

Saft Parameters for Polymers from a New Strategy

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Knowledge of thermodynamic properties and phase equilibria (PE) behavior of polymer systems plays a fundamental role in the design and operation of equipment used in polymer processing and manufacturing. The PE of polymer solutions depends strongly on both free-volume and energetic interactions between the constituent components. Three types of models have been proposed for the description of PE of polymer systems: activity coefficient models (polymer NRTL and UNIFAC-FV), lattice models (Flory-Huggins and Sanchez-Lacombe) and equations of state (polymer-SRK and SAFT). The statistical associating fluid theory (SAFT) was specifically developed to treat systems containing not only long-chain polymers but also associating fluids. However, the modeling of PE of polymer solutions using SAFT-type equations presents mainly two difficulties: (i) the determination of polymer molecular parameters from traditional methods (fitting to vapor pressures and liquid densities data) is not possible as polymers have no detectable vapor pressure and (ii) numerical problems due mostly to large differences in size between polymer and solvent molecules. Three different approaches have been proposed so far to circumvent the difficulties in the estimation of pure-polymer parameters: the group contribution method, the use of binary data and the use of extrapolating equations. In this work, a recent developed parameterization strategy that allows for the estimation of polymer molecular parameters from a pre-defined set of macroscopic properties is used. The parameterization scheme has been developed in terms of the Flory-Huggins interaction parameter, χ , and the Hildebrand parameter, δ , which are readily available in the literature for a large variety of solvents and polymers. The proposed parameterization strategy is demonstrated by reference to the PC-SAFT equation, but might be extended to any molecular-based model. Selected polymer solutions are shown as illustrative examples of the more than 120 polymeric systems studied in this work, that include both associating and non-associating polymers and solvents.