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Phase equilibria and diffusion behavior of high pressure CO_2 in tetra-n-heptyl ammonium bromide

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Abstract: The solid–liquid–gas equilibrium data of the tetra-n-heptyl ammonium bromide ([thepAm][Br])–CO_2 system, and then the solubility and absorption kinetic data of CO_2 in different phases of [thepAm][Br] were measured by a high pressure quartz spring method. Results showed high molar fractions of CO_2 in solid [thepAm][Br] (0.921 at 15.0 MPa and 313.2 K; 0.567 at 5.0 MPa and 313.2 K) which were even higher than those in liquid [thepAm][Br] at same pressures and those in other ionic liquids (ILs) reported in the literature at relatively high pressures. The study also revealed that CO_2 absorption rate was very pressure dependent. The Peng-Robinson equation of state (PR-EoS) with the van der Waals one–fluid mixing rules and the NRTL model were employed to calculate the phase equilibrium data by looking the solid [thepAm][Br] as a special liquid. A 1-D diffusion model with a concentration dependent diffusion coefficient equation combined with the NRTL model was developed to calculate the absorption kinetic data of CO_2 in [thepAm][Br], suggesting that the diffusion coefficient was not a constant at high pressures.

Keywords: Tetra-n-heptyl ammonium bromide; Carbon dioxide; Solid–liquid–gas equilibrium; Solubility; Diffusion model; High pressure