

COUPLED SIMULATIONS OF FAST-SPECTRUM MOLTEN SALT REACTORS

Benjamin Collins¹, Aaron Graham¹, William Dawn², Robert Salko¹, Nicholas Smith², and Cole Gentry¹

¹Oak Ridge National Laboratory
1 Bethel Valley Rd. Oak Ridge, TN.

²North Carolina State University
2500 Stinson Drive. Raleigh, NC.

collinsbs@ornl.gov, wcdawn@ncsu.edu, grahamam@ornl.gov, nickvise@gmail.com,
salkork@ornl.gov, gentryca@ornl.gov

ABSTRACT

The development of a new coupled simulation capability for fast-spectrum molten salt reactors is presented. This paper presents a fast chloride reactor design which has many of the major features of contemporary designs but is based off open literature. The MPACT-CTF molten salt simulation suite is modified to have appropriate cross-section generation, neutron transport, an thermal-hydraulic capabilities for this reactor design. The coupled tool is then used to demonstrate the behavior of this reactor as the core flow rate is varied and as the salt is depleted over the reactor lifetime.

KEYWORDS: VERA, MPACT, CTF, fast spectrum, MSR

1. INTRODUCTION

Molten salt reactor technology has been gaining traction in recent years as can be seen through significant interest from multiple private companies investing in this technology. In response to this interest, Oak Ridge National Laboratory (ORNL) is extending the Virtual Environment for Reactor Applications (VERA) [1] to simulate molten salt reactors (MSRs). Previous work has documented the modifications to VERA to include delayed neutron precursor drift, depletion, and accuracy for a thermal MSR system [2,3]. One reason that molten salt technology has such interest is the diversity of designs that can be used. This work focuses on the development of a similar capability for a fast spectrum chloride salt system which has the interest of companies such as Elysium [4] and TerraPower [5]. In this paper we will first introduce a reactor model loosely based off the Salt reactor Onsite refueling Fast converter Task (SOFT) reactor [6]. Then an overview of the methods used to analyze this reactor will be presented. Finally, a demonstration of capability will be presented which includes benchmarking against Monte Carlo reference solutions and cycle depletion calculations.

Notice: This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy (DOE). The US government retains and the publisher, by accepting the article for publication, acknowledges that the US government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others to do so, for US government purposes. DOE will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan (<http://energy.gov/downloads/doe-public-access-plan>).

2. REACTOR MODEL DESCRIPTION

The reactor model description used in this work is based off the SOFT reactor but modified to represent more contemporary cores. The major modification is to modify the geometry shape to represent a cylindrical core instead of a spherical core. The height to diameter ratio of the cylinder is set to the critical height to diameter ratio for a bare core. The reactor was then sized to have an eigenvalue close to critical with the original SOFT reactor plutonium chloride salt composition. The inlet and outlet of the design are modeled as separate, continuous salt regions above and below the core. The entire core is surrounded by a solid iron reflector. The geometry is summarized in Table 1.

Table 1: Geometry Specification for Simplified Molten Salt Fast Reactor

Radius	160	cm
Height	340	cm
Reflector Thickness	100	cm
Inlet and Outlet Height	80	cm

Figure 1 shows the geometry and outlines the dimensions graphically. It should be noted that the model has 100 cm of iron reflector on the top and bottom of the reactor which is not shown in Figure 1.

