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Recent Development of Thermochimica for Simulations of Nuclear Materials

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The open-source equilibrium thermochemistry library Thermochimica has previously been employed to study uranium dioxide nuclear fuel for light-water reactor applications. Recently, significant improvements to the efficiency and range of applications of Thermochimica have been made. We will discuss these advances and demonstrate applications of Thermochimica for next-generation nuclear technologies, such as Molten Salt Reactors (MSRs) and Tristructural-isotropic (TRISO) fuels. Calculations on popular molten salt fuel materials, such as FliNaK, FliBe and fission product containing salts, have been enabled through the implementation of the quadruplet approximation to the modified quasichemical model in Thermochimica, which takes into account first and second-nearest-neighbor short-range ordering contributions to the Gibbs energies of liquid solution phases. Coupling of Thermochimica to various other software packages, such as the Multiphysics Object Oriented Simulation Environment (MOOSE), Coolant-Boiling in Rod Arrays - Two Fluids(CTF), Virtual Environment for Reactor Applications (VERA), and Oak Ridge Isotope GENeration (ORIGEN) for nuclear fuel applications will also be demonstrated.

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