

# Dortmund Data Bank

Retrieval, Display, Plot, and Calculation

Tutorial and Documentation



## DDBST

Dortmund Data Bank  
Software & Separation  
Technology

DDBST - Dortmund Data Bank Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 441 361819 0

[support@ddbst.com](mailto:support@ddbst.com)

[www.ddbst.com](http://www.ddbst.com)

# Contents

1	Introduction .....	5
1.1	The XDDB (Extended Data).....	6
2	Starting the Dortmund Data Bank Retrieval Program.....	7
3	Searching .....	8
3.1	Building a Simple Systems Query .....	8
3.2	Building a Query with Component Lists.....	8
3.3	Examining Further Query List Functionality .....	9
3.4	Import Aspen Components .....	11
3.5	Import PRO/II Components .....	11
3.6	Import UniSim Design Components.....	11
3.7	Import Simulis Components .....	11
3.8	Import AVEVA SimCentral Components.....	11
3.9	Searching for the Data Sets of a Reference.....	11
3.10	Search Data Sets by Data Set or Reference Numbers .....	13
3.11	Searching Data Sets with Specified Pure Component Properties.....	13
3.12	Searching for Data with Specified Temperatures and Pressures .....	15
3.13	Selectivity Search .....	16
3.14	Search Options.....	17
3.14.1	Data Banks Preselection .....	17
3.14.2	Pure Component Properties Preselection.....	18
3.14.3	Extended Database Properties .....	18
3.14.4	Configurations .....	19
3.14.5	Other Search Options.....	19
3.14.5.1	Salt Solubilities – Handling of Precipitated Components .....	19
3.14.5.2	Demo Data Sets.....	19
3.14.5.3	Retrieve Data Sets Marked as Dubious or Poor or Incorrect .....	19
3.14.6	Search Locations.....	20
4	Exploring the Data Bank – Statistics .....	21
4.1	Set, Points, References .....	21
4.2	Pure Component Properties.....	21
4.3	X Properties.....	21
4.4	Polymer Data.....	21
5	A First Look at Predictions.....	22
6	Using and Understanding the Query Result Window .....	24
6.1	File Menu .....	24
6.2	Edit Menu.....	25
7	Saving and Loading Data Files.....	27
7.1	Open Files .....	27
7.2	Save File.....	27
7.3	Drag and Drop Files .....	27
8	Exploring the Data Set List Grid .....	28
8.1	Data Table Context Menu .....	29
9	Query Result Filters.....	31
9.1	Filter Items .....	31
9.2	Range Filter.....	31
10	Single Data Set Display .....	33
11	Data Set Display Options .....	34
11.1	Display Additional Information.....	34
11.2	Query Result Options .....	37
12	Compact Data Display.....	39
13	Units.....	40
13.1	Mixture Data Banks – Compositions.....	40

13.2	Mixture Data Banks – Properties.....	40
13.3	Pure Component Properties .....	40
14	Consistency Tests .....	41
14.1	Point-to-Point Test.....	41
14.2	Area Test .....	42
14.2.1	Isothermal data .....	42
14.2.2	Isobaric data.....	42
14.3	Automatic Tests.....	43
14.4	Othmer-Tobias and Hand Correlations.....	43
14.4.1	Othmer-Tobias Tie Line Correlation.....	43
14.4.1.1	Equation .....	43
14.4.2	Hand Tie Line Correlation.....	44
14.4.2.1	Equation .....	44
14.4.2.2	Example Data.....	45
15	Modifying and Editing Data Sets .....	47
15.1	Editing Experimental Data .....	47
15.2	Specifying Quality .....	47
15.3	Change LEAR Number .....	47
15.4	Edit Comment.....	48
15.5	Append Comment.....	48
15.6	Change Component Order .....	48
15.7	Add/Modify Extended References .....	49
15.8	Convert GLE Data Sets to HPV Data Sets .....	49
15.9	Convert VLE/HPV TPxy to Pxy(T) Data Sets and Txy(P) Data Sets .....	49
15.10	Create $g^E$ Model Interaction Parameters.....	49
15.11	Apelblat Correlation .....	49
16	Converting Data Sets to ELE Data Sets .....	51
17	Query Result Statistics.....	52
17.1	Summary.....	52
17.1.1	Number of sets/points/references for every database .....	52
17.1.2	Overview over available systems .....	53
17.1.3	Details of pure component properties data .....	53
17.1.4	Details of the polymer related data.....	54
17.2	Systems List.....	54
17.3	Triangle for Binary Systems.....	55
17.3.1	List.....	55
17.3.2	Settings .....	55
17.4	Pure Component Properties Overview .....	57
18	Predict.....	58
18.1	ACM.....	58
18.2	ACT.....	58
18.2.1	Selectivity Calculation.....	59
18.3	AZD.....	60
18.4	ELE.....	60
18.5	GLE .....	60
18.6	HE.....	60
18.7	VLE/HPV .....	60
18.7.1	Predict with EOS .....	61
18.7.2	Calculation of the Solubility of Solids in Supercritical Fluids .....	61
18.7.3	Deviation Plot.....	63
18.7.4	Phase Envelope Calculation .....	63
18.7.4.1	Options .....	64
18.8	LLE.....	64
18.9	PCP.....	65
18.10	POW .....	65
18.11	SLE.....	66
18.11.1	SLE Calculation Options .....	66

18.11.2	Solubility in Binary Solvents.....	66
18.12	VE.....	67
18.13	VIS.....	67
18.14	MFLP.....	67
18.15	MTCN.....	68
18.16	Entering $g^E$ Model Parameters.....	68
18.16.1	Copying Parameters to the Aspen Simulator.....	70
18.17	Checking Availability of Model Parameters .....	71
18.18	Third-Party Thermodynamics Calculations.....	73
18.18.1	Introduction .....	73
18.18.2	Step 1: Read components from a project file.....	73
18.18.3	Step 2: Search for experimental data in the DDB.....	73
18.18.4	Step 3: Calculate VLE using Third-Party Thermodynamics .....	73
19	Fit Equation Parameters.....	75
19.1	AAE.....	75
19.2	Binary VE and VIS.....	75
19.2.1	Redlich-Kister.....	75
19.2.2	Sum of Symmetrical Functions .....	75
19.2.3	Fit Result .....	75
19.3	Ternary LLE .....	77
19.4	PCP .....	80
19.5	Ternary VLE/HPV.....	80
20	Simultaneous Fit – Regression Mix.....	81
21	Plot.....	82
21.1	Plot Selected Sets.....	82
21.2	Plot Current System.....	82
21.3	Plot Current System Incl. Subsystems.....	82
21.4	Quick Plot.....	82
21.5	Sets From Multiple Data Banks.....	83
22	Data Export.....	85
22.1	PPDX format .....	85
22.2	Aspen INP Format .....	85
22.3	Data Points Export.....	87
22.3.1	Export Mixture Data.....	87
22.3.2	Export Pure Component Properties .....	88
23	Appendix – GLE Conversion .....	89
23.1	Overview .....	89
23.1.1	Ostwald Special Treatment.....	89
23.2	Conversion to Henry.....	90
23.2.1	Mole of Gas Calculation.....	90
23.2.2	Solvents Weight Calculation .....	90
23.2.3	Mole Fraction of Gas Calculation.....	90
23.2.4	Partial Pressure Calculation.....	91
23.2.5	Henry Coefficient Calculation.....	91
23.3	Conversion to TPxy .....	91
23.3.1	Converting Solvents Molarity .....	91
23.3.2	Converting Solvents Weight Percent.....	91
23.3.3	Total Mole Fractions Calculation .....	92
23.3.4	Total Pressure Calculation.....	92

# 1 Introduction

This document describes the main program for searching and using experimental data from the Dortmund Data Bank (DDB).

The Dortmund Data Bank is actually not a single database but contains over a dozen different data banks for different data types. The data banks are

<i>Short Term</i>	<i>Data Bank Description</i>
<b>X</b>	Extended data (for a description see chapter 1.1)
<b>VLE</b>	Vapor-liquid equilibria for systems containing components with boiling points above 0 °C
<b>VIS</b>	Mixture viscosities
<b>VE</b>	Excess volumes, volumes, densities
<b>SLE</b>	Solid-liquid equilibria for systems without salt
<b>POW</b>	Octanol-Water partition coefficients
<b>POLYMER</b>	Thermodynamic data of polymer containing systems
<b>PCP</b>	Pure component properties – P-v-T, caloric, transport
<b>MSFT</b>	Surface tension of mixtures
<b>MFLP</b>	Flash points of mixtures
<b>MSOS</b>	Speeds of sound of mixtures
<b>MTCN</b>	Thermal conductivities of mixtures
<b>MPVT</b>	Mixture P-v-T data
<b>MDEC</b>	Mixture dielectric constant
<b>LLE</b>	Liquid-liquid equilibria
<b>HPV</b>	Vapor-liquid equilibria for systems containing components with boiling points below 0 °C
<b>HE</b>	Heats of mixing
<b>GLE</b>	Gas solubilities
<b>GHD</b>	Gas hydrate data
<b>ESLE</b>	Salt solubilities
<b>ELE</b>	Vapor-liquid equilibria for systems containing solved salts
<b>EGLE</b>	Gas solubilities of electrolyte-containing systems
<b>ECND</b>	Electric conductivity
<b>DIF</b>	Diffusion coefficients
<b>CRI</b>	Critical Data of Mixtures
<b>CPE</b>	Excess heat capacities
<b>AZD</b>	Azeotropic/zeotropic information
<b>ACT</b>	Activity coefficients at infinite dilution – binary systems
<b>ACM</b>	Activity coefficients at infinite dilution – ternary systems
<b>AAE</b>	Adsorbent/adsorptive equilibria

The short terms (VLE etc.) are used extensively in this tutorial.

This document tries to be a tutorial but also tries to cover every function at least cursorily. It is organized in chapters – every chapter describing a typical approach for using the DDB in a productive and efficient way.

This document does not cover all features if they are part of other standalone programs – like the component management and the editors.

## 1.1 The XDDB (Extended Data)

The XDDB has been originally created to store complex data which do not follow the strict rules the older DDB parts enforce and to store data which haven't been stored at all.

If such data couldn't be converted into standard formats or do not fit into existing data banks DDBST stored such data simply in Excel files for future usage.

With the introduction of the XDDB DDBST found a way to store such data unmodified and unconverted but accessible, retrievable, plottable and exportable in the DDB main retrieval software. However, some restrictions apply because of the complexity of some data.

The XDDB contains a wide variety of data which is shown in the table below. Many of the new data types could be summarized under one label. For example, many properties give information about gas hydrates. This led to the conclusion that some parts of the XDDB could be shown under such a label.

These XDDB derived data banks are currently:

- Gas hydrate data (GHD)
- Mixture viscosities (VIS)
- Mixture dielectric constants (MDEC)
- Electrical conductivities (ECND)
- Diffusion coefficients (DIF)
- Mixture flash points (MFLP)
- Mixture P-v-T data (MPVT)
- Mixture speeds of sound (MSOS)
- Mixture thermal conductivities (MTCN)
- Mixture surface tensions (MSFT)

These data banks are all extracts of (or views on) the XDDB and are not physically available. These partial data banks currently represent about 75 % of all data in the XDDB. The remaining 25 % are data for other properties or very complex data which couldn't be entered into the standard data banks. Although the majority of data in the XDDB is for mixtures, some data for pure components are also stored. Most pure component properties, including, for example, viscosities, dielectric constants, electrical conductivities, flash points, etc., are stored in the pure component properties data base (PCP).

## 2 Starting the Dortmund Data Bank Retrieval Program

The program itself starts with a query definition dialog. Possible queries can be

- Search for systems (built of components and of component lists)
- Search for references (literature information)
- Search for single sets (data set numbers)
- Search for pure component properties
- A special query for selectivity searches in the database for limiting activity coefficients (ACTDDB).

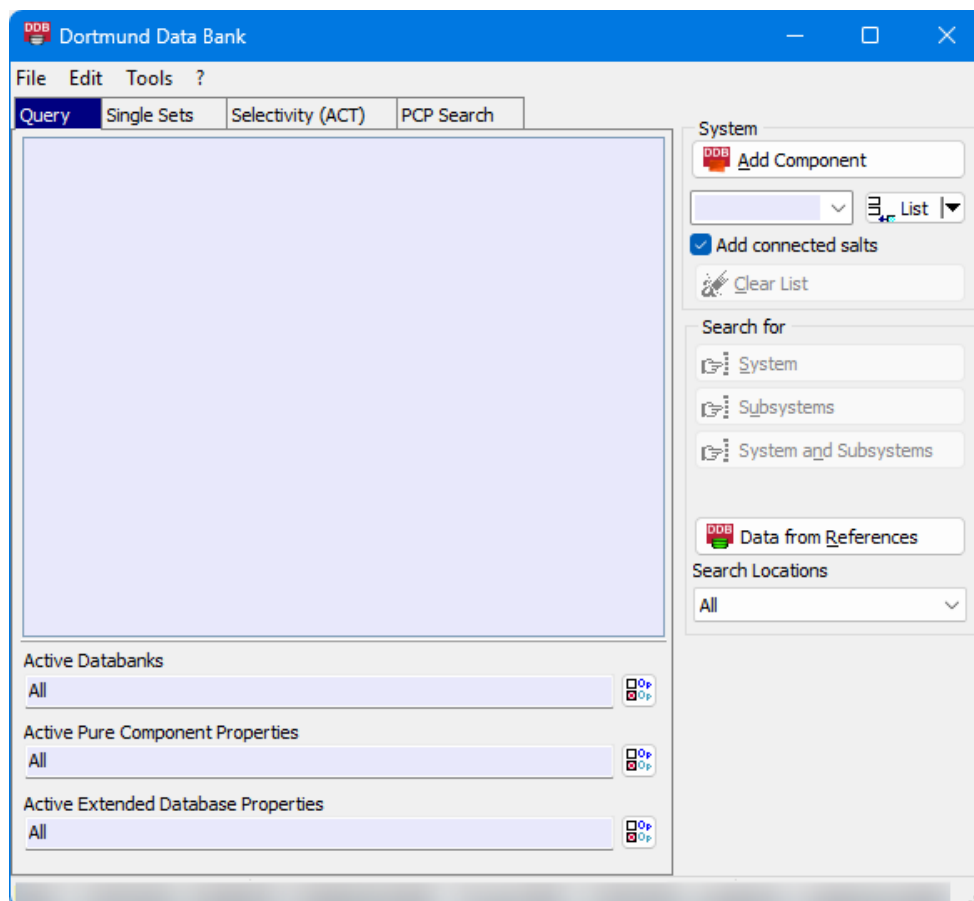


Figure 1: Dortmund Data Bank Start Dialog (Query Definition Dialog)

## 3 Searching

### 3.1 Building a Simple Systems Query

In this step, we will build a systems query for a three components system and take a look at the different search options for such a system.

A *system* in our terms means a list of DDB specific components. DDB components are stored in a component definition file, which can be searched with *DDB Components* application.

Press the *Add Component* button and the *DDB Components* application will be displayed.

The program is described in detail in its documentation (Components.pdf).

After adding the components “Acetone”, “Methanol” and “Nonane” the query list looks like this:

Number	Type/ Count	Loc.	Remove	Name
[4]	C	DDB	Remove	[Acetone]
[110]	C	DDB	Remove	[Methanol]
[398]	C	DDB	Remove	[Nonane]

The system related search buttons are now enabled.

The single buttons perform different type of searches:

Button	Function
<i>System</i>	A system search finds only data sets build of the three collected components.
<i>Subsystems</i>	A subsystems search finds all data sets build of the three collected components plus all data sets with these components and any other (quaternary and higher systems).
<i>System and Subsystems</i>	A system and subsystems search finds all data sets build of the three components and all data sets build by the binary (acetone/nonane, acetone/methanol, nonane/methanol) subsystems and data sets for the pure components.

An exact match search of this three-component-system yields the following data sets for LLE.

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	Publ.Year	Reference
[14163 0 0]	DDB	13	3	[ C4 Acetone] [ C110 Methanol] [ C398 Nonane]	278 (const.)		n.a.		13 tie lines, 2 Ph.		2003	[53809] T
[14164 0 0]	DDB	10	3	[ C4 Acetone] [ C110 Methanol] [ C398 Nonane]	288 (const.)		n.a.		10 tie lines, 2 Ph.		2003	[53809] T
[14165 0 0]	DDB	8	3	[ C4 Acetone] [ C110 Methanol] [ C398 Nonane]	298 (const.)		n.a.		8 tie lines, 2 Ph.		2003	[53809] T

### 3.2 Building a Query with Component Lists

Besides single components like Acetone it is also possible to introduce component lists in the query list.

Component lists can be built in DDB Components by selecting multiple components and send them as list to the DDB Dortmund Data Bank

The resulting query window is



Number	Type/ Count	Loc.	Remove	Name
<a href="#">[110]</a>	C	DDB	<input type="button" value="Remove"/>	<a href="#">[Methanol]</a>
<a href="#">[398]</a>	C	DDB	<input type="button" value="Remove"/>	<a href="#">[Nonane]</a>
<a href="#">[List]</a>	3	-	<input type="button" value="Remove"/>	Component List

If a component list is available on disk (e.g., “\*.ddbpr” files) it is also possible to load these files by the *Load Component List* item in the *File* menu.

The component is treated like a single component. This means that a system search now finds ternary systems with Nonane/Methanol and any the three components of the list Acetone/Ethanol/Diethyl Ether.

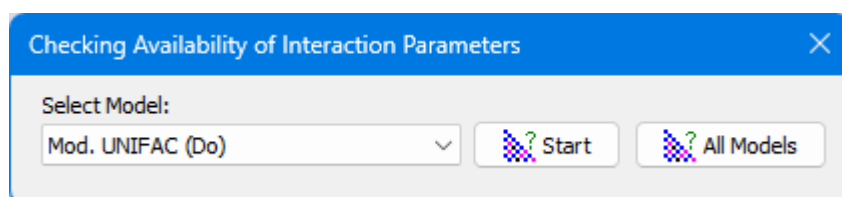
### 3.3 Examining Further Query List Functionality

The component list contains three active areas.

1. The 'Number' column contains hyperlinks, which allow the content to display of the line in DDB Components. This allows the user to display and modify list members and to replace components. If the mouse hovers over the “[List]” hyper link the Dortmund Data Bank displays the content of the list in a hint window – if the list contains less than 10 components.
2. The *Remove* button removes the component or component list.
3. The 'Name' column contains hyperlinks which allow component details to display in DDB Components (see DDB Components documentation).

The component list also has a context menu with the following functions:

- “Main” resp. “Alternative” Names allows switching between the two main synonyms stored in the component basic file.
- 'Display/Edit Compound List Entries' displays the current line in DDB Components (same function as the hyper link in the 'Number' column).
- 'Combine Entries to Single List' builds a single list from all components (disregarding lists or single components) currently in the query list (in the current example the result is a single list with five components).
- 'Expand List to Single Entries' breaks a list into pieces.
- 'Search for data with only component(s) from line' finds sets for the components in that marked line. If this line only contains a single component, only pure component data sets will be found.
- 'Display Component/List Related Statistics' starts a sub list search for the selected component or list and display a detailed list of available data sets.
- 'Display Availability of Interaction Parameters' starts a search for the availability of parameters for some group contribution models used in the Dortmund Data Bank:



This function searches for the parameters for all binary pairs from a list. Currently the models UNIFAC, UNIFAC 2.0, Modified UNIFAC (Dortmund), Modified UNIFAC 2.0, Modified UNIFAC (Lyngby), PSRK, PSRK 2.0, VTPR, COSMO-RS(OI), COSMO-SAC, MOSCED (1984

and 2025), NIST-modified UNIFAC, as well as the UNIFAC Consortium models are supported (see chapter 18.17 “Checking Availability of Model Parameters” for more information).

- 'Display Detailed Pure Component Properties Overview' shows a detailed statistic over the available data for a component.

The edit field below the *Add Component* button list allows the user to directly enter DDB component numbers and add the components either separately or as a list. This field is only useful for experienced users knowing DDB codes for at least some components.

If non-normal components (such as salts, polymers and adsorbents) have to be typed the data type can be switched to salts, adsorbents or polymers by pressing the 's', 'a', or 'p' key. In this special case, the salt numbers will be displayed as salt number plus one million, the adsorbent numbers as adsorbent number plus two millions and the polymer number plus three millions.

After adding the line, the query list looks like

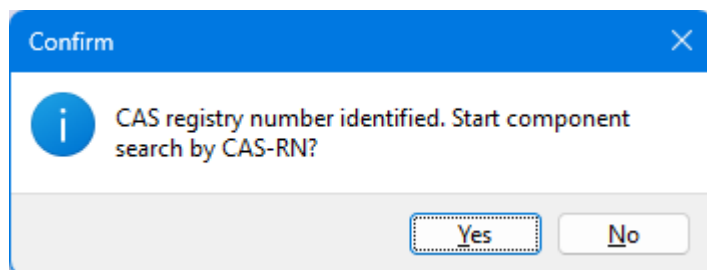
Number	Type/ Count	Loc.	Remove	Name
[11]	C	DDB	Remove	[Ethanol]
[11]	S	DDB	Remove	[Beryllium fluoride]
[11]	A	DDB	Remove	[Molecular sieve carbon]
[11]	P	DDB	Remove	[polyisobutylene]

The “Add connected salts” check box is useful for adding components, which are stored as normal components as well as salts.

The DDB maintains currently four component lists (normal components, salts, adsorbents, polymers) and almost all salts are having entries also in the normal component list. To find all occurrences of a salt (as a salt in the ESLE and the ELE data banks and as a normal component in all other data banks) it is necessary to create a list of both manifestations. If this check box is checked, the program automatically creates this list.

This feature is not available for adsorbents because this type of components does not have duplicate entries in two lists. For polymers, the association is performed automatically during the search.

The program recognizes valid CAS registry numbers and allows starting a direct search for that number.



The text field has a history function where the last sixteen entries are stored.

### **3.4 Import Aspen Components**

The Dortmund Data Bank program can read component information from an Aspen backup file (“\*.bkp”) by using the *Import Aspen Components* button in the *File* menu.

The most important column is the “DDB Number” column. If a component has been identified the DDB number is displayed. If the component is not known, a “0” is displayed. In this case, the button “Change the DDB Number” can be used to search for an already existing DDB component and use its number.

### **3.5 Import PRO/II Components**

The Dortmund Data Bank program can import components from a PRO/II project file (“.prz” file) by using the *Import PRO/II Components* button in the *File* menu.

The import dialog lists all components found in the PRO/II project file and displays the found matching DDB components.

The automatic assignment can be overwritten by changing the DDB number manually (“Change DDB Number” button).

### **3.6 Import UniSim Design Components**

The Dortmund Data Bank program can import components from a UniSim Design project file (“\*.usc” file) by using the *Import UniSim Design Components* button in the *File* menu.

The import dialog lists all components found in the UniSim Design project file and displays the found matching DDB components.

The automatic assignment can be overwritten by changing the DDB number manually (“Change DDB Number” button).

### **3.7 Import Simulis Components**

The Dortmund Data Bank program can import components from a Simulis Thermodynamics calculator file (\*.calculator) by using the *Import Simulis Thermodynamics Components* button in the *File* menu.

The import dialog lists all components found in the Simulis Thermodynamics calculator file and displays the found matching DDB components.

The automatic assignment can be overwritten by changing the DDB number manually (“Change DDB Number” button).

### **3.8 Import AVEVA SimCentral Components**

The Dortmund Data Bank program can import components from an AVEVA SimCentral simulation library file (\*.libx) by using the *Import AVEVA SimCentral Components* button in the *File* menu.

The import dialog lists all components found in the AVEVA SimCentral simulation library file and displays the found matching DDB components.

The automatic assignment can be overwritten by changing the DDB number manually (“Change DDB Number” button).

### **3.9 Searching for the Data Sets of a Reference**

All data sets in the DDB are referenced. Sources are articles, theses, private communications, company data, deposited documents like VINITI, proceedings and so on. These papers have been retrieved, evaluated and the experimental data are now building the DDB.

The literature management program (DDB Literature) is a separate program but the dialogs are incorporated seamlessly. The literature search is started by pressing the *Data from References* button.

DDB Literature provides two search modes, one for experienced users with many possible search items and possible combinations and one easier quick search mode, which we will use here. The dialog has six fields where authors, publication year, first page, journal number, volume, title words, and LEAR record numbers can be entered. Any non-empty field must be found for a successful match – e.g. if authors and a year are specified only articles from these authors published in the specified year will be found. The “Libraries to be Searched” field contains one or two literature data banks – one public (DDBST) database and one private (customer) database if available.

Number	Title	Authors	Publication Year
[82]	Solubilities of nitrogen in heavy normal paraffins from 323 to 423 K at pressures to 18.0 MPa	Tong J.; Gao W.; Robinson R.L.; Gasem K.A.M.	199
[1387]	Determination of Infinite Dilution Activity Coefficients for Organic-Aqueous Systems Using a Dilute Vapor-Liquid Equilibrium Method	Bader M.S.H.; Gasem K.A.M.	199
[6528]	Phase Behavior in the Nitrogen+Ethylene	Gasem K.A.M.; Hiza M.J.; Kidnay A.J.	198

Figure 2: Literature Search Result


The search result is a list with the found articles. The details of the article can be displayed by a double click and the reference is selected by pressing the  button. The search is started now automatically and all data sets from the specified reference or references are displayed.

Figure 3 shows a query result for reference 48664 (Wittig et al.):

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	PublYear	Reference
[VLE 22766 0 0]	DDB	30	2	[ C174 Water] [ C292 Methyl formate]	298 (const.)		3	78	Ex(T)		2001	[48664] Wittig R., L
[VLE 22767 0 0]	DDB	34	2	[ C16 Formic acid ethyl ester] [ C174 Water]	298 (const.)		3	34	Ex(T)		2001	[48664] Wittig R., L
[VLE 22768 0 0]	DDB	52	2	[ C174 Water] [ C288 Formic acid butyl ester].	298 (const.)		3	7	Ex(T)		2001	[48664] Wittig R., L
[VLE 22769 0 0]	DDB	61	2	[ C8 1,2-Ethandiol] [ C161 Toluene]	323 (const.)		<1	13	Ex(T)		2001	[48664] Wittig R., L

Figure 3: Data Sets from Specified Literature

### 3.10 Search Data Sets by Data Set or Reference Numbers

Figure 4: Search by Data Set Numbers

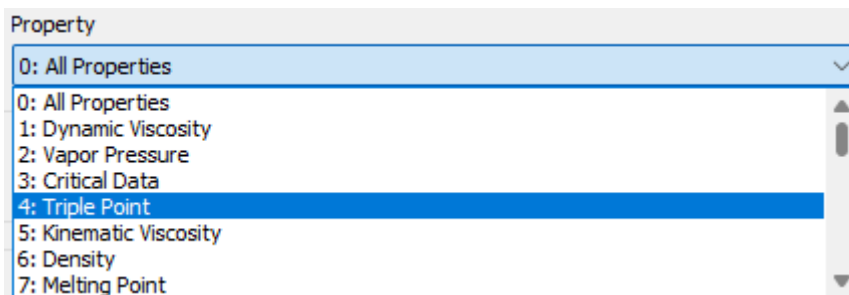
Data set and Literature numbers are the most basic identifiers of a DDB data set.

The input edit fields allow multiple numbers to enter separated by spaces or semicolons and it is possible to define ranges of numbers by writing “lower number slash upper number” (“1/99”). If ranges are used blanks are not allowed as separators.

### 3.11 Searching Data Sets with Specified Pure Component Properties

Figure 5: Pure Component Properties Search

The property search dialog allows specifying the property, to restrict the search to a list of components and states, and you can specify if a wanted value only needs to be present in a data set or if all data points of a set must meet the given criteria.



