Phase Equilibrium Calculations in the Sulfur-Iodine Thermochemical Cycle Process using Electrolyte NRTL Model

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Hydrogen is well-known energy carrier for future application to energy consuming sector. Currently, hydrogen is produced by steam reforming of natural gas generating carbon compounds. With this respect thermochemical processes which produce hydrogen from water splitting are very attractive, extremely if they are powered by renewable main energy sources. The Sulfur-Iodine thermochemical cycle process accomplishes water splitting through the three chemical reactions, carried out at much lower temperature than direct thermal water decomposition. In order to assess process efficiency such as energy consumption, phase equilibrium calculations are of importance. Therefore, we focus on modeling of the phase equilibria, which are relevant to the Section II and Section III, in order to provide reliable simulation results for performing mass and energy balances of the separation processes. In this work, two different chemical reaction models with electrolyte-NRTL were adopted to produce phase equilibrium behavior of Section II and III, respectively.