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Author: Meng Wang, Tim M. Becker, Carlos A. Infante Ferreira

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*Corresponding author.

Email address: M.Wang-2@tudelft.nl (Meng WANG)

Assessment of Vapor-Liquid Equilibrium Models for Ionic Liquid based Working Pairs in Absorption Cycles

Meng WANG*, Tim M. BECKER, Carlos A. INFANTE FERREIRA

Process and Energy Department, Delft University of Technology, Leeghwaterstraat 39 2628 CB Delft, The Netherlands

Highlights

- RK EOS is recommended in correlating VLE data and estimating mixing enthalpies in absorption cycles.
- The mixing of liquid NH_3 with IL is less exothermic than that of H_2O with IL.
- The total enthalpy of the studied NH_3/IL solution is less sensitive to VLE models than that of the studied $\text{H}_2\text{O}/\text{IL}$ solution.
- A lower estimation of the mixing enthalpy leads to an overestimated cycle COP.

Abstract

This paper assesses the performance of vapor-liquid equilibrium (VLE) models in ionic liquid based absorption cycles with natural refrigerants. Frequently used equation-of-state (EOS) based models, activity coefficient based models, and generic Clausius-Clapeyron relations are evaluated. Working pairs considered are $\text{H}_2\text{O}/[\text{emim}][\text{DMP}]$ and $\text{NH}_3/[\text{bmim}][\text{BF}_4]$. Firstly, experimental VLE data of those working pairs are correlated by using the models. Mixing enthalpies are then estimated using the models and corresponding correlated parameters. Performances of the different models in reproducing VLE data and estimating mixing enthalpies are compared with each other. Subsequently, total enthalpies and thermodynamic performances of absorption refrigeration cycles are predicted based on the different models. The assessment reveals that the RK-EOS and the NRTL model perform best in reproducing VLE data. In addition, the RK-EOS and the UNIFAC model show the best performance in estimating mixing enthalpies. Hence, the RK-EOS is recommended in correlating VLE data and estimating mixing enthalpies in absorption cycles.

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