# Phase Equilibrium Calculations of the System Polystyrene-Methylcyclohexane with the Sanchez-Lacombe Equation of State Using Continuous Thermodynamics

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The system polystyrene (PS) in methylcyclohexane has been studied many times [1-7] and a lot of experimental data exist for this system. Narita et al. [3] determined a semi empirical equation of Gibbs free energy of mixing ($\Delta G$) for the system based on the Flory-Huggins equation. The equation of $\Delta G$ was used to prepare microcapsules of controlled size distribution. Vanhee et al. [4] used a nearly monodisperse PS. They applied a pressure-pulse – induced scattering (PPIS) technique and found spinodal and cloud-point curves. They observed the pressure-concentration diagram shows upper critical point (UCP) and lower critical point (LCP) behavior for some temperatures. These curves come closer and turn into hour-glass shaped curves by lowering the temperature. Browarzik et al. [7] studied the mentioned system by using the SWP (Sako-Wu-Prausnitz) equation of state which is suitable for polymer solutions. They also discussed the transition of the UCP/LCP behavior into the hour-glass diagrams for polydisperse polymer and studied the polydispersity effect on stability and phase equilibria. Koak et al. [6] reported experimental cloud-point data for PS-MCH systems in the vicinity of the upper critical solution temperature (UCST) and phase equilibria were measured in the glass tube Cailletet apparatus for two samples of polystyrene. One was nearly monodisperse and the other was polydisperse.

In the present work the Sanchez-Lacombe equation of state is used to model the stability and cloud-point curves of polystyrene (PS) in methylcyclohexane (MCH) systems. An algorithm based on the work of Browarzik and Kowalewski [7] is applied. Three different polymers are studied. Two of them are monodisperse and the third one is polydisperse. To describe the polydispersity of polystyrene, the Schulz-Flory distribution function is considered. One of the monodisperse systems shows lower critical point (LCP) and upper critical point (UCP) curves at a certain temperature region, which turn into hour-glass shaped cloud-point curves by lowering the temperature. Excellent agreement between modeling and experimental data was observed.

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