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Development and Implementation of a Thermochemical Database, MSTDB, for Simulating Fuel Behavior in Molten Salt Reactors

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Molten salt reactors (MSRs), with salt as the fuel/coolant or solely the coolant, require a close understanding of salt properties to be able to simulate normal and off-normal operations. Among the most important are the thermochemical properties of the salt, that is the Gibbs energy relations for the complex liquid and solid solutions as these provide thermal properties as well as critical phase equilibria such as solidus and liquidus. Models for the pseudo-binary and -ternary fluoride and chloride salt systems are being compiled, and where necessary developed, to provide a thermochemical resource. The molten salt thermochemical database (*MSTDB*) is being implemented with the thermochemical solver THERMOCHIMICA in prospective MSR codes for use in reactor design, simulating reactor operations, and assessing of off-normal scenarios to support regulatory activities.

The *MSTDB* is a collection of thermochemical descriptions involving existing data in addition to those found through first principles methodologies and experimental measurements. Density functional theory and related methods are being used to obtain solid salt phase stabilities, along with efforts to extend the approaches to the molten salts. Measurements include determining phase equilibria including melting points, crystalline phase structures, and heat capacities, among other properties. This information together with available reported data are being used in thermochemical assessments to obtain consistent and accurate models and values for Gibbs energy relationships in complex, multi-component salt systems provided to *MSTDB*. The thermochemical database is publicly accessible via an on-line code-sharing protocol. In this presentation, a description of the development and state of the database will be provided along with examples of system assessments and demonstrations of applications of resulting equilibrium calculations within developing MSR codes.

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