Phase equilibria of 1,4-butanediol in supercritical CO_2

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The reuse of carbon dioxide (CO_2) in new processes has been one of the means used to apply this substance reducing its concentration of the atmosphere, minimizing it contribution on the greenhouse effect. Its use in supercritical conditions as solvent has several advantages due to its green properties. Recent research shows that valorization of the raw biomass by successive catalytic hydrogenations is a promising route for obtaining products of commercial value for the industry such as 1,4-butanediol (BDO). The use of supercritical CO_2 (SC-CO_2) promotes a better conversion as well as greater selectivity and safety for the large-scale process, facilitating the separation of the desired product since the reaction medium occurs in biphasic system. In order to optimize the separation step of BDO in hydrogenation of biomass, a phase equilibrium study is necessary to understand the system behavior under the operating conditions. In this sense, this work evaluated the phase equilibria of BDO + H_2O + SC-CO_2 at 313.15 and 333.15 K, in different pressures conditions. The experimental results indicated that the BDO partition for the gas phase is low, at pressures of 160, 200, and 280 bar, however, the addition of H_2O in the medium increases the solubility of BDO in SC-CO_2 at 280 bar. The increase in temperature also increases the solubility of BDO in SC-CO_2.Through this study, it is possible to define the best condition for the BDO separation, minimizing operating costs in the industry when carried out on a large scale.