

# **Physical Property Data in Process Technology @ BASF - From Basic Chemicals to Complex Molecules**

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BASF chemicals are used in almost all industries. The BASF segments Oil & Gas, Chemicals, Functional Materials & Solutions, Performance Products and Agricultural Solutions are covering a wide diversity from basic chemicals to complex molecules. Correspondingly physical property data requirements for chemical research, process design and unit operations are challenging with regard to quality and complexity.

Physical Property Data and Thermodynamics are the basis for process development from the first draft to the optimized plant. The point of origin are and remain in foreseeable future experimental data, a comprehensive physical property database is therefore essential. In addition to traditional fitting equations molecular based modelling methods are applied progressively in industrial process development and design. PC-SAFT- type equations of state enable a physically sound extrapolation for multicomponent systems. With quite high effort the Molecular Simulation, based on customized force fields, is so far only feasible for important systems and enables access to a complete set of physical property data and structural dynamic properties of fluids mixtures.

Thermodynamic screening of process and functional additives and solvents enables a drastic reduction of the experimental effort and the costs for the additive selection. The screening approach by shortcut physical property data criteria and the data compilation is outlined. By means of examples the options and also the limitations are addressed.