# Edit Mixture Data

Entering Experimental Data of Mixtures in the Dortmund Data Bank

DDBST - Dortmund Data Bank Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 441 361819 0

support@ddbst.com

www.ddbst.com

# Contents

# 1 Introduction

## 1.1 Supported Data Banks

DDB Edit Mixture Data is the single editor for the mixture data banks in the Dortmund Data bank (DDB).

The supported data banks are currently:

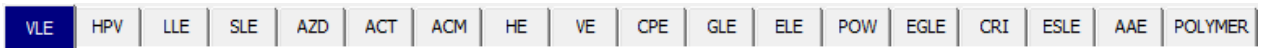



*Figure 1: Data Bank Pages*

| Data Bank | Description |
|---|---|
| VLE | Vapor-liquid equilibria for high boiling substances (above 0°C) |
| HPV | Vapor-liquid equilibria for low boiling substances (below 0 °C) |
| LLE | Liquid-liquid equilibria (miscibility gaps) |
| SLE | Solid-liquid equilibria |
| AZD | Azeotropic and zeotropic data |
| ACT | Activity coefficients at infinite dilution for pure solutes in pure solvents |
| ACM | Activity coefficients at infinite dilution for pure solute in binary solvents |
| HE | Heats of mixing |
| VE | Excess volumes (volume effects of mixing), densities and volumes of mixtures |
| CPE | Excess heat capacities and heat capacities of mixtures |
| GLE | Gas-liquid equilibria (gas solubilities) |
| ELE | Vapor-liquid equilibria for electrolyte containing systems |
| POW | Octanol/Water partition coefficients |
| EGLE | Gas-liquid equilibria (gas solubilities) in electrolyte containing systems |
| CRI | Critical data of mixtures |
| ESLE | Solid-liquid equilibria for electrolyte containing systems (salt solubilities) |
| AAE | Adsorbent/adsorptive equilibria |
| POLYMER | Polymer data |

Pure component properties are stored in the PCPDDB data base and the editor is DDB Edit Pure Data, a separate program described in its own manual.

Many newer data banks, summarized under the term “Extended Data Bank” (XDDB), have also their own editor, the DDB X-Editor.

## 1.2 Working Mode

DDB Edit Mixture Data is directly working on the data banks – no intermediate files are involved. This is contrary to DDB Edit Pure Data, which primarily works on files.

Additionally, it is possible to load and store intermediate files in binary or formatted formats. These formats are not intended for editing in external editors.

This working mode has some advantages and some disadvantages:

- No extra step is needed for updating the data bank.
- Original data in original units are not available any more – we recommend to use a spreadsheet program (Microsoft Excel, OpenOffice Calc, LibreOffice Calc for example) for keeping original data. DDB Edit Mixture Data can easily exchange data with these programs by copy and paste.

## 1.3 DDB Structure

As this document uses some terms referring to the structure of the DDB some general information about the structure is given here.

There's a global *configuration* that contains information used by all applications of the Dortmund Data Bank (DDB).

| *Sample configuration*: | A sample contents of this file is shown here: |
|---|---|
| `@DDBPTH=F:\DDB\`<br>`@DDBPRV=F:\PRIVATE\`<br>`@DDBSCR=F:\SCRATCH\` | The entry `DDBPTH` points to *public folder*, the directory holding *public data* (provided by DDBST GmbH).<br><br>The entry `DDBPRV` is set to the location of the *private folder* (containing data maintained by customers only).<br><br>The entry `DDBSCR` determines the *clipboard directory*, which will be used by DDB applications to exchange input and output files as well as temporary files. Sometimes files created there contain additional information not displayed by the programs. |

The configuration can be viewed and altered with the program "DDB Configuration".

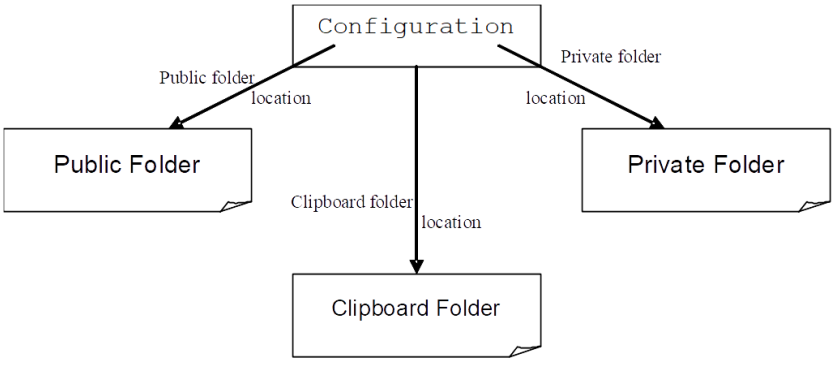



*Figure 2: Rough Structure of the DDB Folders*

Figure 3 shows in more detail how the mixture data banks are organized within the DDB. Published experimental data refer to *components* (defining the system) and *literature data* (representing the paper containing the data). The DDB contains a large component list as well as a large list of literature data sets. These are physically organized outside the mixture data banks.

Experimental data provided by DDBST will refer to public components and public literature only. Customer's data may also refer to private (user-defined) components and private literature.

