Phase Behavior of Polymer-Supercritical Fluid Mixtures

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Abstract

The unique solvent characteristics of supercritical fluids (SCF)* are of great interest in the area of polymer processing. Significant challenges remain for developing the same level of understanding of polymer-SCF solution behavior than for polymer-liquid mixtures. In principle, it is possible to describe the phase behavior of polymer-SCF mixtures using a model including an equation of state. But these equations of state for polymer solutions suffer from certain limitations because they are still not well adapted to describe the unique characteristics of a long-chain polymer in solution. In addition, SCF-polymer solutions are highly compressible mixtures which precludes the application of a rigid lattice description of solution properties.

Our deal with modeling is to predict the changes in phase behavior with a minimum number of fitted parameters. Several different equations of state can be used to calculate polymer-SCF solvent phase behavior. We are interested in understanding three models : Flory-Huggins, Sanchez-Lacombe and SAFT (Statistical Associating Fluid Theory) in order to program the code for each approch including MM, MD and QM techniques. Our research project is based on the phase behavior description of two different mixtures : poly-ε-caprolactone (PCL) and polylactides in supercritical carbon dioxide. The objective of this study is to optimize the synthesis parameters taking these two systems as examples.

* in this work, SCF stands for SuperCritical Fluid (and not Self Consistent Field).

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