NEUP Nuclear Energy University Programs

U.S. Department of Energy

in situ Measurement and Validation of Uranium Molten Salt Properties at Operationally Relevant Temperatures

PI: Wilson K. S. Chiu, University of Connecticut

Program: RC-2.3: Understanding the Structure and Speciation of Molten Salt at the Atomic and Molecular Scale

Collaborators:
Theodore M. Besmann, University of South Carolina
Kyle S. Brinkman, Clemson University
Jacob. W. McMurray, Oak Ridge National Laboratory
John Bargar, Stanford Synchrotron Radiation Lightsource

ABSTRACT:

Since the Generation IV International Forum recognized the unique capabilities of molten salt reactors (MSR), the U. S. Department of Energy has been supporting its development. A major technical hurdle to the deployment of MSR is the lack of understanding of how the structure and dynamics of molten salts impact their physical and chemical properties such as viscosity, solubility, volatility, and thermal conductivity. Specifically, the local and intermediate structure as well as speciation of the salt components at operationally relevant temperatures must be determined. To address this challenge, this project proposes to use advanced spectroscopic and scattering methods to provide information at the atomic and molecular scale. In this project, synchrotron-based x-ray absorption fine structure (XAFS) spectroscopy and Raman spectroscopy will be used at operationally relevant temperatures to measure the local and intermediate structure as well as speciation of chloride fuel salts (NaCl, ZrCl, UCl_3) for fast-spectrum applications and fluoride fuel salts (^7LiF, UF_4) primarily for thermal spectrum applications. Uranium chloride and fluoride materials will be provided through an informal collaboration with ORNL. Speciation of oxidation state in uranium fuel salts will be performed by examining the x-ray absorption near edge structure (XANES) across the uranium L3 absorption edge. The interatomic spacing and coordination of the molten salt will be determined by measuring its extended x-ray absorption fine spectra (EXAFS). Synchrotron access and high temperature heater design will be performed through an informal collaboration with SSRL. Raman spectroscopy will be used by this project to measure and confirm the local structural coordination of molten salt species. To take advantage the greater understanding of the structure of the molten salt systems, the modified quasi-chemical model of the thermodynamics of solutions will be extended to utilize realistic types of species and their concentrations as provided by the measurements. The results will be used to demonstrate thermodynamic models for complex solutions with the next level of fidelity in representing molten salts as well as providing immediately useful properties for compositions of interest, such as viscosity, solubility, volatility, and thermal conductivity. This approach is expected to generate theories and concepts that would allow models to predict behavior, and develop the means for in situ monitoring. Development of this method will leverage the work conducted on molten salts at ORNL, synchrotron-based x-ray spectroscopy measurements by SSRL, as well as team efforts on synchrotron x-ray spectroscopy and molten salt research by the team in past NEUP projects and DOE Energy Frontiers Research Centers.