

Improving Model Parameters with the Help of DECHEMA Thermophysical Databases and Engineering Software Packages

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Inaccurate thermophysical property 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. Inadequate or unavailable data may cause that a promising and profitable process can be delayed or in the worst case be rejected, only for the reason that it was not properly modelled in a simulation. So the most sophisticated software will not lead automatically to the most cost-effective solution in order to save effectively energy, if there is not a background with a correspondent accurate database of physical and thermodynamic data as well as a full featured data regression package. One example for a valuable source of data is the DETHERM database, which provides thermophysical property data for about 36,500 pure compounds and 124,000 mixtures. DETHERM contains literature values, together with bibliographical information, descriptors and abstracts. The DETHERM database is produced from the DECHEMA e.V. in cooperation with the DDBST GmbH, Oldenburg and the FIZ CHEMIE in Berlin. At the time 7.5 million data sets are stored. The database is updated yearly and grows continually with around 8 % per year. The following properties are stored:

- phase equilibrium data
- vapor pressures, critical data
- thermodynamic properties
- transport properties
- surface tensions
- electrolyte data

The user friendly interface enables even unskilled users a rapid and easy access of desired data. The graphical display of data gives an overview on the distribution of the different data sets. For further processing the data can be exported in various formats (XML, CSV, IK-CAPE PPDx). Users of MS/Excel can cut & paste the data also directly. Seamless interfaces exist to a variety of process simulation and data like Aspen Properties or Simulis. The user's own data can be readily handled with the data maintenance module. Following up to the database retrieval the DECHEMA Data Preparation Package will be used to close the gap between raw thermophysical data and model parameters, as used in any process simulation package. Besides selection und graphical display of data sets the package permits the regression of model parameters as well as the comparison of models with each other (e.g. comparison of the gamma models NRTL vs. Wilson vs. UNIQUAC or comparison of vapor pressure equations like Antoine vs. Wagner).