Fluid-Fluid Equilibria of Carbon Dioxide - Aromatic and Carbon Dioxide - Dichlorobenzoate Binary Mixtures

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In this work, the capabilities and usefulness of a molecular-based equation of state, PC-SAFT and several cubic equations of state (PR, SRK, SOFPR, SOF-RK) were explored. Specifically, the two-phase fluid-fluid regions (VLE, LLE) of several demanding binary mixtures of aromatics as well as dichlorobenzoates (alkyl and semi-fluorinated) with supercritical CO_2 were evaluated. Group contribution approaches were used to estimate the pure-fluid parameters for the alkyl and semi-fluorinated dichlorobenzoates needed for each equation of state. We showed that these models can capture many important features of the complex phase behavior of highly asymmetric systems composed of supercritical CO_2 and alkyl (nonfluorinated or semifluorinated) 2,5-dichlorobenzoates. For example, the presence of VLE and LLE regions for the propyl 2,5- dichlorobenzoate system at 323.15 K is clearly predicted from both molecular based and cubic equations of state. It was found that the LLE envelope narrows in mole fraction and the upper critical solution pressure increases with the growing alkyl chain. The present results are open to quantitative improvement, and in this sense our work must be seen as a first effort toward a fully predictive treatment. As more experimental data become available, however, we are confident from these results that thermodynamic modeling can be perfected to provide reliable correlation and prediction of the phase behavior of these and related systems.