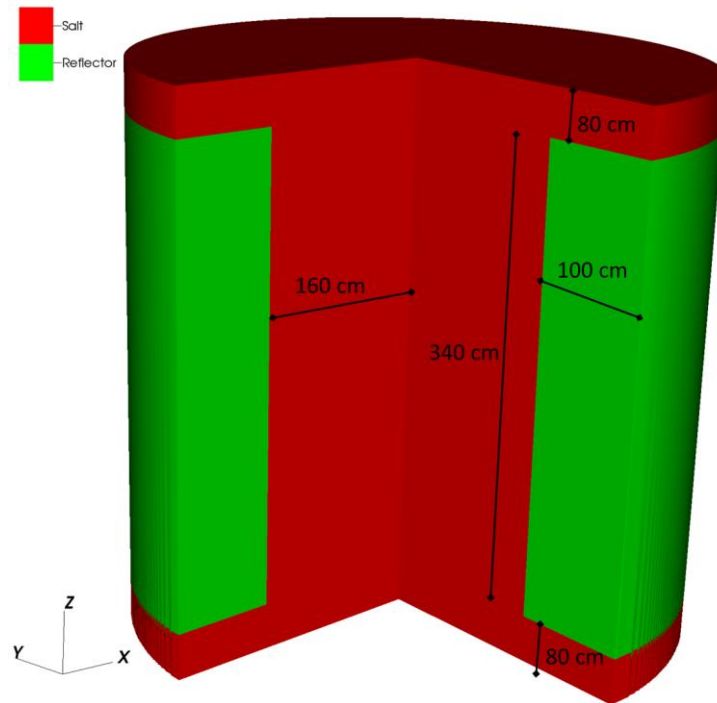


Figure 1: Geometry for Simplified Molten Salt Fast Reactor

The salt composition used comes directly from the SOFT reactor and is given in Table 2. Here 100% enrichment of chlorine is assumed. The reflector is solid iron-56 at a density of 7.874 g/cm³.

Table 2: Initial Salt Composition

Isotope	Atom %
U-235	1.02E-03
U-238	1.41E-01
Pu-239	1.33E-02
Pu-240	1.78E-03
Pu-241	8.92E-04
Pu-242	1.78E-03
Na-23	1.81E-01
Cl-37	6.59E-01

Because this simulation will be coupled with thermal hydraulics, thermophysical properties of the salt are also defined based on values found in open literature and are documented in Table 3. Here all properties are assumed constant except the density, which is a linear function of temperature.

Table 3: Thermophysical Properties of the Salt

Specific Heat	0.95	kJ/kg-K
Density	$6.639 - 3.05 \cdot 10^{-3}T$	g/cc
Viscosity	0.0217	g/cm-s
Thermal Conductivity	0.007	W/cm-K

Other parameters of interest are given in Table 4, which includes the thermal power generation, the velocity through the core, the cold leg temperature, and the effective length of piping outside the reactor core which is used to compute the concentration of delayed neutron precursors returning into the inlet of the core.

Table 4: Reactor Parameters

Power	2500	MW
Axial velocity	100	cm/s
Cold Leg Temperature	740	K
Effective Pipe Length outside Core	480	cm

3. SOLUTION METHODOLOGY

The coupled simulations will be performed using the MPACT-CTF coupled code system which has been widely used for LWR applications and demonstrated for thermal molten salt reactor designs. MPACT contains a collection of deterministic transport solvers for three-dimensional reactor problems. The first step is to obtain a cross-section library that MPACT can use for its calculations. For this work, MC**2-3 [7] was used to generate the cross-sections for the salt and reflector in its 33-group microscopic cross-section library at temperatures of 300, 600, 900, and 1200 K. MPACT is modified to read the ISOTXS file generated by MC**2-3 and then interpolate to the exact temperature for each isotope. While the fuel and fission product cross-sections are generated using a homogeneous medium of the salt, the reflector

cross-sections are generated by using the reference SERPENT flux spectrum in the reflector region to account for the significant spectral changes in the reflector. Further research will be performed to determine a more direct methodology to generate reflector cross-sections inside MPACT.

Once the cross-section libraries are generated, MPACT can solve full core transport problems. The traditional transport methodology that MPACT uses for calculations has been the 2D/1D method [8], but for this work, a 3D S_N sweeper is implemented on a superimposed Cartesian grid. Because of the cylindrical shape of the fuel/reflector interface, the cartesian grid overlay will require homogenization of the materials. This is done using volume homogenization, which should be a good approximation if the mesh is sufficiently small compared to the average mean free path of the neutron. A mesh sensitivity study will look at this impact in the results section. To obtain closure in the finite volume S_N sweeper, the diamond-difference scheme is employed [9]. This scheme defines the cell average flux as the average of the surface fluxes on two opposing surfaces in any of the three directions. MPACT performs the S_N sweeps in a spatially decomposed framework with a Coarse Mesh Finite Difference (CMFD) [10] acceleration technique to improve the overall convergence of the algorithm.

