POLYSTYRENE MIXTURES PHASE EQUILIBRIA: A STATISTICAL ASSOCIATION THEORY APPROACH

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In the present work the phase equilibria of polystyrene with a number of solvents is modeled with the molecular based soft-SAFT Equation of State (EoS)[1]. The SAFT EoS has mainly three parameters characterizing each substance: m, the number of molecular segments, σ, the molecular size of each segment and ε, its the energy.
For small molecular weight substances this is a valid approach, but when modeling polymers when modeling polymer systems, the wide number of average molecular weights for the same polymer has to be taken into account. Thus usually the energy (ε) and the size of segment (σ) are kept constant for a given polymer and only the number of segments changes with molecular weight. Several approaches have been analyzed in a recent work [2] to find the best way to calculate molecular parameters for a polymer.
In this work a method previously tested for the PC-SAFT EoS [3] is used to model polystyrene solutions. It consists on fitting the polymer parameters to a mixture data, along with the binary interaction parameter. Some polymer-solvent mixtures were modeled with this procedure and the validity of the parameters for different polymer molecular weights was checked.
Phase equilibria calculations were performed for polystyrene mixtures with very large ($M_n = 2.70 \times 10^6$ g/mol) and very small ($M_n = 1241$ g/mol) average molecular weight. The obtained results show that both liquid-liquid and vapor-liquid modeling of these mixtures with soft-SAFT EoS was successful for very large molecules. However, the polystyrene parameters considered have prooved to be inadequate when describing the liquid-liquid phase equilibria of polystyrene of very low molecular weight with n-alkanes.

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