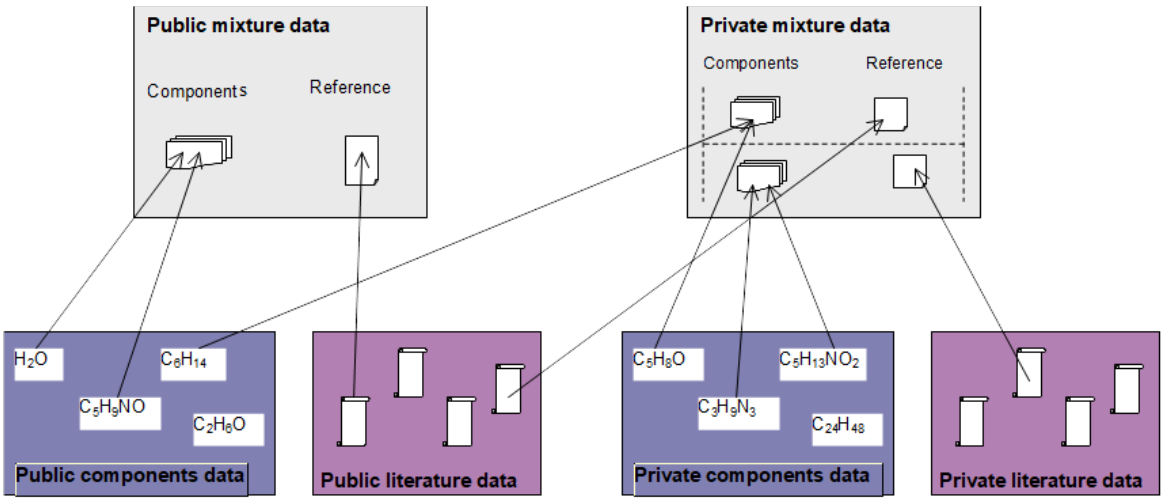



*Figure 3: Organization of Literature Data*

As everything denoted as *public* is provided by DDBST and all (unreported) changes done to public data will be eradicated with an update this document will focus on the maintenance of *private data*.

# 2 Data Input

Since the data sets only contain references to components and literature information it is necessary to add component and literature information prior to the experimental data.

Adding new literature information is described in the DDB Literature documentation. Adding new component information is described in the *Components* documentation.

# 3 Common Options of DDB Edit Mixture Data

## 3.1 Searching for Components

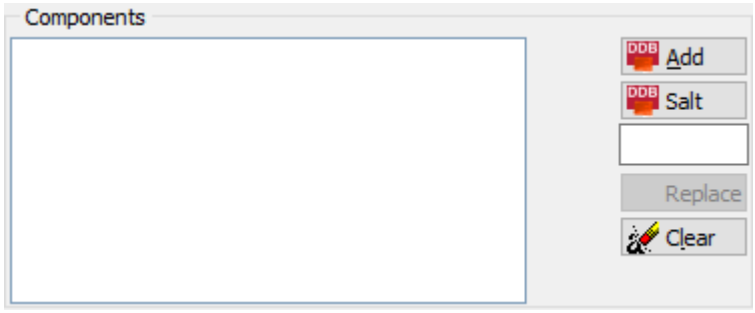



*Figure 4: Component Box*

Pressing the *Add* or the *Salt* button invokes the *DDB Components* application either for all supported component types or for salts.

The edit field below the 'Salt' button allows typing DDB component numbers if they are known.

The *Replace* button calls the *DDB Components* application and replaces the component of the currently selected line.

The selection of components is described in the DDB Components documentation.

After selecting two normal components and a single salt the component box looks like this:

| | | | | |
|---|---|---|---|---|
| 4 | C | DDB | Remove | Acetone |
| 44 | C | DDB | Remove | 1-Chloro-2-methylpropane |
| 7 | S | DDB | Remove | Barium bromide |

The first column contains the component numbers, the second column contains the component type: a “C” (component), an “S” (salts), an “A” (adsorbent), or a “P” (polymer).

The *Remove* button removes the selected component. The fifth column contains the component name.

Depending on the currently selected data bank type not all components will be used for input. All unused components will be marked by a gray color.

| | | | | |
|---|---|---|---|---|
| 4 | C | DDB | Remove | Acetone |
| 44 | C | DDB | Remove | 1-Chloro-2-methylpropane |
| 7 | S | DDB | Remove | Barium bromide |

The order of the components can be changed by drag-and-drop (moving the mouse while keeping the left mouse key pressed).

| | | | | |
|---|---|---|---|---|
| 4 | C | DDB | Remove | Acetone |
| 44 | C | DDB | Remove | 1-Chloro-2-methylpropane |
| 7 | S | DDB | Remove | Barium bromide |

*Figure 5: Start*

| | | | | |
|---|---|---|---|---|
| 4 | C | DDB | Remove | Acetone |
| 44 | C | DDB | Remove | 1-Chloro-2-methylpropane |
| 7 | S | DDB | Remove | Barium bromide |

*Figure 6: Move/Drag*

| | | | | |
|---|---|---|---|---|
| 4 | C | DDB | Remove | Acetone |
| 7 | S | DDB | Remove | Barium bromide |
| 44 | C | DDB | Remove | 1-Chloro-2-methylpropane |

*Figure 7: Drop/Result*

The same reordering can be performed by the arrow keys <▲> and <▼> while holding down the Control (Ctrl) key.

## 3.2 Searching for Literature

If a literature is already available it can be searched via the search button (  ) in the “Reference” block. The search query dialog contains two search modes, a quick search mode and an advanced search mode.

We will show a quick search for the author “Gasem” and the year 2001 (see Figure 8).

