ABSTRACT

Increasing energy demand, gradual depletion of fossil resources and environmental regulations on greenhouse gas emissions have stimulated intensive research in finding a potential raw material for hydrogen production. In this light, water splitting in sulphur-iodine (SI) thermochemical cycle has emerged as a promising approach, whose hydroiodic (HI) acid section (Section 3) greatly influences the thermal efficiency of the SI cycle. This Section 3 that comprises of HI-H_2O-I_2 (HIx system) is proposed to treat by a reactive distillation (RD) that allows the simultaneous separation and reaction in a single unit. Prior to designing the RD column, a deep knowledge of the thermodynamic behavior of the HIx system is inevitable. It is with this intention that the present work has been undertaken.

In this contribution, at first, the vapor-liquid equilibrium (VLE) model is proposed to estimate the bubble pressure of the highly nonideal complex HIx system. For this, we develop an artificial neural network based model followed by a simple non-random two liquid (NRTL) model, disregarding all side reactions commonly considered in previous studies. Getting reasonable accuracy, we extend our work to predict the phase equilibrium more rigorously in terms of compositions, along with bubble pressure, which are required for RD simulation. For this, three VLE models, namely NRTL, SRK (Soave-Redlich-Kwong) and PR (Peng-Robinson), have been formulated for a ternary (HI-H_2O-I_2), and four VLE models, namely NRTL, SRK, PR and NRTL-SRK, for a reactive quaternary (HI-H_2O-I_2-H_2) system. Experimental validation is made for all these phase equilibrium models. It is observed for the reactive quaternary system that the homogenous equation of state (EoS) models (i.e., SRK and PR) with no side reactions are capable of showing close performance, if not better, with the relatively complicated model of Murphy and O'Connell (2010).

Finally, a configuration for the RD column is constructed for simulation with using the developed SRK equation of state model and a kinetic model for the HI decomposition reaction. It is investigated that the proposed RD shows a close result, particularly in terms of H_2 production, with the simulation result reported by Murphy and O'Connell (2012), and Roth and Knoche (1989).

Keywords: SI thermochemical cycle; HIx system; vapor-liquid equilibrium; modeling and experimental validation; reactive distillation; hydrogen production