An algorithm for calculation fo cloud point of polydisperse polymers using NLFHB EOS

이주호, 이철수*, 강정원
고려대학교
(cslee@korea.ac.kr*)

An algorithm was proposed to calculate high pressure liquid-liquid equilibria of solvent-polydispersed polymer systems, ethylene-HDPE, ethylene-LDPE and 1-butene-Polybutene at various temperatures. All constituents of polydispersed polymers were regarded as a one pseudo component characterized by two parameters. The proposed algorithm is divided into two loops – inner and outer loop. In inner loop, the two parameters of pseudo component is obtained by satisfying some material and equilibrium equations at given P. Outer loop adjusts pressure to satisfy all equilibrium equation. To test the applicability of the proposed algorithm, cloud point pressure was calculated of some systems using NLF(Non-random lattice fluid theory). NLF equation of state was shown to be formulated with the parameters of pseudo component regardless of the number of polymers in polydispersed polymer like SAFT(Statistical Associating Fluid Theory). We tried to find the parameter of equation of states for polymer species by optimizing both PVT data of polymers and cloud point data of polymer-monomer. Calculation result showed that optimized parameters for NLFHB EOS exists however it doesn't correctly predicts critical point of polydisperse-solvent system.