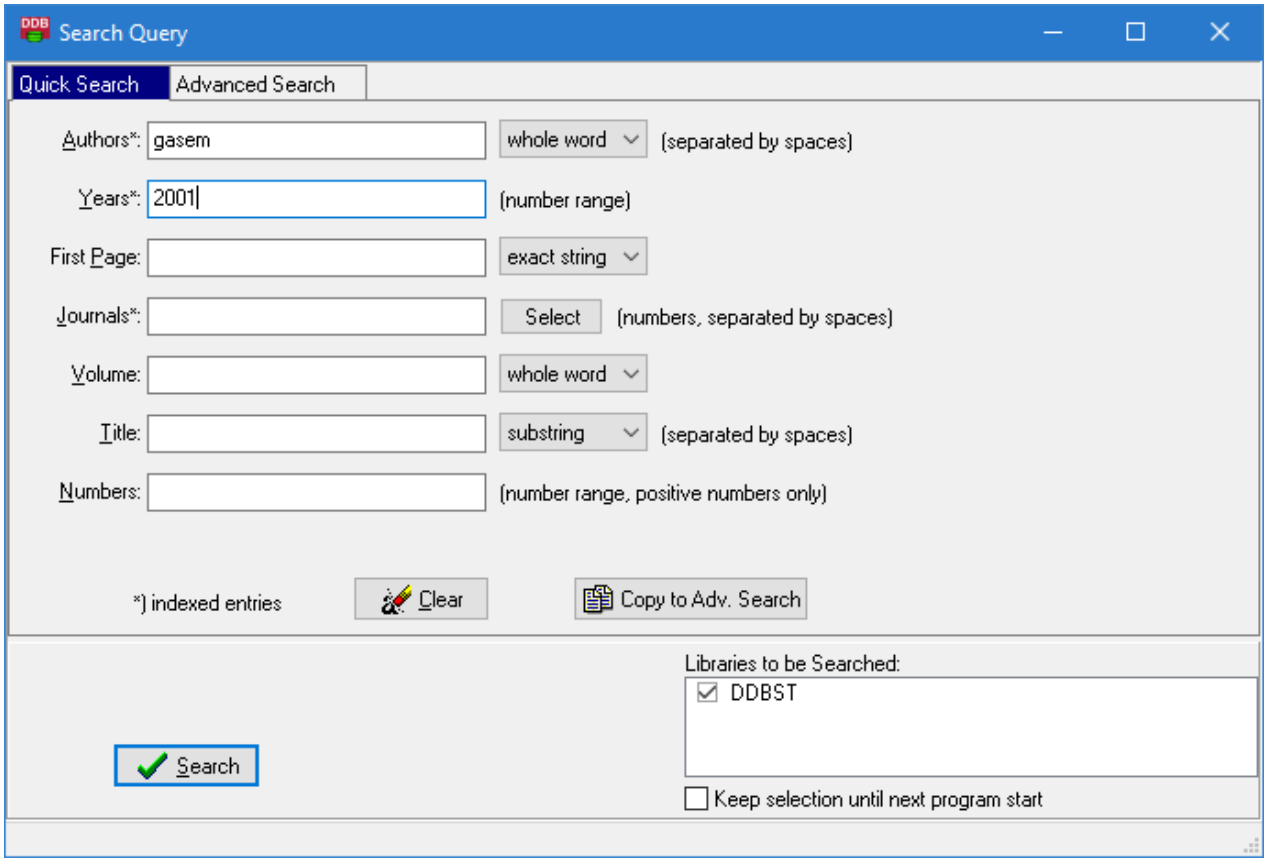


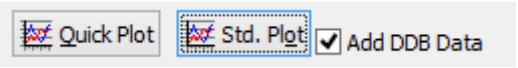

*Figure 8: Quick Search Query*

After selecting one of the found data sets ( ) DDB Edit Mixture Data will display the LEAR number and some information about the selected reference.

| LEAR # | | Details |
|---|---|---|
| 30608 | | [30608] Shaver R.D., Robinson R.L., Gasem K.A.M., Fluid Phase Equilib., 179, 43-66, 2001 |

If a LEAR number is known it can be directly typed in the “LEAR#” edit field. After accepting the input by pressing enter DDB Edit Mixture Data shows the details.

## 3.3 Plot Options



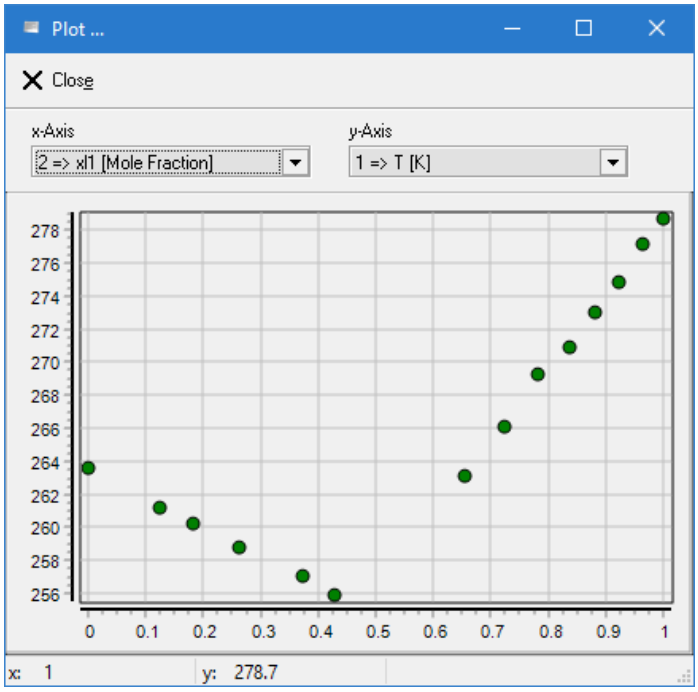
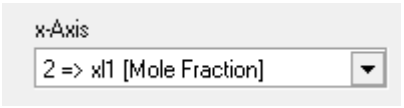




*Figure 9: Quick Plot*

To receive a quick overview about the just edited data the *Quick Plot* button can be used.

