

Predicting CO₂ solubility in aqueous and organic electrolyte solutions with ePC-SAFT advanced

CO₂ solubility is predicted, and solvent-specific and ion-specific effects are evaluated

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CO₂ solubility in aqueous and organic electrolyte solutions is of special interest for carbon capture and storage (CCS) or utilization (CCU) processes. Unfortunately, the experimental determination at such conditions is rather laborious. Therefore, the ion-based model ePC-SAFT advanced was used in this work to predict the CO₂ solubility in such systems. We found that the model predictions were accurate. For the first time the salt effect on CO₂ solubility was predicted without the use of parameters that correlate the ion-CO₂ interactions. The mixtures under investigation were binary systems of CO₂ + solvent and higher systems comprised of water + organic solvent + salt (NaCl, KCl, CsCl, MgCl₂, CaCl₂, NaNO₃, KNO₃, Mg(NO₃)₂, Ca(NO₃)₂, Na₂SO₄, K₂SO₄, MgSO₄, NaHCO₃, and K₂CO₃).

Knowledge on CO₂ solubility is of crucial importance for process engineering. As the experimental determination is expensive, we used ePC-SAFT advanced to predict CO₂ solubility in various aqueous and organic electrolyte solutions. First, systems of CO₂ + solvent were considered (Figure 1), showing that the CO₂ solubility is highest in non-polar solvents. In a next step, more complex systems containing solvent mixtures and additional salts were studied.

The nature of the considered systems required including dissociation reactions of carbonic acid (H₂CO₃/HCO₃⁻/CO₃²⁻) in the modeling framework, most importantly for the systems containing carbonate salts. The results showed that all salts caused salting-out effects on the CO₂ solubility except carbonates (an apparent salting-in due to a pH shift), as shown in Figure 2. The strength of the salting-out effect is related to the charge density of the ions. ePC-SAFT advanced was found to accurately predict the CO₂ solubility in aqueous and organic electrolyte solutions while accounting for solvent-specific effects and ion-specific effects for a broad range of conditions.

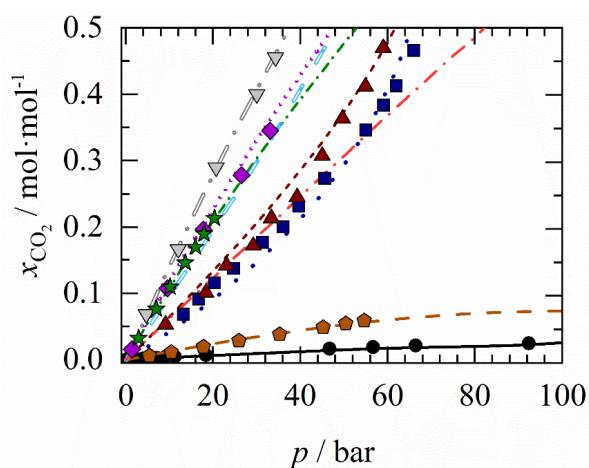


Figure 1: CO₂ solubility in mole fraction in different solvents plotted against the pressure at constant temperature $T = 313.15$ K. Symbols represent experimental data from the literature (solid circles: water, solid hexagons: GVL, solid squares: methanol, solid up-triangles: ethanol, solid stars: NMP, solid diamonds: DMF, and solid down-triangles: THF). Lines are modeling results (solid line: water, long-dashed line: GVL, dotted line: methanol, long-dash-dotted line: DMSO, short-dashed line: ethanol, empty-dashed line: MeCN, short-dash-dotted line: NMP, empty-dotted line: DMF, and empty-long-dash-dotted line: THF).

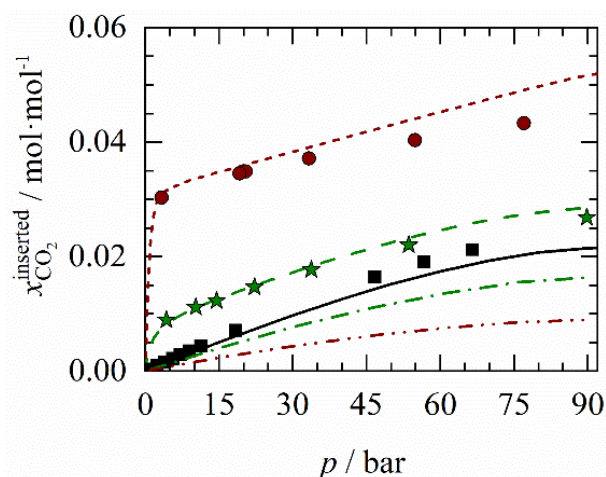


Figure 2: CO₂ solubility in aqueous electrolyte solutions in mole fraction plotted against the pressure at constant temperature $T = 313.15$ K. Symbols represent experimental data from the literature (solid squares: salt-free system, solid stars: 0.42 mol kg⁻¹ K₂CO₃, and solid circles: 1.71 mol kg⁻¹ K₂CO₃). Lines represent predictions (solid line: salt-free system, dash-dotted line: 0.42 mol kg⁻¹ K₂CO₃ and dash-double-dotted line: 1.71 mol kg⁻¹ K₂CO₃ while neglecting the dissociation of carbonic acid, dashed line: 0.42 mol kg⁻¹ K₂CO₃ and dotted line: 1.71 mol kg⁻¹ K₂CO₃ including the dissociation of carbonic acid).

Publications:

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