DDBST
Dortmund Data Bank
Software & Separation
Technology

DDB Model Parameter Estimator

Fitting g^E and EOS Model Parameter from Group Contribution based Estimation Methods

For the calculation of the multicomponent mixture behavior using different g^E and EOS models the knowledge of the binary interaction parameters is required.

If these parameters are not available, they are usually derived from experimental vapor-liquid equilibrium data or other mixture data. If these data are also not available, group contribution methods can be used for the estimation of activity coefficients. Binary interaction parameters can then be derived from these values by non-linear regression.

The **DDB Model Parameter Estimator** employs such a regression with a sophisticated and safe approach for homogeneous and heterogeneous systems. The package allows generating binary interaction parameters for the **Wilson**, **NRTL**, **UNIQUAC** and **EOS** models.

These parameters may be constant or temperature dependent. The models **UNIFAC**, **UNIFAC 2.0**, **mod. UNIFAC (Dortmund)**, **mod. UNIFAC 2.0**, **mod. UNIFAC (Lyngby)**, **mod. UNIFAC (NIST)**, **PSRK**, **PSRK 2.0**, **VTPR**, **COSMO-RS(Ol)**, **COSMO-SAC**, **COSMO-SAC 2010** and **COSMO-SAC 2013** are available for data estimation.

The software comes with

- the latest published parameter matrices for the estimation methods.
- structural group lists
- r and q values (UNIQUAC)
- liquid densities (Wilson)
- critical data and acentric factors (EOS)

Members of the UNIFAC-Consortium (see www.unifac.org) have access to the latest UNIFAC, mod. UNIFAC, PSRK and VTPR parameters.

Parameters can be saved in the internal parameter database or exported to Microsoft Excel or Aspen® (via "inp"-file). The complete fit information can be saved in a ddbpr file.

For the supported Process Simulators **Simulis Thermodynamics**, **Aspen** and **AVEVA SimCentral** the fit can directly be done with the internal parameterization and thermoengine. The resulting parameters can be saved in the project file.

Changes and errors are possible regarding all information and prices.