The integrated plot of *DDB Edit Mixture Data* only allows plotting two data columns against each other.

The selected columns can be changed by the combo boxes:





The status bar displays the x and y data for the point which is next to the mouse cursor indicated by a rubber band.

The "*Std. Plot*" button calls the normal plot program. This plotting program automatically selects the generally used plot types for the current data sets.

It displays the components, the reference and also the point's data which is next to the mouse cursor in the status line.

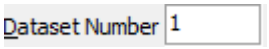
For this plot it is possible to include already stored data. Check "*Add DDB Data*" to activate this option.

## 3.4 Loading from and Storing to the DDB

DDB Edit Mixture Data stores and reads data sets directly from the data banks.

There are two database access areas, one for the private (customer's) and the public (DDBST's) database.

To change an existing data set (or to use its data as basis for a new data set) use the appropriate *Load* button. Before loading a data set from the (private) DDB be sure that the correct data bank tab is selected. "Load" will always fetch the data set specified in the




field.

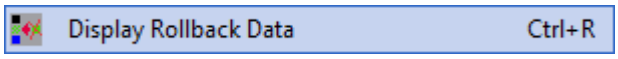
There are two possibilities to put a data set directly into the private DDB: A data set can either replace an existing data set or it can be appended to the data bank, leaving all other data sets untouched.

The *Replace* option is intended for corrections of existing data sets. But it is, of course, possible to replace an existing data set by a completely new data set. Before replacing a data set a confirmation dialog will prevent the user from accidentally messing up the data bank and additionally every overwritten data set is saved in a "Roll Back" file.

To add a new data set to the private DDB use the *Append* option. If the data bank does not exist so far, a brand new will be created and the current data set will be added as first (and only) data set. Anyway, the *Data Set Number* field will be updated to the new number.

The public DDB cannot be modified.

## 3.5 Restoring Overwritten Data Sets




Every replaced and overwritten data set is saved in a roll-back file. These saved data sets can be restored from this list.

The dialog displays the entire list of overwritten sets. The view on the list can be restricted to single data banks, single users, single locations (private or public DDB) and, the most effective filter, the data set number.

Data bank, data set number, location, data and time of overwriting, and the user is displayed.

The *Restore* button allows restoring the selected data set. The data set which is now replaced by the old data set will be stored in the roll-back file.

## 3.6 Import/Export Options

Use the *Open* button to load data sets from a query result file (*.qrx or *.qr). Some legacy file formats are also supported.

If a file is loaded, a dialog displays the complete list of found data sets. The dialog shows the database, the given number of data points, the component list (as DDB numbers) and the reference number.

It is possible to edit the single data set (using the *Edit* button) or to append all sets to the private data bank. If the loaded data sets contain valid data set numbers, it is also possible to replace existing (private) data sets by switching the *Mode* to *Replace*.

Use the *Save* button to store the current data set to a query result file (*.qrx). These files can be loaded in the *Dortmund Data Bank* application.

## 3.7 Units and Qualities

The input unit information – also containing a selection option for data quality and source descriptions – is displayed in the lower right area of the main window (“Units/Qualities").

When switching to another database the program displays the standard units initially.

Some databases have their own unit description (GLE for example). In this case, the selection box is grayed out.

## 3.8 Display Data Set in Dortmund Data Bank

This function transfers the currently edited data set to the *Dortmund Data Bank* application without storing it to the data bank before-hand.

This allows the usage of the entire functionality of the *Dortmund Data Bank* program like extended plotting, estimation, fitting, exporting, and more.

# 4 Input Options Separated by Data Bank

It is recommended to select the appropriate data bank before selecting components or literature.

## 4.1 VLE – Vapor-Liquid Equilibrium Data of Normal Boiling Substances

Select the VLE tab above the edit field to enter vapor-liquid equilibrium data for systems containing components with a boiling point above 0 °C. The number and heading of the input columns will be set automatically by (de-)selecting of components and the other options described below.

The maximum number of components in a system is four.

In the *Data Type* area, the desired data type of the data has to be selected.

There are currently nine data types defined. They specify which phases are given and if there's a constant pressure or temperature for the whole data set.

The liquid phase is denoted 'x' and the vapor phase is denoted 'y'.

For data types 1 to 8 a constant value has to be entered. The value's unit is selected in the "Units/Quality" area.

A composition is always given in mole fractions. The value for the last component in the system has to be omitted.

If no constant temperature or pressure is given for the whole data set, then data type 9 has to be selected. With this selection a second "Non-Constant Unit" field will appear. It is also possible to specify which measured quantity is really given. In this case a special option can be used to define a (pseudo) constant column. By this it is allowed either to specify a constant value for one phase or to state that the deviation of the values of one column is small.