The questions (criteria) are simply upper and lower limits for a specific table item and are entered through a simple dialog.

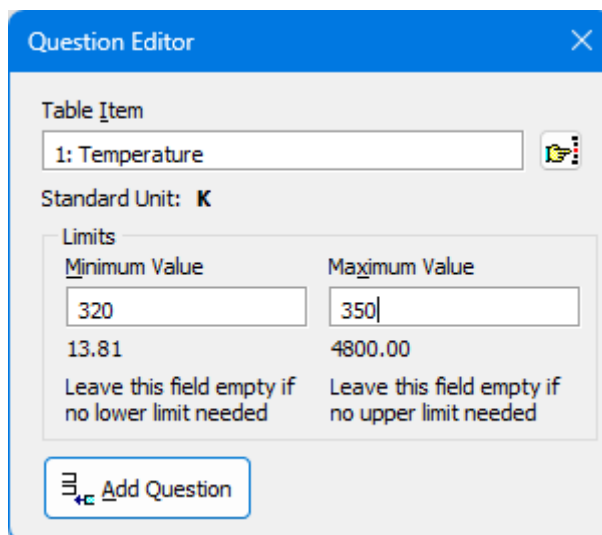


Figure 6: Question Dialog

It is possible to add several conditions which all have to be fulfilled for a matching data set.

Table Item	Minimum Value	Maximum Value	Unit	Remove?
1 T	320	350	K	Remove
7 VSK	0.05	0.11	m <sup>2</sup> /s	Remove

Figure 7: List of Questions

The results of a search are two lists, a component list and a data set list.

The component list can be saved to file or directly used in subsequent searches and the data set list can be displayed as a Query Result window in the Dortmund Data Bank program.

#	Data Set ID	Property	Component
9	844 [0]	VIS	Pentadecane
10	1212 [0]	VIS	Trifluorobromomethane [R13B1]
11	1213 [0]	VIS	Trifluorobromomethane [R13B1]
12	1248 [0]	VIS	Benzene
13	1251 [0]	VIS	Benzene
14	1252 [0]	VIS	Benzene
15	1253 [0]	VIS	Benzene
16	1254 [0]	VIS	Benzene
17	1255 [0]	VIS	Benzene
18	1294 [0]	VIS	Hexane
19	1295 [0]	VIS	Hexane
20	1296 [0]	VIS	Hexane
21	1297 [0]	VIS	Hexane
22	1298 [0]	VIS	Hexane
23	1299 [0]	VIS	Hexane

1753 data sets found.

Figure 8: Property Search - Data Set List

#	#DDB	Name
1	1	Acetaldehyde
2	3	Acetonitrile
3	4	Acetone
4	7	Ethyl bromide
5	11	Ethanol
6	12	Diethyl ether
7	21	Ethyl acetate
8	22	2-Butanol
9	25	Ethylbenzene
10	27	Chlorobenzene
11	29	Benzonitrile
12	30	Nitrobenzene
13	31	Benzene
14	39	1-Butanol
15	41	2-Butanol

218 components found.

Figure 9: Property Search - Component List

### 3.12 Searching for Data with Specified Temperatures and Pressures

This function is accessible through the “File” menu of the main window of the Dortmund Data Bank program.

VLE/HPV/AZD/SLE Temperature/Pressure Search

Both the VLE and the HPV data bank contain saturated vapor-liquid equilibrium temperature/pressure data values for specific compositions of binary or higher mixtures. The AZD (azeotropic data) contains also many data points where pressures and temperatures are given.

The SLE (solubilities) data bank contains mainly only melting temperatures of mixtures without a given pressure. For this reason, it is possible to exclude the pressure limits from the search criterion.

VLE/HPV/AZD/SLE T/P Search ✕

Please enter temperature and pressure limits:

Lowest Temperature	Highest Temperature
<input type="text" value="300"/> K	<input type="text" value="400"/> K
Lowest Pressure	Highest Pressure
<input type="text" value="100"/> kPa	<input type="text" value="200"/> kPa

Ignore Pressure Limits for SLE Search

Figure 10: VLE/AZD/SLE Temperature/Pressure Search Criteria

A standard query result window shows all the found data sets.

### 3.13 Selectivity Search

Figure 11: Selectivity Search

This selectivity search is specific search for ACT data bank. This data bank contains activity coefficients at infinite dilution of a single solute in a single solvent.

This dialog allows three different tasks to perform:

1. Specification of two solutes and a single solvent. The resulting query result can be plotted (plot button or context menu). The diagram displays the usability of the solvent as entrainer in separation process mainly used to break azeotropes. This is useful if a specific solvent is known.

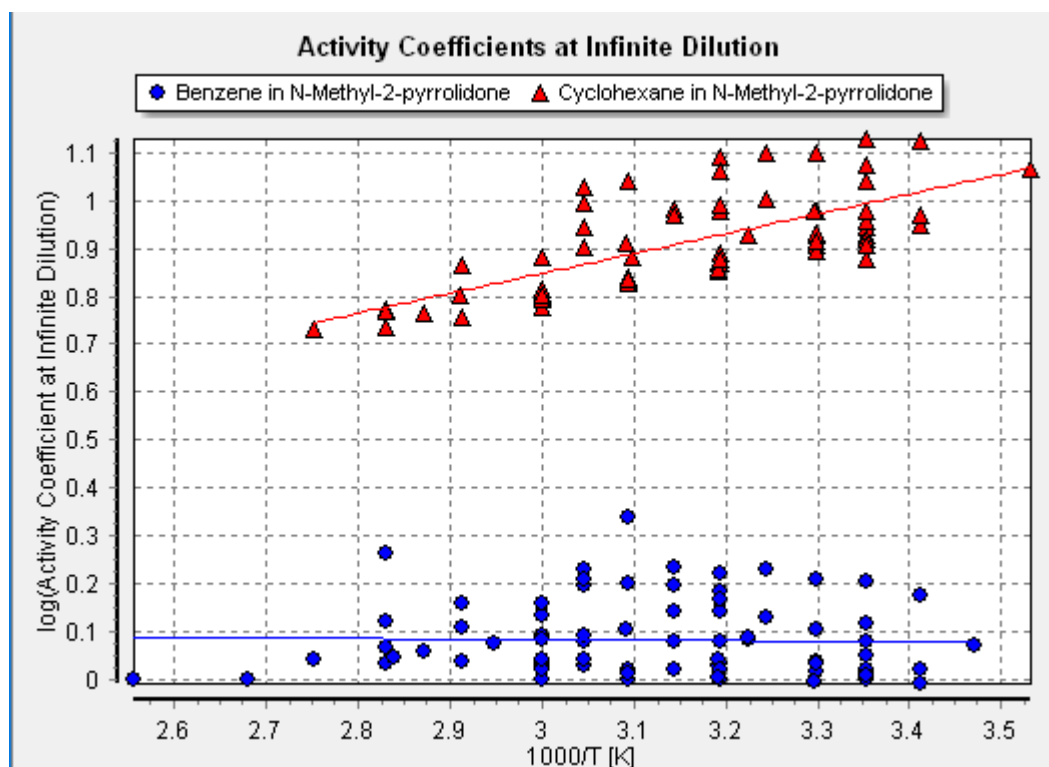


Figure 12: Selectivity Diagram

2. Search for all data sets for two solutes. This leads to a list of all solvents stored in the ACT data bank which can be further examined.



- Predicting selectivity. The prediction calculates activity coefficients at infinite dilution for both solvents in a single solvent. The results can be displayed as a table output, as a query result or as a plot. The resulting plot is the same as for the data set search with the exception that only predicted data are displayed.

## 3.14 Search Options

### 3.14.1 Data Banks Preselection

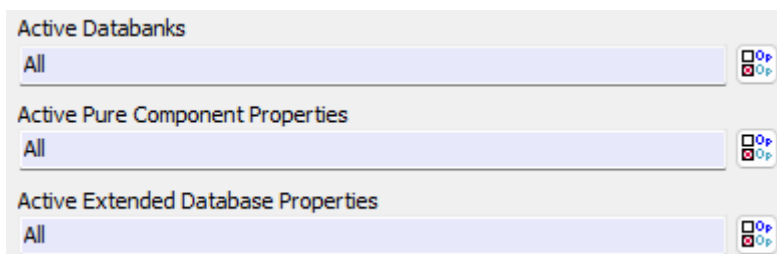


Figure 13: Data Banks and Pure Component Property Preselection

The search can be restricted to specified data banks.

Search?	DDB	Description
<input checked="" type="checkbox"/> Yes	AAE	Adsorbent/adsorptive equilibria
<input checked="" type="checkbox"/> Yes	ACM	Activity coefficients at infinite dilution (ternary systems)
<input checked="" type="checkbox"/> Yes	ACT	Activity coefficients at infinite dilution (binary systems)
<input checked="" type="checkbox"/> Yes	AZD	Azeotropic/zeotropic information
<input checked="" type="checkbox"/> Yes	CPE	Excess heat capacities
<input checked="" type="checkbox"/> Yes	CRI	Critical data of mixtures
<input checked="" type="checkbox"/> Yes	EGLE	Gas solubilities (electrolyte containing systems)
<input checked="" type="checkbox"/> Yes	ELE	Vapor-liquid equilibria for systems containing solved salts
<input checked="" type="checkbox"/> Yes	ESLE	Salt solubilities
<input checked="" type="checkbox"/> Yes	GLE	Gas solubilities
<input checked="" type="checkbox"/> Yes	HE	Heats of mixing
<input checked="" type="checkbox"/> Yes	LLE	Liquid-liquid equilibria
<input checked="" type="checkbox"/> Yes	PCP	Pure component properties
<input checked="" type="checkbox"/> Yes	POLYMER	Thermodynamic data for polymer containing systems
<input checked="" type="checkbox"/> Yes	POW	Octanol-Water partition coefficients
<input checked="" type="checkbox"/> Yes	SLE	Solid-liquid equilibria (mainly organic compounds)
<input checked="" type="checkbox"/> Yes	VE	Densities and (excess) volumes of mixtures
<input checked="" type="checkbox"/> Yes	VLE	Vapor-liquid equilibria

Figure 14: Data Bank Preselection

The list shows always all possible parts of the Dortmund Data Bank. If a data bank is not available, it is marked as “n. a.” and cannot be selected.

### 3.14.2 Pure Component Properties Preselection

Number	Search?	Property
1	<input checked="" type="checkbox"/> Yes	VIS Dynamic Viscosity
2	<input checked="" type="checkbox"/> Yes	VAP Vapor Pressure
3	<input checked="" type="checkbox"/> Yes	CRI Critical Data
4	<input checked="" type="checkbox"/> Yes	TRI Triple Point
5	<input checked="" type="checkbox"/> Yes	VSK Kinematic Viscosity
6	<input checked="" type="checkbox"/> Yes	DEN Density
7	<input checked="" type="checkbox"/> Yes	MPT Melting Point
8	<input checked="" type="checkbox"/> Yes	HCP Molar Heat Capacity (cP)
9	<input checked="" type="checkbox"/> Yes	BII Virial Coefficients
10	<input checked="" type="checkbox"/> Yes	HVP Heat of Vaporization
11	<input checked="" type="checkbox"/> Yes	HFS Heat of Fusion
12	<input checked="" type="checkbox"/> Yes	TCN Thermal Conductivity
13	<input checked="" type="checkbox"/> Yes	TBP Boiling Point
14	<input checked="" type="checkbox"/> Yes	SFT Surface Tension

Figure 15: Pure Component Properties - Property Preselection

The search for pure component properties can be restricted to specified properties. Single properties can be selected with a right-click with the mouse.

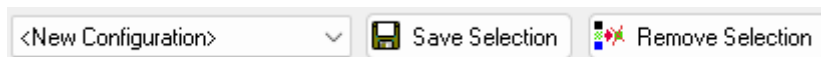
### 3.14.3 Extended Database Properties

Number	Search?	Property
1	<input checked="" type="checkbox"/> Yes	DIJ Diffusion Coefficients (I in J)
2	<input checked="" type="checkbox"/> Yes	SVLE Solid-Liquid-Vapor Equilibrium (XL = XLVL, YL = YLVL)
3	<input checked="" type="checkbox"/> Yes	PVT Pressure-Volume/Density-Temperature(-T)
4	<input checked="" type="checkbox"/> Yes	n_IoR Index of Refraction
5	<input checked="" type="checkbox"/> Yes	VLE Vapor-Liquid Equilibrium (XL = XLVL, YL = YLVL)
6	<input checked="" type="checkbox"/> Yes	dHDil Heat of Dilution
7	<input checked="" type="checkbox"/> Yes	dHSol Heat of Solution/Solvation
8	<input checked="" type="checkbox"/> Yes	GLE Gas Solubilities
9	<input checked="" type="checkbox"/> Yes	hE Heat of Mixing
10	<input checked="" type="checkbox"/> Yes	Lw-H(I) Liquid-Hydrate(Type I)-Equilibrium
11	<input checked="" type="checkbox"/> Yes	IHFT Initial Hydrate Formation Temperature
12	<input checked="" type="checkbox"/> Yes	LLE Liquid-Liquid-Equilibrium
13	<input checked="" type="checkbox"/> Yes	LLE/LCST LLE, Lower Critical Solution Temperature

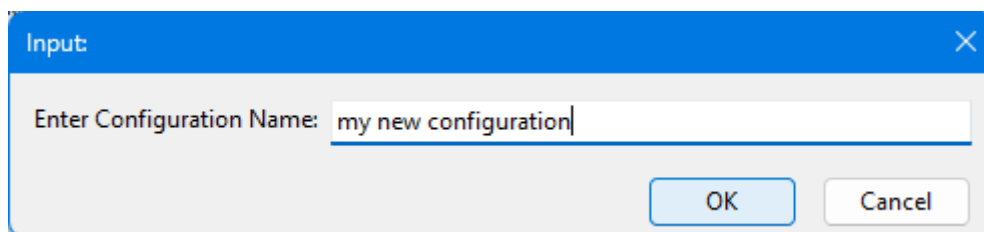
Figure 16: Extended Database - Property Preselection

The extended database contains multiple properties. The preselection allows limiting the search to single or some properties. Single properties can be selected with a right-click with the mouse.

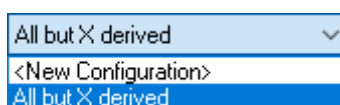
### 3.14.4 Configurations



Search options can be stored and restored through configuration files. If such a configuration has not been stored yet, a “New Configuration” can be saved.



Stored configurations are shown in the configuration combo box and are activated simply by selecting the appropriate line.



“Remove Selection” will remove a selection from the list of configurations.

### 3.14.5 Other Search Options

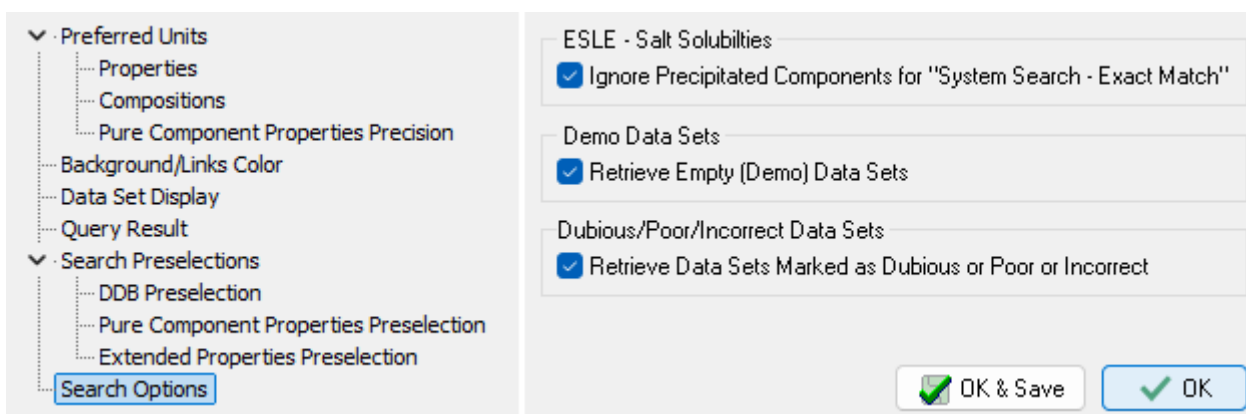


Figure 17: Other Search Options

#### 3.14.5.1 Salt Solubilities – Handling of Precipitated Components

Salt solubility data contain solved and precipitated components and salts. The number of precipitated components and salts can be very large because mainly of many different hydrates and other associates. The search for an exact match of such a system containing seven or even more components is very difficult. The option “Ignore Precipitated Components” allows to neglect the precipitated components.

#### 3.14.5.2 Demo Data Sets

The DDB is delivered with empty sets if a specific database is not licensed. These data sets only contain a list of components but no experimental data. These data sets are normally searched and displayed together with licensed data sets. It is then possible to hide the demo data sets in the search query result form. This option now allows avoiding the retrieval of demo data sets during initial search.

#### 3.14.5.3 Retrieve Data Sets Marked as Dubious or Poor or Incorrect

This option allows excluding data sets marked as being of low quality from the data bank search.

### 3.14.6 Search Locations

The Dortmund Data Bank is typically divided into a public DDB provided by DDBST and a private DDB maintained by customers. The switch allows the user to use a single location or all locations for the search.

## 4 Exploring the Data Bank – Statistics

The Statistic option in the File Menu allows starting different analyze tools:

### 4.1 Set, Points, References

The DDB statistics main page (“Sets/Points/Refs”) shows the number of data sets, data points, and references for public and private data banks. The list will be shorter if not all data banks are available.

Because many references are used in more than one database the real number of references is lower and shown at the bottom of the table.

The second and third pages are more detailed statistics. They display the number of different systems in the data banks separated in a summary and in binary and higher systems. The row with the title “=All=” is shown on the top of all other data base specific lines and show the entire list of systems. The values are not the sum of the single line because many systems are present in two or more data banks.

The “Pure Component Properties” statistics shows the data sets and points for all the single properties.

The “Components” column shows the number of components for which the DDB contains data.

### 4.2 Pure Component Properties

The pure component properties grid has a context menu that contains commands to save list of components, references, and data sets for single properties. “Show Data Sets” display all data sets of the property of a marked line.

### 4.3 X Properties

The “X Properties” page shows detailed information about the properties stored for sets of complex data, which can be summarized under the corresponding properties.

### 4.4 Polymer Data

The “Polymer Data” page shows detailed information about the properties stored for polymers and their mixture in the Dortmund Data Bank.

## 5 A First Look at Predictions

This part of the DDB software contains lot of dialogs for the different data banks and is explained in other chapters in more details. In this step we'll focus on some common features.

Predicting using *Tools* → *Predict Mix* from the main window has been introduced to obtain thermophysical data where no experimental data sets are available. This 'direct' prediction creates artificial – predicted – data sets, which will be added to a query result just like experimental data.

The menu item displays a dialog where a system of components has to be specified.

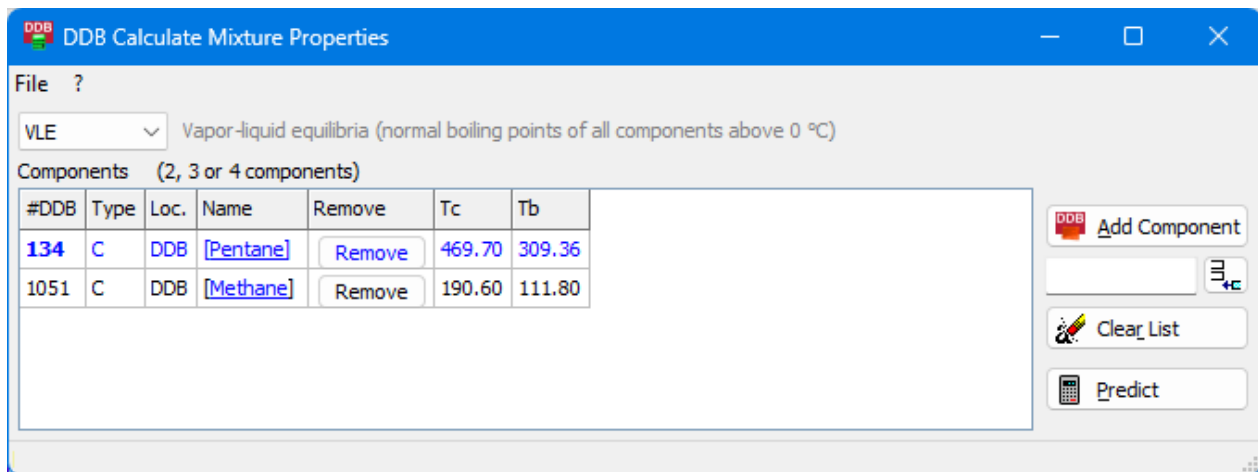


Figure 18: Mixture Prediction, Main Dialog

If components already have been specified in the query definition dialog they will be inserted here automatically. Direct predictions are currently possible for the data banks

- VLE, HPV (vapor-liquid equilibria)
- LLE (liquid-liquid equilibria)
- ACT, ACM (limiting activity coefficients)
- ACTCOEFF (activity coefficients)
- AZD (azeotropy)
- SLE (solid-liquid equilibria)
- HE (heats of mixing)
- CPE (excess heat capacities)
- VE (excess volumes and densities)
- GLE (gas solubilities)
- ELE (vapor-liquid equilibria of electrolyte-containing mixtures)
- ESLE (salt solubilities)
- POW (octanol-water partition coefficients)
- VIS (mixture viscosities)
- JTC (Joule-Thomson coefficients)
- MTCN (mixture thermal conductivities)
- MFLP (mixture flash points)

Special calculations for selectivities and P/T curves (phase envelopes) complete the list.

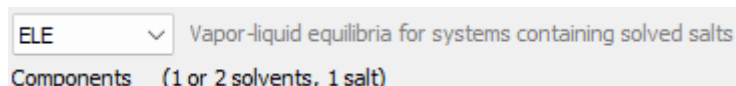
New components can be added by the DDB Components application using the “Add Component” button. If the DDB component numbers are known, they can be typed in directly. The button “Clear List” clears the entire list.

The “Predict” button shows the prediction dialog for the current data bank.

Some databases are requiring special component orders.

- GLE (gas solubilities) predictions need one gas and one solvent with the gas on top position.
- ACM (activity coefficients at infinite dilution of pure solutes in binary solvents) need three components with two solvents on the top and the solute below.
- ELE (vapor-liquid equilibria for electrolyte containing systems) needs one or two solvents at the top and one salt following.
- Selectivity needs three components, two solutes first and a single solvent.

The programs display a short help text above the component list showing these requirements.



The component grid can be sorted either by clicking in the first (fixed) row of the grid or by manual drag and drop of the components.

#DDB	Type	Loc.	Name	Remove	Tc	Tb
134	C	DDB	<a href="#">[Pentane]</a>	<a href="#">Remove</a>	469.70	309.36
1051	C	DDB	<a href="#">[Methane]</a>	<a href="#">Remove</a>	190.60	111.80

A repeated click in the sort row reverses the sort order. Sorting is possible by DDB number, name, T<sub>c</sub>, and P<sub>c</sub>.

The single dialogs for the single data banks are described in the chapters below.

## 6 Using and Understanding the Query Result Window

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [K]
[278 0 0]	DDB	1	3	[ C4 Acetone] [ C110 Methanol] [ C174 Water]	n.a.		101 (
[416 0 0]	DDB	1	3	[ C4 Acetone] [ C47 Chloroform] [ C110 Methanol]	331 (const.)		101 (
[4882 0 0]	DDB	1	3	[ C4 Acetone] [ C70 Dichloromethane] [ C110 Methanol]	n.a.		101 (
[4883 0 0]	DDB	1	3	[ C4 Acetone] [ C47 Chloroform] [ C110 Methanol]	331 (const.)		n.a.
[11487 0 0]	DDB	1	3	[ C4 Acetone] [ C50 Cyclohexane] [ C110 Methanol]	298 (const.)		n.a.
[18525 0 0]	DDB	1	3	[ C4 Acetone] [ C110 Methanol] [ C134 Pentane]	373 (const.)		n.a.
[19294 0 0]	DDB	1	3	[ C4 Acetone] [ C47 Chloroform] [ C110 Methanol]	323 (const.)		76 (c

DDB: AZD Data Set: 4882 Source: 0 (Public DDB) Counter: 0

1 data set/s marked.

Figure 19: Query Result

### 6.1 File Menu

The “File” menu contains typical functions like loading from disk and saving to disk.

'Append Datafiles' resp. the 'Save Data' menu entries allow loading and saving data in different DDB specific formats. The single formats are described in the next steps (see chapter 7, “Saving and Loading Data Files”).

'Save Grid' saves only the “Data Set List” grid content.

'Show' allows displaying the single data sets in different ways.

The 'Show List' entries display the same content as the single data set display but all data sets in a row. The 'Current View' shows all sets from the currently displayed data bank.

The 'Compact' displays are only showing some descriptive information – like components, references, data set count, and value ranges.

'Show References' display the references of the data sets in the literature management program LEAR.

'Show Components' display the component of the data sets in the compound list editor.

'Show Difference' compares two data sets and shows all differences in a table. These functions make most sense when an experimental and a predicted set are compared.

'Show PCP Data Overview (Selected Sets)' produces a statistic for pure component property data sets.



'**Check Available Parameters for Prediction Methods**' searches the parameter files of several models for the availability of parameters for all the systems of marked sets. The model has to be selected first.

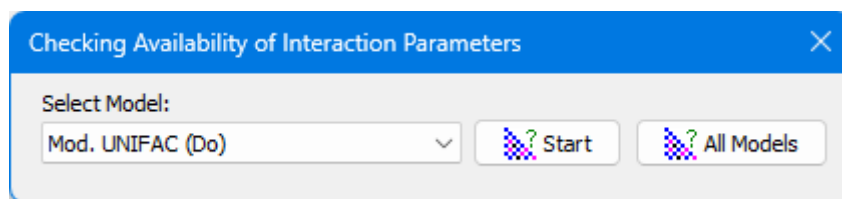


Figure 20: Checking Interaction Parameter Availability

“All models” is only enabled if a single system is selected.

This function does not check if every needed data types are available – it only checks for the model specific parameters but not, for example, the availability of critical data which are needed for PSRK, for example.

'**Check for Needed Basic Data for Calculations**' checks for critical temperature and pressure, for the acentric factor, the melting temperature, and the heat of fusion. The functions behind the buttons “Check Data for Equations of State” and “Check Data for SLE Calculations” check the data sets accordingly. Use the tool button “Remove Sets with Unused Component from the Query Result” to remove all data sets where needed basic data are missing.

'**Export in PPDX Format**' exports (saves) the data sets to the PPDX format – the format and this export feature are described in a separate document.

'**Export in Aspen INP Format**' allows storing the data sets in the Aspen INP format – still the standard data exchange format in Aspen.

'**Export Data Points**' allows writing a table containing all data points

'**Close All**' closes all query result window

'**Close All Query Results Except This**' closes all query result windows with the exception of the current window

'**Close**' closes only the current query result window.

## 6.2 Edit Menu

The 'Edit' Menu contains typical functions like copying and editing.

'**Select**' contains functions to select all data sets in the current result grid or to select data sets for the current system or the current system and subsystems.

'**Copy to Clipboard**' copies the selected part of the data grid to the Windows clipboard. This function only copies the data grid not any additional data.

'**Export Data Points**' allows writing experimental data to files in text and Excel format. Please see chapter 22.3 “Data Points Export” on page 87 for more information.

'**Retrieve Datasets**’ assembles four functions to start new searches related to the current search result.

- Retrieve data sets for the reference
- Retrieve data sets for the system(s)
- Retrieve data sets for binary subsystems
- Retrieve data sets for a pure component

'**Modify**' allows changing data sets. This is explained in chapter 15 “Modifying and Editing Data Sets” on page 47ff.

