

Thermophysical Property Databases in Chemical Engineering - A Survey of Existing Data Bases with the Focus on Electrolyte Solutions

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For the design and modeling of chemical plants, process calculations are carried out during the whole process life cycle. Especially in the case of the synthesis, simulation and optimization of separation processes, the phase equilibrium of the system to be separated has to be known exactly. Chemical and process engineers are nowadays able to model or even predict a vapour-liquid-equilibrium, the density or viscosity of a multicomponent mixture containing numerous different species with sufficient reliability. But these calculations depend heavily on availability and reliability of thermophysical property data of the pure components and mixtures involved, mainly when in a later status of a process design the accuracy of models as equations of state or group contribution methods are not sufficient anymore. This is especially true when salts are contained in the mixtures. In that case even traces of salts have the consequence that nearly all models work with less accuracy or even tend to fail. Another area influenced greatly by electrolyte modeling is biochemical engineering. For example nobody knows how to predict quantitatively salting-out effect of proteins. Nevertheless modeling results have a great impact on the design and construction of single chemical apparatus as well as whole plants or production lines. Inaccurate data may lead to very expensive misjudgments whether it is to proceed with a new process or modification of it or not to go ahead. So even today, where the usage of process simulation packages is a standard feature, many improvements can be done for the precision of the models in using experimental thermophysical properties. Therefore chemical engineers developing new production processes are having a pressing need to access reliable thermophysical property data. In the following an actual survey on the worldwide existing and still maintained collections and databases is given, with a special focus on data for electrolyte solutions or, more generally, for liquids containing a fraction of electrolytes.