Properties Modeling and Process Synthesis of the Sulfur-Iodine Cycle for Thermochemical Water Decomposition to Hydrogen

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Contemporary scenarios for future energy supply include using enormous amounts of hydrogen as an energy carrier for fuel cells and as a reagent for upgrading heavy oils and converting coal to liquid fuels. The Sulfur-Iodine (S-I) cycle is a continuous, all fluid-phase, thermochemical process for decomposing water into hydrogen and oxygen that may be the most energy efficient among the many proposed. Current process simulation studies suggest that the energy requirements are unacceptably high, especially in the section where H_2 is formed from HI and separated from the recycled I_2 by reactive distillation (Section III). The reliability of these analyses with regard to the ultimate feasibility of the S-I process, and the testing of creative alternatives for improvement, is hampered by the lack of an accurate thermodynamic properties model for the HI-I_2-H_2O system. A new properties model, based on alternative speciation reactions and parameters for the Electrolyte-NRTL model, has been developed and utilized to find optimal configurations and conditions for Section III of the S-I process. Significantly different results are found compared to the literature; these suggest that while the stream flow rates are greatly reduced, the energy requirements are not. This outcome arises because of a smaller positive heat effect when concentrated streams are mixed, and a larger temperature difference between the reboiler and condenser which heat pumps must overcome. While uncertainties in the analysis have been reduced by improved modeling, experimental data do not yet exist under the extreme operating conditions of the process to provide complete validation. Thus, the reliability of these findings can be further enhanced with support for our assumed speciation reactions via quantum calculations and spectroscopic data comparisons. This paper will also describe the results of an ab-intio study for the formation of atomic clusters of water and iodine in aqueous solutions of HI and I_2.