'**Consistency Tests**' allows calling consistency tests for VLE data (see chapter 14 “Consistency Tests” on page 41ff for detailed information).

'**Plot**' shows diagrams of the selected data sets (see chapter 21 “Plot” on page 82 for more information).

'**Fit**' is described in chapter 20 (“Simultaneous Fit – Regression Mix”) on page 81 and in a separate manual “Regression Mix”.

'**Show Query Window**' brings the main query definition window to front.

'**Options**' are explained in chapter 11 “Data Set Display Options” on page 34ff.

'**Statistics**' menu entries are display in chapter 17 “Query Result Statistics” on page 52ff.

'**Rename this Query Result**' allows changing the caption of the query result window.

## 7 Saving and Loading Data Files

### 7.1 Open Files

Data sets can be loaded in the query result window and in the query definition window. Loading multiple files in the main window will open multiple query result files, loading multiple files in a query result window allow collecting all the data in that window.

'**Append Datafiles**' resp. the '**Load Data Files**' menu entries allows loading data in different formats – but all only in DDB specific formats.

**Save Grid**' only stores the 'Data set List' grid content, not the data themselves.

### 7.2 Save File

'**Save Data**' allows storing the data sets in different formats – but all only in DDB specific formats. The formats are

- “**Save Marked Sets**”: This format is the free formatted but extended by database names. Its extension is “.qrx”. It stores all data sets from all databases in the current query result (and allows it to restore). We now use it as standard exchange format.
- “**Save Single Set**”: This function stores a single data set in the “.qrx” format.
- “**Save All Sets – All Data Banks**”: The format is also the “.qrx” format but allows storing the entire query result in one file.
- “**Data Set Identifiers**”. This format only stores the database name and data set identifiers (data set numbers, data bank location).
- “**Literature Numbers**”. This file (“.stx”) stores the literature numbers of the data sets. This file can be loaded in the literature management program (LEAR).
- “**Component Numbers**”. This file (“.ddbpr”) stores the DDB numbers of the components. This file can be loaded in different programs (Component Management, Dortmund Data Bank, etc.).

There are two types of saved data file.

1. Files containing the complete experimental data (Query Result data sets, .qrx format).
2. File containing only data descriptors (Data set identifiers, literature numbers, raw data set numbers and component numbers).

The files containing only descriptors are damageable by data bank changes because the descriptor might point to a replaced or deleted data set. Please consider these files only for *temporary* storage.

### 7.3 Drag and Drop Files

All files that can be opened through the menu commands can also be loaded by dragging and dropping the files from the Windows explorer to the main dialog of the Dortmund Data Bank program.

## 8 Exploring the Data Set List Grid

The grid contains the list of data sets found in a specific database.

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	Publ.Year	Reference
[45 0 0]	DDB	1	2	[ C4 Acetone] [ C110 Methanol]	329 (const.)		101 (const.)		homEmax		1950	[408] Chu J.
[101 0 0]	DDB	1	2	[ C4 Acetone] [ C110 Methanol]	329 (const.)		101 (const.)		homEmax		1976	[1405] Derni
[123 0 0]	DDB	1	2	[ C4 Acetone] [ C110 Methanol]	329 (const.)		103 (const.)		homEmax		1973	[1600] Campb
[158 0 0]	DDB	1	2	[ C4 Acetone] [ C110 Methanol]	328 (const.)		101 (const.)		homEmax		1977	[1899] Ochi

Figure 21: Query Result Grid

The grid contains the following columns:

- **“Set No.”**: A set number is a combination of data set number, database location, and an additional number if both previous numbers are the same – for duplicate entries. The location is '0' for the public (DDBST) database and '1' for the private (customer) data bank. Other numbers are used for predicted data – the numbers are model specific in that case. The set numbers are hyperlinks. A single-click opens the single data set display window (see next steps). The 'Links Details' window below the grid displays the data set id details when the mouse cursor hovers above a link.
- **“Pts.”**: Number of points in the data set.
- **“#DDB”**: DDB component numbers. The prefix 'C' determines normal components, an 'S' salts and electrolytes, an 'A' an adsorbent, a 'P' a polymer. The 'Details' window below the grid displays the component names when the mouse cursor hovers above a component number.
- **“Tmin [K]”** and **“Tmax [K]”**: Temperature range of the data set. For the PolymerDDB the temperature and pressure columns are used to display mean molecular weights and the polydispersity index (PD)
- **“Pmin [kPa]”** and **“Pmax [kPa]”**: Pressure range of the data set.
- **“Comment”**: Further database-dependent details for the data set.
- **“Reference”**: Author, Journal, and some other details of the reference. The number in brackets is the main literature number – database independent.

The literature numbers are hyperlinks and allow displaying a special literature detail dialog that has the following functions:

- Search for all data sets for the current reference. The result will be displayed in a new query result window.
- Display a dialog in DDB Literature with all available details for the current reference (“Further Details”).
- Display linked files (“Linked Info” button, see “Literature Management” manual for more details)

LEAR Dataset

Search Datasets | Further Details | Linked Info

L22261 L118610

Dataset Number: 22261

Title: Liquid-Vapour-Solid Phase Equilibria. III. The Acetone-Methanol-Lithium Chloride System

Authors: Tatsievskaya G.I. Vitman T.A. Kushner T.M. Serafimov L.A.

Journal: Russ.J.Phys.Chem.

Pages: 1668 to 1669 Publishing Years: 1982

Volume: 56 Issue: 11

Reference: [22261] Tatsievskaya G.I., Vitman T.A., Kushner T.M., Serafimov L.A., Russ.J.Phys.Chem., 56(11), 1668-1669, 1982

Figure 22: Reference Details

The data set grid allows the data sets to sort by clicking in the first – fixed – row. A repeated click reverses the sort order.

Set No.	Source	PI
[1632 0 0]	DDB	1
[8082 0 0]	DDB	1
[8083 0 0]	DDB	1
[8084 0 0]	DDB	1

Figure 23: Sort Order

The reference column has a special sort order. It is sorted alphabetically after the first author and not by the numbers.

## 8.1 Data Table Context Menu

The data set grid has a large context menu. This menu repeats several functions from the main menu, and from tool bars. Some features are unique.

“**Show Data Set**” displays the set in the single data set display.

“**Show Reference Details**” shows the complete reference information.

“**Show List**” displays a list of sets in the single data set or in a compact format. It can either show the data sets currently shown or just the marked data sets. It is also possible to list all loaded data sets from all data banks and it can show the content of the parameter data base (ParameterDDB).

“**Component Details**” allows displaying the component's basic data (like names, formula, CAS registry number etc.).

“**Plot Selected Sets**” plots the marked data sets.

“**Plot Current System**” marks automatically all data sets build of the same components and plots them together.

“**Plot Current System Incl. Subsystems**” can be used for data sets of ternary systems and will plot all the data sets of the ternary and all three binary subsystems together.

“**Quick Plot**” opens a plot dialog where the properties on the x, y, and z axes can be arbitrarily selected.

“**Predict**” the prediction routines. This function is described in another step.

The “**Query Result Grid**” sub menu allows the

- selection of all data sets in the grid
- selection of all data sets build of the same components
- selection of all data sets build of the same components including subsystems
- adjusting the columns widths to the content's width
- selecting which columns are visible
- copying the grid content to the Windows clipboard
- saving the grid content to a CSV (comma separated values) file
- saving the grid to a HTML formatted file
- switching between different display modes for names and DDB numbers, these switches are also available in the 'options' dialog

“**Create New Query Result From Selected Sets**” builds a new query result windows only from the marked sets.

“**Retrieve Data Sets for Reference**” performs a new search for the current reference. This allows collecting all data sets for a specific article.

“**Retrieve Data Sets for System**” performs a new search on the current system.

“**Retrieve Data Sets for Binary Subsystems**” performs a search for the data of a specified binary subsystem of a ternary or higher data set.

“**Retrieve Data Sets for Pure Components**” performs a search for the data of specified component of a binary or higher mixture.

The “**Save Data**”, “**Export**”, and “**Modify**” entries are clones of the main menu function for saving, exporting and modifying data sets and described in other chapters.

“**Plot AZD as LLE**” shows azeotropic points in a diagram of existing LLE data (max. ternary system).

“**Consistency Tests**” starts the two consistency tests for VLE data.

“**Remove Selected/Additional Sets From Query Result**” deletes the data sets from the search result but leaves the databases unchanged.

“**Retrieve Linked Sets**” is only available for XDDB data sets. It shows all linked records.

## 9 Query Result Filters

The query result can be filtered for each data type separately. The filters are applied in two steps.

The upper area (left from the result grid) contains all possible filter categories. Some categories are not available for all data types.

To use (or change) a filter click on the category name (e.g. “Reference”). Then the lower area will contain all available filter items (e.g. all references available in the currently visible grid). Use the filter items to include or exclude data sets (or points).

It is possible to use multiple filter categories for a further restriction of the data set list. For example, use the *System Size* category to display only binary data sets. Afterwards use the *System* category to include or exclude specific binary systems.

If any filter item is selected for a specific category, then all selected items can be disabled (or enabled again) using the category checkbox. Categories without selected items cannot be selected.

The query result window displays separate statistics on the full data set list and the currently filtered data set list.

All Sets	All Points	All Ref's	All Sys.	Sets	Points	Ref's	Systems
359	4466	152	106	222	2497	99	91

### 9.1 Filter Items

Each filter item row can contain the following fields:

- a checkbox to enable, disable or exclude the item (see below)
- the key (e.g. containing the reference or component number)
- an input field for the minimum and maximum value (see *Range Filter*)
- the number of data sets
- further information (e.g. the reference text or the component name)

Enable a filter item (with a left-click on the checkbox) to include only those data sets matching the selected filter. The corresponding category will be enabled automatically (if required). Usually it is possible to select multiple filter items. With a left-click inside a row (not the checkbox) the clicked item is exclusively selected (all other items will be unselected automatically). Use the down resp. up key to have the next resp. previous item exclusively selected.

It is also possible to *exclude* a filter item with a *right-click* on the checkbox. Now all data sets meeting the item condition will be excluded, no matter if they meet any other condition. If no other filter item is selected, then all other items will be selected automatically. Excluded items have a different checkbox state than included items.

The filter items can be sorted with a left-click on the column header. This does also apply to the checkbox column.

The filter items can be copied to the clipboard. For references and components, the list can be saved to a file.

### 9.2 Range Filter

If available for the specific data type, it is possible to filter the data by a given temperature and/or pressure range. For binary VLE also a range for component concentration values can be specified.

Enter the minimum and maximum value in the according item field to change the allowed range. If only one value is given, the minimum = maximum is assumed. The filter is applied to every data point. Therefore, a filtered data set may have less data points than the original data set.










Use the *Add* button to specify more than one temperature or pressure range.

If neither data set matches the range filter(s), then the data set grid will be empty.



## 10 Single Data Set Display

The tool bar functions are

-  **“Save”**: Saves the window content as normal text.
-  **“Print”**: Prints the window content (shows the standard printer dialog).
-  **“Copy”**: Copies the window content to the Windows clipboard.
-  **“Plot”**: Plot the current data set (for details see chapter 21 “Plot”, page 82).
-  **“Predict”**: Predicts the current data set (for details see chapter 18 “Predict”, page 58).
-  **“Edit”**: Allows modifying the currently shown data set (temporarily).
-  **“Options”**: Calls the options dialog (details in other chapters).
-  **“Export”**: Creates a data point table
-  **“Reference”**: Display reference details

## 11 Data Set Display Options

### 11.1 Display Additional Information

The DDB retrieval program allows adding some calculated values to the data tables with experimental data sets.

Figure 24: Data Set Display Options

These options are

1. **Display excess cP values from cP data sets.**

If pure component heat capacities are available it is possible to display the excess heat capacities as well.

cp [J/mol*K]	cpIdeal [J/mol*K]	cpE [J/mol*K]	x1 [mol/mol]
75.2000	75.2000	0.0000	0.000000
79.5000	75.9300	3.5700	0.020166
83.0000	76.7074	6.2926	0.041640
86.6000	77.5368	9.0632	0.064553
90.8000	78.4238	12.3762	0.089055
93.7000	79.3745	14.3255	0.115317
95.8000	80.3960	15.4040	0.143535
97.8000	81.4965	16.3035	0.173937
99.3000	82.6857	16.6143	0.206787
102.1000	85.3764	16.7236	0.281115
104.5000	88.5834	15.9166	0.369708
107.1000	92.4713	14.6287	0.477107
111.4000	111.4000	0.0000	1.000000

2. **Always try to convert ESLE data sets for plots**

The ESLE data bank contains data in the originally published unit. For being able to combine data sets with different units, many ESLE data sets can be converted to a standard form. If this option is not set, all data sets are shown in the original units and in different windows.

### 3. GLE Data Bank Options

The GLE database contains data sets in many different forms and units. These options allow these multiple formats to convert into two standard forms.

1. "Display converted GLE to T-Henry data."
2. "Display converted GLE to TPxy data."

Ptot [kPa]	x gas *10 <sup>4</sup> [mol/10kmol]	recalc. Henry [kPa]	recalc. P [kPa]	recalc. xgas [mol/mol]
33,104	50,8900	4970,088	33,104	0,005089
56,995	100,3000	4907,572	56,995	0,010030
77,300	143,4000	4850,892	77,300	0,014340
100,698	194,1000	4791,328	100,698	0,019410

### 4. VE Data Bank Options

1. "Display converted densities from excess volume data sets"  
Densities will be calculated from excess volume data sets. Pure component densities are additionally needed and taken from the ParameterDDB.
2. "Display converted excess volumes from density data sets"  
If a density data set contains pure component densities then the program calculates the excess density/volume.

### 5. VLE/HPV Data Bank Options

1. "Display relative volatility in VLE/HPV data sets."

$$Rel. Vol. = \frac{y_1/x_1}{y_2/x_2}$$

As the equation shows relative volatilities can only be calculated for binary systems.

2. "Display K factors"

$$K = \frac{y}{x}$$

K factors displayed for every component if vapor and liquid composition are given.

T [K]	x1 [mol/mol]	y1 [mol/mol]	Rel.Vol. [-]	K-factor1 [-]	K-factor2 [-]
349.75	0.006300	0.048000	7.9528	7.6190	0.9580
348.25	0.012500	0.098800	8.6609	7.9040	0.9126
346.85	0.018900	0.153000	9.3769	8.0952	0.8633

3. "Display Activity Coefficients"  
Additional columns with activity coefficients are displayed. This is only possible for complete data sets containing pressure, temperature, vapor and liquid compositions. The program uses the simplified equation:

$$x_i \gamma_i P_i^s = y_i P$$

For some systems with associating carboxylic acids chemical theory is applied.

## 6. VLE/HPV/SLE Data Bank Options

### 1. Display Complete Mole Fractions

The databases normally only contain mole fractions for n-1 components. For a binary system only a single mole fraction is stored and displayed. This option allows displaying the mole fraction of all components.

## 7. PCP Data Bank Options

### 1. Display Molar Densities

This option allows displaying the molar density together with the specific density (which is the standard in the pure component properties data bank).

P [kPa]	DEN [kg/m <sup>3</sup> ]	DEM [mol/l]
4910.000	588.200	7.936
9810.000	598.000	8.068
19620.000	611.300	8.247

## 8. PCP/POW Data Bank Options

### 1. Display Structure in Single Set Display

This option allows appending the molecular structure of the component to the single set display.

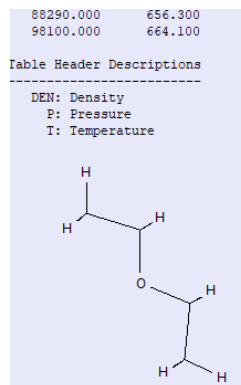


Figure 25: Structure appended to Single Set Display

## 9. VIS Data Bank Option

### 1. Display converted viscosity deviations from viscosities

The deviations (sometimes called excess viscosities) can be calculated if pure component viscosities are available

## 10. LLE Data Bank Options

### 1. Display K Factors

$$K = \frac{x_r}{x_l}$$

The K factors show the distribution of single components in the two liquid phases. Values can only be calculated for tie lines.

### 2. Sort Point by T

This option improves the readability of some sets.

## 11.2 Query Result Options

The query result display can be changed by two different options.

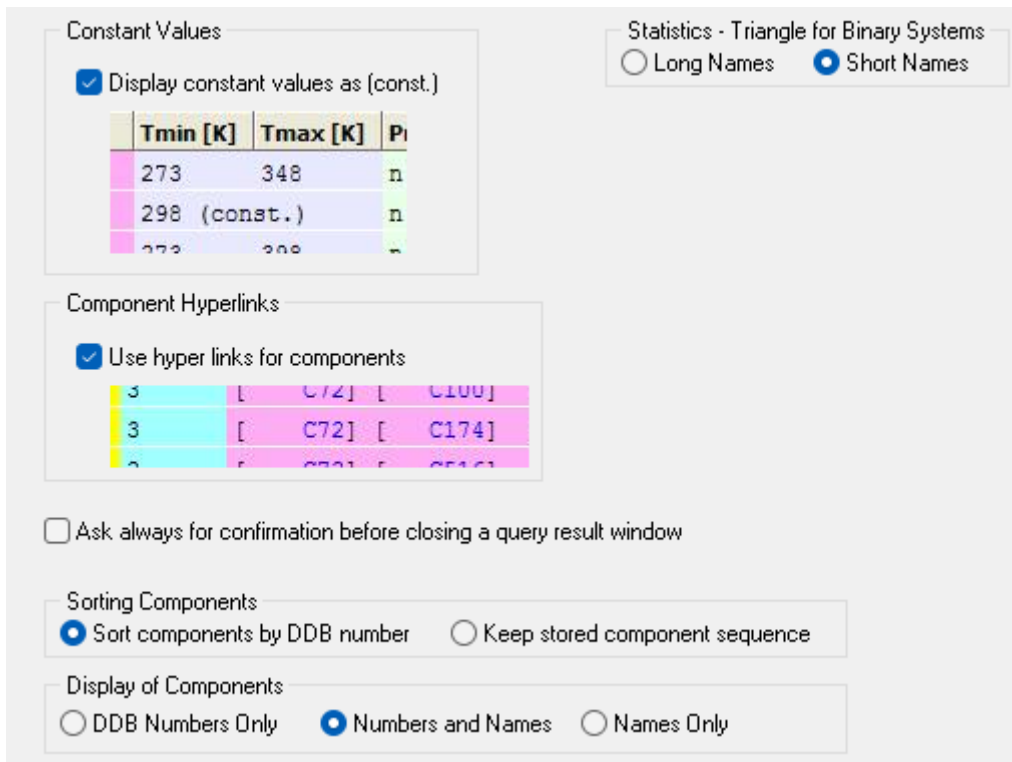


Figure 26: Query Result Display Options

### 1. Display of constant temperatures and pressures

Normally constant temperatures and pressures are displayed as e. g. “274 (const.)” in a single grid cell and ranges are display as “274 313”. This option allows to show constant values like range values.

Tmin [K]	Tmax [K]	Pi	Tmin [K]	Tmax [K]	Pi
273	348	n	273	348	n
298 (const.)		n	298	298	n
273	348	n	273	348	n

### 2. Display of hyperlinks for components

The grid is able to display hyperlinks for the components which makes it easier to call the component details dialog.

3	[ C72 ]	[ C100 ]	2	C91	C125	37
3	[ C72 ]	[ C174 ]	2	C74	C125	35
2	C82	C84	2	C125	C84	30

### 3. “Ask always for confirmation before closing a query result window”

Setting this option will let a confirmation dialog pop up every time a query result windows is closed.

### 4. Sorting Components

The components can either be sorted by ascending DDB numbers or displayed as they are stored in the data sets.

### 5. Display of Components

There are three options available. The “DDB numbers only” option delivers the most compact display and all component numbers are shown in a single row. Both other options will display the components in their own lines.

## 6. Statistics – Triangle for Binary System

This switches between the output of full component names and the usage of short names which are of the type “C” + DDB number like “C234”.

#DDB
[ C12] [ C73]
[ C12] [ C73]
[ C12] [ C73]

Figure 27: DDB Number Only

#DDB
[Diethyl ether] [Dimethoxymethane]
[Diethyl ether] [Dimethoxymethane]
[Diethyl ether] [Dimethoxymethane]

Figure 28: Names Only

#DDB
[ C12 Diethyl ether] [ C73 Dimethoxymethane]
[ C12 Diethyl ether] [ C73 Dimethoxymethane]
[ C12 Diethyl ether] [ C73 Dimethoxymethane]

Figure 29: Numbers and Names

## 12 Compact Data Display

The compact display (Show List in context menu or tool bar) can be used to get a compact overview on a list of data sets. The displays are only showing some descriptive information – like components, references, data set count, and value ranges. An exception is the output for pure component properties, see below.

A typical output for VLE is

VLE - Vapor-Liquid Equilibrium Data								
(1) C11	C2H6O	Ethanol						
(2) C12	C4H10O	Diethyl ether						
References:								
1 [475] Gordon A.R., Hornibrook E.J., Can.J.Res.Sec.B, 24, 263-267, 1946								
2 [476] Kireev V.A., Khachadurova E.M., Zh.Prikl.Khim., 7(4), 495-496, 1934								
3 [866] Moeller W.P., Englund S.W., Tsui T.K., Othmer D.F., Ind.Eng.Chem., 43(3), 711-717, 1951								
4 [3229] Borisova I.A., Erlykina M.E., Sokolov N.M., Mikhailov V.A., Zakharov D.L., Gorbunov A.I., Onitekhim, Code 308 KHP - D82, 1-12, 1982								
5 [4581] Wüllner A., Ann.Physik, 205(11), 353-366, 1866								
no.	type	values	T(min) [K]	T(max) [K]	P(min) [kPa]	P(max) [kPa]	ref	data set
1	Txy(P)	10	342.15	377.65	287.48	287.48	3	175 0 0 VLEDDB
2	Txy(P)	10	378.15	400.15	721.85	721.85	3	176 0 0 VLEDDB
3	Txy(P)	10	363.15	382.55	515.01	515.01	3	177 0 0 VLEDDB
4	Txy(P)	8	391.35	417.95	963.17	963.17	3	178 0 0 VLEDDB
5	Pxy(T)	19	298.15	298.15	8.80	69.62	1	636 0 0 VLEDDB
6	Txy(P)	29	308.85	351.25	101.32	101.32	2	637 0 0 VLEDDB
7	Txy(P)	20	307.90	350.79	101.32	101.32	4	11357 0 0 VLEDDB
8	PTx(x)	8	280.35	298.65	24.40	52.36	5	20637 0 0 VLEDDB
9	PTx(x)	10	280.35	304.55	28.66	75.71	5	20638 0 0 VLEDDB
10	PTx(x)	10	280.35	307.75	30.88	90.03	5	20639 0 0 VLEDDB

The compact output is composed of three main parts.

1. System or component
2. List of references where data of this system or component has been entered
3. List of data sets with some descriptive entries.

The compact data set display is, of course, quite different for the different data banks but these three parts can be always found.

The output for pure component properties is an exception, as mentioned, because it does contain all available data points in a single table and so contains significantly more information than the compact views for the different mixture properties.

PCP - Pure Component Properties					
Component:					
( 1)	134 C5H12	Pentane			
Property:					
[ 1]	Dynamic Viscosity				
References:					
1 (31441) Rastorguev Yu.L., Grigorev B.A., Prisyazhnyuk S.I., Keramidi A.S., Onitekhim, Code 919 KHP - 87, 1-24, 1987					
2 (31442) Grigorev B.A., Keramidi A.S., Prisyazhnyuk S.I., Onitekhim, Code 217 KHP - 89, 1-25, 1989					
T	P	VIS	State	Prop:	Ref:
K	kPa	mPas			
146.15	100.000	3.2300	L	1	[31441]
148.15	100.000	3.0210	L	1	[31441]
148.15	9910.000	3.4720	L	1	[31441]
148.15	19720.000	3.9070	L	1	[31441]
148.15	24630.000	4.1900	L	1	[31441]
154.15	100.000	2.3630	L	1	[31441]
154.15	9910.000	2.6370	L	1	[31441]
154.15	19720.000	2.9330	L	1	[31441]
154.15	29530.000	3.2710	L	1	[31441]
154.15	39340.000	3.6630	L	1	[31441]
154.15	49150.000	4.1170	L	1	[31441]
154.15	58960.000	4.6590	L	1	[31441]
173.15		1.2510	L	1	[31441]
173.15	100.000	1.2620	L	1	[31441]
173.15	9910.000	1.3980	L	1	[31441]
173.15	19720.000	1.5540	L	1	[31441]
173.15	29530.000	1.7740	L	1	[31441]
648.15	2086.000	0.01505	G	1	[31442]
648.15	3062.000	0.01539	G	1	[31442]
648.15	4042.000	0.01596	G	1	[31442]

(stripped some lines)

## 13 Units

### 13.1 Mixture Data Banks – Compositions

Compositions can be displayed in original units, mole based (mole fraction or mole percent) or mass based (mass fraction or mass percent).

It is also possible to display both mole and mass fractions. This option does not add columns – it shows a second table.

### 13.2 Mixture Data Banks – Properties

Only for the properties temperature, pressure, enthalpy (heats of mixing), heat capacity, density, volume, excess volumes, and viscosity it is possible to change the display and plot unit. The “Disable Conversion” check box allows showing the DDB data sets in original database specific units.

The temperature and pressure units are also used in the query result.

### 13.3 Pure Component Properties

Every property in the pure component properties database has a list of units. The “Precision” column allows specifying the number of digits behind the decimal separator.

The *Standard* button resets all setting to DDB standard settings.



## 14 Consistency Tests

Consistency tests are checking VLE data sets for thermodynamic correctness. For vapor-liquid equilibria data sets two consistency tests are available.

### 14.1 Point-to-Point Test

The first consistency test offered is the so-called “point-to-point test of “van Ness et al.”<sup>1</sup> in the version of “Fredenslund et al.”<sup>2</sup>.

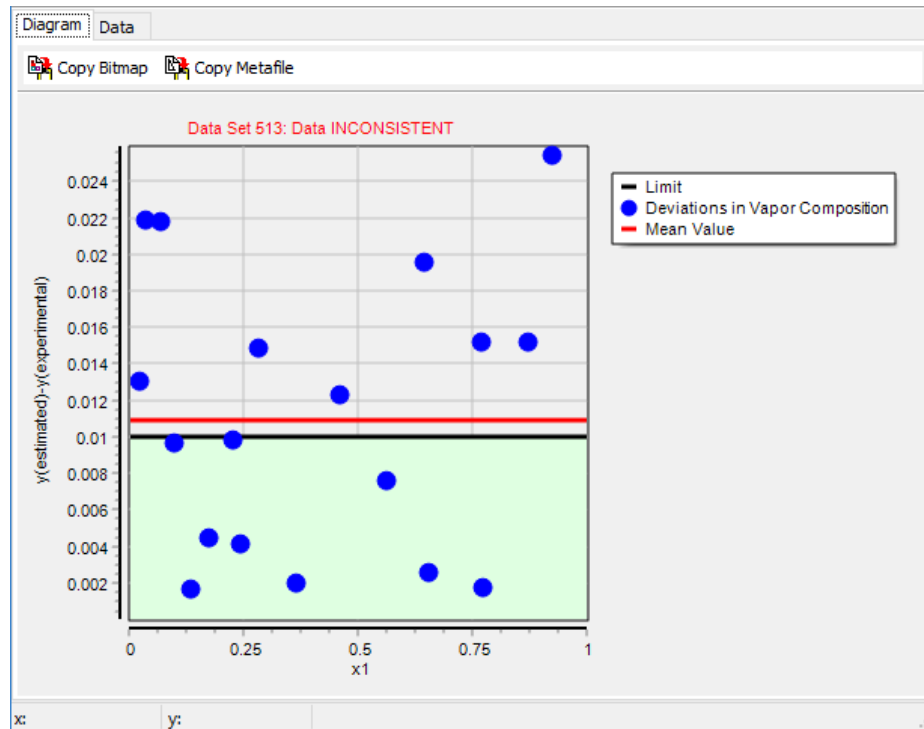


Figure 30: Point-to-Point Consistency Test

The method applied in this program uses a flexible expression for the excess Gibbs energy for fitting experimental  $x$ ,  $P$ ,  $T$ -data. With the aid of the fitted parameters the vapor composition  $y$  for each experimental point ( $x$ ,  $P$ ,  $T$ ) in a data set is calculated and compared with the experimental value. If the mean deviation between experimental and calculated  $y$ -values is smaller than  $0.01 \text{ mol/mol}$ , the data set is considered to be consistent.

