Extension of *MSTDB* to Provide a High-Quality, Validated Thermochemical Database for Predicting/Simulating Corrosion in Molten Salt Reactor Systems

PI: Theodore M. Besmann, University of South Carolina

Collaborators: Ming Hu, University of South Carolina
Stephen S. Raiman Oak Ridge National Laboratory
Jacob W. McMurray, Oak Ridge National Laboratory
Ruchi Gakhar, Idaho National Laboratory

Program: NEAMS

ABSTRACT:

The use of molten salts as heat transfer and storage media, as electrolytes/solvents for electrochemical/separations processes, and, most recently, once again as nuclear fuels reflect their substantial utility. Yet, molten salts are notoriously corrosive, challenging the ability of design alloys that have adequate mechanical and high temperature properties, acceptable cost, and sufficient resistance to corrosive attack. An important goal under the current program to support domestic molten salt reactor development is the generation of an understanding of corrosion and the ability to model and simulate that behavior. Thermochemical models of salts that include corrosion products, and potentially corrosion accelerating contaminants such as moisture, will allow computing of key interactions and potentials of interest for even the most complex, many-component systems.

It is the objective of the research to obtain and develop as necessary thermochemical models and values for corrosion-related systems (i.e., primarily systems with chrome, iron, and nickel plus others as needed), expanding the scope of a general thermodynamic database that is under development in the broader molten salt reactor program. The effort to include corrosion components will build on the base salt systems already available, and those that will be added under that project. The database, when used with computational thermochemical equilibrium codes under conditions of temperature, pressure and elemental composition, will predict stable phase formation/precipitation, vapor pressures, and other important conditions in a molten salt reactor. The database and related information will be available via a controlled project website. A unique and important additional objective is the development of a provision for integrating uncertainties in database values, and a means for propagating them to larger scale. This will then allow users of the database to understand the bounds of the predicted phenomena and therefore make decisions with confidence.

The effort to develop thermochemical information is utilizing well-developed approaches in modeling complex thermochemistry. It will entail assessment of multiple element systems, where thermodynamic information allows generation of free energy relations, the fundamental energy properties of materials, that have assured accuracy and consistency. These are subsequently incorporated in the broader database, and when all are used together for calculation the chemical state of a system, they can provide a comprehensive set of results. In this way, basic values needed to calculate the chemical state within a molten salt reactor under essentially all conditions will be available, assuring accurate control and overall safety.