DDBST
Dortmund Data Bank
Software & Separation
Technology

Model Parameter Estimator

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

For the calculation of the multicomponent mixture behavior using different g^E-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.

In most cases, the parameters are directly calculated from only few estimated activity coefficients at infinite dilution. This procedure may in several cases result in very unreliable parameters.

The **DDBSP Model Parameter Estimator** employs a more complex and safe approach for homogeneous and heterogeneous systems. The package allows generating binary interaction parameters for the **Wilson**, **NRTL** and **UNIQUAC** model.

These parameters may be constant or linearly or quadratic dependent on temperature. The models **UNIFAC**, **mod. UNIFAC (Dortmund)**, **mod. UNIFAC (Lyngby)**, **mod. UNIFAC (NIST)**, **ASOG**, **COSMO-RS(Ol)** and **COSMO-SAC** 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)

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

Component lists can be entered by hand or imported directly from the Aspen simulation object (OLE) or the "bkp" project file. Parameters can be exported to Microsoft Excel or Aspen® (via "inp"-file).

Changes and errors are possible regarding all information and prices.