<sup>1</sup> van Ness H.C., Byer S.M., Gibbs R.E., *AIChE J.* 19, 238 (1973)

<sup>2</sup> Fredenslund A., Gmehling J., Rasmussen P., *Vapor-Liquid Equilibria Using UNIFAC, A Group Contribution Method*, Elsevier, Amsterdam 1977

## 14.2 Area Test

The second consistency test is the so-called integral or area test using the method of Redlich-Kister<sup>3</sup> and Herington<sup>45</sup>. In this test for each experimental point the logarithm of the ratio of the activity coefficients is calculated. These values are then fitted by a third-order polynomial and the areas above and below the abscissa are determined by integration of the polynomial. The resulting area deviation is evaluated in various ways.

### 14.2.1 Isothermal data

If A and B denote the areas above and below the abscissa, then the deviation D is given by:

$$D = | ( A - B ) / ( A + B ) * 100 | [ \% ]$$

If D is smaller than 10%, the data are considered to be consistent.

### 14.2.2 Isobaric data

For this type of data, the influence of the excess enthalpy on the Gibbs-Duhem equation must be taken into account. In this program, this is done by an empirical parameter, which was introduced by Herington.

For nearly ideal systems this test is not applied, as areas above and below the abscissa become very small and their relative deviation can become very large due to small experimental errors.

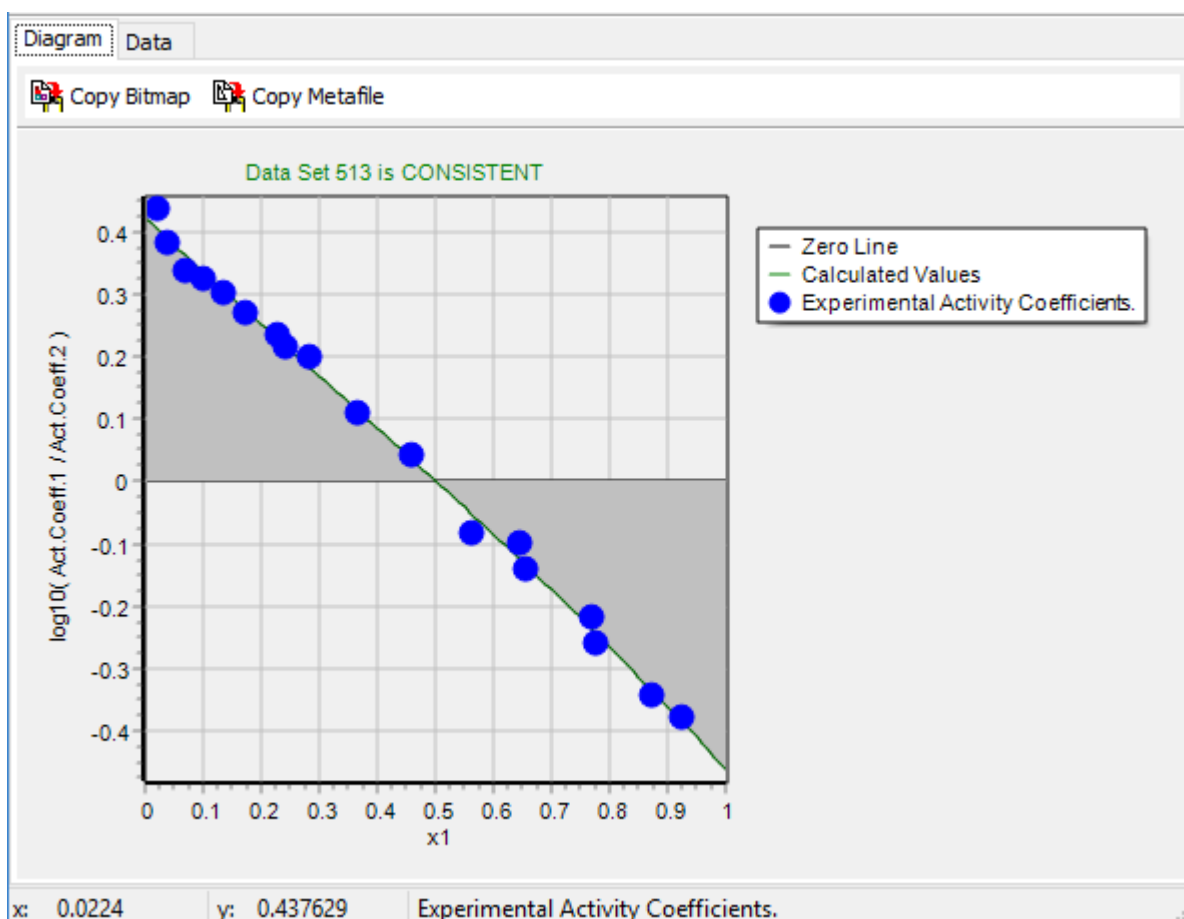


Figure 31: Area Test

<sup>3</sup> Redlich O., Kister A.T., Ind. Eng. Chem. 40, 345 (1948)

<sup>4</sup> Herington E.F.G., Nature 160, 610 (1947)

<sup>5</sup> Herington E.F.G., J. Inst. Petrol. 37, 457 (1951)

### 14.3 Automatic Tests

<p>“Automatic Tests” starts the consistency tests for all marked sets in the background and displays their results in the “Comment” column of the data set grid.</p> <p>“-” denotes an inconsistent data set.</p> <p>“+” denotes a consistent set.</p> <p>“?” denotes consistency test failure.</p> <p>“*” shows that the consistency test hasn't been performed.</p>	Comment
	{--} T <sub>X</sub> Y (P)
	{-?} T <sub>X</sub> Y (P)
	{--} T <sub>X</sub> Y (P)
	{-?} T <sub>X</sub> Y (P)
	{+-} P <sub>X</sub> Y (T)
	{--} T <sub>X</sub> Y (P)
{++} P <sub>X</sub> Y (T)	
{++} P <sub>X</sub> Y (T)	

### 14.4 Othmer-Tobias and Hand Correlations

These correlations are used to check the consistency of the tie lines in ternary LLE data. Both correlations yield a straight line if the data are consistent.

#### 14.4.1 Othmer-Tobias Tie Line Correlation

Othmer and Tobias<sup>6</sup> published a correlation which can be used to check tie lines in ternary mixture with two immiscible components and a single co-solvent for their consistency.

##### 14.4.1.1 Equation

The equation is

$$\log \frac{1-a_1}{a_1} = n \log \frac{1-b_2}{b_2} + S$$

with

Index 1: Aqueous phase (typically)

Index 2: Organic phase (typically)

a<sub>1</sub>: Weight fraction of solvent “a” in the solvent “a” rich phase (typically Water)

b<sub>2</sub>: Weight fraction of solvent “b” in the solvent “b” rich phase (typically an organic compound)

n: Slope

S: Constant

<sup>6</sup> Othmer D.F., Tobias P.E., "Tie Line Correlation ", Indian Chem.Eng., 34, 693-696, 1942

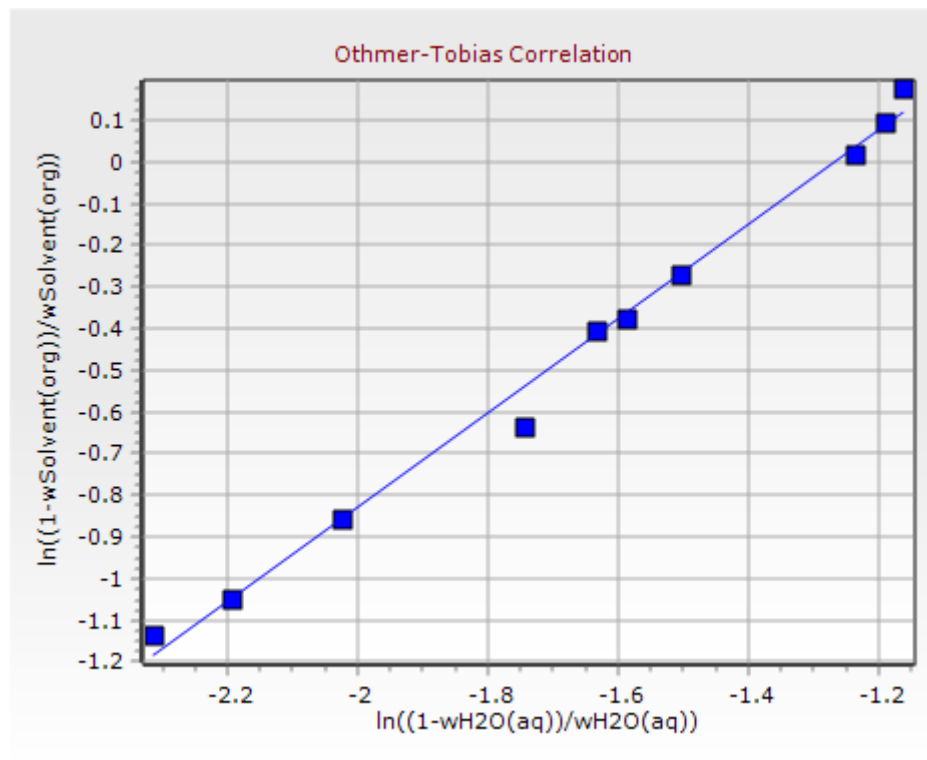


Figure 32: Othmer-Tobias Correlation

#### 14.4.2 Hand Tie Line Correlation

Hand<sup>7</sup> published a correlation which can be used to check tie lines in ternary mixture with two immiscible components and a single co-solvent for their consistency.

##### 14.4.2.1 Equation

The equation is

$$\log \frac{c_2}{b_2} = n \log \frac{c_1}{a_1} + S$$

with

Index 1: Aqueous phase (typically)

Index 2: Organic phase (typically)

$c_2$ : Weight fraction of third component in solvent "b" rich phase

$b_2$ : Weight fraction of solvent "b" in the solvent "b" rich phase (typically an organic compound)

$c_1$ : Weight fraction of third component in solvent "a" rich phase

$a_1$ : Weight fraction of solvent "a" in the solvent "a" rich phase (typically water)

$n$ : Slope

$S$ : Constant

<sup>7</sup> Hand D.B., "Dimeric Distribution. I. The Distribution of a Consolute Liquid Between Two Immiscible Liquids", J.Phys.Chem., 34, 1961-2000, 1930

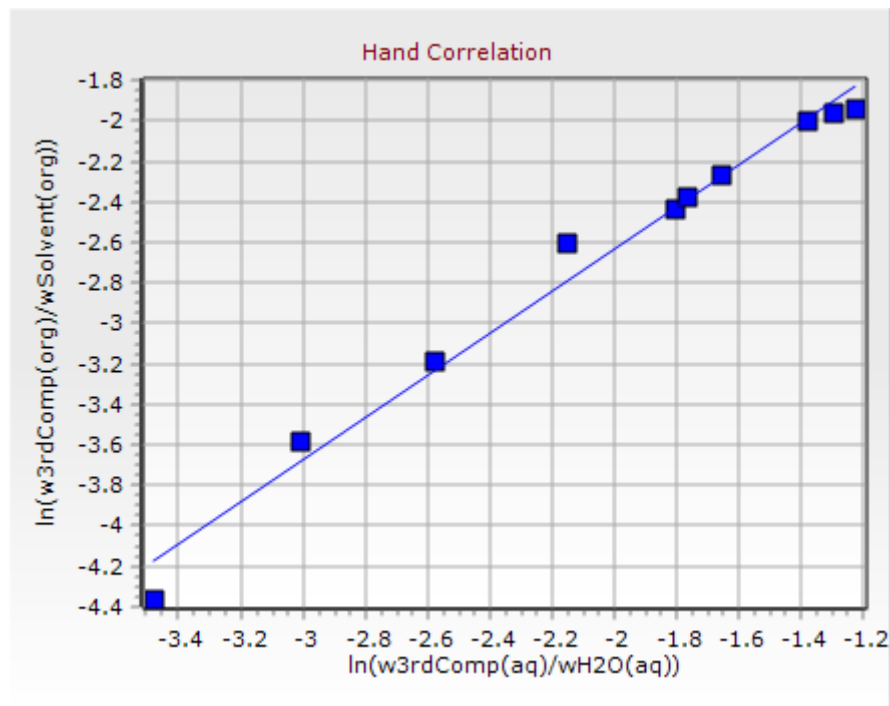


Figure 33: Hand Correlation

#### 14.4.2.2 Example Data

LLE data set no. 1367 has an aqueous phase with small amounts of Benzene and an organic phase rich of Benzene and small amount of Water. The third component (co-solvent) is acetic acid.

	W't Fract. (Aq.) Water	W't Fract. (Aq.) Acetic Acid	W't Fract. (Aq.) Benzene	W't Fract. (Org.) Water	W't Fract. (Org.) Acetic Acid	W't Fract. (Org.) Benzene
Equation Terms	$a_1$	$c_1$	$b_1$	$a_2$	$c_2$	$b_2$
	0.95401	0.04562	0.00038	0.00001	0.00150	0.99849
	0.82101	0.17702	0.00197	0.00040	0.01400	0.98560
	0.70600	0.29000	0.00399	0.00110	0.03270	0.96620
	0.39799	0.56900	0.03301	0.00400	0.13302	0.86298
	0.36799	0.59200	0.04001	0.00500	0.15002	0.84498
	0.29599	0.63901	0.06500	0.00700	0.19902	0.79398
	0.27500	0.64801	0.07699	0.00850	0.22802	0.76348
	0.16100	0.65802	0.18098	0.01900	0.31003	0.67097
	0.14400	0.64502	0.21099	0.02500	0.35303	0.62197
	0.13200	0.63401	0.23399	0.03000	0.37803	0.59197
	0.10700	0.59303	0.29997	0.04600	0.44703	0.50697

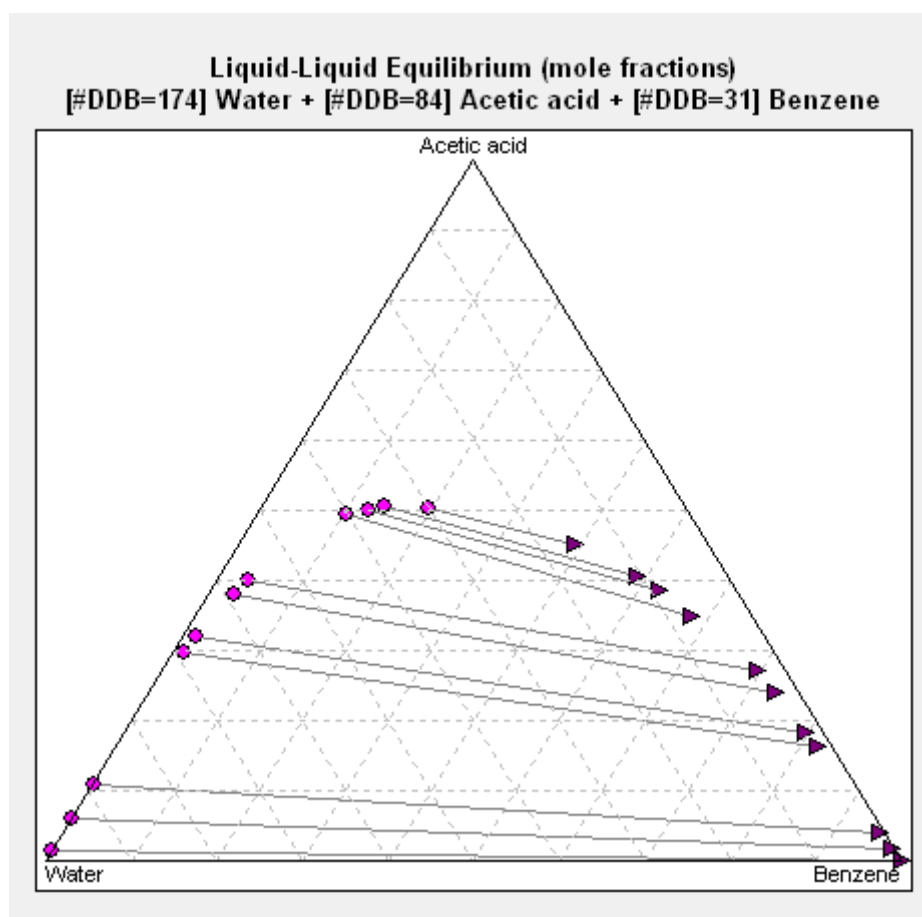


Figure 34: LLE Data Set No. 1367

## 15 Modifying and Editing Data Sets

### 15.1 Editing Experimental Data

A detailed description of the pure component properties and the mixture properties editors can be found in other documentation documents.

Modifications of data sets from the main retrieval program are not changing database content. It only allows the currently loaded data set to edit. The changes are lost if a query result window is closed because all data sets are removed from memory.

It is possible to edit data sets via an OLE call to the standard editors DDB Edit Pure Data resp. DDB Edit Mixture Data. These programs work in a special mode allowing temporary changes.

For people knowing the free formatted file format it is also possible to use an internal or external text editor. The external editor has to be configured in the *DDB Configuration* program.

### 15.2 Specifying Quality

The qualities settings are used to comment on special weaknesses. The type of comment is rather widespread since further tests are mentioned, changes, sources, problems with the references and so on.

These should not be changed by customers. They are additional information provided by DDBST on data sets. Customers can use the comments but normally they don't fit well on a new problem.

### 15.3 Change LEAR Number

This function allows changing the reference to the reference for all marked sets.

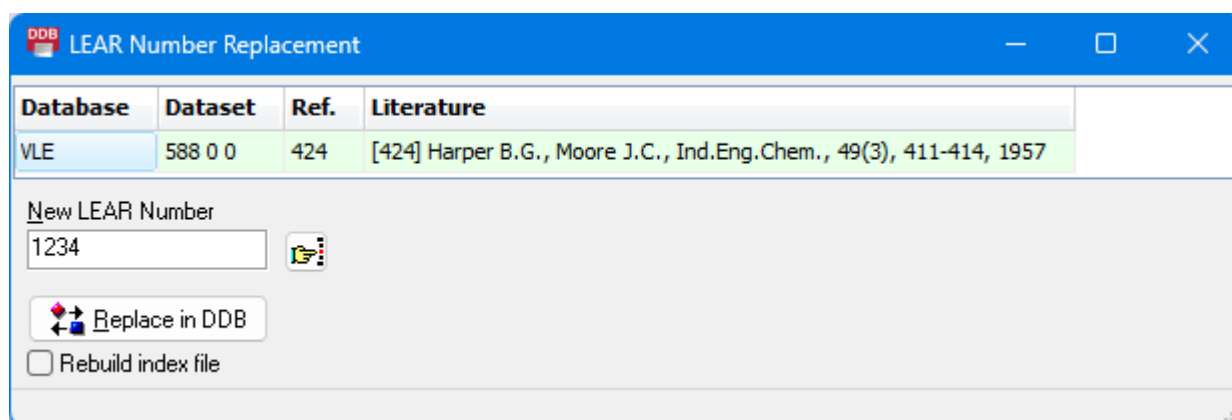


Figure 35: Changing Literature Number

The dialog lists all marked data sets together with the references which will be exchanged. The “Rebuild index file” option allows updating the data bank index. Otherwise the index has to be updated separately later.

## 15.4 Edit Comment

This command allows specifying comments for single sets.

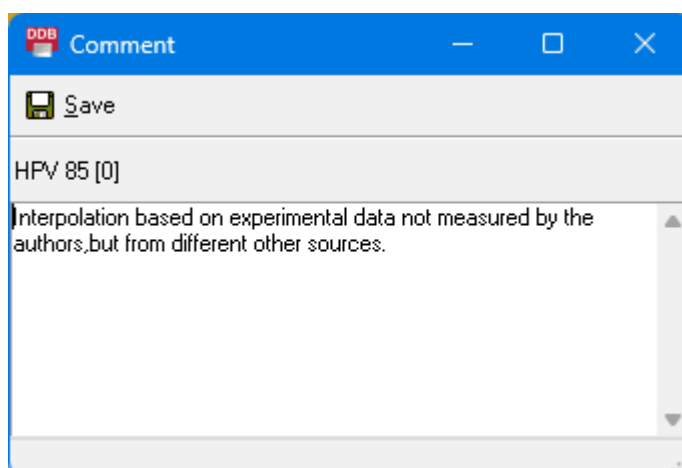


Figure 36: Comment Dialog

## 15.5 Append Comment

This command allows a single comment to enter for all selected data sets. Existing comments are not overwritten – the new comment is appended. These comment are displayed in the single-set display and, sometimes, in diagrams.

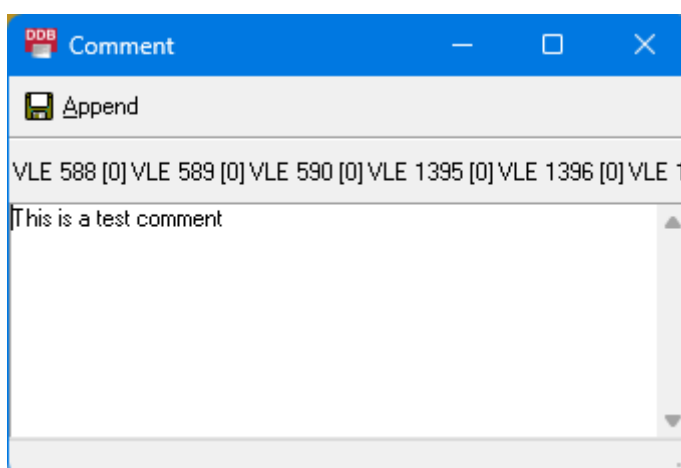


Figure 37: Append Comment Dialog (Multiple Sets)

## 15.6 Change Component Order

Changing the component order is useful if data sets for the same systems are stored (published) in different orders making it difficult to compare the tables. The same is true for comparing diagrams with different component sequences.

To change the sequence the button “Up” and “Down” can be used but it is also possible to drag and drop the components with the mouse.

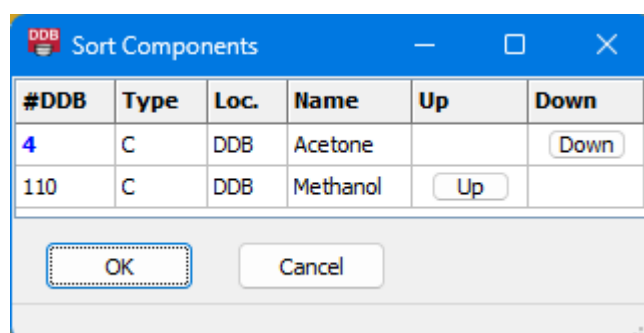


Figure 38: Change Component Order



## 15.7 Add/Modify Extended References

This is a function mainly intended for internal use at DDBST. It allows multiple references to specify to a single data set. This is normal only useful for sets published in different publication like, e.g., scientific papers and GPA reports.

## 15.8 Convert GLE Data Sets to HPV Data Sets

Many gas-solubility data sets are containing TPxy data or can be converted to this form. This function allows convertible GLE data sets to add to the HPV data bank page. This does not change any data banks, neither GLE nor HPV. It only copies data sets inside the query result list. The sense of this function to be able to use GLE data sets for plotting and fitting as vapor-liquid equilibrium data.

## 15.9 Convert VLE/HPV TPxy to Pxy(T) Data Sets and Txy(P) Data Sets

VLE/HPV “TPxy” data sets are data sets without any constant value. Since most DDB programs need at least a constant pressure or a constant temperature this function allows you to convert these data sets to single point data sets. This makes the data sets accessible and usable mainly for the DDB fitting programs.

## 15.10 Create $g^E$ Model Interaction Parameters

This function allows the calculation of Wilson and UNIQUAC parameters directly from activity coefficients at infinite dilution.

11 Ethanol 174 Water	
11 solved in 174	174 solved in 11
<input type="radio"/> 3.18000 at T=283.15	<input type="radio"/> 3.28000 at T=298.15
<input type="radio"/> 4.38000 at T=283.15	<input checked="" type="radio"/> 2.90000 at T=373.15
<input type="radio"/> 4.81000 at T=293.15	<input type="radio"/> 2.50000 at T=324.86
<input type="radio"/> 6.51000 at T=293.15	<input type="radio"/> 2.47000 at T=331.05
<input checked="" type="radio"/> 4.74000 at T=297.45	<input type="radio"/> 2.47000 at T=336.03
<input type="radio"/> 3.27000 at T=298.15	<input type="radio"/> 2.52000 at T=342.15

**Wilson**

Δ<sub>12</sub>= -109.5565 cal/mol  
 Δ<sub>12</sub>= 1186.16 cal/mol

**UNIQUAC**

τ<sub>12</sub>= 479.707 cal/mol  
 τ<sub>12</sub>= -136.0501 cal/mol

Figure 39:  $g^E$  Model Parameters from Activity Coefficients at Infinite Dilution

The dialog shows all available limiting activity coefficients. If one data point for component 1 solved in component 2 and one data point for component 2 in component 1 is selected the parameters  $\Lambda_{12}/\Lambda_{21}$  for Wilson and  $\tau_{12}/\tau_{21}$  for UNIQUAC are calculated immediately. The selected coefficients should be measured at similar temperatures.

The parameters can be saved in the parameter data bank (ParameterDDB) or directly used to calculate activity coefficients and to show the result in a diagram.

## 15.11 Apelblat Correlation

The modified Apelblat equation for solid-liquid equilibria (SLE)

$$\ln x = A + \frac{B}{T} + C \ln T$$

is used to correlate solubilities expressed as change of mole fractions  $x$  with temperature. Enthalpies and entropies of dissolution can be calculated from its parameters.

$$\Delta H_{\text{Sol}} = R T \left( C - \frac{B}{T} \right)$$

$$\Delta S_{\text{sol}} = R \left( C - \frac{B}{T} \right)$$

The Apelblat equation can only be used for small solubilities. An example is the solubility of Norfloxacin in some alcohols, Water and Acetone. The program shows a table output

x [mol/mol]	T [K]	Delta(sol) H [kJ/mol]	Delta(sol) S [J/mol*K]	A	B	C	R
26521 [0]	Norfloxacin			Water			
0.000020	293.150	14.19	48.4	Apelblat Equation Parameters			
0.000023	298.150	16.85	56.5	-433.471	17095.88	64.1379	0.99991
0.000025	303.150	19.52	64.4				
0.000029	308.150	22.18	72.0				
0.000034	313.150	24.85	79.4				
0.000039	318.150	27.52	86.5				
0.000047	323.150	30.18	93.4				
37472 [0]	Norfloxacin			1-Octanol			
0.000052	293.150	37.00	126.2	Apelblat Equation Parameters			

Figure 40: Apelblat Regression - Table Output

and a diagram with the regression results.

