MOLTEN-SALT REACTORS AND THEIR FUEL CYCLES

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EXECUTIVE SUMMARY

The Advanced Reactors and Fuel Cycles Group (ARFC) at the University of Illinois at Urbana–Champaign models and simulates nuclear reactors and fuel cycles with a goal of improving the safety and sustainability of nuclear power. In the context of high-performance computing, this work couples multiple physics at multiple scales to improve the design, safety, and performance of advanced nuclear reactors. In particular, thermal–hydraulic phenomena, neutron transport, and fuel reprocessing couple tightly in nuclear reactors. Detailed spatially and temporally resolved neutron flux, temperature distributions, and isotopic compositions can improve designs, characterize performance, inform reactor safety margins, and enable validation of numerical modeling techniques for those unique physics. In this work conducted on Blue Waters, ARFC has demonstrated the capability to simulate coupled, transient neutronics, thermal hydraulics, and fuel reprocessing in multiple advanced, molten-salt-fueled nuclear reactor designs.

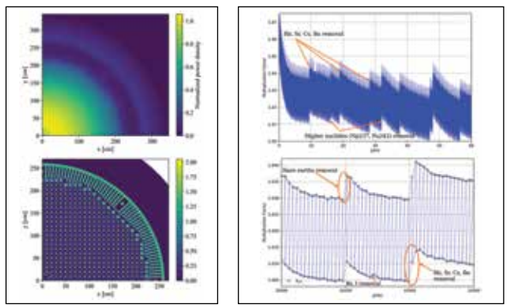

Figure 1 (left): Normalized power density (above) and ^{232}Th neutron capture rate normalized by total flux (below), both at the equilibrium fuel salt composition in the molten-salt breeder reactor [6]. Figure 2 (right): Reactor criticality dynamics for a full-core molten-salt breeder reactor over a 60-year reactor operation lifetime (above) and a zoomed time interval (below) at three-day time resolution. These were obtained using SaltProc and SERPENT 2, which simulate reprocessing and online refueling [5–7].

RESEARCH CHALLENGE

Nuclear power is an emissions-free, safe source of electricity with unparalleled energy density, baseload capacity, and land-use efficiency, so the world's energy future increasingly depends on improved safety and sustainability of nuclear reactor designs and fuel cycle strategies. The current state of the art in advanced nuclear reactor simulation focuses primarily on traditional light-water reactor designs. ARFC's work extends that state of the art by enabling similar modeling and simulation capability for more advanced reactor designs that have the potential to improve the already unparalleled safety and sustainability of nuclear power. High-fidelity simulation of dynamic advanced reactor performance requires development of models and tools for representing unique materials, geometries, and physical phenomena. In particular, insights coupling feedback between the reactor scale and the fuel cycle scale are essential to the deployment and scalability of these innovations in the real world.

METHODS & CODES

Blue Waters has enabled ARFC to develop and test two new significant software solutions: Moltres and SaltProc. Moltres is a first-of-its-kind finite-element application simulating the transient neutronics and thermal hydraulics in a liquid-fueled molten-salt reactor design [1–4]. SaltProc is a highly capable Python tool for fuel salt reprocessing simulation [5–7].

Moltres is a collection of physics kernel extensions and material definitions for the highly scalable, fully implicit, multiphysics, object-oriented simulation environment (MOOSE) framework from Idaho National Laboratory [9]. These physics kernels enable Moltres to solve arbitrary-group neutron diffusion, temperature, and precursor governing equations in up to three dimensions and on an arbitrary number of processing units.

Moltres is built on top of the MOOSE framework, which itself leans on the LibMesh [9] finite-element library and the PETSc [10] toolkit for solving systems of discretized partial differential equations (PDEs). MOOSE and LibMesh handle translation of Moltres-defined weak PDE forms into residual and Jacobian functions that PETSc solves simultaneously via Newton–Raphson routines. All codes use MPI for parallel communication and are easily deployed on Blue Waters. MOOSE applications such as Moltres use monolithic and implicit methods that are ideal for closely coupled and multiscale physics.

SaltProc includes fission product removal, fissile material separations, and refueling for time-dependent analysis of fuel-salt evolution. It relies on full-core high-fidelity Monte Carlo simulations to perform depletion computations that require significant computational time and memory. This capability enables unprecedented fidelity in dynamic fuel cycle analysis for liquid-fueled reactors. The analysis requires thousands of full-core simulations for relevant timescales. With Blue Waters, the research team accomplished this high-fidelity fuel cycle simulation and provided the field with unprecedented detail in the dynamics of fuel processing for molten-salt reactors.

Figs. 1 and 2 show the effective multiplication factors (criticality) obtained using SaltProc and SERPENT 2. The criticality values were calculated after removing fission products listed and adding the fertile material at the end of cycle time (three days for this work) over the full 60-year lifetime of this reactor concept. The simulation demonstrated in detail how the effective multiplication factor fluctuates significantly as a result of the batch-wise nature of this online reprocessing strategy.

The workflow begins when SERPENT calculates the effective multiplication factor for the beginning of the cycle (there is fresh fuel composition at the first step). Next, it computes the new fuel salt composition at the end of a three-day depletion. The corresponding effective multiplication factor is much smaller than the previous one. Finally, SERPENT calculates k_{eff} for the depleted composition after SaltProc applies feeds and removals. The k_{eff} increases accordingly since major reactor poisons (*e.g.*, Xe, Kr) are removed, while fresh fissile material (^{233}U) from the protactinium decay tank is added.

RESULTS & IMPACT

Current interest in advanced nuclear energy systems and molten-salt reactor (MSR) concepts has illuminated a need for tools that model these systems. By developing such applications in the open, ARFC enables both transparency and distributed collaboration on promising nuclear reactor concepts. Detailed spatially and temporally resolved neutron fluxes, temperature distributions, and changing isotopic compositions can improve designs, help characterize performance, inform reactor safety margins, and enable validation of numerical modeling techniques for unique physics.

ARFC has conducted simulations of multiple molten-salt reactor designs. Steady state, transient, and fuel cycle analysis simulations have been run in 2D as well as 3D by leveraging the Moltres and SaltProc tools developed in the research group.

Recently, fuel cycle dynamics were obtained from depletion and SaltProc reprocessing simulations for a 60-year time frame. A molten-salt breeder reactor full-core safety analysis was performed at the initial and equilibrium fuel salt compositions for various reactor safety parameters such as effective multiplication factor (shown in Fig. 2), neutron flux distributions, temperature coefficients, rod worths, power, and breeding distributions [5–7].

WHY BLUE WATERS

Simulations that faithfully capture this coupling at realistic spatial and temporal resolution are only possible with the aid of high-performance computing resources. To assess nuclear reactor performance under a variety of conditions and dynamic transients, the ARFC group must conduct myriad 2D and 3D finite-element simulations using the MOOSE framework and their in-house-developed modules. Such simulations commonly occupy tens of thousands of CPU cores at a time and vary in completion time. The MOOSE framework has been shown to scale very well up to 10,000 cores. The ARFC group has demonstrated appropriate scaling for MSR simulation above 20,000 CPU cores (600 Blue Waters nodes). Transient and multiscale simulations, which require greater capability per simulation, are on the horizon for this work. These may occupy up to 100,000 CPU cores at a time. Only a few of those larger simulations will be necessary to enable better understanding of the dynamics in these reactor systems.

PUBLICATIONS & DATA SETS

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