

# A Novel Standard Gibbs Energy of Formation Model for High-Enthalpy Water Systems

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Recent developments in high-enthalpy geothermal systems, ultra-deep oil and gas reservoirs, and biowaste-to-fuel processes emphasize the need to predict chemical reactions closer to water's critical temperature (374°C). Traditional Gibbs energy of formation models fail in such extreme conditions due to their empirical nature. Herein, we present an advanced standard molar Gibbs energy of formation model, informed by molecular statistical thermodynamics (MST), and validated by mineral solubility and ion association reactions. This new model aligns with experimental data within uncertainties and highlights the role of specific MST interactions around the critical point. The MST interactions evaluated include hard sphere, ion-dipole, and dipole-dipole interactions via the mean spherical approximation. In regions of interest, this new model shows good alignment with experimental findings compared to the established Helgeson-Kirkham-Flowers model, while utilizing fewer adjustable parameters. The model's robustness is further validated by accurately deriving standard thermodynamic values for key ion pairs in supercritical water, marking a significant leap in our understanding and predictive capabilities of solute behavior in high enthalpy environments. Our hope is that this work will provide a reliable tool for the optimization of industrial processes operating at the edges of the supercritical domain.