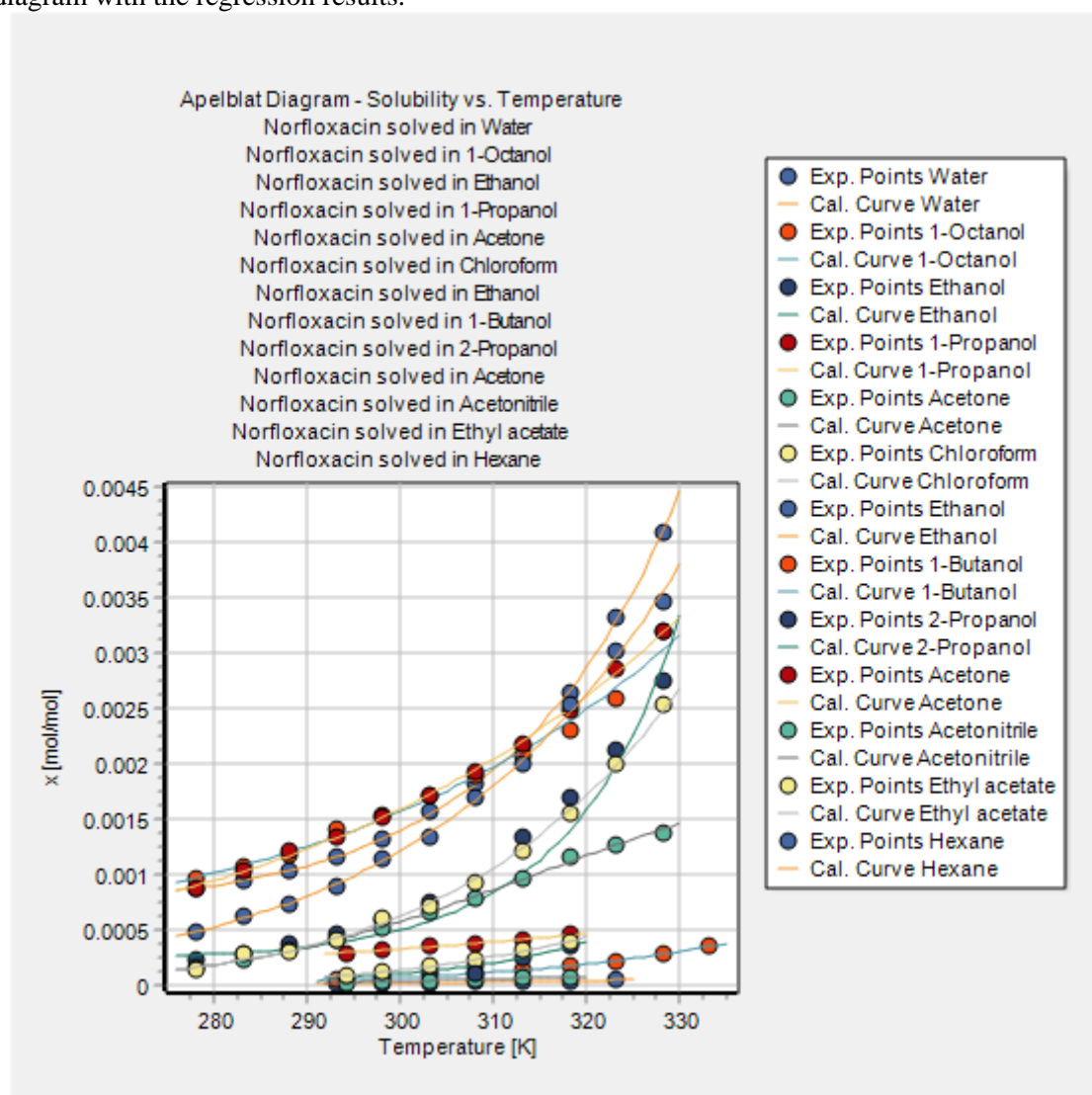
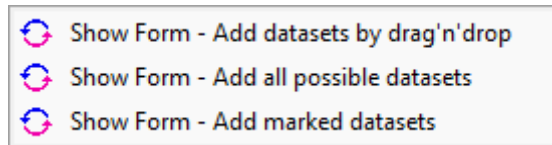


Figure 41: Apelblat Regression - Plot Output

## 16 Converting Data Sets to ELE Data Sets



This function can convert

- VLE and HPV (vapor-liquid equilibria),
- GLE and EGLE (gas solubilities)

data sets to ELE data sets. The ELEDDB contains vapor-liquid equilibrium data of electrolyte-containing mixtures. The different options in the menu allow collecting data sets from the source data types (vapor-liquid equilibria and gas solubilities) in a dialog and convert the collected sets in a batch.

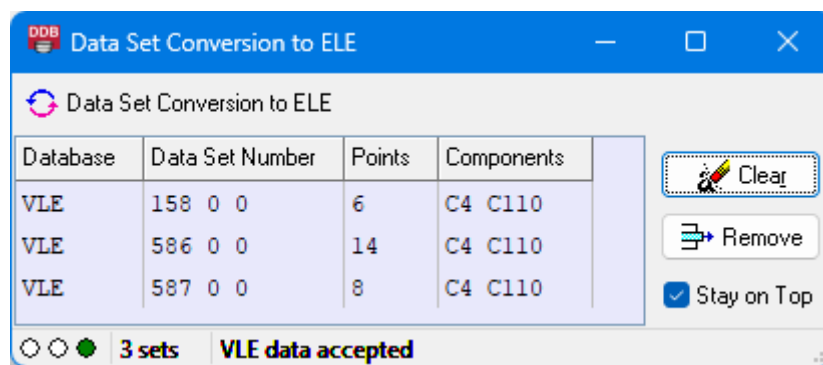


Figure 42: Data Set Conversion to ELE Format

The result is a list of ELE data sets which can be plotted together or used in the prediction mainly by the LIFAC model.

## 17 Query Result Statistics

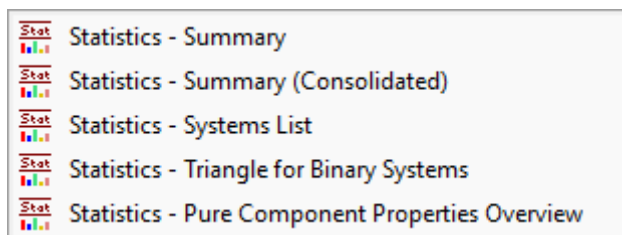


Figure 43: Statistics Sub Menus

### 17.1 Summary

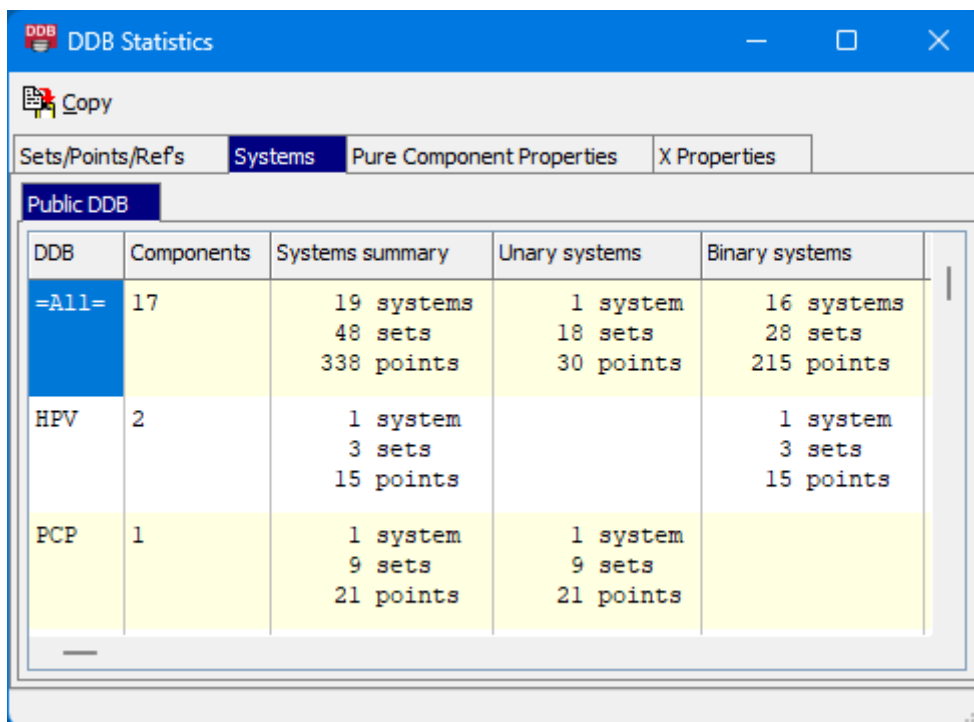
The “Statistics – Summary” for a query result grid shows approx. the same information as the statistics for the complete list of data banks.

#### 17.1.1 Number of sets/points/references for every database

Databank	Sets	Points	References	DDB Description
HPV	3	15	1	Vapor-liquid equilibria (normal boil
PCP	9	21	4	Pure component properties
POW	9	9	1	Octanol-Water partition coefficients
SLE	23	285	7	Solid-liquid equilibria (mainly orga
X	4	8	2	Different thermodynamic properties
Total	48	338	11	Consolidated

Figure 44: Data Bank Statistics

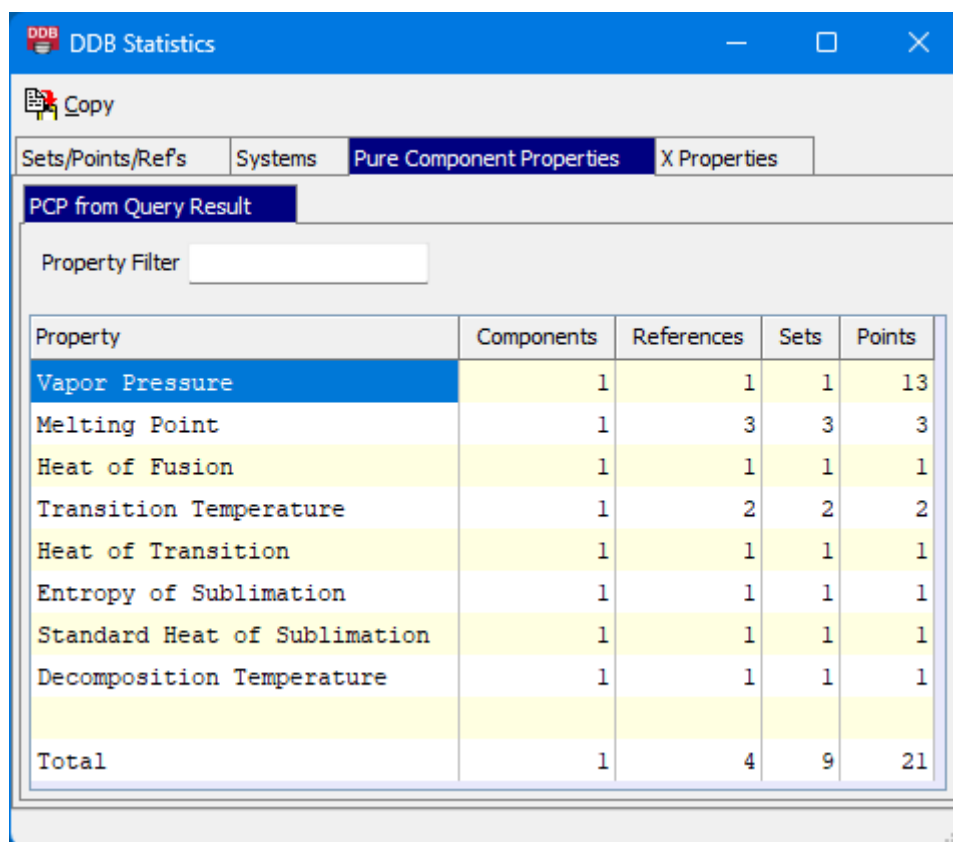
### 17.1.2 Overview over available systems



DDB	Components	Systems summary	Unary systems	Binary systems
=All=	17	19 systems 48 sets 338 points	1 system 18 sets 30 points	16 systems 28 sets 215 points
HPV	2	1 system 3 sets 15 points		1 system 3 sets 15 points
PCP	1	1 system 9 sets 21 points	1 system 9 sets 21 points	

Figure 45: Systems Statistics

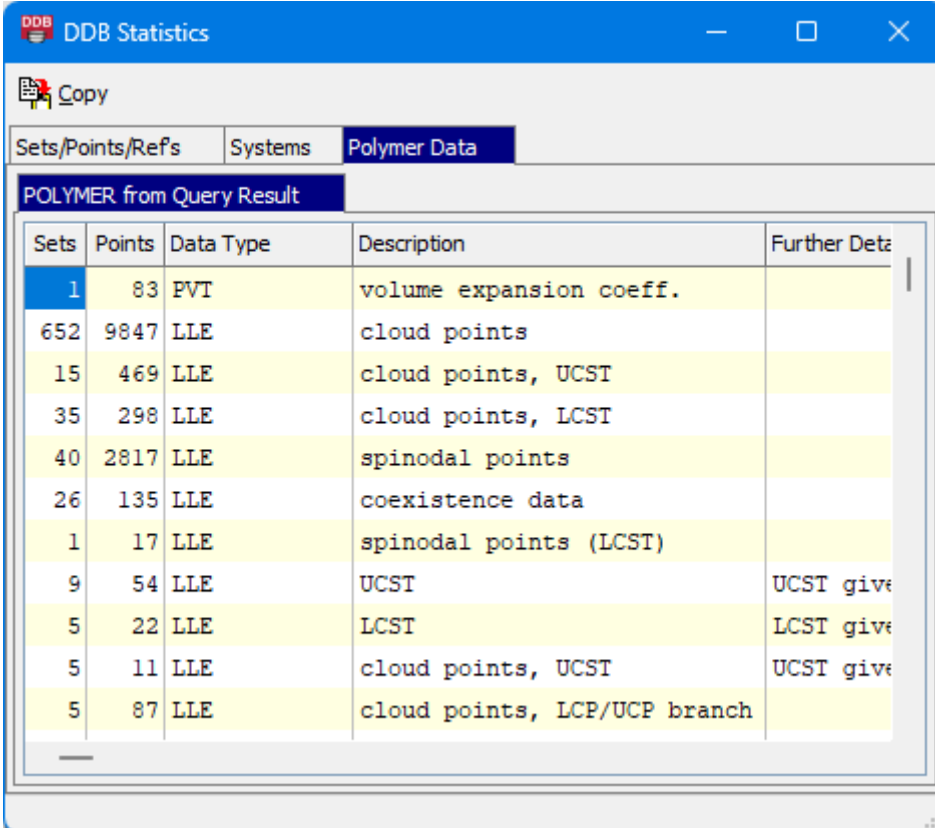
### 17.1.3 Details of pure component properties data



Property	Components	References	Sets	Points
Vapor Pressure	1	1	1	13
Melting Point	1	3	3	3
Heat of Fusion	1	1	1	1
Transition Temperature	1	2	2	2
Heat of Transition	1	1	1	1
Entropy of Sublimation	1	1	1	1
Standard Heat of Sublimation	1	1	1	1
Decomposition Temperature	1	1	1	1
Total	1	4	9	21

Figure 46: Pure Component Properties Statistics

### 17.1.4 Details of the polymer related data

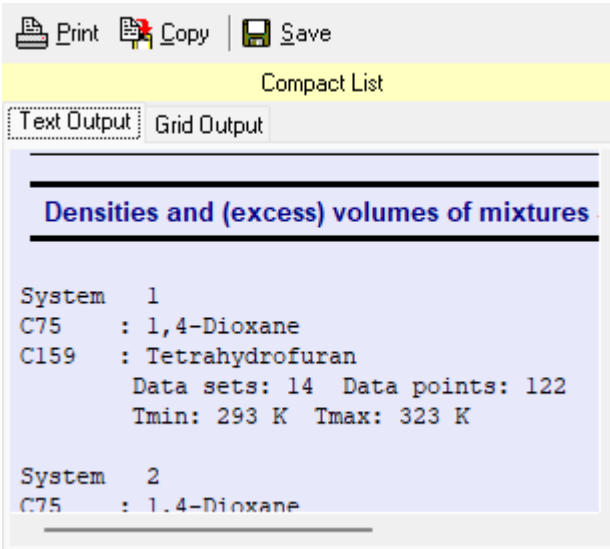


Sets	Points	Data Type	Description	Further Data
1	83	PVT	volume expansion coeff.	
652	9847	LLE	cloud points	
15	469	LLE	cloud points, UCST	
35	298	LLE	cloud points, LCST	
40	2817	LLE	spinodal points	
26	135	LLE	coexistence data	
1	17	LLE	spinodal points (LCST)	
9	54	LLE	UCST	UCST give
5	22	LLE	LCST	LCST give
5	11	LLE	cloud points, UCST	UCST give
5	87	LLE	cloud points, LCP/UCP branch	

Figure 47: Polymer Data Statistics

## 17.2 Systems List

The “Statistics – Systems List” is a list of all systems found in the data sets including the number of data sets and points and the temperature range.



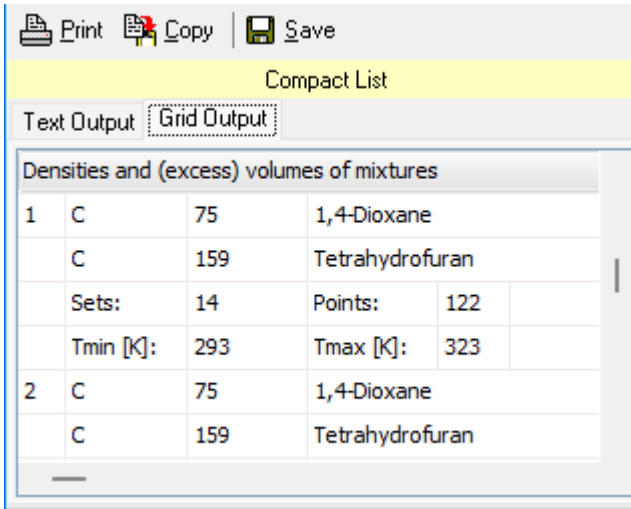
```

Densities and (excess) volumes of mixtures

System 1
C75 : 1,4-Dioxane
C159 : Tetrahydrofuran
Data sets: 14 Data points: 122
Tmin: 293 K Tmax: 323 K

System 2
C75 : 1,4-Dioxane
  
```

Figure 48: Systems List - Text Output



Densities and (excess) volumes of mixtures			
1	C	75	1,4-Dioxane
	C	159	Tetrahydrofuran
	Sets:	14	Points: 122
	Tmin [K]:	293	Tmax [K]: 323
2	C	75	1,4-Dioxane
	C	159	Tetrahydrofuran

Figure 49: Systems List - Table Output

### 17.3 Triangle for Binary Systems

This kind of display has been added to allow a quick view on how many binary systems are available for a given list of components.

The names in the binary triangle can short (in the form "C" plus DDB number, "C77" as an example) or the full component names can be used.

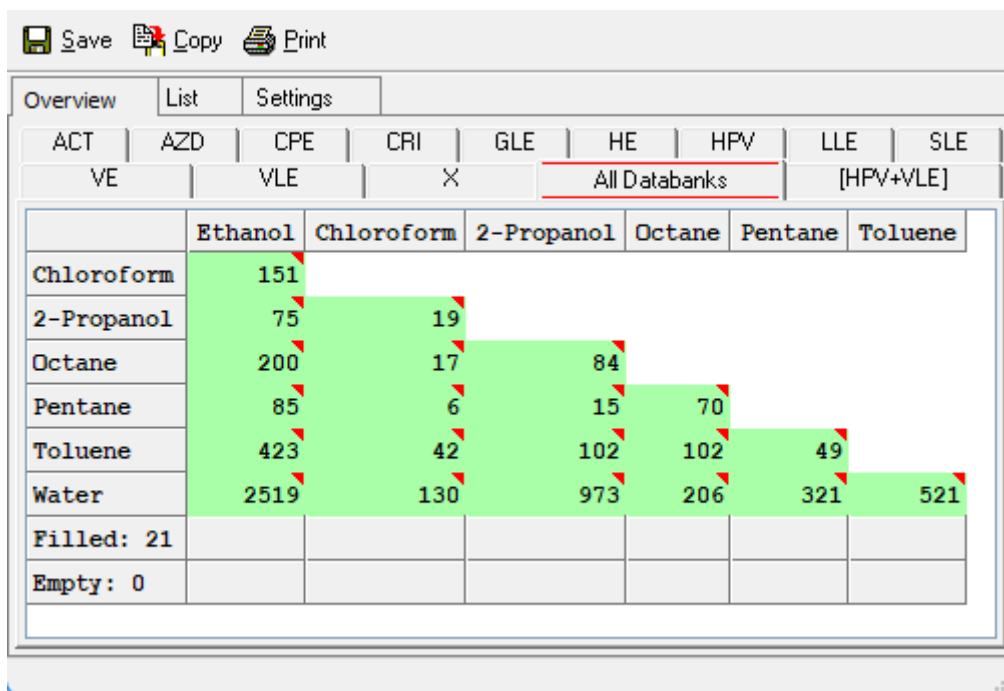


Figure 50: Triangle Diagram for Binary Systems

#### 17.3.1 List

"List" provides an overview of the number of binary systems in the respective databases.

#### 17.3.2 Settings

Besides showing the number of sets per binary system only, it is also possible to add the number of points and the temperature range to the triangle.

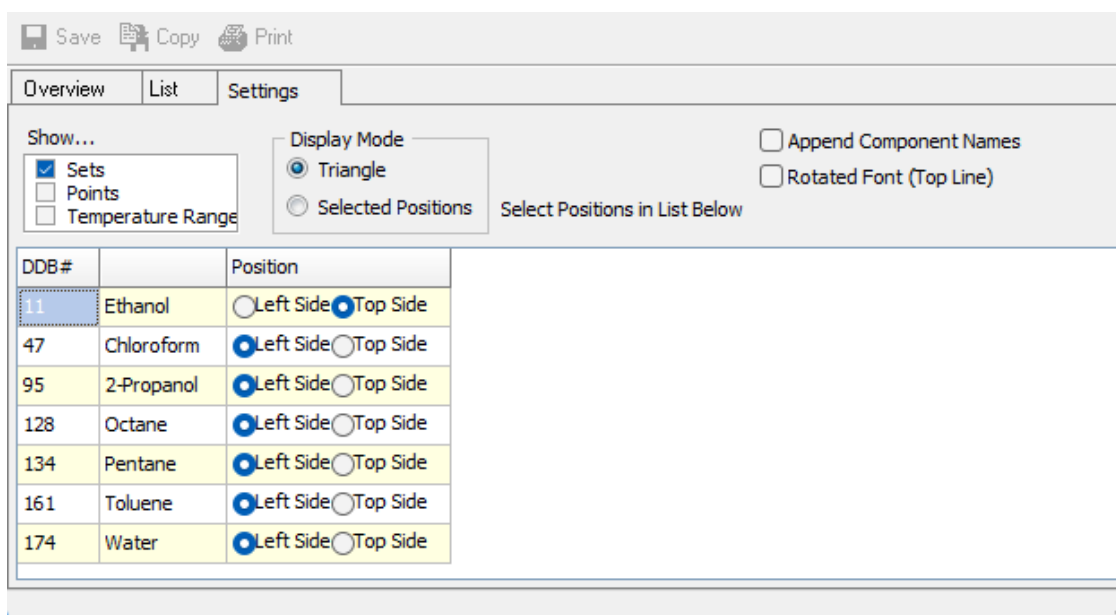


Figure 51: Triangle for Binary Systems - Settings

The “Display Mode” allows the triangle mode to switch and a tabular mode with freely selected positions of the components on top or left side.

	Norfloxacin
Acetonitrile	1
Acetone	2
Ethanol	2
Ethyl acetate	1
1-Butanol	1
Chloroform	1
N,N-Dimethylformamide (DMF)	1
Hexane	1
2-Propanol	1
1-Propanol	1
Water	3
1-Octanol	2
Carbon dioxide	3
Nicotinic acid	3
Polyethylene glycol 400	1
Metronidazole	4
Filled: 16	
Empty: 0	

Figure 52: Binary Systems - Tabular Display

“Append Component Names” determines whether a list of component names is appended or not and “Rotated Font” determines whether the upper component names are show rotated or not.

Component Name
Acetonitrile
Acetone
Ethanol
Ethyl acetate
1-Butanol
Chloroform

Figure 53: Rotated Component Names



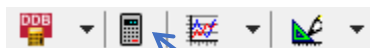
## 17.4 Pure Component Properties Overview

	Dynamic Viscosity	Vapor Pressure	Critical Data	Triple Point
98 Isoprene	1 set/s 9 point/s 273.50/305.17 K	59 set/s 176 point/s 215.55/373.11 K		
99 Methyl iodide	9 set/s 37 point/s 207.05/363.15 K	52 set/s 211 point/s 176.20/413.15 K	1 set/s 1 point/s 528.00/528.00 K	
100 1-Hexene	50 set/s 317 point/s 158.15/473.15 K	100 set/s 320 point/s 253.43/504.05 K	11 set/s 11 point/s 502.25/516.65 K	1 set 1 poi

Figure 54: Statistics - Pure Component Properties Overview

This function gives a quick overview over the available properties especially if data have been retrieved for multiple components.

## 18 Predict



Prediction routines are available for many data banks and data types. If started from the query result window using the *Predict* button, then the components and some data ranges are already set. Almost every prediction creates artificial data sets that are returned to the retrieval program and displayed in a new data set grid together with the used data set.

### 18.1 ACM

This is the prediction of activity coefficients at infinite dilution of a single solute in a mixture of two solvents.

The ACM prediction allows the selection between some  $g^E$  model, some group contribution models, the COSMO-SAC model, and third-party thermodynamics engines. The data sets can be calculated either at a constant composition over a specified temperature range or at a constant temperature over a composition range.

The buttons allow to produce a table and a plot output and to return the estimated data sets to the retrieval program.

### 18.2 ACT

This is the prediction of activity coefficients at infinite dilution of a single solute in one solvent.

The activity coefficients models are the same as for the ACM database plus the two group-contribution equation of state models PSRK and VTPR and the two MOSCED<sup>8,9</sup> models.

Two calculation types are possible:

1. Calculation of activity coefficients over a temperature range with given start and end temperature and a step width
2. Re-calculating the temperatures in the given experimental data sets.

---

<sup>8</sup> Thomas E.R., Eckert C.A., "Prediction of Limiting Activity Coefficients by a Modified Separation of Cohesive Energy Density Model and UNIFAC", *Ind.Eng.Chem. Process Des.Dev.*, 23(2), 194-209, 1984

<sup>9</sup> Lazzaroni M.J., Bush D., Eckert C.A., Frank T.C., Gupta S., Oslon J.D., "Revision of MOSCED Parameters and Extension to Solid Solubility Calculations", *Ind.Eng.Chem.Res.*, 44(11), 4075-4083, 2005

## 18.2.1 Selectivity Calculation

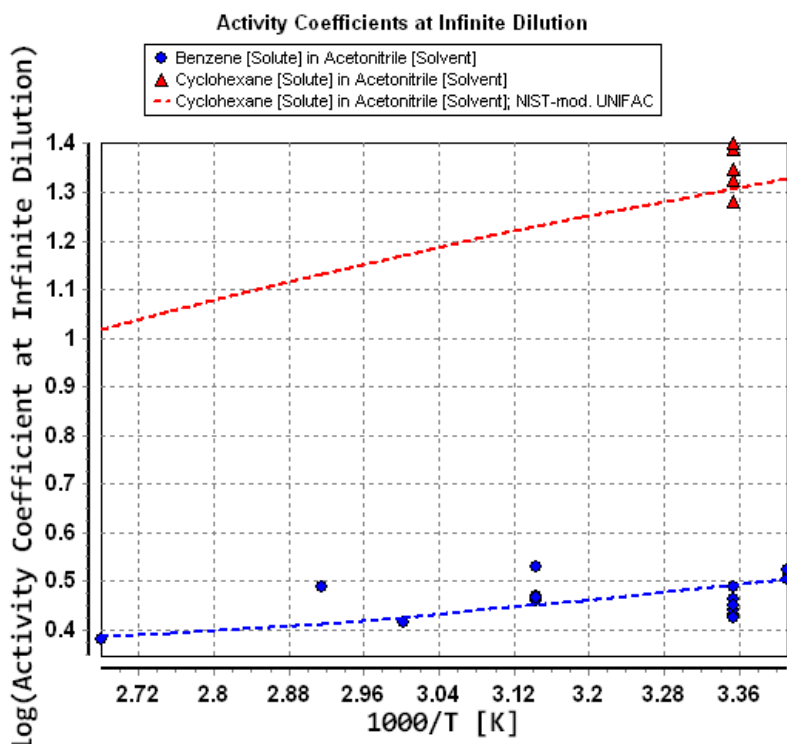


Figure 55: Activity Coefficient Diagram

This dialog contains an additional part “Selectivity Calculation” if two solutes in a single solvent have been specified. This dialog is used to calculate activity coefficients at infinite dilution of two solutes in a single solvent. If the resulting data are shown in a query result and plotted together the different gradients give information about the selectivity of the solvent for the separation of the binary mixture of the both solutes.

