Phase Equilibrium Calculation of Mixtures containing Polymer, Supercritical Fluids and Cosolvent using Lattice Fluid EOS

알렉산더, 유기풍, 임종성, 이철수[1], 강정원[1,*]
서강대학교; [1]고려대학교
(jwkang@korea.ac.kr[*])

Supercritical fluids are considered as an alternative media for polymer processing since they exhibit considerable solubility and gas−like viscosity. For simple polymers such as polyolefins, supercritical carbon dioxide can be a good media for separation and reaction because they show high solubility even just above the critical pressure of carbon dioxide. However, polymers with complex structures exibit limited solubility. Cosolvents can be introduced to enhance solubility of supercritical fluids for polymer processing. The choice of the cosolvent for specific polymer processing requires experience and a significant amount of experiments among a broad spectrum of solvent candidates. In this study, phase equilibrium calculation have been performed for polymer + supercritical fluid + cosolvent systems and accuracies of calculation and effect of cosolvents are discussed. The nonrandom lattice fluid equation of state with hydrogen bonding (NLF−HB EOS) proposed by the current authors were used because they can be extended toward group contribution model and further extended to predict the effect of the solubility enhancement of cosolvents.