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Polymer thermodynamics for pharmaceutical applications

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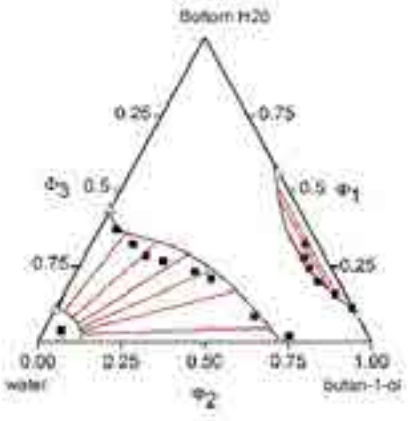
Polymeric carries, which physically entrap molecules of interest (pharmaceutical active ingredient, API) and polymer conjugates, to which such molecules are chemically bound, play an important role in modern pharmaceutical technology. Macromolecular architecture is receiving increasing interest as the search for new tailor-made polymeric materials with strictly specified properties intensifiers. Therefore, the molecular architecture must be taken into account in the thermodynamic framework. The lattice cluster theory (LCT), developed by Dudowicz and Freed, allows the calculation of the thermodynamic properties of a molecule having an arbitrary structure and hence it is possible to take the short-chain branching of the polymer directly into account. The LCT will be utilized to model phase equilibria of polymer containing mixtures. Polymers involved in this research are polyolefins and hyperbranched polymers. In the case of polyolefins, which are semi-crystalline polymers, the chemical composition, the molecular weight distribution, stereoregularity and short-chain branching distributions (SCBD) play the dominant role for the material properties. All these properties show an impact of the related phase equilibria (solid-liquid equilibria, liquid-liquid demixing at high pressure). This contribution demonstrated the possibilities as well as the limitation of the LCT and their modifications for phase equilibria predictions. Hyperbranched polymers carry a large number of polar terminal groups and therefore they are widely applied for increasing the solubility in water and consequently the bioavailability of hydrophobic API. In this contribution the increase of the solubility of the model API quercetin, which has very poor water solubility, by adding a hyperbranched polymer will be discussed. Alcohols are excellent solvents for quercetin, however, quercetin degraded in this solvent. Additionally, the prediction of the relevant liquid-liquid equilibria using the LCT is discussed in detail. One example is the ternary system composed of hyperbranched polymer+water+butanol (Figure-1).



Biography

Sabine Enders leads the Institute of Technical Thermodynamics and Refrigeration Technology at the Karlsruhe Institute of Technology in Germany. Her scientific expertise lies in the field of phase behaviors and interfacial properties of complex mixtures, such as mixtures containing polymers, crude oil, pharmaceuticals or surfactants.

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