

Application of Electrolyte NRTL for Heat Duty Estimation on an Iodine Crystallizer for SI Thermochemical Hydrogen Production Process

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SI thermochemical hydrogen production process converts water into hydrogen and oxygen through three chemical reactions. The process is comprised of three sections and one of them is HI decomposition into H_2 and I_2 called as Section III. The production of H_2 includes processes involving EED for concentrating a product stream from Section I. Additionally the I_2 crystallization would be considered to reduce the burden on EED by removing certain amount of I_2 out of a process stream prior to EED.

In this study, the current thermodynamic model of SI process was briefly described and the calculation results of the applied Electrolyte NRTL model for phase equilibrium calculations were illustrated for ternary systems of Section III. We calculated temperature and heat duty of an I_2 crystallizer and heat duty of heaters using UVA model and heat balance equation of simulation tool. The results were expected to be used as operation information in optimizing HI decomposition process and setting up material balance throughout SI process.