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Modeling of phase behaviors for hydrogen bonding polymer solution using PC-SAFT equation of state

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Modeling of the phase behavior of polymer solutions is a crucial requirement to develop new polymer solution technologies and to design various polymer processes, such as purification, fractionation, devolatilization and polymer production. In particular, the Liquid-Liquid Equilibrium (LLE) calculation is essential for processes design of polymerization. The hydrogen bonding in polymer solutions leads to deviate remarkably from normal solutions behaviors and is a major cause of different phase behaviors. The perturbed-chain statistical association Fluid Theory (PC-SAFT) Equation of State (EoS) is applied to calculate the pressure-volume-temperature (PVT), infinite dilution weight fraction activity coefficient (WFAC), Vapor-Liquid Equilibrium (VLE) and Liquid-Liquid Equilibrium (LLE) of associating polymer mixtures with hydrogen bonding association such as self- and cross-association with various phase behaviors such as Upper Critical Solution Temperature (UCST), the Lower Critical Solution Temperature (LCST) and closed-loop of polymer solutions. The PC-SAFT model shows a satisfactory performance.

Biography

Bong-Seop Lee has his expertise in modeling the phase behaviors on organic molecules, polymers, biological molecules (i.e., amino acid, peptide) and electrolyte solutions (i.e., inorganic salt, ionic liquids). He has received his Master's degree and developed the electrolyte-PC-SAFT equation of state by combining PC-SAFT and primitive mean spherical approximation in his PhD course. In his Post-doctoral studies, he focused on the modeling of physical and chemical properties of ionic liquid mixtures. His research interest is in dissociation phenomena of weak and strong acids and the equilibrium of various materials (polymer, blend, organic solvent) at high pressure condition.

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