

Modeling of Supercritical Carbon Dioxide - Biopolymer Systems

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Biopolymer particle formation is a promising application of supercritical fluid technology [1] and has received much attention in the literature. Use of supercritical CO₂, in particular, has provided a ‘clean’ and effective alternative to liquid solvents such as tetrahydrofuran and methanol that are commonly employed in crystallization and particle formation steps in the pharmaceutical industry. However, efficient development of supercritical fluid technology for biopolymer particle formation suffers from the fact that equations of state used in process simulation software cannot adequately describe the unique characteristics of long polymer chains in supercritical solutions [2].

Recently, Ozkan and Teja [3] described a thermodynamic model for associating polymer solutions based on lattice theory. Their model accounts for specific solute-solvent interactions in supercritical CO₂ –polymer solutions, as well as the compressibility of the lattice. In the present work, we discuss the application of their model to the prediction of phase behavior of supercritical CO₂ and D, L poly lactic acid (PLA) or lactic acid-glycolic acid (PLGA) co-polymers. In situ Fourier transform IR (FT-IR) spectroscopy was employed to investigate the interaction of CO₂ with the above polymers. Shifts in the spectra of polymers exposed to CO₂ were used to obtain one of the model parameters. We also show that the sorption behavior of supercritical CO₂ – biopolymer systems can be a priori predicted using parameters obtained from FT-IR and cloud point data.

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