, this form of the fission source yields the same source as Eq. (10).

For the special case when the velocity is zero and the precursors are stagnant, Eq. (7) shows that the precursor concentration becomes

$$\overline{C}_k = \frac{\beta_k \Psi}{\lambda_k} , \qquad (12)$$

so the fission source simplifies to the standard definition of the fission source:

$$Q_{fission,g} = \left((1-\beta)\chi_g + \chi_{d,g}\beta \right) \Psi \ . \qquad (13)$$

III. RESULTS

The reactor model used in this work is based on the reactor concept being proposed by Transatomic Power Corporation (TAP) [10]. The TAP reactor is a 1,250 MWth MSR with LiF-based uranium fuel. Unlike previous MSR designs such as the Molten Salt Reactor Experiment (MSRE) [11], the TAP reactor uses zirconium hydride moderator rods in the core to control reactivity.

The capabilities developed are demonstrated using the MSR lattice cell model illustrated in Figure 1.
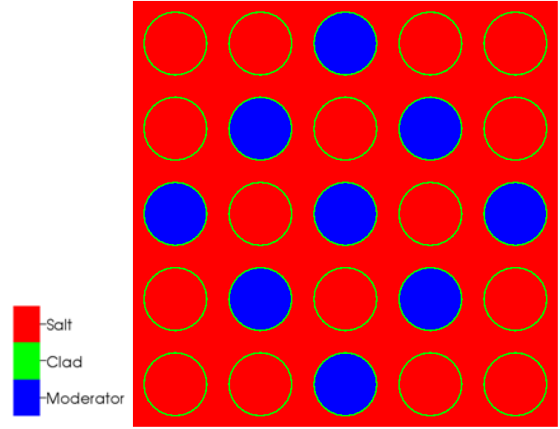

Fig. 1. TAP lattice cell.

1. Liquid Fuel Depletion

The lumped depletion and material transfer components are demonstrated using the TAP lattice cell and fuel addition and fission product removal rates set to sensible values. Figure 2 demonstrates how the employment of the different MSR depletion components influences model k-eff. Using neither the depletion lumping nor the material transfer yields the lowest k-eff. This is to be expected because no material transfer implies that fission product poisons are being retained within the salt, and since no fresh fuel is introduced and no lumping is used, excessive depletion of the high reactivity region occurs. Using lumped depletion while only considering the salt volume within the core (i.e., assuming there is no ex-core salt volume) increases k-eff to some degree due to the dispersal of reaction rates over the entire in-core volume rather than concentrating the reactions within only the high reactivity regions. This is further accentuated when considering lumped depletion with some additional salt volume existing outside the model. The transfer of materials also increases k-eff due to the introduction of fresh fuel material to offset some of what is depleted and the removal of fission product poisons generated during fuel depletion. The combined effects of lumped depletion and material transfer are substantial, with k-eff values over 25,000 pcm lower when neither effect is considered. This demonstrates not only the importance of accounting for material transfers, which is generally self-evident, but also the significance of fuel mixing captured here through the well-mixed approximation. More testing is required to thoroughly benchmark these MPACT components, but the initial results follow expected behaviors.
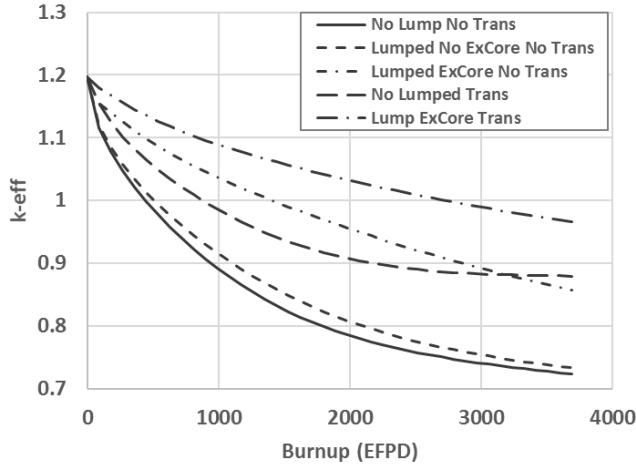
Fig. 2. Depletion components effects.

This assessment of MSR depletion features is also supplemented by Table I, which provides a brief analysis of solution convergence with respect to time discretization. Typical core conditions are expected to change fairly slowly during normal reactor operations, so efforts should be made to determine requisite time mesh fidelity for the sake of modeling efficiency. In MPACT, two time mesh considerations must be taken into account: the depletion macro-step, and the depletion substeps. The depletion macro-step, generally referred to as simply *the depletion step*, follows a predictor-corrector scheme. During the predictor and corrector calculations, the macro-step is divided into several depletion substeps in which microscopic cross sections are maintained constant, but the region fluxes are renormalized to reflect the constant power conditions of the reactor. Currently when the continuous material transfer option is used in MPACT, transfers are performed in small sub-batches based on user-specified rates at the end of each substep. Transfer rates can be based on absolute values, as is typically done for fuel additions, but they may also be based on fractional values, which may be more representative for continuous isotopic removals. As such, the depletion solution can be sensitive to both macro-step size and the number of substeps for each macro-step.