Although any data classified as type 1-8 can be seen as special type 9 data it is recommended to avoid the usage of this data type. The data types one or two should be used as often as possible, because most calculation routines are optimized for them.

The VLE editor allows also performing consistency tests and starting the evaluation if the entered VLE data show azeotropic behavior.

## 4.2 HPV – Vapor-Liquid Equilibrium Data of Low Boiling Substances

Select the HPV tab to edit vapor-liquid equilibrium data for systems containing components with boiling points below 0 °C. The options are mostly the same as for VLE data. Only the pressure and temperature units used in the DDB are different.

The differentiation between the VLE and the HPV data bank is arbitrary and has only some historic and commercial reasons. Data from both data banks are handled the same way throughout the DDB software.

## 4.3 LLE – Liquid-Liquid Equilibrium Data

To edit liquid-liquid equilibrium data (miscibility gap information) the LLE tab has to be selected. It is recommended to select the desired system and literature data set before configuring the data sheet itself. The selected literature data set must be prepared for use with the LLE data bank. The maximum number of components in a system is five.

The input of this kind of data differs much from editing e.g., VLE data. For example, no predefined data types are used. Instead, the table entries are selected directly.

All the settings described below (and the number of components) control the number of columns in the data grid.

The **Table Entries** specify the measured quantities. It is not possible to specify a constant environment condition directly. In this case the constant value has to be entered in any row of the data grid.

If a pressure is given, then the **Pressure Type** has to be specified. If unsure **Not Specified** should be selected.

If there are three or more components in the system, then up to three liquid phases may be specified in the field **Number of Phases**. A possibly given vapor phase is not counted here.

## 4.4 SLE – Solid-Liquid Equilibrium Data

Select the SLE tab above the edit field to enter solid-liquid equilibrium data (solubility information) and add it to the SLE data bank. The number and heading of the input columns will be set automatically by (de-) selecting of components and the other options described below. It is recommended to select the desired system and literature data set before configuring the data sheet itself. The selected literature data set must be prepared for use with the SLE data bank. The maximum number of components in the system is four.

The desired data type can be selected in the *Data Set Entries* field. There are currently nine main types defined which are described below.

'*T*' denotes a temperature is given. '*xl*' is an abbreviation for mole fraction in the liquid phase. '*xs*' means mole fraction in the solid phase. '*y*' is for mole fraction in gas phase. A symbol is listed in brackets denotes an environment condition valid for all data points.

For the data types 1 to 8 a constant condition (either temperature or pressure) is given for all data points. A constant value has to be specified. The value's unit is selected in the "Units/Quality" dialog.

There is a reserved data type (9) to specify that neither a temperature nor a pressure as constant environment condition is given. This data type 9 can also be used if P/T is unknown for any data point. Selecting this data type will make up to two *Non-Constant Unit* fields to appear. Again, it is possible to define one (almost) constant column.

Although any data classified as type 1-8 can be seen as special type 9 data it is recommended to avoid the usage of this data type. Most of the plot and calculation routines will only work with the data types 1-8.

Several classifications are available in the *SLE Type* drop-down list. If unsure "*unknown type"* should be selected. The "Statistics" button reads all SLE data sets and display the number of data sets for the different data types.

## 4.5 AZD – Zeotropic/Azeotropic Data

To edit azeotropic/zeotropic data the AZD tab has to be selected. It is recommended to select the desired system and literature data set before configuring the data sheet itself. The selected literature data set must be prepared for use with the AZD data bank. The maximum number of components in the system is four.

Any data set in the AZD data bank contains just one data point. It is possible to specify a temperature, a pressure and (if an azeotrope exists) a composition. If no temperature, no pressure or no composition is given, then the corresponding option should be unchecked.

Furthermore, some additional information can be specified. These will be described below.

***Type of Azeotrope*:** If beyond the fact that there's an azeotrope no further information is known, then this field should be left empty.

To specify that there's *no azeotrope* (maybe under certain environment conditions) for the given system *none* can be selected. Of course, this will exclude a detailed specification of the azeotrope described below.

*Selecting Pmax* resp. *Pmin* will specify a pressure maximum resp. minimum azeotrope, where *Saddle* specifies a saddle point.

If there a miscibility gap exists under the given environment conditions *MisGap* should be selected.

Enabling *2azd* specifies the existence of two azeotropes.

Select *supercrit* if one of the components is supercritical under the given conditions.

*3 liq.phases* specifies the co-existence of three liquid phases.

*Sep.Fac.~1.0* is a qualitative statement that the separation factor is near 1.

***Measurement Method*:** If the measurement method is unknown or none of the listed, then the first entry in the list should be selected.

Otherwise select *Distillation* if the information has been obtained by distillation or choose *Phase Equilibrium* (based on phase equilibrium measurements).

***Reaction*:** If the system is reactive select *Yes*, otherwise *No* should be chosen.

***Evaluated by*:** The "*Evaluated by* -field" contains information about the person and how the data has been gained. Leaving the first entry unchecked means the evaluation has been done by the author.

If the data has been published as table or in a graphical representation choose the corresponding check box.

Select *VLE* if the information has been provided as VLE data. If the information has been extracted by fitting to published VLE data, then *fitted* should be selected. If furthermore the information has been calculated using the fitted parameters obtained by the published VLE data, then *calculated* should be activated.

