

Reduced Database and Thermodynamic Modeling of the Sulfur-Iodine Thermochemical Cycle

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A plethora of challenging problems have been identified related to the measurement and prediction of thermodynamic properties of the aqueous solutions occurring in the Sulfur-Iodine (SI) thermochemical cycle. Moreover, a series of spectroscopic measurements are currently undertaken in many laboratories in order to identify the species and ionic complexes that exist in the aqueous solutions of this process. These efforts aim at a better understanding of the mechanisms of the reactions that take place during the formation of the acids in the Bunsen reactor, and the decomposition/distillation of acids in the process sections that produce oxygen and hydrogen. However, thermodynamic and kinetic data for aqueous solutions occurring in this process appear to be inconsistent. Data including vapor pressures, vapor-liquid-liquid-solid equilibrium, heats and heat capacities of mixing, as well as speciation measurements, have to be combined to develop a self-consistent database of thermodynamic and speciation data. This would allow validation of experimental results using fundamental thermodynamic equations and detailed reaction schemes embedded within an advanced optimization framework capable of handling a large number of data points. Furthermore, advanced thermodynamic modeling is required to predict the different experimental data available. The model in question should be capable of predicting thermodynamic properties, such as vapor-liquid-liquid-solid equilibrium, using the experimentally identified speciation of the solution and reaction schemes that follow the experimental evidence. This can be done by using a local composition model applicable to electrolyte solutions, such as the electrolyte-NRTL model, modified for application to electrolyte mixtures and to include hydration and complex formation. Particularly, much research is required on the phenomena occurring in the Bunsen section of the SI cycle. A comprehensive thermodynamic framework is developed to address the issues of thermodynamic data inconsistencies and the modeling of thermodynamic properties of multi-electrolyte solutions in which hydration and complex formation is dominant.