Table 1 shows that coarsening the time mesh by using either fewer macro-steps or fewer substeps per macro-step generally leads to less agreement with higher fidelity solutions. One exception is in the single substep cases when reducing the number of macro-steps from 123 to 41, which might be attributed to cancellation of errors. However, solution agreement remains nearly constant when the total number of substeps (i.e. product of number of macro-steps and number of substeps per macro-step) is the same. This indicates greater sensitivity to the degree of material transfers sub-batching rather than the number of flux solution updates resulting from increasing the number of macro-steps. Sensitivity to the amount of sub-batching makes sense when considering fractional transfers upon

which the absolute atom values depend on the amount of material available for transfer. The available amount of material depends on the amount of depletion that has occurred by the end of a given substep, which depends on the substep size and therefore depends on the number of substeps. Insensitivity to the flux solution update frequency is likely due to the combined influence of the well-mixed approximation, removing spatially dependent depletion effects, and fission product poison removal and fuel addition, all of which help maintain near constancy of important salt isotopes. Though a full MSR core model will likely exhibit greater time-dependent heterogeneity with regard to material transfers and reactor configurations (i.e. positioning of control elements), the lack of influence of flux solution update frequency exhibited in this lattice model supports the assumption that operating conditions will generally remain constant and thus justifies using larger macro-step sizes.

Table I. Solution Sensitivity to Time Mesh Refinement in terms of Δk-eff (pcm)

Macro-steps / Substeps per Macro-step	369	123	41
1	287	437	416
3	121	287	439
9	-	-	289
10	ref	108	271
30	-	2	110
90	-	-	8

2. Precursor Drift

The same Transatomic MSR model was extended to a 3D single moderator cell problem that is 300 cm tall with 20 cm of salt reflector at the top and bottom with vacuum boundary conditions. The axial distribution of the precursors is shown in Fig. 3 for the 6 precursor groups at a 50 cm/s flow rate.
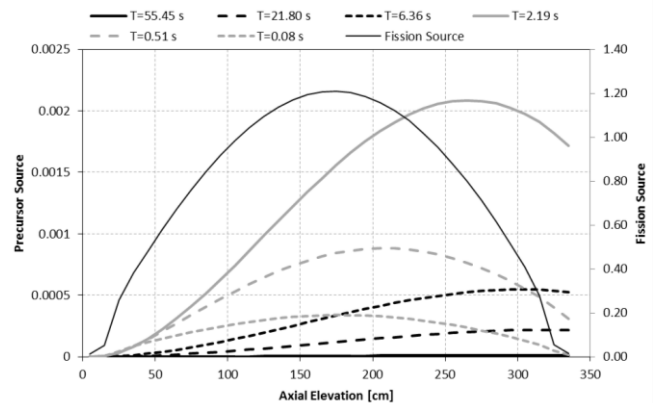

Fig. 3. Precursor source axial distribution.

The short-lived precursors maintain the original shape of the fission source, but the longer lived precursors are

transported upward in the core. The increase in concentration at the inlet for the longest lived precursors is also observed.

The impact of the flow rate on the eigenvalue of the system is of particular interest. As the velocity of the fluid is increased, the amount of precursors leaving the system is increased, which will result in less neutrons in the core. This will decrease the multiplication factor of the reactor. To demonstrate this effect, the eigenvalue is computed for flow rates ranging from 0 to 100 cm/s. The reactivity worth of the precursor drift is shown in Fig. 4 as a function of axial velocity.
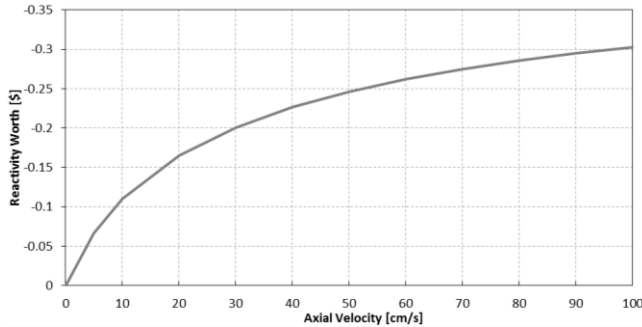

Fig. 4. Reactivity worth of axial flow velocity.

The worth is zero when the flow is zero, but as the flow increases, the worth changes very quickly. Once the flow reaches the nominal value (~50 cm/s), the reactivity loss is 25 cents. Doubling the nominal flow rates only adds an additional 5 cents of reactivity loss in the system, which demonstrates the diminishing impact of flow velocity on core reactivity.

IV. CONCLUSIONS

In this work, modifications that were made to the MPACT whole core reactor simulator in support of MSRs are discussed. First, the ability to model the circulation and mixing of the molten fuel is discussed. This involves modifying the depletion logic, which exists in MPACT to integrate over the entire salt volume and to provide core total reaction rates to ORIGEN. The second component needed is the treatment of the addition and removal of isotopes from the salt. Both of these features are demonstrated by depleting a lattice over a 10 year period. A study was performed to determine the time step size needed to accurately predict the behavior during time. It was concluded that large step sizes are feasible as long as sufficient substeps are used to maintain flux magnitude and to treat continuous feed and removal of isotopes from the reactor.

Another modification made was to simulate the effects of delayed neutron precursors drifting in the system. An axial convection solution was developed to describe the spatial distribution of delayed neutrons in the core. The delayed neutron source is rewritten to scale with the magnitude of the local fission source to maintain a consistent eigenvalue formulation for the transport equation. This results in a method which effectively adjusts the neutron fission spectrum to account for delayed neutrons being born at lower energies and the effects of drift. A series of simulations was run varying the flow velocity which resulted in a function for reactivity worth as a function of velocity. It was found that at nominal flow rates, the decrease is 25 cents.

Future work will focus on coupling MPACT to the subchannel thermal-hydraulics code Coolant-Boiling in Rod Arrays—Two Fluids (COBRA-TF), or CTF [12], to provide thermal feedback to reactor simulations. CTF can provide 3D velocity fields, including mixing between subchannels, and it includes effects of temperature and density changes. The precursor drift model will use this velocity field to more accurately account for the motion of precursors in the system.

ACKNOWLEDGMENTS

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