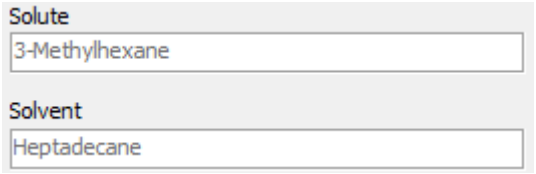
***Precision:*** The precision of a measured value can be specified using the according drop-down list. '=' denotes exact, '<' denotes lower than, '~' denotes about, '>' denotes higher than and '?' denotes a dubious value.

The dialog allows entering several temperature, pressure, and composition points for the current reference and system. Since the data bank itself just stores single points, a data set for each point will be created.

## 4.6 ACT – Activity Coefficients at Infinite Dilution (Binary Systems)

Select the ACT tab to edit activity coefficients at infinite dilution data for binary systems.

The first listed component of the system will be interpreted as *solute*, the second component will be assumed to be the *solvent*. The selected classification will be displayed.




Besides the activity coefficient at infinite dilution a temperature has to be specified.

It is also possible to state the *Measurement Method* that has been used to obtain the activity coefficient. If the method is unknown or none of the listed, then *other techniques* should be selected.

There are several predefined experimental methods like GLC (including specializations), LLC, ebulliometry, dilutor and the Rayleigh distillation method.

If the value has been calculated either the general prediction or the calculated from Henry coefficients can be selected.

Currently every data set contains only one data point. However, it is possible to type more lines. Every line typed here will become a separate data set. It is not possible to load the typed line simultaneously.

## 4.7 ACM – Activity Coefficients at Infinite Dilution (Ternary Systems)

Select the ACM tab to edit activity coefficients at infinite dilution data for ternary systems.

Here the *third* listed component of the system will be interpreted as *solute*. The first two components will be assumed to be the *solvent system*. The right selection can be validated inspecting the *Solvents* and *Solute* field where the DDB component numbers will be displayed.

For any data point a temperature, the composition (for the first component) and the activity coefficient itself has to be specified.

For the entire data set a *measurement method* can be specified.

## 4.8 HE – Heats of Mixing Data

Excess enthalpy data (heats of mixing) can be edited using the HE tab. The maximum number of components in the system is five.

For any selected component the original state before mixing has to be specified next to each component name. If the component has been liquid, 'L' has to be selected (default). If the component has been in the vapor state, then 'V' should to be activated.

For *binary systems* it is possible to edit either data with a constant composition as environment condition or to specify a constant temperature. For ternary systems and higher only the latter may be specified.

If a *constant temperature* is given its value has to be entered. Furthermore, for any data point the excess heat and the composition (in mole fraction) have to be specified.

If a *constant composition* (mole fraction of the first component) is given, then for any data point the excess heat and a temperature has to be specified.

*None (split data set)* is chosen if no constant value is given. Every data point is saved as an individual isothermal data set.

A *constant pressure* may be stated by selecting the corresponding checkbox and entering a valid pressure within the chosen pressure unit.

The *unit* for the specified $h^E$ data can be set using the "*Unit of* $h^E$" selector.

For isothermal data it is possible to state the existence of a *miscibility gap* under the given conditions (temperature and pressure, if given).

## 4.9 VE – Excess Volumes and Densities

Select the VE tab to edit excess volumes data (volume effects of mixing), densities, and volumes of mixtures. The options and restrictions are nearly the same as for mixing enthalpies (HE) except the possibility to set the data type.

- Excess volume [$cm^3/mol$]
- Density [$g/cm^3$]
- Molar Volume [$cm^3/mol$]

The "Statistics" button shows the number data sets and point for the three properties.

## 4.10 CPE – Excess Heat Capacities

To edit excess heat capacities and heat capacities of mixtures the CPE tab has to be selected. The options and restrictions are nearly the same as for HE except the possibility to set the data type.

- Excess heat capacity "$cp^E$" in different units
- Heat capacity "cp" in different units

The "Statistics" button shows the number of data sets and points for both properties.

## 4.11 GLE – Gas Solubility Data

Gas solubility data can be edited by selecting the GLE tab.

This database does not use the temperature and pressure selection from the Units/Quality dialog because it stores the original units inside the database.

Currently one gas in up to three solvents may be specified. The first component will always be assumed to be the gas. So, the maximum number of components in the system is four.

***Constant Property**:* It is necessary to specify an environment condition. It is possible to choose between a partial pressure, a total pressure or a temperature value.

If a (partial or total) pressure has been selected as environment condition, then a temperature has to be specified for any data point. If a constant temperature has been specified, then it is possible to select partial pressure, total pressure or fugacity as table value.

Independent from being specified as constant or table value one of the various units has to be selected both for the pressure and for the temperature value(s).

The *Table Value* group can be used to customize the number and contents of the data table columns. Besides a temperature/pressure value up to two values may be specified.

If there is one gas in one solvent given, then it is possible to specify the mole fraction of the gas in the vapor phase (selecting entry 3).

For two or more solvents the composition in the liquid phase must be specified. Choose entry 5 for mole fraction and entry 9 for kmol/m$^3$ as unit. Usually, the *real* mole fraction of all but the last solvent should be specified if either solubility coefficient no. 10 or no. 12 is selected (see below). Otherwise, the *gas-free* mole fraction should be specified.

## 4.12 ELE – Vapor-Liquid Equilibrium Data of Electrolyte Systems

Select the ELE tab to edit vapor-liquid equilibrium data of electrolyte systems.