In addition to computing the neutron flux distribution throughout the core, MPACT has methods to incorporate homogeneous depletion with continuous feed and removal, delayed neutron precursor drift, and thermal hydraulic coupling with CTF. Details about the depletion and precursor drift methods can be found in [2].

Lastly, the thermal hydraulics solution is obtained using the subchannel code CTF [11]. CTF models the reactor core using multiple parallel channels which have open gaps to allow mixing between the channels. While CTF does not have the detailed turbulence model which would be needed to capture the true flow paths in this reactor design, it captures many of the dominant physics and is useful for understanding the reactor performance in this work.

The coupling scheme is a standard Picard iteration between the neutron transport and the thermal-hydraulics solution. MPACT computes the power generation in all of the CTF channels and passes the power as a direct heat source. CTF then uses these powers to compute the mass, momentum, and energy distributions in the reactor. Once complete, the channel temperatures and densities are passed back to MPACT which will impact the salt number densities and the microscopic cross-sections. This process is continued until both the neutronics and thermal hydraulic fields are sufficiently converged.

4. RESULTS

We are still currently gathering results for the coupled code system, but some preliminary work has been done to obtain solutions for both the neutronic and thermal hydraulic system.

The first step in this comparison is to compare the cross-sections generated by MC²-3 directly to an equivalent model in SERPENT [12]. For a homogeneous medium of the initial salt composition, the eigenvalues agree well. A full core SERPENT model now allows us to assess the impact of the cartesian grid approximation for S_N and to determine the quality of the cross-section library for a case where the spectrum is significantly changing. Figure 2 shows the current MPACT power distribution in the core and fast flux distribution in the reflector regions. The mesh convergence study will be complete in time for final paper submission.

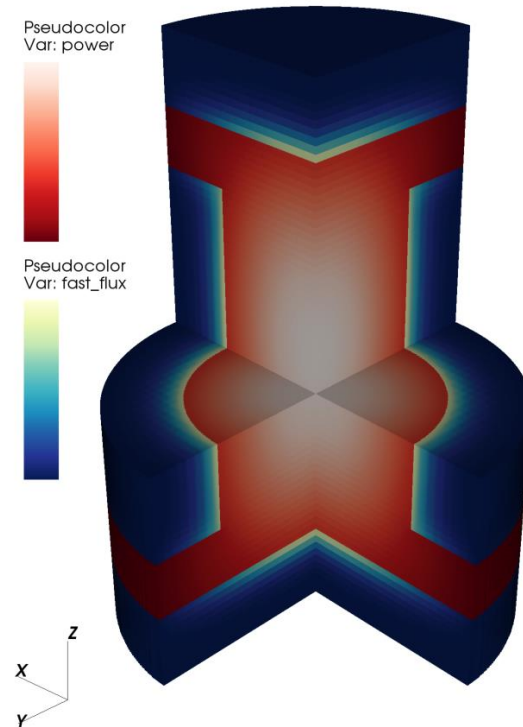


Figure 2: MPACT Power Distribution in the core and Fast Flux Distribution in the Reflector

Now that the errors associated with the MPACT solution are understood, coupling with CTF can be done. The CTF model provides a temperature and density distribution as shown in Figure 3.

