Modeling the CO_2 Solubility in Electrolyte Solutions with ePC-SAFT

CO_2 solubility is predicted as function of pressure, temperature and salt concentration

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Carbon dioxide (CO_2) solubility in aqueous electrolyte solutions is of special interest for carbon capture and storage or utilization, particularly as function of temperature, pressure, and electrolyte concentration. Unfortunately, experimental determination at such multivariable conditions is laborious. Therefore, the ion-based model ePC-SAFT was used to model the CO_2 solubility in such systems in a broad range of conditions. The CO_2 solubility was successfully modeled in water and in aqueous electrolyte solutions containing alkali and earth alkali chlorides and nitrates or mixtures thereof.

Knowledge on the CO_2 solubility in water and in various electrolyte solutions is important in many different applications in the chemical industry. Many data sets exist in the literature, some of them being very old or unreliable, or without knowledge of the experimental uncertainty. Still, thermodynamic models that have been applied do not cover all of the studied experimental conditions in terms of temperature, pressure, and type and concentration of electrolyte. Thus, in this work ePC-SAFT was applied to fill this research gap. First, the basic system CO_2 + water was characterized as shown in Figure 1. For temperatures up to 423 K and pressures up to 150 bar the pH was found to be in a range between 2.5 – 4.0 depending on the amount of dissolved CO_2. In these pH ranges, CO_2 dissociation reactions were found to be negligible. Thus, only the molecular species water and CO_2 were considered and dissociation species were neglected. Accounting for cross hydrogen bonds between water and CO_2 allowed modeling the system quantitatively correct.
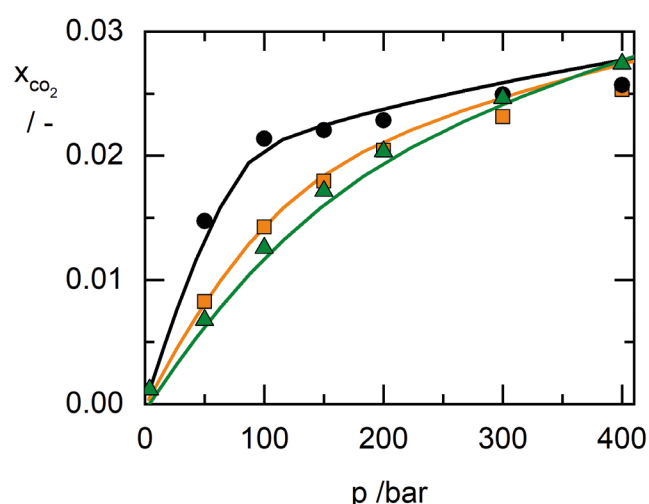
Further, the influence of different concentrations and types of electrolytes (i.e. the salts containing chloride and nitrate alkali and alkaline-earth metals) was investigated. The salting-out effect of NaCl for different concentrations varying from 1 to 5 mol salt per kg water is shown in Figure 2. Compared to the solubility in pure water, adding salt successively increases the salting-out effect, i.e. reduces the CO_2 solubility. This behavior was observed for all investigated systems. ePC-SAFT was found to be able to accurately model the CO_2 solubility in in aqueous systems containing electrolytes over a broad range of temperatures, pressures, and salt concentrations.
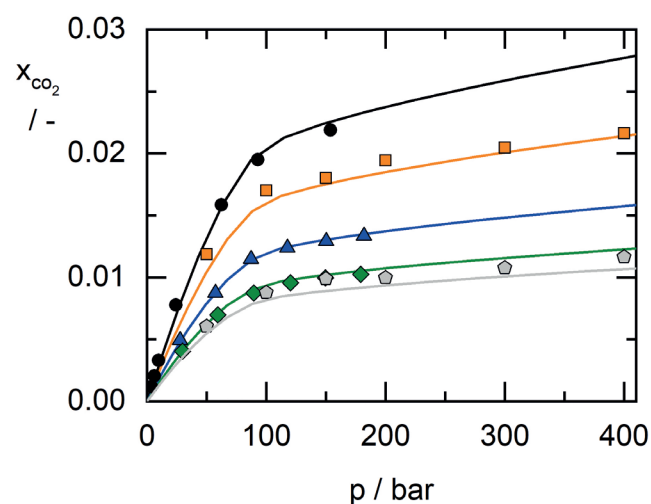

Figure 2: CO_2 mole fraction solubility as function of pressure at T = 323 K for different NaCl molalities (circles salt free), squares $\tilde{m}$ = 1 mol kg^{-1}, up-triangles $\tilde{m}$ = 2.5 mol kg^{-1} , diamonds $\tilde{m}$ = 4 mol kg^{-1} , and pentagons $\tilde{m}$ = 5 mol kg^{-1}. Lines are ePC SAFT modeling results.

To conclude, ePC-SAFT is now available to predict successfully the influence of pressure, temperature and kind and concentration of salt and salt mixtures on the CO_2 solubility.

Figure 1: CO_2 mole fraction solubility as function of pressure at three different temperatures varying from 323 K to 413 K (circles T = 323 K, squares T = 373 K, triangles T = 413 K). Lines are ePC SAFT modeling results.

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