The ELE data bank allows storing information about systems containing up to four solvents and up to four salts. So, the maximum number of components in the system is eight.

The field *Data Set Entries* describes how measured quantities may be combined to be processed. For ternary systems and higher (at least two solvents and at least one salt) the data types lower than 20 and in the thirties have to be used because they allow a solvent composition to specify. For binary systems (single solvent) the data types between 21 and 29 and higher than 40 must be used.

The abbreviation *xs* means the liquid solvent mole fraction (salt-free), *y* represents the vapor mole fraction, and again *T* is for temperature (in °C) and *P* is for pressure (in kPa). For binary systems a molal osmotic coefficient (*osm. coeff.*) or a mean molal activity coefficient (*gamma+-*) may be specified.

***Concentration Scale*:** The abbreviation *conc* in the data set entries list denotes the salt concentration. The selection list *Concentration Scale* can be used to select the desired unit. There are currently five different concentration units available. The units *<m>*, *<w%>* and *<M>* are self-explanatory. If the salt concentration is given in mole fraction without considering the charge of ions, then *<Z>* should be selected. The concentration unit *<X3>* is defined by the mole fraction of ions:

$$X_3 = \frac{n_3}{n_1 + n_2 + \nu n_3}$$

n: moles ($n_1$, $n_2$ for solvents, $n_3$ for salt)

ν: moles ions (referring to one mole completely dissociated salt – e.g. 2 for NaCl)

The value of the constant measured quantity (depending on the selected data type) has to be entered next to the *Concentration Scale* selector.

## 4.13 POW – Octanol-Water-Partition Coefficients

A data point in this database contains

- Temperature
- Logarithmic (base 10) partition coefficient of a single component in the Octanol/Water system

- pH value of the liquid phase
- Experimental error (in log $P_{ow}$ units)
- Measurement method (Normally unused, only predicted values should be marked)
- Quality code.

A data set contains only single points.

## 4.14 EGLE – Gas Solubilities in Electrolyte Containing Systems

The EGLE database structure is the same as the GLE database. Salts and electrolytes are stored not with their special salt number but with their 'normal' component code.

Another slight difference is that reference links are not needed for this database since the normal literature numbers (LEAR) are used directly.

## 4.15 CRI – Critical Data of Mixtures

The CRI database contains temperatures, pressures, densities and compositions describing critical, near-critical or pseudo-critical information of mixtures.

The composition can be given in several different units. The numbers in angle brackets are used as conversion factors.

The concrete type of critical data has to be specified by the “State” selection box.

The complete list of states:

| State No. | Short Term | Description/Transition |
|---|---|---|
| 0 | Not specified | no specification on present/vanishing phases given |
| 1 | Liquid-vapor | Liquid-vapor to vapor/gas (VL > V/G) |
| 2 | UCEP | Upper critical end point |
| 3 | LCEP | Lower critical end point |
| 4 | Liquid-liquid | Liquid-liquid to liquid (LL > L) |
| 5 | to be defined | no specification on present/vanishing phases given |
| 6 | Univariant (undef. phases) | Univariant line (present/vanishing phases not explicitly defined) |
| 7 | VLL | Vapor-liquid-liquid to two phases (VLL > VL, VLL > LL) |
| 8 | DCEP | Double critical end point |
| 9 | SVL TP | Solid-vapor-liquid (univariant) temperature/pressure data |
| 10 | VLL TP | Vapor-liquid-liquid (univariant) temperature/pressure data |
| 11 | Gas-gas | Gas-gas to gas (GG > G) |
| 12 | Near crit. TP (2PHS) | 2-Phase temperature/pressure point near critical point |
| 13 | Univariant SLLV | Univariant point or data, solid-liquid-liquid-vapor phases |
| 14 | VL1L2L3 | Vapor-liquid1-liquid2-liquid3 to three phases (VLLL > VLL, VLLL > LLL) |
| 15 | LLL > LL | Liquid-liquid-liquid to two phases (LLL > LL) |

| State No. | Short Term | Description/Transition |
|---|---|---|
| 16 | LLS TP | Solid-liquid-liquid univariant temperature/pressure data |
| 17 | S1S2LV TP | Solid-solid-liquid-vapor univariant temperature/pressure data |
| 18 | CST (LLE) | Critical solution temperature (LL>L) |
| 19 | LCST (LLE) | Lower critical solution temperature (LL>L) |
| 20 | UCST (LLE) | Upper critical solution temperature (LL>L) |
| 21 | SL1G | Solid-Liquid1-Gas univariant temperature/pressure data |
| 22 | SL2G | Solid-Liquid2-Gas univariant temperature/pressure data |
| 23 | LL > L | Transition from two to one liquid |
| 24 | HL1L2 | Hydrate-liquid-liquid (univariant) temperature/pressure data |
| 25 | HL1G | Hydrate-liquid-vapor/gas (univariant) temperature/pressure data |
| 26 | Quadruple point | Four phases present under given (univariant) conditions |
| 27 | Structural transition point | Hydrate I to Hydrate II transition |
| 28 | L1L2S2 TP | Liquid-liquid-solid-temperature/pressure data |
| 29 | K-point (L1-L2=V) | Liquid-liquid to liquid-vapor (L1L2>L1V) |
| 30 | HL1L2V | Hydrate-liquid-liquid-vapor (univariant) temperature/pressure data |
| 31 | HL2G | Hydrate-liquid-vapor/gas (univariant) temperature/pressure data |
| 32 | HIceG | Hydrate, Ice, Gas |
| 33 | SSG | Solid, Solid, Gas |
| 34 | SLF | Solid, Liquid, Fluid |

The “Table Entries” selection drop-down-boxes allow the specification of up to seven columns. Beside the main data types, it is possible to add errors for them. For every table entry, it is necessary to define the unit.

