Identifying MSR Multiphysics Modeling Challenges

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1 Introduction

Solid fueled nuclear reactors differ from liquid fueled reactors with respect to many physical domains including neutronics, thermal hydraulics, and materials performance. Accordingly, liquid fueled reactors challenge the capabilities of conventional computational tools designed for modeling and simulating the physics of solid fueled reactors.

These challenges compound one another in numerical simulations that model the coupling between physics, particularly in liquid fueled reactors in which the fuel *circulates*. In such reactors, neutron kinetics, fuel depletion, heat transport, and fluid flow couple together much more tightly, stiffening the interdependent system of partial differential equations (PDEs) driving reactor behavior. While solid fueled reactor simulation can accurately couple neutronics and thermal hydraulics through operator splitting techniques and loose coupling, such approaches cannot capture the tightly coupled multiphysics of reactors with circulating liquid fuel.

2 Liquid vs. Solid Fuel

Differences between liquid and solid fueled designs arise primarily from the mobility of the dissolved fuel. This feature impacts neutronics, thermal hydraulics, and the relationship between them. In particular, modeling and simulating time dependent reactor dynamics can require new methods when coupling neutron kinetics, feedbacks, and depletion dynamics with fuel expansion, flow dynamics, heat removal, and system safety.

2.1 Neutronic Differences

In all liquid fueled molten salt reactors, salt movement directly impacts neutron kinetics and control through delayed neutron precursor movement. Since the fissionable material is dissolved in the fuel salt, isotopes produced by fission also move congruously with the salt. Reactor controllability hinges upon delayed neutron precursors, which contribute to β_{eff}, the delayed neutron precursor fraction.

Circulating fuels can additionally be reprocessed during reactor operation. Thus, fuel composition in liquid fueled reactors not only varies with in-core transmutation, but also through out-of-core chemical extraction, gas sparging, mechanical filtering, and other methods. For example, several fission products selectively precipitate onto nickel surfaces in fluoride salt, as documented in [1], allowing those to be removed when the fuel salt is circulated out of the core, reducing unwanted neutron absorption. These dynamics occur on fast timescales (minutes) if the fuel is reprocessed "online" or on slower, discrete timescales if the design involves processing in batches.

Very long fuel residence times in circulating, liquid fueled reactors also presents a challenge regarding depletion dynamics. In contrast to legacy reactors, material damage to the fuel does not limit burnup. Instead, corrosion and fast neutron damage to other structures (e.g. graphite moderation structures) limit burnup. If those structures are protected (as in [1]) reactor operation can continue without opening the vessel for thirty or more years. The buildup and transmutation of fission products in the vessel during that time impacts reaction rates over the course of years or decades. Computational tools to accurately characterise this depletion evolution must incorporate chemical processing logistics as well.

Additionally, fuel temperature reactivity feedback related to salt density is very strong in liquid fueled Molten Salt Reactors (MSRs). Though the fuel salt remains single phase, density variation with temperature impacts fuel isotope number densities, N_i, and corresponding reaction rates $\sigma_x N_i \Phi$, resulting in very strong fuel temperature feedbacks. For example, in fast-spectrum fluoride MSRs, salt expansion contributes approximately half of the total temperature reactivity coefficient [2].

2.2 Thermal Hydraulic Differences

In MSR concepts, the fuel salt remains in a single, liquid phase throughout normal operation. And, in contrast to conventional reactors, MSRs operate at near atmospheric pressures and very high temperatures, frequently with very high Prandtl number flow. Natural circulation in these fluids plays a strong role in reactor performance, and although many designs incorporate pumps to drive fuel circulation, some designs may rely on natural circulation driven flow instead.

Such single-phase flows can typically be modeled with the incompressible Navier-Stokes equations or a weakly compressible lattice-Boltzmann equation. However, in startup, shutdown, off-normal operation, and accident scenarios, simulations may need to capture the solid and gaseous phases as well.