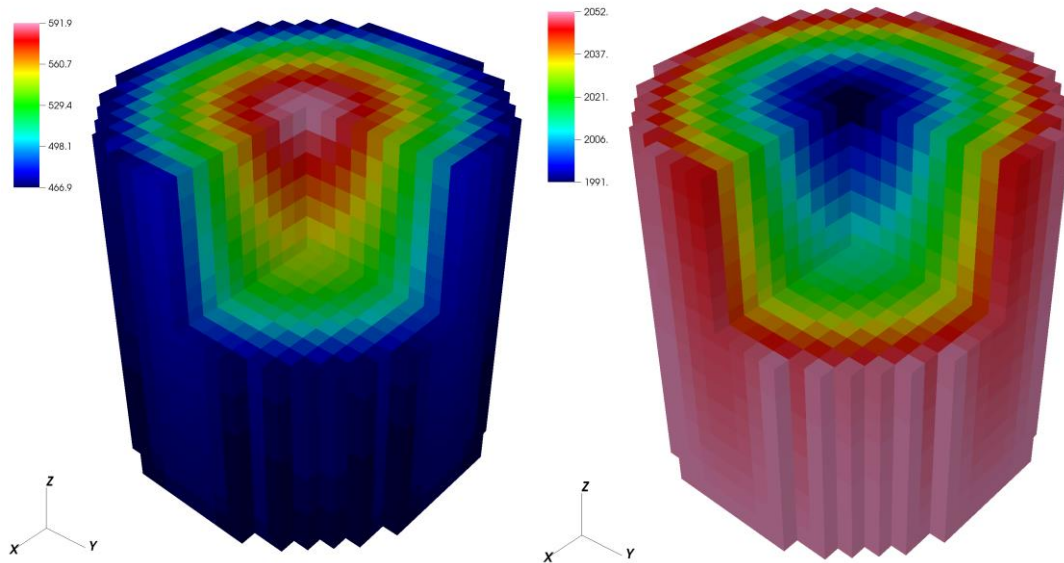


Figure 3: CTF Temperature (left) and Density (right) Distributions

We are currently finishing the channel coupling needed for this reactor. Once the coupling is complete, a series of cases will be run that will look at the impact of changing the core flow rate on reactivity and the impact of depletion with continuous feed and removal on the core performance.

5. CONCLUSIONS

In this paper we present the methodology used to simulate a fast spectrum molten salt reactor with the MPACT-CTF coupled code system. A reactor design is presented that is believed to be representative of contemporary fast spectrum MSR designs. Then the methodology used to solve the whole core coupled system is presented. Results are still being compiled and conclusions on these results will be made in the final paper.

ACKNOWLEDGMENTS

Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

REFERENCES

1. Consortium for the Advanced Simulation of Light Water Reactors. <http://www.casl.gov>.
2. B. Collins, et al. "Molten Salt Reactor Simulations Using VERA-CS," *Proc. M&C 2017*, Jeju, Korea (April 16-20, 2017).
3. B. Collins, et al. "Molten Salt Reactor Simulations using MPACT-CTF," *Trans. Am. Nucl. Soc.*, **116**, pp. 1170-1173 (2017).
4. Elysium Industries. <https://www.elysiumindustries.com/>. (2017)
5. TerraPower. <http://terrapower.com/>. (2017)
6. M. Taube, et al. "Reactors with very low fission product inventory," Swiss Federal Institute of Reactor Technology. EIR-411. <http://moltenalt.org/references/static/downloads/pdf/EIR-411.pdf> (1980)
7. C.H. Lee and W. S. Wang. "MC²-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis," Argonne National Laboratory. ANL/NE-11-41 Rev 1. (2012)
8. B. Collins, et al. "Three-Dimensional Nuclear Reactor Simulations of the Boltzmann Transport Equation with the 2D/1D Method Using MPACT," *Journal of Computational Physics* (2016).
9. B. G. Carlson, "Numerical formulation and solution of the neutron transport problems" Proceedings IBM Scientific Computing Symposium Large-Scale Problems in Physics. New York. (1965)
10. K. SMITH, "Nodal method storage reduction by nonlinear iteration," *Trans. Am. Nucl. Soc.* 44, 265 (1983).
11. R. Salko and M. Avramova, "CTF Theory Manual," Consortium for Advanced Simulation of Light Water Reactors, CASL-U-2016-1110-000, 2016.
12. J. LEPPANEN. "Serpent— a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code", VTT Technical Research Centre of Finland (2012).