Simplified Flory-Dimer Equation of State for Application to Normal Fluids, Polymers and Their Mixtures

양한얼, 배영찬[1,†]
한양대학교; [1]한양대학교 화학공학과
(ycbae@hanyang.ac.kr[†])

A simplified generalized Flory dimer (s-GFD) theory is developed to improve the performance of equation of state (EOS) for long chain molecules. The new EOS is formulated by a combination of the s-GFD theory and perturbed chain statistical associating fluid theory (PC-SAFT). Three pure component parameters were obtained by correlating experimental liquid densities and vapor pressures for pure n-alkanes ranging from methane to eicosane. The pure component parameters of polyethylene (PE) were determined by extrapolating the pure component parameters of a series of n-alkanes. Compared to PC-SAFT, the new equation provides better correlation results for vapor pressures and liquid densities, particularly for long chain molecules and for PE. The proposed model allows phase equilibrium calculations to be conducted for binary and ternary mixtures of volatile components without requiring the use of binary interaction parameters. Correlations were carried out for equilibrium behaviors of PE solutions by using one adjustable parameter, and the calculated results agreed well with experimental data.