The gaseous phase must be considered because gaseous fission product isotopes appear in the liquid fuel during operation. As gaseous fission product inventory evolves, microbubbles may form when these gases coalesce. Aufiero et al. [2] recently showed significant impact to reactor neutronics from compressibility in the salt potentially introduced by such microbubbles. Since these microbubbles cannot be neglected in safety assessment, mass transport must be incorporated into any multiphysics assessment of liquid-fueled MSRs.

In certain designs stationary flow vortices may develop as well, potentially causing the fuel salt in that location to overheat and evaporate. Such voiding can be avoided at the design stage if computational tools can accurately capture such vortical stagnation points in the flow.

Finally, the solid phase may need to be considered when simulating "freeze plugs," solidified salt which may block a channel. Some designs incorporate freeze as an intentional safety valve which melts at a high core temperature, allowing the core salt to drop into a dump tank or other safe configuration [3]. Transition into solid phase (freezing) is most likely to occur in small out-of-core fuel piping under off-normal scenarios.

Toward validation of this software, new experimental flow loops (e.g. [4]), promise to correct a dearth of experimental data regarding thermophysical properties for these salts and their natural circulation behavior.

2.3 Coupling Differences

While loose coupling (e.g. operator splitting) can be sufficient for solid fueld reactors, tight interdependencies among neutronics and thermal hydraulics must be modeled as tightly or fully coupled. A fully coupled approach demands methods which are stable, parallelizable, and multi-scale. Common approximations in both thermal hydraulics and neutronics may need to be used with care. Specifically, methods which neglect density variation (e.g. Boussinesq), rapidly changing isotopics (e.g. cross sections generated a single isotopic composition), or compressibility (Navier-Stokes), may fail to capture important coupled phenomena.

Additionally, simulation of time dependent multiphysics phenomena in MSRs must handle neutronics concerns at many time scales such as density-driven temperature feedbacks, delayed neutron precursor drift, and composition changes due to online reprocessing. Multiphysics modeling must similarly handle thermal hydraulics concerns such as thermal expansion, compressibility due to fission gases, natural circulation, and evaporation or solidification of the fuel salt.

3 Coupled Multiphysics Modeling

Forward looking needs and challenges for modeling and simulation of any molten salt reactor will address separate neutronic and thermal hydraulic modeling challenges as well as unique issues with respect to coupling them.

3.1 Current Tools

With the inclusion of the MSR among the Generation-IV reactor designs [5, 6] and many new nuclear companies proposing both liquid-fueled and solid-fueled commercial MSR concepts [7, 8, 9, 10, 11], corresponding tools for modeling and simulation of the coupled physics are in development internationally.

Standard Monte Carlo [12, 13] and deterministic [14] transport solvers capably handle static neutronic analysis of MSRs However, time dependent kinetics and dynamics analysis cannot be achieved with conventional software. Toward this end, various efforts have extended or created custom tools which incorporate delayed neutron precursor drift. Some solutions have coupled Computational Fluid Dynamics (CFD) with Monte Carlo, while others are built on software packages such as COMmon SOLution (COMSOL) [15] or Multiphysics Object-Oriented Simulation Environment (MOOSE) [16, 17] fundamentally designed for multiphysics coupling.

In 2007, Křepel et al. extended the Light Water Reactor (LWR) diffusion code DYN3D to incorporate delayed neutron precursor drift and fission energy release directly into the mobile coolant. Křepel et al. demonstrated the resulting tool, DYN3D-MSR, via simulation of the Molten Salt Reactor Experiment (MSRE) [18]. Soon thereafter, Kophazi et al. used iterative coupling between in-house three-dimensional neutronic and one-dimensional heat conduction models DALTON and THERM to analyze normal MSRE operation as well as channel-blocking-incident transients [19]. The Kophazi model added entrance effects of heat transfer coefficients as well as thermal coupling between fuel channels through moderator heat conduction.

