

ASSESSMENT OF CONSTITUENT MOLTEN SALT FUEL SYSTEMS AND  
DEMONSTRATION OF RELEVANT MOLTEN SALT THERMOCHEMICAL  
CALCULATIONS

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Reliable and comprehensive thermochemical values for the constituents of molten salt fuels and coolants is a requirement to adequately simulate molten salt reactor systems. However, no publicly available, single-site collection of benchmarked thermochemical data has been heretofore available. In response to this requirement, a comprehensive thermochemical database for uranium/thorium-based fuel salts, the Molten Salt Thermochemical Database (MSTDB), is being developed at UofSC in collaboration with Oak Ridge National Laboratory. The MSTDB is a collection of thermochemical descriptions involving existing data in addition to those found through first principles methodologies and experimental measurements. The thermochemical data will be publicly accessible in website format along with assessed, consistent Gibbs energy relationships for potential fuel salt systems. In this presentation, a description of the state of the database will be provided with examples of system assessments and demonstrations of applications of resulting equilibrium calculations. These include prediction of liquidus temperature, phase stability, precipitate phases, and effects of actinide fission products including UF<sub>3</sub>-UF<sub>4</sub> behavior and prototypical fuel-fission product salts.

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