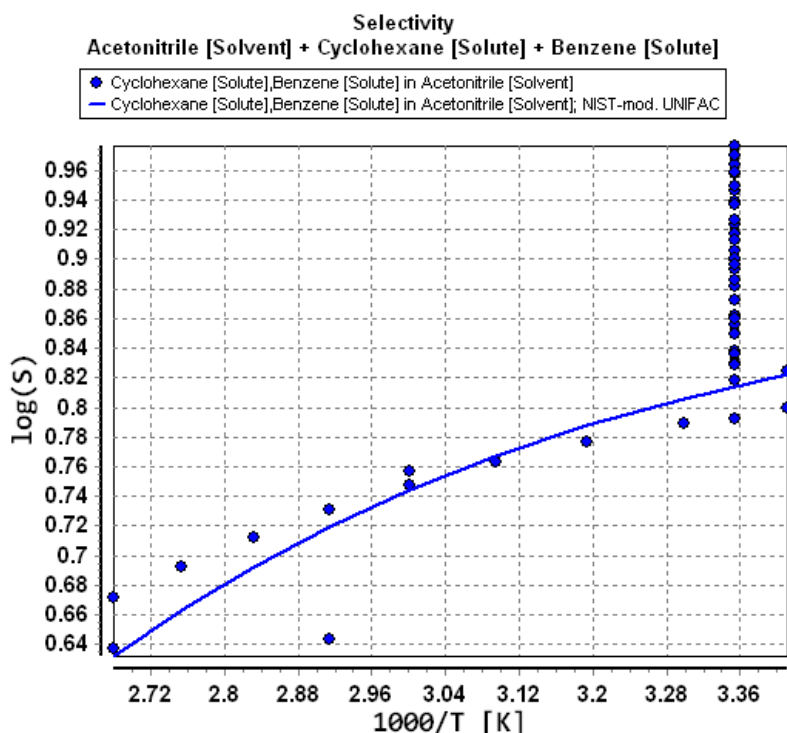


Figure 56: Selectivity Diagram

The selectivity itself is the ratio between both limiting activity coefficients.

### 18.3 AZD

This is the prediction of azeotropic points for binary or ternary mixtures.

The azeotropic prediction uses VLE calculations to determine the points where the vapor and liquid composition are equal ( $x=y$ ).

Either a temperature or a pressure range can be specified.

The selection of the vapor pressure equation, the vapor phase fugacity model, and (optional) the Poynting correction model is possible.

### 18.4 ELE

This is the prediction of vapor-liquid equilibria for electrolyte-containing systems.

The available ELE models are Electrolyte-NRTL (“eNRTL”) and LiFAC (by Hans-Martin Polka). These models can also handle binary solvents.

The models Pitzer, Chen, and Bromley can only handle pure solvents.

The checkbox “Water Normalization” is only valid for eNRTL and switches between the normalization of compositions based just on water or on all solvents.

### 18.5 GLE

This is the prediction of gas solubilities.

If the gas solubility data sets contain pressure, temperature and liquid compositions, or if they are convertible to such data, it is possible to transfer the data to the vapor-liquid equilibrium prediction dialog (see page 60) using the “VLE Prediction” button.

### 18.6 HE

This is the prediction of heats of mixing.

Heats of mixing deliver quantitative information about the temperature dependency of activity coefficients.

Heats of mixing can be calculated from activity coefficient models and models based on an equation of state (like PSRK and VTPR), and using third-party thermodynamics engines.

### 18.7 VLE/HPV

This is the prediction of vapor-liquid equilibria.

Vapor-liquid equilibria can be calculated by  $g^E$  models and by models based on equation of states and mixing rules, and by third-party thermodynamics engines.

Models based on simple  $g^E$  equations are Wilson, UNIQUAC, NRTL, Margules, and van Laar. These equations need binary interaction parameters for all binary subsystems. These parameters can be fitted by the *Regression Mix* application.

These  $g^E$  models have been the basis for group contribution models which are replacing the component specific parameters by group specific parameters. These group contribution methods are original UNIFAC, modified UNIFAC (Lyngby) and modified UNIFAC (Dortmund). The UNIFAC models are based on UNIQUAC.

These activity coefficient models are calculating the difference to the ideal vapor pressure curve. Therefore, these models need pure component vapor pressure data for the VLE equation – these vapor pressure data are provided by Antoine or DIPPR 101 equation parameters.

The PSRK and the VTPR models are based both on equations of state and a group contribution method and allow VLE data sets to predict even if components are super-critical.

COSMO-SAC and its variants published in 2010 and 2013 is a method based on molecular structure and the charge distribution of the molecular surface. This model needs component specific “ $\sigma$ -profile” files.

“Recalculate Data Points” allows the user to calculate the data points of given experimental data sets. If the option is activated the text output will contain the deviations for temperature, pressure and/or vapor composition (depending on the type of data set).

For gamma-based models it is possible to select the vapor pressure equation, the vapor phase fugacity model, and (optional) the poynting correction model. The vapor phase description can be done by Raoult's Law (“Ideal”), by equation of states, by the Hayden-'O'Connell method, or by the VPA method.

### 18.7.1 Predict with EOS

The prediction of VLE with EOS requires interaction parameters for all binary component pairs in the system. If any required data is missing the text “EOS” in the “Active Models” grid will become red and a hint will explain the error.

Component DDB#157 missing in EOS project file.  
Component DDB#11 missing in EOS project file.

Figure 57: Error hint for EOS predictions

Click on the EOS “Edit” button to open the *VLE Calculation by EOS* dialog. There the equation of state, the mixing rules, the  $g^E$  model (if required) and the alpha function can be selected. Furthermore, binary interaction parameters for all binary component pairs can be entered manually, retrieved from an EOS project file or retrieved from the parameter DDB.

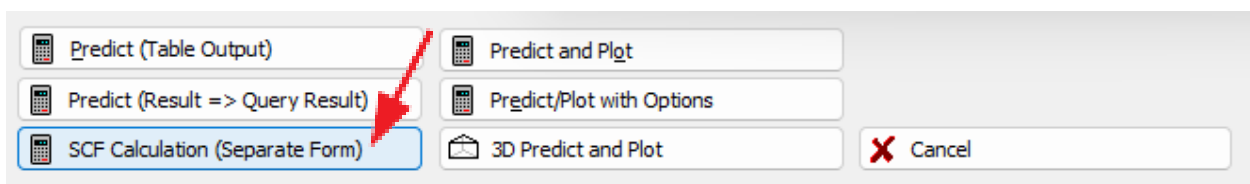
EOS      EOSPool\_01\_0...      Edit

If all data is available the text “EOS” turns black and the hint will contain information about the selected model.

EOS model: 1 - Soave-Redlich-Kwong  
Mixing rule: 1 - Quadratic  
Alpha Function: 1 - Mathias-Copeman

Now the EOS can be used like any other model.

### 18.7.2 Calculation of the Solubility of Solids in Supercritical Fluids



This type of calculation allows the prediction of the solubility of solids like anthracene in a supercritical solvent like carbon dioxide.

Additionally needed data are sublimation equation parameters either for the Antoine equation or vapor pressure parameter for either the Mathias-Copeman (PSRK) or the Twu-Bluck-Cunningham-Coon equation (VTPR). For the latter equation additionally a heat of fusion value and a melting temperature are needed.

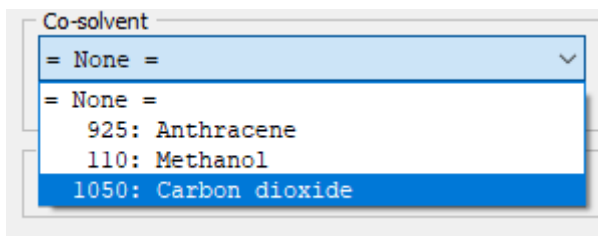
Antoine parameters in mmHg and °C can be entered directly in the edit control if parameters are not available from the Dortmund Data Bank.

Antoine Parameters: 8.4004 2771.1 176.02

The solid volumes in liters per square meter are directly read from the Dortmund Data Bank (pure component properties). If this data bank is not available or doesn't contain the necessary data it is possible to enter data directly.

Solid Volume (Solute): 0.14259 dm<sup>3</sup>/mol at 2

The “Cosolvent” combo box allows the specification of a single additional solvent.



The only necessary information is the mole fraction of this co-solvent.

A data table and a diagram are the results of a SCF calculation.

P[bar]	VV[l/mol]	Y (2)	log (y2)	PHI (2)	POYN (2)	Y (1)
2.00	14.47	0.19903E-05	-5.7011	0.93463	1.0090	0.99999801
4.00	7.192	0.10748E-05	-5.9687	0.87313	1.0180	0.99999893
6.00	4.767	0.77423E-06	-6.1111	0.81531	1.0272	0.99999923
8.00	3.554	0.62773E-06	-6.2022	0.76097	1.0364	0.99999937
10.00	2.826	0.54314E-06	-6.2651	0.70990	1.0457	0.99999946
.....						

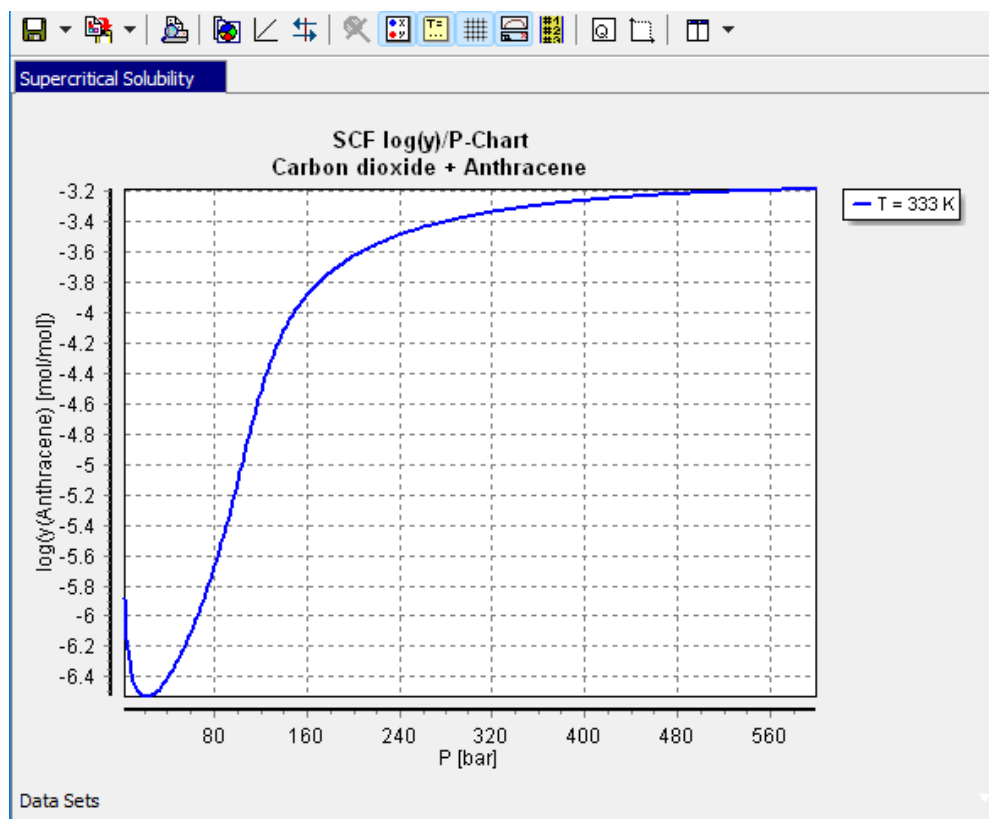


Figure 58: Solubility in a Supercritical Fluid

The table contains the solubility of the high-boiling component in the “Y (2)” column as mole fraction. The

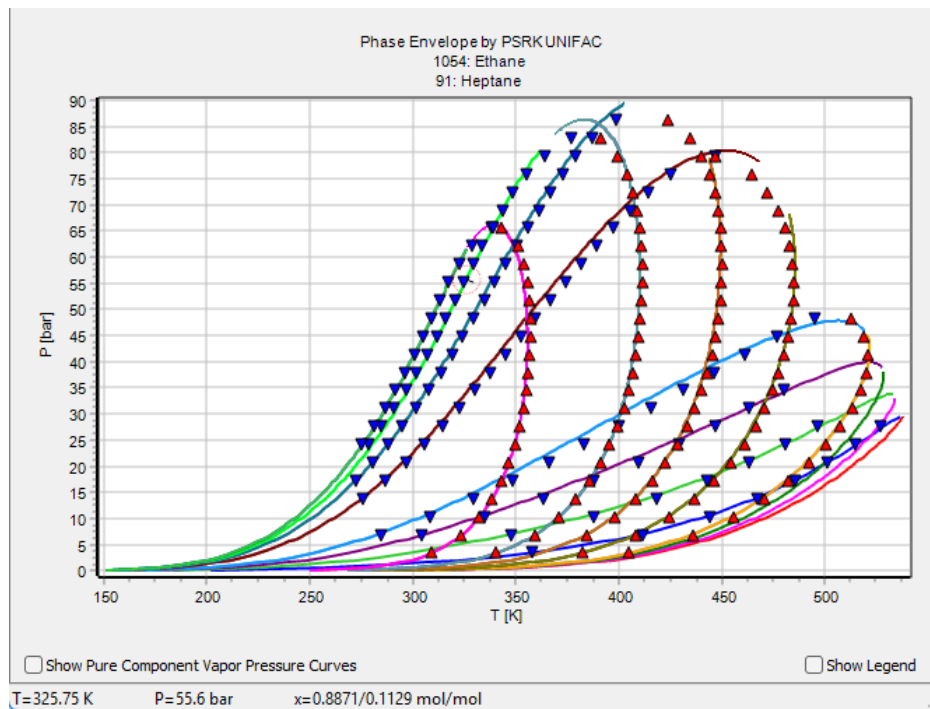
calculation is automatically for a pressure range from 2 to 600 bar. “VV” is the vapor volume, “PHI” is the fugacity, and “POIN” the Poynting factor.

Besides the table a diagram showing the pressure-dependency of the (logarithmic) solubility is displayed.

### 18.7.3 Deviation Plot

The deviation diagrams focus on the difference between the experimental pressure (isothermal data sets) or temperature (isobaric data sets).

### 18.7.4 Phase Envelope Calculation



If VLE or HPV data sets with constant compositions have been selected a dialog for the phase envelope calculation is (additionally) opened.

Phase envelopes are calculated at constant compositions and consist of a dew point and a boiling point curve. Ideally, both lines are connected close to the critical point of the mixture but in many cases the calculation stops before closing the curve completely because of iteration problems.

These P/T curves can be calculated with the equation of state group contribution methods PSRK and VTPR.

Use the option “Return Result” to create a new Query Result window with the calculation results. Otherwise, the results will be shown in the current dialog only.

Additional composition can be added manually into the data grid. The last entry, in the example

Mole Fraction	
0.887100	0.321
0.112900	0.679

it is the second line, is filled in automatically so that the sum of compositions is 1.

The function “Check Parameter” is described in the chapter 18.17 “Checking Availability of Model Parameters”.

### 18.7.4.1 Options

“Show Pure Component Vapor Pressure Curve” switches the display of the pure component's vapor pressure and the critical points (circles).

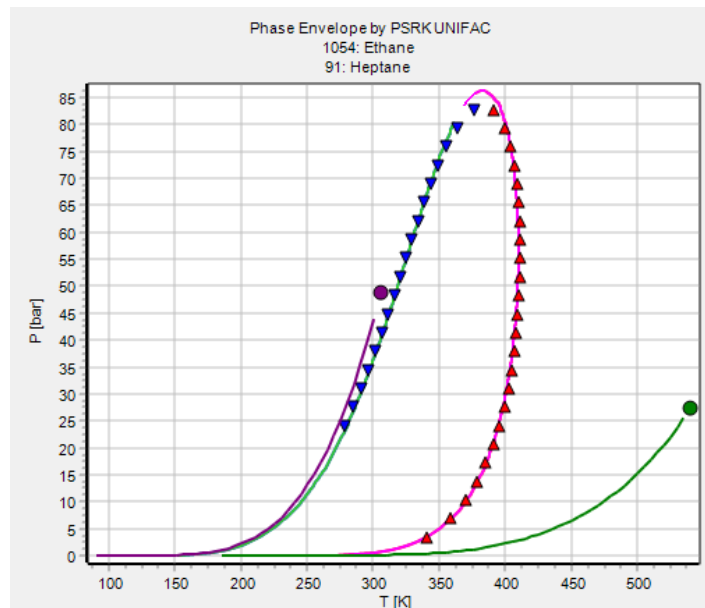


Figure 59: Phase Envelopes: Pure Component Vapor Pressures

“Show Legend” shows descriptions of the curves in the diagram.

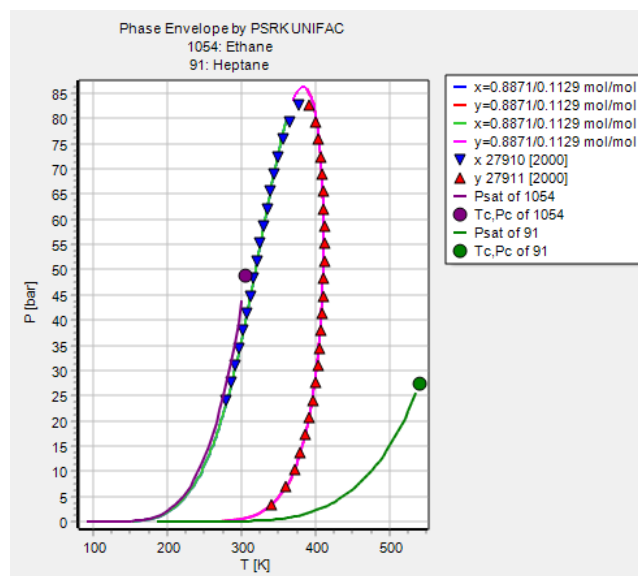


Figure 60: Phase Envelopes: Show Legend

The plot options are “Zoom”, “Rotate” (3D), “Move”, “Depth” (3D), “Chart Editor”, “Print”, “Copy”, “Save”.



## 18.8 LLE

This is the prediction of miscibility gaps.

Liquid-liquid equilibria can be predicted with several models.

For the  $g^E$  models UNIQUAC and NRTL as well as for cubic equation of states (EOS) component-specific interaction parameters are needed. These parameters can be obtained by DDB Regression Mix.



Also, the group contribution models original UNIFAC, modified UNIFAC (Dortmund, Lyngby and NIST), PSRK and VTPR can be used. Here group specific interaction parameters are required.

The usage of third-party thermodynamic engines is also supported.

Since 2013 the COSMO based models are supported.

## 18.9 PCP

This is the prediction of pure component properties.

The PCP prediction works in a quite different way. Since the PCP database contains multiple properties the program has to determine the property and the state (e. g. VLE for vapor pressures) before the model selection is possible.

The list of models comes from two main sources. One source is the Artist package providing mainly estimation models based on group contributions methods. Parameterized equations are the other source where the parameters have been fitted in advance ("PCP Equation Fit" and ParameterDDB).

Vapor pressures and some other properties can also be calculated with the Aspen thermodynamic engine using Aspen projects. Therefore, it is possible to select an Aspen project file for vapor pressures.

## 18.10 POW

Prediction of Octanol/Water partition coefficients

For Octanol/Water partition coefficient the UNIFAC model developed by Wienke and Gmehling (1998)<sup>10</sup> is implemented and additional the "normal" activity coefficient models original, modified UNIFAC, and NIST-modified UNIFAC as well as COSMO-RS(OI), PSRK, and VTPR.

---

<sup>10</sup> Wienke G., Gmehling J., "Prediction of Octanol-Water Partition Coefficients, Henry Coefficients and Water Solubilities Using UNIFAC", *Toxicol. Environ. Chem.*, 65, 57-86, 1998

## 18.11 SLE

SLE calculations can be performed via standard activity coefficient models but need heats of fusion for the pure components. Other supported models are the equation of state group contribution models PSRK and VTPR. The prediction methods always assume that the system shows eutectic behavior.

### 18.11.1 SLE Calculation Options

- **“Calculation Mode”**

The calculation modes, either Schröder/van Laar or Neau, use slightly different equations for the determination of the solubility.

Neau: 
$$\ln x_i = -\ln y_i - \Delta_{\text{fus}} \frac{H}{RT_M} \ln \left( \frac{T_M}{T} \right)$$

Schröder/van Laar: 
$$\ln x_i = -\ln y_i - \Delta_{\text{fus}} \frac{H}{R} \left( \frac{1}{T} - \frac{1}{T_M} \right)$$

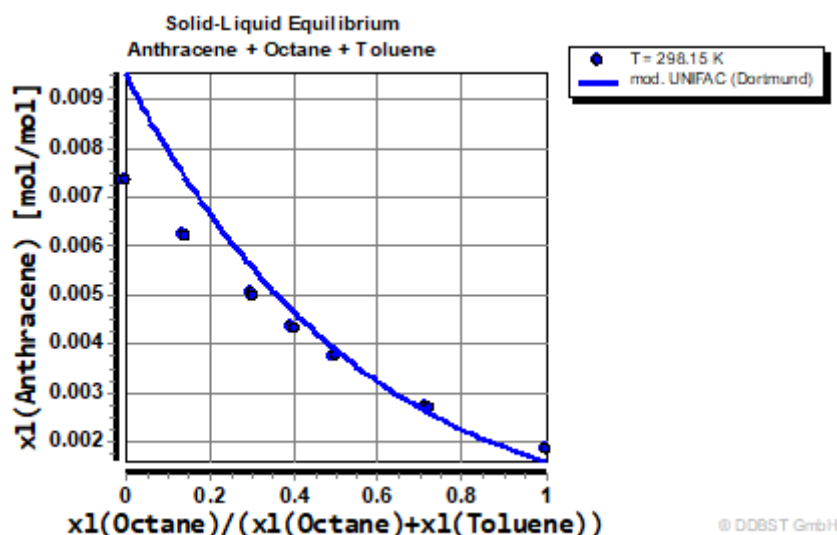
- **“Use Experimental Melting Points”**

This option allows to switch from a “standard” melting point stored in the basic component file to a melting point specified in the experimental SLE data sets. This causes a shift in the predicted melting points and improves matching of predicted and experimental data.

- **“Allow Calculation with Incomplete Data”**

The SLE calculation normally needs pure component melting points and heats of fusion. The calculation is still possible with missing heats of fusion but will give unreliable results. This option is only useful if not all heats of fusion are missing so that at least the branches with an existing heat of fusion can be calculated correctly.

### 18.11.2 Solubility in Binary Solvents



A special prediction for the solubility of a high-boiling and high-melting component in a binary mixture at constant pressure can be called by the button “Solubility in Binary Solvents”.

This calculation leads to a diagram where the solubility of the high-melting component is plotted against the solute-free composition of the binary solvent mixture.

## 18.12 VE

This is the prediction of excess volumes and densities

The excess volume can be calculated by the equation of state group contribution methods Predictive Soave-Redlich-Kwong (PSRK) and Volume-translated Peng-Robinson (VTPR).

“Redlich-Kister” and “Sum of Symmetrical Functions” are both equations where parameters can be fitted and stored inside the DDB system (see 19.2 “Binary VE and VIS”, page 75).

The “Deviation Plot” displays the difference between estimated and experimental excess volumes or densities.

## 18.13 VIS

This is the prediction of mixture viscosities.

Mixture viscosities can be predicted by the two methods Grunberg/Nissan/Isdale<sup>11</sup> and UNIFAC-VISCO<sup>12</sup> and the three simple mixing rules from Arrhenius, Kendall, and the linear mixing rule.

All these methods only estimate the excess viscosity (the reality) and need pure component viscosities at the given temperatures. These can be calculated by the pure component equations Andrade, Vogel, DIPPR101, PPDS9, and extended Andrade. Parameters for these equations can be made with the DDB Regression Pure program. The equation forms are described in the manual of that program.

Important note: The two predictive methods Grunberg/Nissan/Isdale and UNIFAC-VISCO both have a very limited applicability because of few supported functional groups.

## 18.14 MFLP

This is the prediction of mixture flash points.

Mixture flash points can be predicted by the commonly available activity coefficient models.

The flash point calculation uses the method of Gmehling and Rasmussen.<sup>13</sup>

The needed basic data are taken from DDB files with recommended values (pure component flash point and heats of combustion from the data file used in the stand-alone flash point calculation software and pure component vapor pressures are provided by the Antoine equation with the parameters stored in the ParameterDDB).

A description of the used techniques is available in the manual of the stand-alone flash point calculation software tool.

---

<sup>11</sup> Isdale J.D., MacGillivray J.C., Cartwright G., "Prediction of Viscosity of Organic Liquid Mixtures by a Group Contribution Method", Report, 1-21, 1981

<sup>12</sup> Gaston-Bonhomme Y., Petrino P., Chevalier J.L., "UNIFAC-VISCO Group Contribution Method for Predicting Kinematic Viscosity: Extension and Temperature Dependence", Chem.Eng.Sci., 49(11), 1799-1806, 1994

<sup>13</sup> Gmehling J., Rasmussen P., "Flash Points of Flammable Liquid Mixtures Using UNIFAC.", Ind.Eng.Chem. Fundam., 21(2), 186-188, 1982

## 18.15 MTCN

This is the prediction of mixture thermal conductivities.

Mixture thermal conductivities can be calculated by pure component thermal conductivities calculated with two equations (polynomial and PPDS8) and three different rather simple mixing rules.

The parameters for the pure component equations are read from the ParameterDDB.

## 18.16 Entering $g^E$ Model Parameters

If a  $g^E$  model (NRTL, UNIQUAC, Wilson, van Laar or Margules) has been selected for the prediction, parameters for the binary component pairs have to be entered.

The starting dialog displays the system or systems for which the parameters are needed. The “Edit Parameters” buttons opens a dialog where the single binary parameters can be edited.

