Aromatic VOCs absorption with phenyl–based deep eutectic solvents: A molecular thermodynamics and dynamics study

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Abstract

The suitability of phenyl–based deep eutectic solvents (DESs) as absorbents for toluene absorption was investigated by means of thermodynamic modeling and molecular dynamics (MD). The thermodynamic models PC–SAFT and COSMO–RS were used to predict the vapor–liquid equilibrium (VLE) of DES–toluene systems. PC–SAFT yielded quantitative results even without using any binary fitting parameters. Among the DESs consisting of three different HBAs and three different HBDs (phenol, levulinic acid, ethylene glycol), [TEBAC][PhOH] was considered as the most suitable absorbent. Systems with [TEBAC][PhOH] had lowest equilibrium pressures of the considered DES–toluene mixtures, the best thermodynamic characteristics (i.e., Henry's law constant, excess enthalpy, free energy of solvation of toluene), and the highest self–diffusion coefficient of toluene. The molecular–level mechanism was explored by MD simulations, indicating that [TEBAC][PhOH] has the strongest interaction of HBA–/HBD–toluene compared to the other DESs under study. This work provides guidance to rationally design novel DESs for efficient aromatic VOCs absorption.

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