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Bridging the gap between experiments and modeling to improve the design of molten salt reactors

PI: Massimiliano Fratoni, UC Berkeley

Program: NEAMS

Collaborators:
Mark Asta, Peter Hosemann, Raluca Scarlat—UCB
Izabela Szlufarska—UWM
Alexandra Navrotsky, Hongwu Xu—ASU
Marisa Monreal—LANL
Abdalla Abou Jaoude—INL
Carolyn Burns, Thomas Hartmann—PNNL
Nader Satvat—Kairos Power, LLC
Karl Britsch—TerraPower, LLC

ABSTRACT:

Design and analysis of molten salt reactors (MSRs) mostly rely on thermophysical and corrosion properties of clean salts. In reality, salts carry impurities from the manufacturing process or can acquire impurities from residues on other reactor components such as fuel. Furthermore, during reactor operation fission products (FPs) and activation products can be produced or released in the salt. The effect of impurities and fission products on salt properties and consequently on reactor behavior during normal and transient conditions remain largely unknown. In this regard it is important to differentiate between the different types of MSRs. There are, indeed, two main categories of MSRs: liquid fuel and solid fuel. In liquid fuel MSRs, fuel, in the form of fluorides or chlorides, and the salt are intimately mixed with no barrier between the two. This means that FPs are produced and accumulated in the salt. Unless an active cleanup and removal of FPs is employed, most FPs can reach concentrations in the salt that are much greater than those of impurities and can potentially alter the thermal physical properties of the salt. In solid fuel MSRs, instead, FPs are contained in the fuel; only small amounts can be released in the salt from a small fraction of failed fuel. Therefore, it is expected that the impact on thermal physical properties of the salt is negligible. Nevertheless, original impurities contained in the salt pose a different challenge. Differently from the ideal case of clean salt, impurities, and among those actinides such as uranium greatly contribute to salt activation and ultimately have a detrimental impact on the expected source term that could be released in an accident scenario; therefore, activity from dilute species in the salt is a key component of the licensing process.

The scope of this project is to improve our understanding of the role of impurities and fission products on the operational performance of MSRs as well as potential impact on accident scenarios. A key target is to contribute to the development of MSRs solving real world issues and for this reason we will work closely with two MSRs vendors representing the two different categories. TerraPower Molten Chloride Fast Reactor (MCFR) is the selected case study for liquid fuel MSRs. In this case the project will assess the role of FPs in changing chloride salt thermal physical properties such as density, thermal conductivity/diffusivity, viscosity, and heat capacity. TerraPower will provide salt specimens for experimental measurements to be conducted at ASU, UCB and LANL. Kairos Power Fluoride-cooled High-temperature Reactor (FHR) will instead be the case study for solid fuel system. In this case the project will focus on the activation products and FPs from salt impurities and their retention in the salt.

The project will develop along multiple tracks in order to complete a comprehensive assessment of the role of impurities and FPs within the limited timeframe and resources available. The experimental effort will focus on measurements of key properties identified together with the industrial partners both for clean salt (if needed) and salt with added solutes (fission products as well as impurities and

activation products). Molecular dynamics simulations in combination with machine learning methodologies will be employed to elaborate and supplement the experimental data in order to identify trends in the selected properties with characteristics of solutes in the salt and with operating conditions. The correlations between properties and salt composition will then integrated into NEAMS tools as input to engineering scale modeling to assess the impact on the reactor performance. It is understood that a systematic evaluation of any FPs and any combination of them is an impossible task for the time and resources of this project, therefore, we will focus on a small subset of elements. These representative elements will be determined in the initial phase of the project combining information from engineering scale modeling, high-throughput experiments, and clustering elements based on fundamental properties (e.g., coordination number, oxidation number, fluoroacidity when known). Sensitivity analysis will be performed varying salt’s properties to determine how changes in density, thermal conductivity/diffusivity, viscosity and heat capacity impact MSRs operational parameters such as burnup, power peak, temperature peak, pressure drop, reactivity coefficients, etc., as well as response in an accident scenario (e.g., unprotected loss of flow). Burnup analysis and activation analysis will inform which elements and in which concentration are present in the salt at any stage. In addition to operational performance and salt properties of MSRs, this project also aims to address the impact of impurities and FPs on the corrosion kinetics of structural materials. We are concerned about conventional corrosion as well as localized corrosion and cracking associated with the presence of FP, corrosion products, transmutation products as well as stress at operating temperature. Direct interaction between neutronics, chemistry and materials will lead to a comprehensive understanding of individual phenomena that can have potential catastrophic effects. This project aims to provide more value as a whole than what individual efforts can do to collaboration and interaction.