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# DECHEMA
# Thermophysical databases and engineering software packages.

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The numerical database DETHERM provides thermophysical property data, which are indispensable for construction and design of chemical apparatus, plants and processes.

The DETHERM database provides thermophysical property data for about 31,600 pure compounds and 115,200 mixtures. DETHERM contains literature values, together with bibliographical information, descriptors and abstracts. At the time 7 million data sets are stored. The database is updated yearly and grows continually with around 8 % per anno. The follo-wing properties are stored:

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

The DETHERM database is produced from the DECHEMA e.V. in cooperation with the DDBST GmbH, Oldenburg and the FIZ CHEMIE in Berlin.

A DETHERM Inhouse installation consists of a SQL database server in combination with the retrieval package DETHERM-ORS. 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. Running in Client-Server-Mode assures that all users of the system use identical data sets. Multiple data sets and the use of differing values from user to user can thus be avoided.

## B) Data Preparation Package DPP

The DECHEMA Data Preparation Package (DPP) closes the gap between raw thermophysical data as stored in the DETHERM database and model based process simulation packages like Aspen Properties or Simulis. 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).