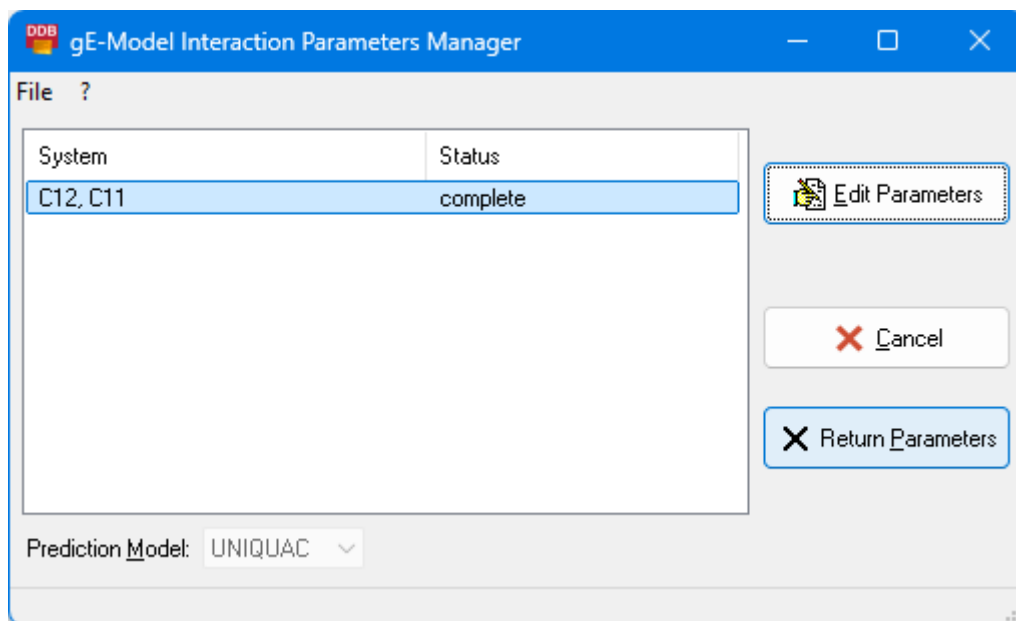


Figure 61: Main Dialog for Entering  $g^E$  Model Parameters

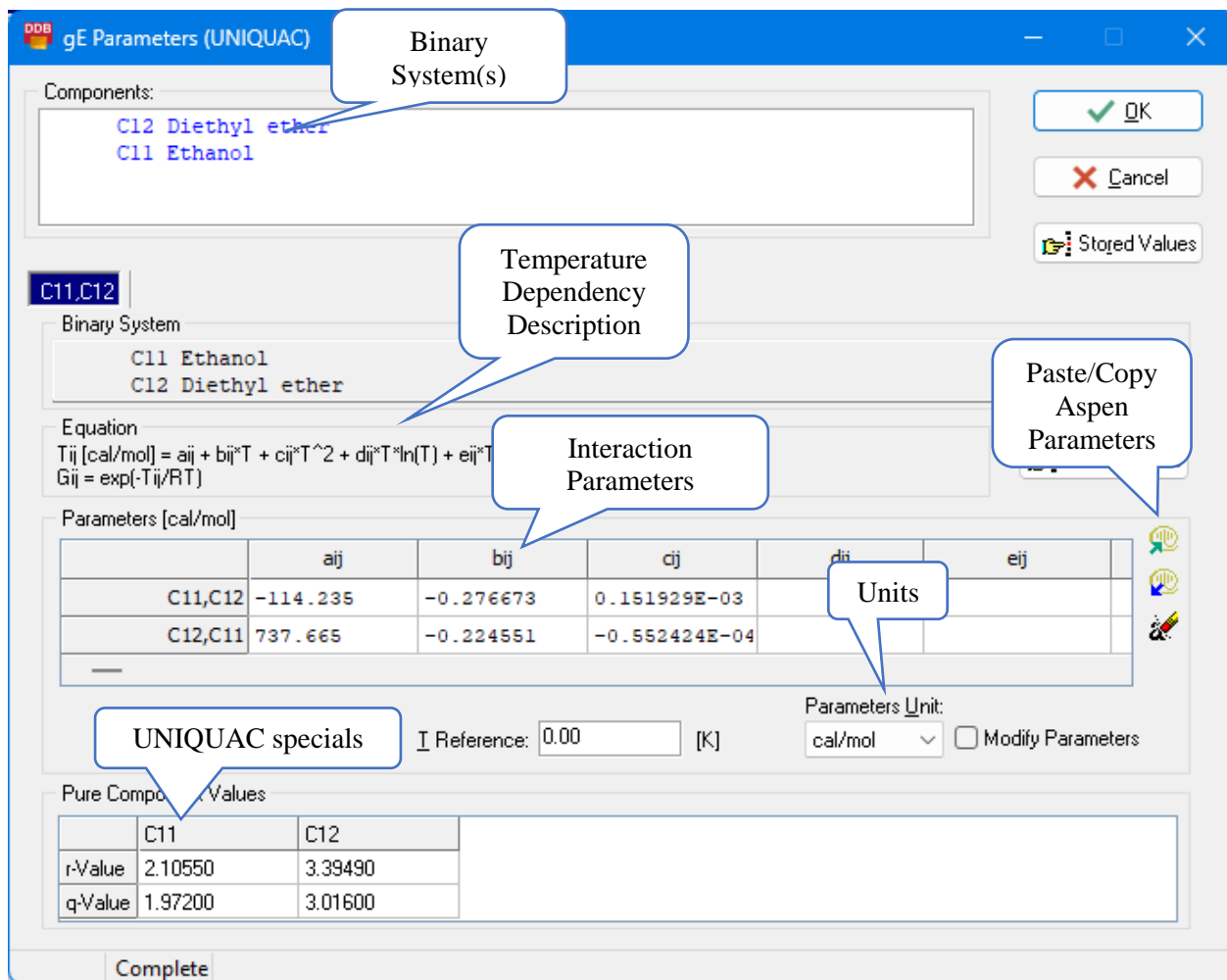


Figure 62: gE Model Parameters Editing Dialog

This list can be different for different phase equilibria. The “Stored Values” buttons allows loading parameters from the ParameterDDB if data are available.

The dialog has a “Load?” column where the wanted parameter set has to be checked.

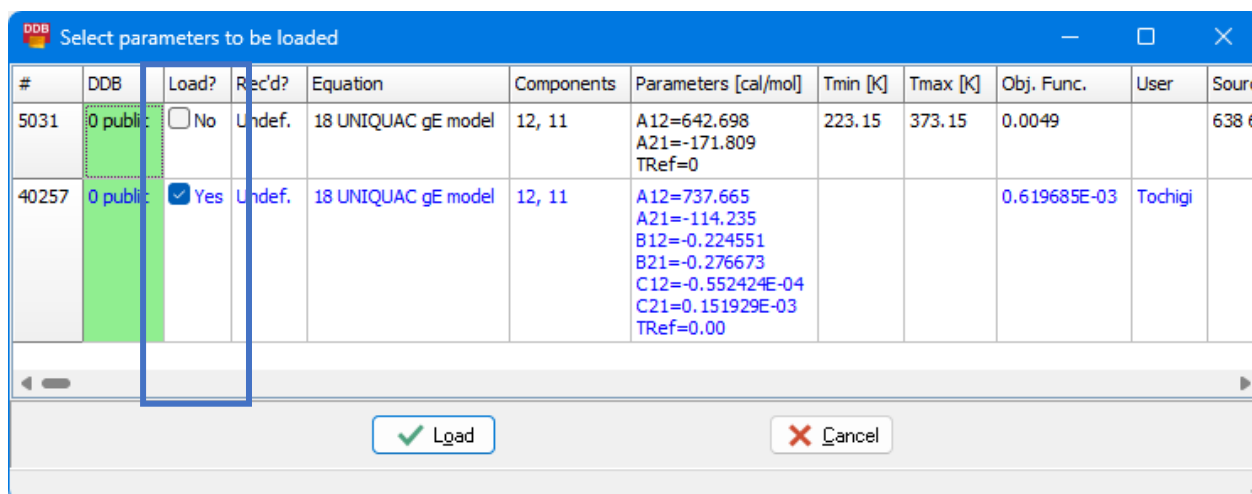

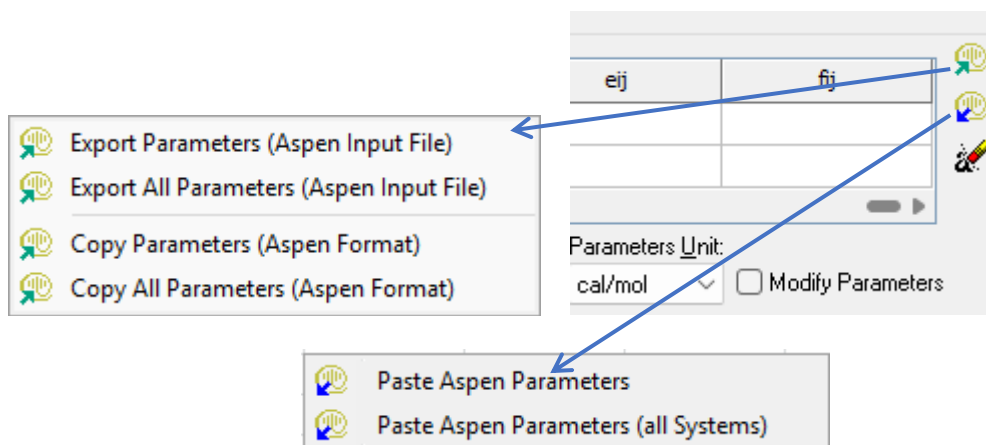


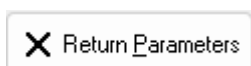
Figure 63: Parameter Set Selection

The button with the AspenTech icon  allows the entered parameters to export to an Aspen INP (“.inp”) file. This file can be loaded in the Aspen simulator. If Aspen compatible data are available in the Windows clipboard (copied from inside Aspen) it is also possible to insert these parameters.

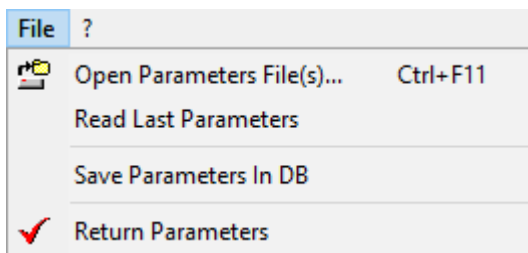


Parameters can be entered either in [ $\text{cal}/\text{mol}$ ], [ $\text{J}/\text{mol}$ ] or in [K].

Being back in the main dialog it is now possible to return the parameters to the calculation program:



It is also possible to save entered parameters to the ParameterDDB (“Save Parameters in DB”).



The “Read Last Parameters” allows to re-use the parameters used previously.

### 18.16.1 Copying Parameters to the Aspen Simulator

The exchange dialog shows the currently selected  $g^E$  model parameters either entered by the user or read from the ParameterDDB and allows to copy them in an Aspen simulator compatible format into the Windows clipboard. It is important to know that only the selected lines are actually copied. This allows to copy the entire table shown in the right pane (select all lines) or just few, for example, just the parameters.

Aspen Parameter Exchange

Model: **UNIQUAC**

DDB No.	DDB Name	Aspen Name
11	Ethanol	DDB11
12	Diethyl ether	DDB12

Aspen Parameters: Aspen Version: 10.0

Component i	DDB11
Component j	DDB12
Source	K
Temperature units	
Aij	0.1392269
Aji	0.1129981
Bij	57.485123
Bji	-371.20640
Cij	0
Cji	0
Dij	-7.6453427e-0
Dji	2.7798977e-05
TLOWER	
TUPPER	
Eij	
Eji	

Copy Selection Close

Figure 64: Aspen Parameter Exchange

Source	
Aij	0.1392269
Aji	0.1129981
Bij	57.485123
Bji	-371.20640
Cij	0
Cji	0
Dij	-7.6453427e-0
Dji	2.7798977e-05
TLOWER	

Figure 65: Copying Parameters

The format of the parameters the Aspen simulator is different in different Aspen versions. The correct Aspen version can be chosen by a drop-down box.

Aspen Version: 2004 - 7.1

DDB11	2004 - 7.1
DDB12	7.2 - 9.0
	10.0

Figure 66: Aspen Version

### 18.17 Checking Availability of Model Parameters

The glasses button opens a dialog with a short and a detailed display of available model specific parameters for the group contribution methods and for the COSMO models.

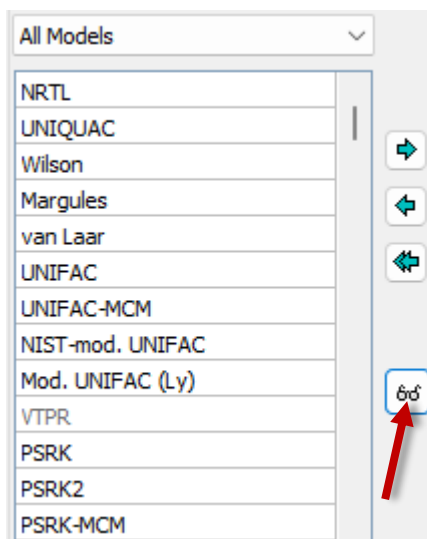


Figure 67: Checking Availability of Parameters

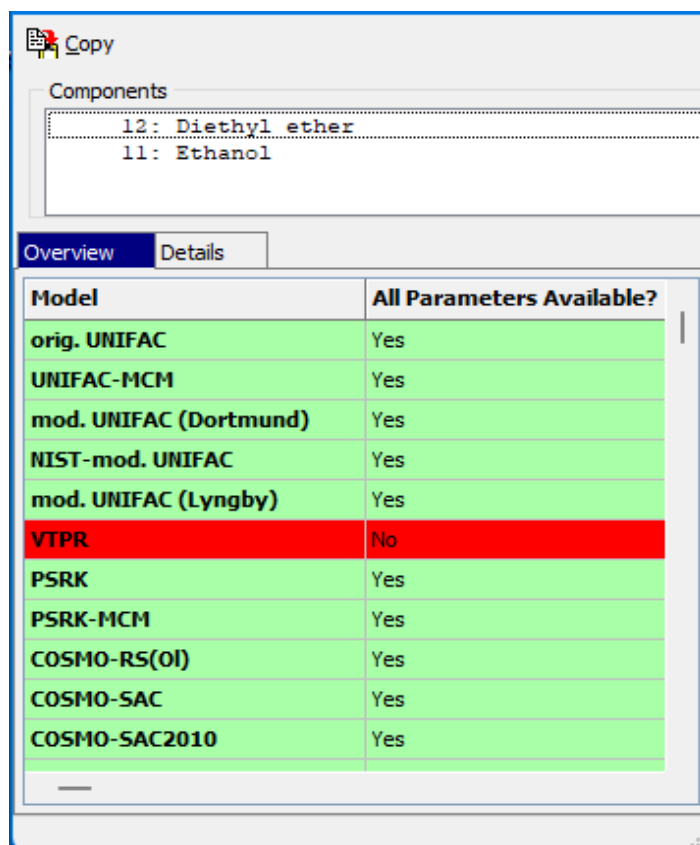


Figure 68: Checking Availability of Parameters of Group Contribution Methods

The “Overview” page gives a quick overview if model specific parameters are available. Green lines indicate that all data are available, red lines indicate missing parameters.

The “Details” page shows the available and missing required data.

**UNIFAC**

Component 17: Aniline  
Subgroups: 9 (ACH ) 36 (ACNH2 )

Component 49: 3-Methylphenol  
Subgroups: 9 (ACH ) 11 (ACCH3 ) 17 (ACOH )

List of Main Groups  
Maingroups: 3 (ACH ) 4 (ACCH2 ) 8 (ACOH ) 17 (ACNH2 )

Interaction parameters  
3 - 4: 1 parameter/s  
3 - 8: 1 parameter/s  
3 - 17: 1 parameter/s  
4 - 8: 1 parameter/s  
4 - 17: 1 parameter/s  
8 - 17: 1 parameter/s

*System has all parameters available.*

**mod. UNIFAC (Lyngby)**

Component 17: Aniline  
Subgroups: 10 (ACH ) 11 (AC ) 30 ((A)NH2 )

Component 49: 3-Methylphenol  
Subgroups: none given



## 18.18 Third-Party Thermodynamics Calculations

### 18.18.1 Introduction

This section describes briefly in a step-by-step tutorial how to use third-party thermodynamic engines in the DDB software. Currently supported are the Aspen simulator, PRO/II, UniSim Design, Simulis Thermodynamics and AVEVA SimCentral.

The supported features are:

- Reading components from a project file
- Calculation of mixture thermodynamic properties (like VLE, LLE) using the thermodynamics defined in a project file

The following files are used for the different thermodynamic engines:

- Aspen backup file (\*.bkp)
- PRO/II database file (\*.prz)
- UniSim Design case file (\*.usc)
- Simulis Thermodynamics calculator file (\*.calculator)
- AVEVA SimCentral simulation library file (\*.libx)

### 18.18.2 Step 1: Read components from a project file

In order to compare the experimental data stored in the DDB with a third-party thermodynamics model the components in a project file must be identified and assigned to DDB components (see sections 3.4-3.8).

The system tries to assign the components automatically. This is done by a predefined mapping. Make sure all required components are identified or newly defined.

After all assignments have been done, the components can be added to the query using the *Add Components to Query* button.

Additional components can be added to the list the same way. Unwanted components can be removed from the list using the *Remove* button.

### 18.18.3 Step 2: Search for experimental data in the DDB

After the components of interest have been defined within the *Dortmund Data Bank* program, the DDB can be searched for experimental data. Click on the button *System (Exact Match)* in the *Search* area to find data for the selected system.

The result is grouped by data types. To see the result for vapor-liquid-equilibrium data click on the *VLE* tab.

### 18.18.4 Step 3: Calculate VLE using Third-Party Thermodynamics

The experimental data in a query result can be used as basis for a calculation.



Select the data of interest and press the *Predict selected data sets* button. The *VLE/HPV Prediction* dialog will be displayed. The components of the first selected data set will be used as system for the prediction.

Scroll down the list of available models. Then double-click on the third-party thermodynamic engine (or use the right arrow button) to make the model active.

The project file, which has been opened most recently within the DDB software, is selected as default file to be used for a calculation.

If the mouse is over the third-party model field in the *Active Models* area, then some additional information is displayed.

Use the *Edit* button next to the displayed file name to select a different file for the calculation. Then a component assignment dialog will be displayed. For some engines, the active model can be changed.

Use the *Predict and Plot* button to display the experimental data together with the calculated results in a plot with several diagrams.

For a text output, the *Predict (Table Output)* button can be used. The button *Predict (Result => Query Result)* will send the predicted data to the Dortmund Data Bank program.

## 19 Fit Equation Parameters



For some data types special fitting dialogs are used.

### 19.1 AAE

Adsorbent-adsorptive equilibria data sets with isothermal and single adsorptive data sets can be fitted. The following isotherms are supported:

1. Freundlich-Isotherm
2. Langmuir-Isotherm
3. Brunauer-Emmett-Teller-Isotherm
4. Mixed-Langmuir-Freundlich-Isotherm
5. Toth-Isotherm
6. Statistical combined Langmuir-Isotherm
7. Modified Langmuir-Isotherm for SSTM
8. Virial-Isotherm-Equation (SPD)
9. Vacancy Solution Model
10. Dubinin-Astakhov-Isotherm for MI/RAST

### 19.2 Binary VE and VIS

The data banks contain excess data or data that be converted to an excess property (excess volumes, viscosity deviations). All these excess values have a similar curvature and therefore the type of fit is the same. Two equations are implemented, “Redlich-Kister” and “Sum of Symmetrical Functions” with different number of parameters.

#### 19.2.1 Redlich-Kister

$$\frac{v^E}{x_1 x_2} = \sum_{i=1}^n A_i (2x_1 - 1)^{i-1}$$

n=1..6

#### 19.2.2 Sum of Symmetrical Functions

$$v^E = \sum_{i=1}^m \frac{A_i x_1 x_2}{\left(\frac{x_1}{a_i} + x_2\right)^2}$$

m=1..3

#### 19.2.3 Fit Result

The button “Fit/Table/Plot Best Model” automatically fit the data with both equations and *all possible parameter count* and displays the result with the lowest deviation. A table with the numerical results is displayed in a second window.

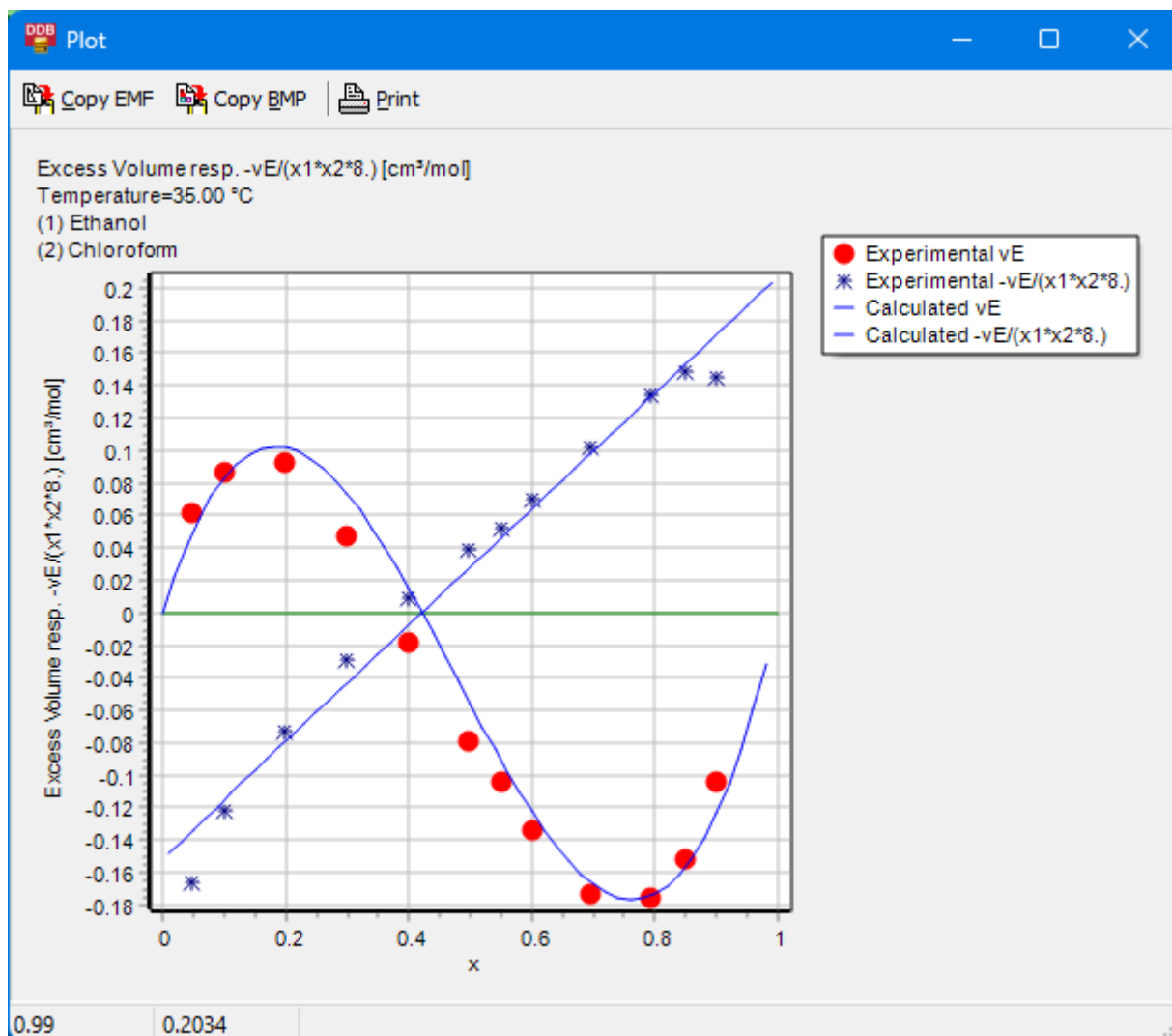


Figure 69: Plot Result for Excess Properties' Fit (Volume)

If the check box “Prepare Storing Results in Parameter Database” is checked, a dialog with the fitted parameters is shown which allows storing the values in either the public or private parameter data base.

The stored parameters can then be used to predict the property they describe.

A typical fit result table shows the components, the parameters, and the data table with experimental data from the DDB and recalculated values by the selected equation.

```

Excess Volume      Data Set(s): 13476 [0]
=====
Components:
(1) Diethyl ether          C4H10O          60-29-7
-----
(2) Ethanol                C2H6O           64-17-5
-----

Temperature=25.00 °C

Sum of Symmetrical Functions
=====
Par1 =      -2.6486
Par2 =    1039.9436

Experimental Data
vE cm³/mol          x1 Diff vE cm³/mol          SSF
                    x1 Diff vE cm³/mol          vE Calc'ed cm³/mol
-0.1138             0.0432             -0.0119             -0.1019
-0.1981             0.0839             -0.0074             -0.1906

```

### 19.3 Ternary LLE

In case of ternary data sets temperature independent parameters can be fitted for all binary combinations for UNIQUAC and NRTL.

The screenshot shows the 'Ternary LLE gE Model Parameter Fit' window. The 'System' table lists three components: Toluene (DDB Code 161, Formula C7H8, R=3.9228, Q=2.9680), Acetone (DDB Code 4, Formula C3H6O, R=2.5735, Q=2.3360), and Water (DDB Code 174, Formula H2O, R=0.9200, Q=1.4000). The 'Fitting' tab is active, showing a table of experimental data points. The table has columns for component number (#), mole fractions (x1, x2, x3, x4, x5), and excess volume (vE). The data points are numbered 1 through 12. A dropdown menu for the model is open, showing options for NRTL, UNIQUAC, and NRTL. The 'Fit Parameters' button is also visible.

#	x1 [mol/mol]	x2 [mol/mol]	x3 [mol/mol]	x4 [mol/mol]	x5 [mol/mol]	vE
1618 [0]						
1	0.99587	0.00158	0.00255	0.00010	0.00010	
2	0.98110	0.01637	0.00253	0.00010	0.00010	
3	0.96558	0.02938	0.00504	0.00010	0.00010	
4	0.95497	0.04001	0.00502	0.00010	0.00010	
5	0.94612	0.04887	0.00501	0.00010	0.00010	
6	0.91710	0.07796	0.00494	0.00010	0.00010	
7	0.88300	0.10969	0.00731	0.00021	0.00021	
8	0.83486	0.15558	0.00956	0.00022	0.00022	
9	0.80002	0.18820	0.01178	0.00033	0.00033	
10	0.76752	0.21854	0.01394	0.00034	0.00034	
11	0.72635	0.25768	0.01597	0.00046	0.00046	
12	0.66126	0.31880	0.01994	0.00059	0.00059	

Figure 70: Fitting Ternary LLE Data Sets

The “Fit Parameters” Button opens a parameter grid.

