

Generating Reliable Thermodynamic Model Parameters with the Help of DECHEMA Software Suite

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Process synthesis, design and optimization, and detail engineering for chemical plants and equipment depend heavily on availability and reliability of thermophysical property data of the pure components and mixtures involved. Inaccurate data may lead to very expensive misjudgments on whether or not to proceed with a new process or modification. Inadequate or unavailable data may cause the delay or even rejection of a promising and profitable process, only because it was not properly modeled in a simulation. The most sophisticated software will not automatically lead to the most cost-effective energy saving solution, unless there is a background with an accurate correspondent database of physical and thermodynamic data, as well as a full featured data regression package.

One example of a valuable source of data combined with an adequate software tool is the DETHERM Software Suite, which consists of the numerical database DETHERM and the data regression and optimizer tool Data Preparation Package. DETHERM now contains more than 5.6 million data sets for more than 115,000 pure components and mixtures. The data are collected and updated by well-known research groups, e.g. the Universities of Oldenburg and Regensburg, the DDBST, and the FIZ CHEMIE. The properties stored include mainly phase equilibrium data (VLE, LLE, SLE, VLLE), vapor pressures, critical data, thermodynamic properties, transport properties, surface tensions, and electrolyte data. Following a database retrieval, the DECHEMA Data Preparation Package can be used to close the gap between raw thermophysical data and model parameters, as used in any process simulation package. Data retrieved in DETHERM or otherwise generated data sets can be displayed, compared, and selected. Afterwards, parameters for pure component as well as binary models can be regressed and displayed in comparison with the data. The regression module is capable of simultaneously correlating different data types using different error functions. For example the simultaneous correlation of VLE, LLE, HE, gamma, gamma infinity, and azeotropic data is possible. The package is not restricted to its built-in thermodynamic models. Thermodynamic calculations are performed using a standardized Interface. In many cases, this enables users to simply plug in any thermodynamic package and/or model of their choosing.