

Model Development in Section III of the Sulfur–Iodine Cycle for Hydrogen Manufacture

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The Sulfur–Iodine cycle (SI cycle), use the nuclear energy as the heat source for hydrogen production by thermochemical water splitting, is a promising candidate. Because the section III of SI cycle determines the yield of hydrogen, accurate prediction of phase behaviors of the HI mixture(HI–H₂O–I₂) is the most crucial section. To explain the phase behavior of HI mixture, two main thermodynamic models have been used for the design and simulation of the section III in SI cycle, namely, the GA model and UVa model. In recent study, to solving the problem that two models can't explain the phase behaviors of the HI mixture system accurately, a new KIER–2K model have been proposed along with the regression of binary interaction parameters between molecules and ions for electrolyte NRTL model. In this study, the further development of KIER–2K model is carry out with the pure components or the multi components parameters for preferably represent the interactions between species in the HI mixture.