FY2020 Nuclear Energy University Programs

CINR Webinar – August 7, 2019

PROGRAM SUPPORTING: FUEL CYCLE TECHNOLOGIES

ELIGIBLE TO LEAD: UNIVERSITIES ONLY

MATERIAL RECOVERY AND WASTE FORM DEVELOPMENT (FC-1)

- **FC-1.1: NUCLEAR FUEL CYCLE CHEMISTRY**
- **FC-1.2: ELECTROCHEMICAL SEPARATIONS**
- **FC-1.3: WASTE FORMS DEVELOPMENT AND OFF-GAS CAPTURE**
  - **FC-1.3a: Iodine Immobilization from Caustic Scrubber Solution**
  - **FC-1.3b: Salt Waste Recycle and Immobilization**

FC-1.1: Nuclear Fuel Cycle Chemistry – Complexation Chemistry, Actinides Chemistry, Radiation Induced Degradation and Chemistry

Fundamental knowledge and understanding of the complexation chemistry of actinides and competing metal ions (e.g. lanthanides, fission products) will expand our ability to predict actinide behavior under relevant conditions in fuel recycling. This knowledge will enable enhanced separation and recovery efficiencies of the actinides over fission products and transition metals. These data will also be important in the development of improved (non-empirical) models to predict speciation and separation factors.

There is also a need for an improved understanding of the fundamental processes that affect the formation of radicals and ultimately control the accumulation of radiation-induced damage to separation systems. For example, gamma radiation is known to produce radicals that can affect the oxidation states of multivalent cations in solution. Fundamental knowledge of the chemical speciation and partitioning of multivalent cations (e.g. actinides, Tc, Zr) in advanced extraction processes under high irradiation fields will improve process flowsheet design and reduce actinide losses.

Proposals are requested to enhance fundamental understanding of fuel cycle chemistry and to enable the development of novel new approaches for advanced reactor used fuels treatments and recycling.

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(UP TO 3 YEARS AND $600,000)

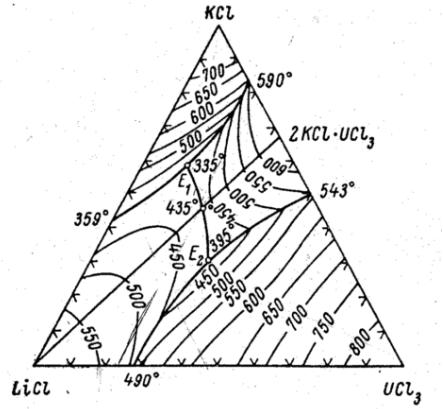
FC-1.2: Electrochemical Separations (Pyroprocessing)

Fission product solubility in molten chloride salts impacts the timing for salt treatment and recycle, or disposal.

- Solubility data as a function of temperature and composition is available for many binary and ternary chloride systems especially those that contain alkali and alkaline earth chlorides
- Similar data is lacking for complex multicomponent chloride salt systems especially those involving the lanthanide and actinide elements

Proposals are requested to establish fundamental thermochemical data in chloride salt systems with an emphasis on multicomponent solubility of the fission product chlorides.

- Experimental work may be supplemented by thermodynamic data simulation to yield a more complete understanding and predictive models of the solid-liquid equilibria in the complex chloride systems.



Example *phase diagram for ternary LiCl – KCl – UCl_3 system*

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MISSION SUPPORTING: FUEL CYCLE TECHNOLOGIES – FUNDAMENTAL MOLTEN SALT CHEMISTRY

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MS-FC-1:
UNDERSTANDING, PREDICTING, AND OPTIMIZING THE PHYSICAL PROPERTIES, STRUCTURE, AND DYNAMICS OF MOLTEN SALT (UP TO 2 YEARS AND $400,000)

MS-FC-2:
UNDERSTANDING THE STRUCTURE AND SPECIATION OF MOLTEN SALT AT THE ATOMIC AND MOLECULAR SCALE (UP TO 3 YEARS AND $600,000)

MS-FC-1: UNDERSTANDING, PREDICTING, AND OPTIMIZING THE PHYSICAL PROPERTIES, STRUCTURE, AND DYNAMICS OF MOLTEN SALT

Thermodynamic models are needed to predict critical salt characteristics such as melting points, heat capacity, free energies for potential corrosion reactions, and solubilities for fission and corrosion products as function of temperature and composition.

Proposals are requested to better understand, predict, and optimize the physical properties and thermochemical behavior of molten salts. Our goal is to develop and use first-principles molecular dynamics simulations and computational electronic structure method to extend the limited experimental data sets in covering a broader range of chemical evolution and environments.

- Apply molecular dynamics simulations to predict thermophysical and transport properties;
- Build multi-component models for prediction of phase diagrams; and
- Develop advanced models to guide the experimental efforts to manipulate the molten salt thermophysical properties are especially encouraged

(UP TO 2 YEARS AND $400,000)

MS-FC-2: UNDERSTANDING THE STRUCTURE AND SPECIATION OF MOLTEN SALT AT THE ATOMIC AND MOLECULAR SCALE

To understand how the structure and dynamics of molten salts impact their physical and chemical properties—such as viscosity, solubility, volatility, and thermal conductivity—it is necessary to determine the speciation of salt components as well as the local and intermediate structure at operationally relevant temperatures.

Proposals are requested to take advantage of recent breakthroughs in advanced characterization tools and instrumentation methods to provide information at the atomic and molecular scale. Our goals are to determine the local structure and bonding of chemical species in salt solution and to develop innovative real-time analytical methods for microscopic and macroscopic property measurements.

- Determine salt molecular structure using scattering and spectroscopic methods;
- Develop novel electrochemistry and spectroscopy methods for in-situ monitoring and predictive modeling; and
- Develop molten salts optical basicity scale to determine corrosivity and solubility of actinides

(UP TO 3 YEARS AND $600,000)