More recently, Cammi et al. performed a 2D-axisymmetric single-channel analysis of the Molten Salt Breeder Reactor (MSBR) using the commercial finite element package COMSOL Multiphysics [20]. That work directly solved for the fuel salt velocity field, used heterogeneous group constants in fuel and moderator regions, and employed the COMSOL software package intrinsically designed for coupled multiphysics simulation. Fiorina, Lathouwers, and their colleagues conducted a benchmarking exercise [21] in which this Politecnico di Milano approach was expanded to a multi-channel model of the Molten Salt Fast Reactor (MSFR) and compared to code from the University of Delft [22, 23] based on the 2009 DALTON/THERM iterative coupling approach in [19]. These models showed good agreement for multiple accident transients. Meanwhile, leveraging lessons learned from these efforts resulted in a multiscale approach from Zanetti et al. in 2015 [24] successfully combines high and low geometric fidelity for graphite-moderated MSRs.

The most recent developments in this area leverage open frameworks such as the multiphysics MOOSE framework [16, 17] or the CFD framework OpenFOAM[25]. In concert with the Idaho National Laboratory (INL) MOOSE framework, Lindsay et al. [26, 27] developed and demonstrated a finite element based application, Moltres, with full coupling between multi-group diffusion neutronics with delayed neutron precursor drift and the Navier Stokes equations. Moltres is in continued active development [28] at the University of Illinois alongside the helper utility SaltProc [29, 30] which simulates online fuel reprocessing via depletion with SERPENT2[12]. The processing flow chart for SaltProc v.1.0 appears in Figure 1.

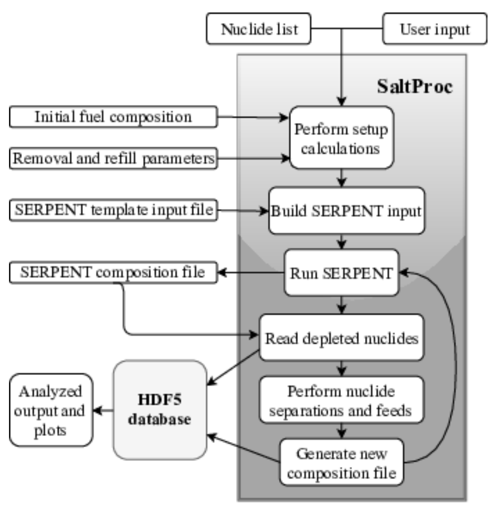

Figure 1: SaltProc couples to Serpent to add and remove specific isotopes from the core at the appropriate reprocessing intervals, mass rate, removal efficiency to simulate fuel management. Figure reproduced from [29, 30].

Very recently, Aufiero et al. [31] have begun to approach transient simulations in the MSFR within the finite volume OpenFOAM CFD toolkit [25]. This approach benefits from pre-implemented turbulence models available in the OpenFOAM library and captures the full-core three-dimensional geometry of the reactor primary circuit. OpenFOAM CFD has additionally been shown by Laureau et al. [32] to couple well with Transient Fission Matrix neutronics within the MSFR. This OpenFOAM coupling approach also enabled the first analysis of compressibility effects in the MSFR by Aufiero et al. [2]. That work has been extended this year by Cervi et al., who incorporated modeling of a helium bubbling system envisioned for fission product removal in the MSFR and assessed the impacts of that system on coupled thermal hydraulics and neutronics with respect to compressibility [33]. As shown in Figure 2, reproduced from [33], this simulation approach uses tight, but not full coupling, in order to incorporate the fidelity awarded by Monte Carlo neutronics.

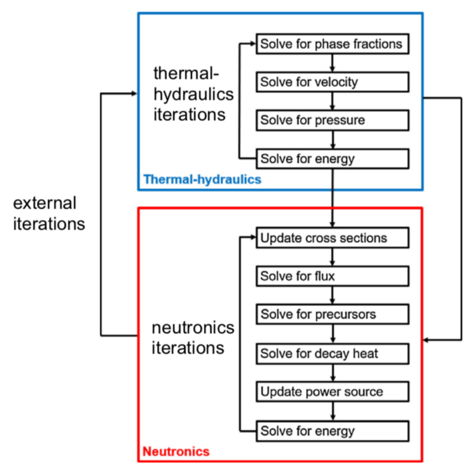

Figure 2: In this figure reproduced from [33], the structure of the coupling between Serpent and OpenFOAM is shown. Picard iterations seek convergence of the thermal hydraulic solution, then proceeds to solve the neutronics iterations.

