Modeling the Vapor-liquid and Liquid-liquid Equilibria of Polymer Solutions

N. Pedrosa[S], J.A.P. Coutinho, and I.M. Marrucho[C]
Chemistry Department, University of Aveiro CICECO, Aveiro, Portugal

L.F. Vega
Institut de Ciència de Materials de Barcelona, Bellaterra, Cataluña, Spain

In industrial environment, polymer solutions are very common, as they appear in the polymerization process, the separation and purification processes. Although there are nowadays a number of models to describe such solutions, it is very difficult to have a universal treatment in terms of their modeling due to highly non-ideal behavior caused by the co-existence of large molecules (polymers) with small molecules (solvents and unreacted monomers).
In this work, the soft-SAFT (Statistical Association Fluid Theory) equation of state (EoS) was extended to model the phase behavior of polymer systems, in particular, vapor-liquid and liquid-liquid equilibria of polyethylene (PE) mixtures. In the context of the soft-SAFT EoS, a set of molecular parameters is needed for each substance: m, to describe the length of the chain of segments; σ to describe the size of each segment and ε being the energy of that segment. The molecular parameters for the PE were determined by extrapolation of the correlation of parameters established for the alkanes. However, a different correlation was used to calculate the energy parameter. The molecular parameters for the solvents have already been published before.

In this work the modeling of the vapor-liquid and liquid-liquid equilibria of binary mixtures of polymers and solvents.