Systematic Investigation of the Influence of Additives on Polymer Solution

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Polymer solution are often modelled with the Flory-Huggins approach or the Sanchez- Lacombe equation of state. In the last decade the Statistical Association Fluid Theory (SAFT) gained more attention. Comparisons of calculations with the SAFT model have shown that it is more appropriate for the description of polymer solutions [1]. Based on our biquadratic equation of state for chain molecules [2], which accurately reproduces the more complicated SAFT model, a fourth oder equation for long chain molecules has been developed [3]. Using this equation we performed a systematic investigation of the phase behavior during a polymerisation.

The solubility of polymers over a wide range of temperature and pressure decreases with increasing molecular weight. At some point in a polymerisation the polymer precipitates from the solution because of the increasing molecular weight. In order to avoid the precipitation one can increase the pressure in the reactor. An alternative way to increase the solubility is the introduction of additives. With co-solvents the polymerisation can be continued towards higher molecular weight without increasing the pressure. The opposite effect can be accomplished by adding anti-solvents such as compressed carbon dioxide [4]. This can be used for separating the polymer.

In this investigation the connection between molecular processes and macroscopic variations of the phase behavior is accomplished by global phase diagrams. The investigated system consists of monomers mixed with oligomers or monodisperse polymers. With paths in the global phase diagram the effect of co-solvents on the self-attraction and the cross-attraction is investigated separately.

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