Regarding thermal hydraulics, Leandro et al. [34] demonstrated MSRE systems analysis with the Nuclear Energy Advanced Modeling and Simulation (NEAMS) System Analysis Module (SAM) module. Pressure drop predictions compared well to results from the MSRE as well as RELAP5-3D simulation comparisons. Meanwhile, the existing MSR multiphysics simulation tools mentioned in the previous section each capture some, but not all thermal hydraulic phenomena of importance in these reactors. With regard to thermal hydraulic modeling challenges, none of the current multiphysics tools capture one key operational safety challenge for these reactor types. Preliminary analysis indicates that serious local power density concerns may arise from *stagnation points* in liquid fueled MSRs. When flow vortices arise in the core, fuel may become trapped in the vortical stagnation points, driving temperature increase which could damage reactor components or initiate boiling. Quantifying the likelihood of stagnation points for the many operational states expected in these designs (e.g. load-following transients) is currently beyond the capability of existing molten salt multiphysics tools.

3.2 Multiphysics Coupling Needs

For stability, modeling multiphysics modeling and simulation approaches in MSR regimes should use stable, fully coupled PDE solver methods such as Jacobian-Free Newton Krylov (JFNK). To capture the multi-scale nature of these systems simulations should incorporate adaptive meshing in both time and space. For parallelizability, mesh handling methods such as domain decomposition must be available in the multiphysics framework or if the mesh is not domain decomposed, then the framework must scale well in memory. Applications built on the MOOSE and COMSOL frameworks both satisfy all of these requirements.

3.3 Conclusion

To summarize, the main modeling and simulation needs for successful coupled multiphysics MSR simulation stem from neutronic and thermal hydraulic behaviors unique to circulating molten salt fuels. While state-of-the-art MSR simulation approaches now handle treatment of delayed neutron precursor drift, many tools lack treatment of salt compressibility, potential formation of vortical stagnation points, fuel composition variability due to online reprocessing, and treatment of natural circulation flow for mildly compressible high temperature high Prandtl number flows. Furthermore, some high fidelity methods (e.g. Monte Carlo transport) challenge implementation within multiphysics simulation frameworks enabling full coupling. Finally, a dearth of experimental data limits validation of all of these tools, though new natural circulation flow loops, corrosion studies, and fission product removal experiments promise to improve validation capabilities.

4 Opportunities

Tools such as Moltres [26] can be improved by incorporating compressibility into their thermal hydraulic models and by introducing higher fidelity methods for neutron transport into MOOSE applications.

All existing tools could benefit from composition modeling that incorporates isotopic changes on the minute-to-minute, and hour-to-hour timescales inherent to online reprocessing systems.

And, all existing multiphysics tools are lacking stagnation point modeling and simulation. One option is to leverage high fidelity thermal hydraulic and neutronics tools to improve coupled neutronics-and-thermal-hydraulics multiphysics capabilities, predictively simulate vortices and similar thermal hydraulic phenomena, identify experimental data needs, and clarify the licensing pathway for these designs. High order fluid dynamics simulations of these vortices could rely on methods in a spectral element code such as Nek5000 [35]. Reduced order models, informed by such simulations could be implemented in the MOOSE [17] application, Moltres [26] which captures coupled multi-group neutronics, simplified thermal hydraulics, and delayed neutron precursor drift in liquid fueled MSRs. Additionally, geometrically detailed power distributions (needed by Nek5000) and few-group cross sections (needed by Moltres) can be generated with the high fidelity Monte Carlo neutron transport software, Serpent [12].

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