High-pressure phase equilibrium studies of multicomponent (alcohol+water+ionic liquid+CO_2) systems

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Climate change poses one of the major problems and challenges worldwide and is predominantly caused by an increasing amount of greenhouse gasses emissions. In this context, CO_2 capture will very likely be a practical reality, generating large amounts of compressed CO_2 in high purities, which will have to be stored or used as raw material in the production of chemicals and fuels [1]. One of the most promising route to the systematic use of CO2 as a chemical raw material is in the synthesis of low energy molecules, such as organic carbonates. The reaction between CO2 and alcohols has been subject of intensive research and is very promising, although it has a severe equilibrium limitation caused by the formation of high quantities of water as a by-product [2].

In this work the utilization of highly hydrophobic ionic liquids with a high CO2 up-take, e.g. fluoroalkylphosphate- and tetracyanoborate-based [3,4], were explored in order to remove the water and shift the reaction equilibrium towards product formation. For that purpose, it is essential to determine the phase behaviour of such a multicomponent reaction system containing substrate (diol), ionic liquid, water and organic carbonate, under high CO_2 pressures. Vapour-liquid equilibrium measurements were performed with a static analytical method at various temperatures and pressures up to 18 MPa. A proof-of-principle reaction was performed and the role of highly hydrophobic ILs as in-situ dehydrating agents is discussed.

References :

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