The Purities button opens a dialog where the purities of the used pure component properties can be specified.

The measurement method can be specified as free text.

The data are stored in original units and in original notation.

## *4.16 ESLE – Salt Solubilities*

The ESLE database contains information on the solubility of salts and electrolytes in pure components and mixtures.

There is a special *Components* and *Salts* area where each substance has to be classified as solved, precipitated, or both.

Use the “*Hide Components*” button to hide the information. Use the “Show Components” buttons to make the information visible again.

An ESLE data set also contains information in the measurement method.

It is possible to define a constant temperature and a constant pressure. For both properties it is necessary to define the unit.

Pressure and temperature can either be constant or in the data table when they change for every data point.

The data table can be built from the selection box "*New Table Entry*".

Use the "*Add*" button to add a new column.

Use the "*Repl.*" button to change the currently selected column.

Use the "*Clear*" button to clear the entire grid.

The "*Delete Column…*" button opens a popup-menu to select a column to be deleted.

Possible table entries are

- Temperature (T)
- Pressure (P)
- Salt solubility (SOLUB) in molar- and mass-based units
- Solvent composition (COMPOS)
- Component and salt number of precipitated component or salt (SALT_PREC, COMP_PREC)
- Time needed for equilibrium (EQTIME)
- Liquid density (LIQDEN)
- Salt solubility (SOLUBV) in volume-based units
- Component solubility (SOLUBC)

Experimental data are stored in original units.

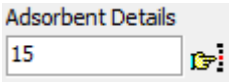
A special feature is the possibility to read and save a tagged file format. These files must have the extension ".sle" and are pure text files.

## 4.17 AAE – Adsorbent/Adsorptive Equilibria

The AAE database contains data on standard components adsorbed on zeolites, coals, molecular sieves etc.

The database content is specified by data type number.

These data types determine the content of the data table.




The adsorbent is defined by two entries. One number is a coarse specification of the adsorbent type, zeolite x, activated carbon etc. This number is selected in the common components/salts/adsorbents list of DDB Edit Mixture Data. The other number references an entry in an adsorbent details list where quantitative data for the special adsorbent is specified.

The *adsorbent details* list contains:

1. Adsorbent number (class)
2. Unit cell molecular weight – if available
3. Reference number/s
4. Four fields with details. These fields are pure text, but contain some tags listed in the "Short Terms" box. For some historic reasons empty fields are filled with the string "E-M-P-T-Y".
5. Two text fields reserved for kinetic information – which are currently unused.

An item can be selected by selecting the “Select” button or by double-clicking the appropriate line.

The database contains information on adsorption and desorption. The process type has to be specified in the “Data Type” selector.

The “Original Unit” selection boxes specify the units of pressure, temperature, and amount in the original publication. The database itself only stores temperatures in [K], pressures in [kPa], and adsorbed amounts in [mmol/g].

## 4.18 Polymers

The polymer data bank contains

- Vapor-liquid equilibria
- Liquid-liquid equilibria (mixing gaps)
- Solubilities
- Excess and dilution enthalpies
- Densities and volumes
- Swelling
- Partition coefficients
- and few other data

for polymers and polymer containing systems.

The “Data Type” is a number specifying the properties of the data set. The edit field has a context menu where available data types are listed.

This data type describes the content of the data set but the table items can be selected independent of this number. This is a possible pitfall since table items might be specified which have no meaning for the specified data type.

### 4.18.1 Constants

A polymer data set might contain as many constants as needed.

A constant is defined by its property, phase, related components, a unit, and its value. All data have to be entered via context menus.

The component description is not a direct relation to a specific component but rather a sort of index. This index (“Polymer B”, “Additive A” etc.) are specified in the “Polymer/Component Details” page.

This table also allows several details to enter for the polymers like mean molecular weights and a polydispersity index. Two fields are reserved for any additional information and one field is for a trade name.

The “#Index” column is used for specifying a component or polymer specific index and the entries are selected via context menus.

Only valid entries are selectable. The “Comment” page is a place for entering arbitrary text which does not fit into any other place.

The “Polymer Values” is twin of the “Constants” page but intended for polymer specific values only.

### 4.18.2 Specifying the Columns of the Table

The buttons “*Add Column*”, “*Add Qualifier Column*”, and “*Delete Column*” allow the user to add and remove columns. The “*Add Column*” function adds always the same column type.

These four entries represent the property, the phase, the compound or compounds, and the unit of the property.

The ellipsis buttons (…) allow the values to change by context menus.

The "*Add Qualifier Column*" button adds a special column containing only unspecified values, text or numbers. Only a single qualifier column can be added.

The "*Delete Column*" button displays a context menu with the column numbers.

### 4.18.3 Exploring the Definition Lists

The polymer data bank uses in several cases indexes instead of a complete and repeated storage of some data.

The index numbers are pointing to entries in the definition lists for

- Component Specification (index code)
- Data Types (like VLE, LLE, SLE, etc.)
- Phases (liquid, vapor, solid, etc.)
- Properties (Temperature, Concentration, etc.)
- Units (specific lists for all properties)

These lists are currently not extendable.