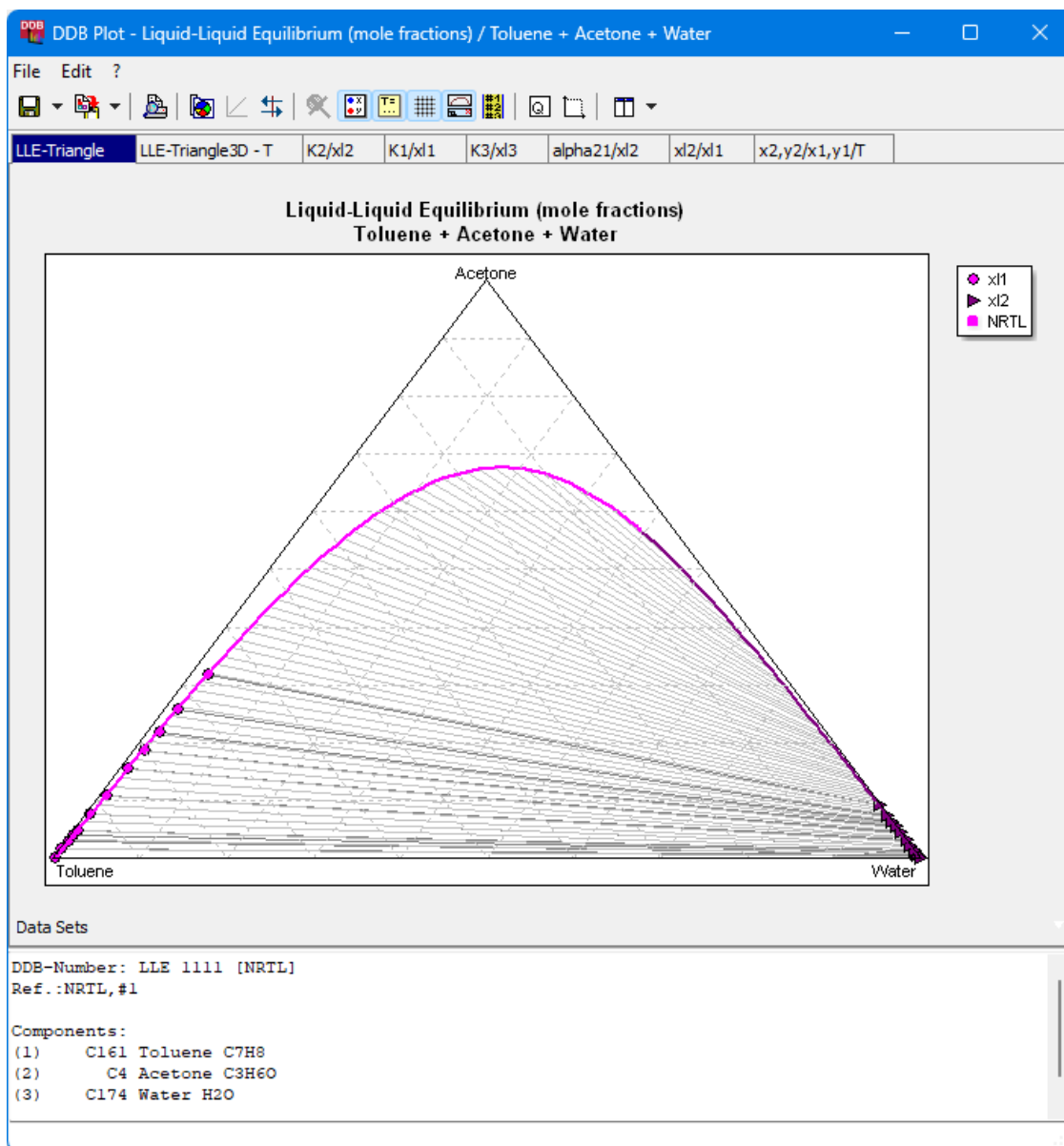
Parameter	Start Value	Initial Step	Constant?	min.	max.	Limits
a 161 4	50	500	<input type="checkbox"/> Constant			<input checked="" type="checkbox"/> Respect
a 4 161	60	500	<input type="checkbox"/> Constant			<input checked="" type="checkbox"/> Respect
alpha 161 4	0.2	0	<input checked="" type="checkbox"/> Constant	0.01	1	<input checked="" type="checkbox"/> Respect
a 161 174	50	500	<input type="checkbox"/> Constant			<input checked="" type="checkbox"/> Respect
a 174 161	60	500	<input type="checkbox"/> Constant			<input checked="" type="checkbox"/> Respect
alpha 161 174	0.2	0	<input checked="" type="checkbox"/> Constant	0.01	1	<input checked="" type="checkbox"/> Respect
a 4 174	50	500	<input type="checkbox"/> Constant			<input checked="" type="checkbox"/> Respect
a 174 4	60	500	<input type="checkbox"/> Constant			<input checked="" type="checkbox"/> Respect
alpha 4 174	0.2	0	<input checked="" type="checkbox"/> Constant	0.01	1	<input checked="" type="checkbox"/> Respect

Optimizer: LM + SNM      Fit Lev. Steps: 400

Use Expert Modus

This menu sets the starting values of the fit. It also allows specifying if a parameter should be constant or has to be in a limit range during the fit. This option also allows the optimizer to choose for this fit. Either Simplex-Nelder-Mead (minimum 3 tie lines), Levenberg-Marquardt (minimum 6 tie lines) or a combination of both can be used. The “Ok” button starts the fit. Results are shown in a plot form. The exact numbers can be found in the “Results” Tab Sheet.

Fitting Results Parameters															
Copy															
NRTL	#	x1l [mol/mol]	x2l [mol/mol]	x3l [mol/mol]	x1r [mol/mol]	x2r [mol/mol]	x3r [mol/mol]	T [K]	P [kPa]	x1l_calc [mol/mol]	x2l_calc [mol/mol]	x3l_calc [mol/mol]	x1r_calc [mol/mol]	x2r_calc [mol/mol]	x3r_calc [mol/mol]
	1618	[0]													
	1	0.99587	0.00158	0.00255	0.00010	0.00056	0.99934	283.150	0.000	0.99722	0.00000	0.00278	0.00051	0.00000	0.99949
	2	0.98110	0.01637	0.00253	0.00010	0.00537	0.99453	283.150	0.000	0.98190	0.01498	0.00311	0.00056	0.00496	0.99448
	3	0.96558	0.02938	0.00504	0.00010	0.00918	0.99072	283.150	0.000	0.96649	0.03003	0.00348	0.00060	0.00986	0.98954
	4	0.95497	0.04001	0.00502	0.00010	0.01227	0.98763	283.150	0.000	0.95099	0.04514	0.00388	0.00065	0.01470	0.98465
	5	0.94612	0.04887	0.00501	0.00010	0.01484	0.98506	283.150	0.000	0.95099	0.04514	0.00388	0.00065	0.01470	0.98465
	6	0.91710	0.07796	0.00494	0.00010	0.02324	0.97666	283.150	0.000	0.91967	0.07553	0.00480	0.00075	0.02417	0.97508
	7	0.88300	0.10969	0.00731	0.00021	0.03270	0.96709	283.150	0.000	0.88795	0.10615	0.00590	0.00086	0.03339	0.96575
	8	0.83486	0.15558	0.00956	0.00022	0.04599	0.95379	283.150	0.000	0.83957	0.15248	0.00795	0.00104	0.04674	0.95222
	9	0.80002	0.18820	0.01178	0.00033	0.05516	0.94451	283.150	0.000	0.80677	0.18360	0.00963	0.00117	0.05533	0.94351
	10	0.76752	0.21854	0.01394	0.00034	0.06432	0.93534	283.150	0.000	0.77351	0.21488	0.01161	0.00130	0.06368	0.93502
	11	0.72635	0.25768	0.01597	0.00046	0.07470	0.92484	283.150	0.000	0.72274	0.26201	0.01525	0.00151	0.07581	0.92268
	12	0.66126	0.31880	0.01994	0.00059	0.09158	0.90783	283.150	0.000	0.65336	0.32501	0.02163	0.00181	0.09134	0.90685



The fitted parameters are stored in the “Parameters” Tab Sheet. The Parameters can be saved as XLS or INP format. They can also be stored in the DDB by the “Save in Parameter DDB” Button and the results can be copied to the clipboard by the “Copy” button.

#	DDB	Store?	Rec'd?	Equation	Components	Parameters [cal/mol]	Tmin [K]	Tmax [K]	Obj. Func.	Source	Comment
1	1 private	<input checked="" type="checkbox"/> Yes	Undef.	17 NRTL gE model	161, 4	A12=-228.99154 A21=440.37344 Alpha=0.2000000 TRef=0.0	283.15	283.15	Error=0.00567569901	DDB	Fit by RecF
2	1 private	<input checked="" type="checkbox"/> Yes	Undef.	17 NRTL gE model	161, 174	A12=2190.5227 A21=3067.0619 Alpha=0.2000000 TRef=0.0	283.15	283.15	Error=0.00567569901	DDB	Fit by RecF
3	1 private	<input checked="" type="checkbox"/> Yes	Undef.	17 NRTL gE model	4, 174	A12=581.68798 A21=421.37857 Alpha=0.2000000 TRef=0.0	283.15	283.15	Error=0.00567569901	DDB	Fit by RecF

Figure 71: Storing Fitted LLE Parameters

## 19.4 PCP

For pure component data the external program DDB Regression Pure is started.

This program is described in a separate manual.

## 19.5 Ternary VLE/HPV

Ternary vapor-liquid equilibrium data sets can be fitted by  $g^E$  models (Wilson, NRTL, UNIQUAC). The objective function of the fit can be defined in the “Property” combo box. Also, the vapor phase model, the vapor pressure equation and the poynting correction can be chosen. Point specific options can be found in lower left corner.

The “Fit Parameters” button allows entering starting values for the fit. It is also possible to define if there are limits for the parameters or if some of them are constant. The “OK” button starts the fit.

The Results are given in the “Results”- Tab Sheet.


NRTL	#	x1 [mol/mol]	x2 [mol/mol]	x3 [mol/mol]	y1 [mol/mol]	y2 [mol/mol]	y3 [mol/mol]	T [K]	P [kPa]	Calc. Act.Coeff.1	Calc. Act.Coeff.2	Calc. Act.Coeff.3	Calc.y1 [mol/mol]	Calc.y2 [mol/mol]	Calc.y3 [mol/mol]	Calc.T [K]
	26167	[0]														
	1	0.21670	0.62670	0.15660	0.35500	0.53070	0.11430	343.350	101.325	1.14356	1.17973	2.41038	0.38233	0.51802	0.09965	342.726
	2	0.40000	0.48000	0.12000	0.58920	0.32330	0.08750	338.450	101.325	1.06351	1.27852	2.07967	0.57960	0.36357	0.05682	338.789
	3	0.60000	0.32000	0.08000	0.75050	0.21640	0.03310	334.650	101.325	1.02075	1.39282	1.82942	0.74452	0.22639	0.02909	335.268
	4	0.80000	0.16000	0.04000	0.89040	0.09820	0.01140	331.650	101.325	1.00375	1.50376	1.64627	0.88185	0.10655	0.01160	332.200
	5	0.20000	0.48000	0.32000	0.36400	0.47200	0.16400	344.750	101.325	1.02463	1.41910	1.71568	0.33327	0.51242	0.15431	344.426
	6	0.40000	0.36000	0.24000	0.57160	0.33500	0.09340	339.750	101.325	1.00571	1.48665	1.64791	0.57069	0.33483	0.09449	340.056
	7	0.60000	0.24000	0.16000	0.74120	0.20560	0.05320	335.550	101.325	0.99973	1.54244	1.59503	0.75155	0.19586	0.05259	336.193
	8	0.80000	0.13000	0.07000	0.90020	0.08130	0.01850	332.150	101.325	1.00003	1.56157	1.57161	0.88901	0.09135	0.01965	332.553
	9	0.20000	0.32000	0.48000	0.35250	0.46360	0.18390	346.350	101.325	1.01292	1.83428	1.33018	0.34372	0.46755	0.18873	345.807
	10	0.40000	0.24000	0.36000	0.60120	0.27920	0.11960	341.050	101.325	1.00348	1.78448	1.37293	0.59303	0.28304	0.12393	341.342
	11	0.60000	0.16000	0.24000	0.78540	0.14620	0.06840	336.550	101.325	1.00014	1.72930	1.41828	0.77484	0.15246	0.07270	337.120
	12	0.80000	0.08000	0.12000	0.91760	0.05390	0.02850	332.750	101.325	0.99974	1.66848	1.46253	0.90626	0.06166	0.03208	333.138
	13	0.20000	0.16000	0.64000	0.39500	0.37790	0.22710	349.150	101.325	1.10317	2.52112	1.12177	0.40663	0.35925	0.23412	348.540
	14	0.40000	0.12000	0.48000	0.65390	0.19810	0.14800	342.950	101.325	1.05220	2.20866	1.19482	0.65749	0.18885	0.15367	343.126
	15	0.60000	0.08000	0.32000	0.85000	0.07500	0.07500	337.950	101.325	1.02089	1.96233	1.28385	0.81811	0.09054	0.09135	338.168
	16	0.80000	0.04000	0.16000	0.92770	0.03380	0.03850	333.350	101.325	1.00470	1.76454	1.38719	0.92534	0.03331	0.04135	333.617

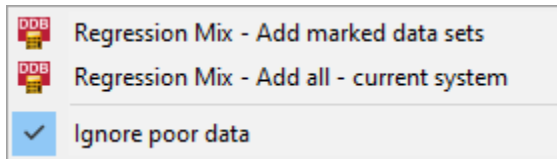
Figure 72: Result Sheet

The fitted parameters are stored in the “Parameters” Tab Sheet. The parameters can be saved as XLS or INP format. They can also be stored in the DDB by the “Save in Parameter DDB” Button and the results can be copied to the clipboard by the “Copy” button.



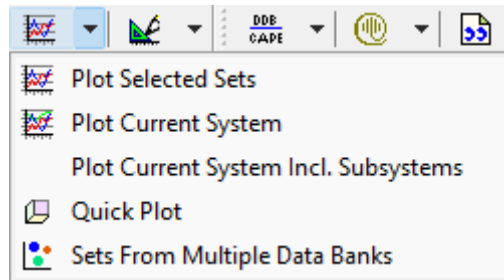
## 20 Simultaneous Fit – Regression Mix

 DDB Regression Mix can fit binary VLE/HPV, HE, ACT, LLE, AZD, CPE and SLE data simultaneous. Either the marked data or all possible data can be transferred to Regression Mix with the fit options in the fit button.



A full description is available in separate documentation.

## 21 Plot



The main functions of the plot utility are explained in the DDB Plot documentation.

### 21.1 *Plot Selected Sets*

This function displays the marked data sets.

### 21.2 *Plot Current System*

This function searches for all data sets for the currently selected mixture or pure component, marks these data sets, and then display these data sets together in one diagram.

### 21.3 *Plot Current System Incl. Subsystems*

This function is mainly intended for the use with ternary data where all the data of binary sub systems are added as pseudo-ternary data.

### 21.4 *Quick Plot*

The quick plot allows to show the data with arbitrarily selected x, y, and depth axis.

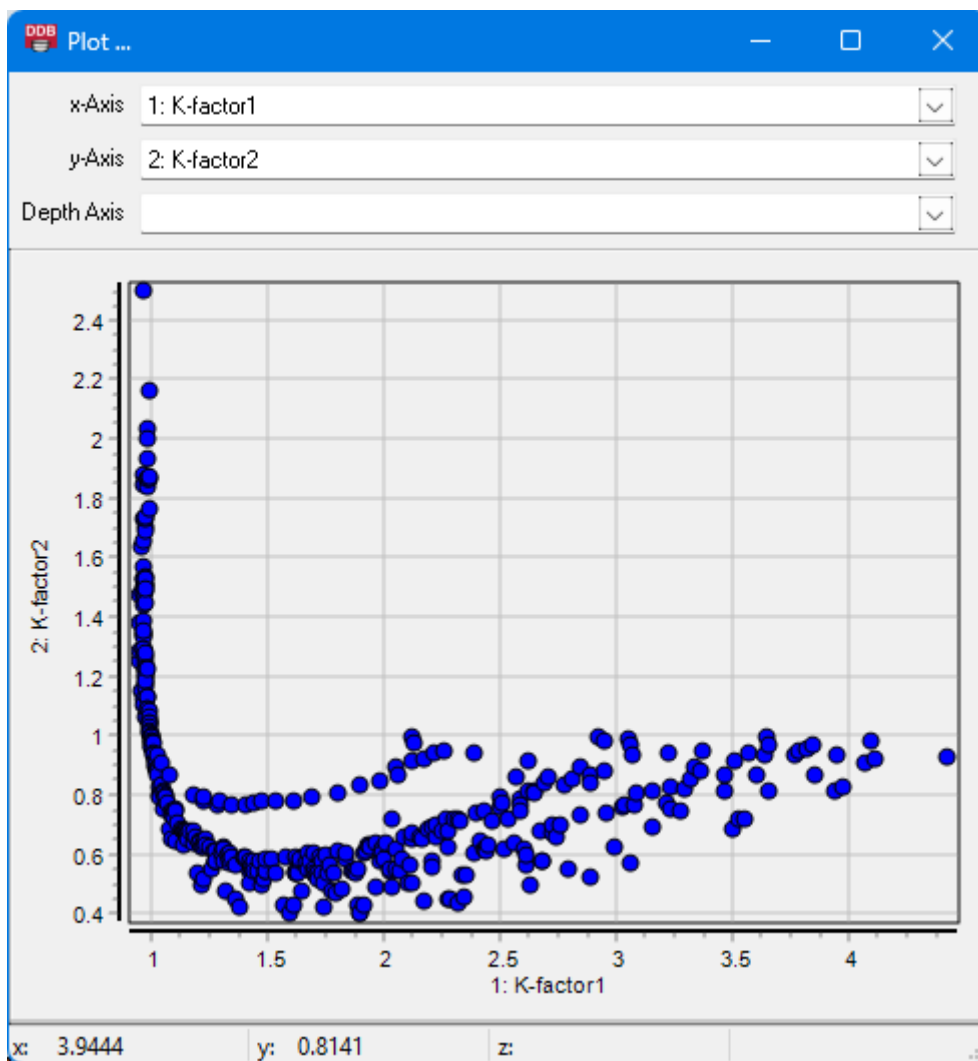


Figure 73: Quick Plot

## 21.5 Sets From Multiple Data Banks

This function allows plotting experimental data from different data banks together in one diagram. This is especially useful for combining VLE, LLE, and SLE data to see all phase equilibria in one diagram.

A first step in showing these diagrams is collecting the data sets. A dialog

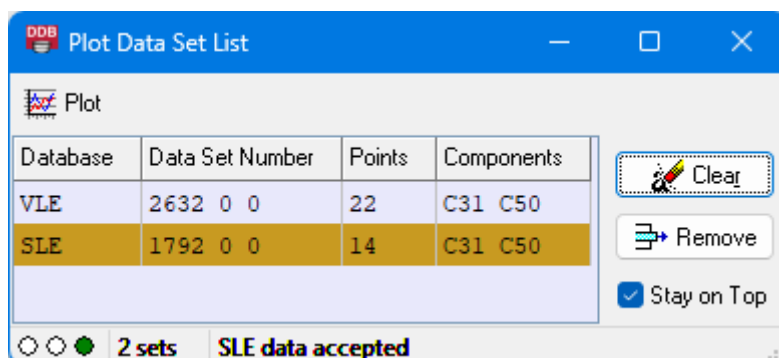


Figure 74: Data Set Collector

is shown where the data sets can be collected by drag'n drop operations. An example for a final diagram for some VLE, LLE, and SLE sets of 1-butanol and water is shown in Figure 75.

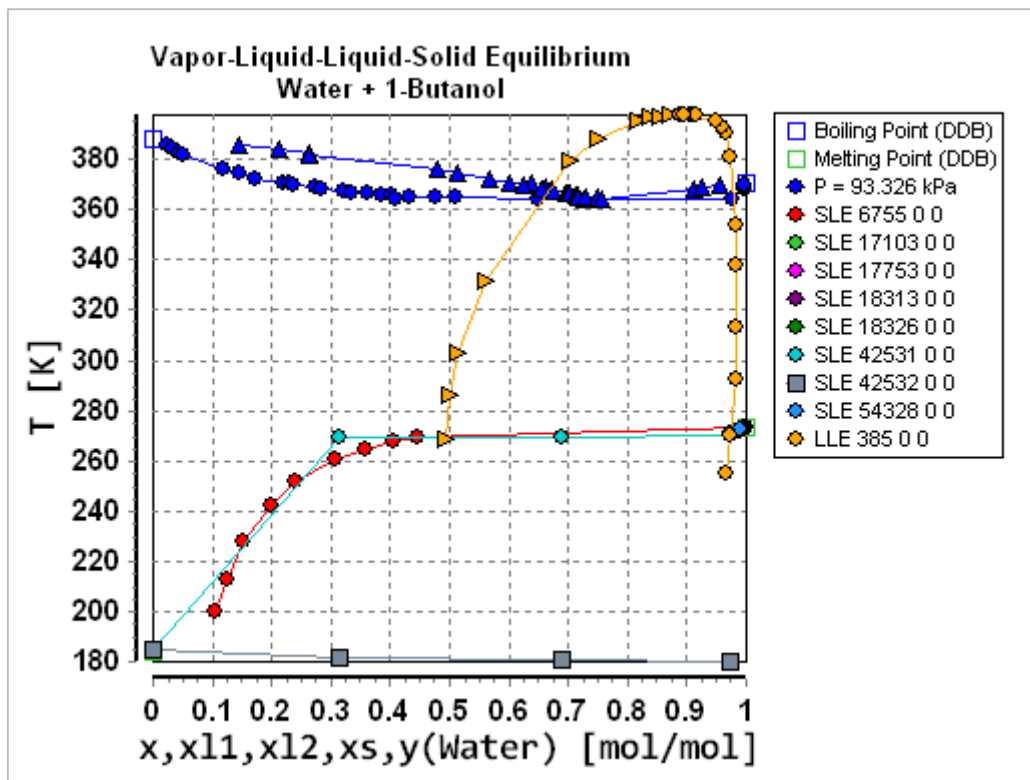
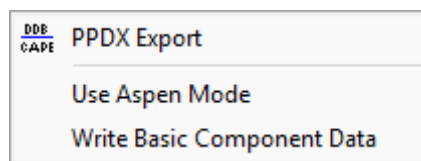


Figure 75: Vapor-liquid-liquid-solid Equilibrium of 1-Butanol and Water

## 22 Data Export

### 22.1 PPDX format



The **Physical Properties Data eXchange** file format is a result of a joined committee of several people from mainly German chemical industry and is intended as a standard file format for the exchange of experimental data and parameters between programs from independent vendors. It is part of the efforts to provide some kind of standard for information exchange in the computer-aided process engineering (CAPE) area.

The PPDX format is purely text based and uses tags for identifying data types. It is easy to read by humans but unfortunately quite difficult to write and read correctly by computer programs since it lacks some necessary definitions and information. A more detailed description of the format and its problem is available in a separate document.

The current definition document can be obtained from the [DECHEMA](#).

PPDX data files always carry the extension “.IKC”. All marked sets are exported together in a single file.

The option “Use Aspen Alias” can be used to export the Aspen alias for components in the FORMULA block instead of the normal empirical formula. Aspen aliases are available for approx. 1500 components. Using this alias allows the Aspen simulator software to match the imported components easily to its own component system.

The option “Write Basic Component Data” adds some data from the DDB's component definition file like critical data and more.

In addition to the experimental data some basic pure component information is exported.

Supported data banks are

- VLE and HPV – vapor-liquid equilibria
- LLE – liquid-liquid equilibria
- HE – mixing enthalpies
- GLE – gas solubilities
- VE – (excess) volumes and densities
- PCP – pure component properties
- ACT – activity coefficients at infinite dilution
- AZD – azeotropic information
- SLE – solid-liquid equilibria
- CPE – (excess) heat capacities

### 22.2 Aspen INP Format

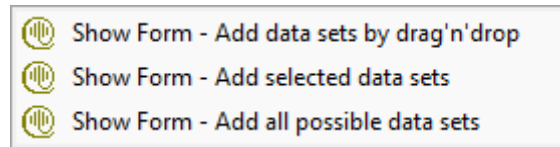
The Aspen INP format is the format for the AspenTech simulator and other related software. A detailed description can be found in the AspenTech documentation.

Supported data banks are

- VLE and HPV – vapor-liquid equilibria
- LLE – liquid-liquid equilibria

- HE – enthalpies of mixing
- GLE – gas solubilities
- AZD – azeotropic information
- ACM and ACT – activity coefficients at infinite dilution
- PCP – selected pure component properties.

Pure component and mixture properties cannot be exported in the same file.



Data sets have to be collected before they can be exported. This “collection” is done by drag 'n' drop from the data set list in the query result window to the Aspen window.

The drop-down-dialog provides two other modes.

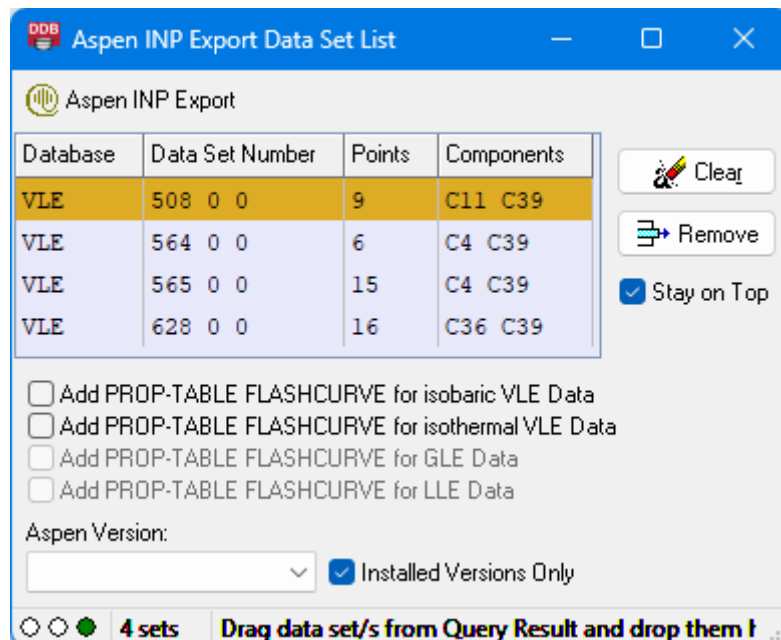


Figure 76: Aspen INP Export - Data Set List – Mixture Data Banks

- “Add selected sets”  
The collection dialog is opened and all marked sets are inserted.
- “Add all possible data sets”  
The collection dialog is opened and all exportable data sets from all supported data banks are inserted. If the pure component properties (PCP) data bank has been active this collector dialog only contains PCP data and won't accept mixture property data sets. If any supported mixture properties data bank is active only mixture properties will be added to the collector dialog and PCP data won't be accepted.

The export function can write additional property table for some data types (VLE, GLE, LLE). Adding these flash-curve blocks forces the Aspen simulator to perform some calculations after loading the file.

Aspen INP normally has the extension “.INP” but can also have the extension “.APRINP”.

The following pure component properties are supported:

- Normal boiling point (normal boiling points are extracted from saturated vapor pressure (VAP) data sets – temperature at atmospheric pressure).
- Critical pressure, temperature, and volume.
- Heat for formation
- Melting temperature

Another limitation is that a single export can contain only data for a single component and only a single value of a specific property. A file might contain a normal boiling point and a critical temperature but not two normal boiling points. The collector dialog therefore has been extended by a selection column allowing data sets to specify.

Database	Data Set Number	Points	Components	Export?	Property	Table Item	Value
PCP	17820 0 0	1	39	<input type="checkbox"/>	VAP	T	390.71 K
PCP	17913 0 0	1	39	<input type="checkbox"/>	VAP	T	390.75 K
PCP	19473 0 0	1	39	<input type="checkbox"/>	VAP	T	390.55 K
PCP	22103 0 0	1	39	<input checked="" type="checkbox"/>	VAP	T	390.23 K
PCP	39961 0 0	1	39	<input checked="" type="checkbox"/>	CRI	T	564.15 K
PCP	44562 0 0	1	39	<input type="checkbox"/>	HFO	ENTH	-332837.00 J/mol
PCP	45126 0 0	1	39	<input type="checkbox"/>	HFO	ENTH	-325808.00 J/mol
PCP	45254 0 0	1	39	<input checked="" type="checkbox"/>	HFO	ENTH	-332837.00 J/mol

Aspen Version:   Installed Versions Only

8 sets Drag data set/s from Query Result and drop them here

Figure 77: Aspen INP Export - Data Set List – Pure Component Properties Data Bank

## 22.3 Data Points Export

### 22.3.1 Export Mixture Data

#### Export Datapoints

This export creates a large data table where all data from all data banks are collected.

It is possible to export marked sets directly but it also possible to collect data before exporting.

If collecting data, a very similar collector dialog like used for the Aspen export.

The export creates a table where all columns of all data sets are presented. This table can become rather bulky if many different data have been added. The table can be copied to the Windows clipboard in a spreadsheet (like Microsoft Excel) compatible format. Supported file formats are the “.csv” format (comma separated values), the Microsoft Excel format, and an HTML based format.

Database	Data Set Number	Points	Components
VLE	35 0 0	9	C110 C39
VLE	46 0 0	5	C110 C39
VLE	119 0 0	11	C78 C131
VLE	120 0 0	9	C78 C131
VLE	133 0 0	30	C110 C89
VLE	223 0 0	9	C110 C39

6 sets VLE data accepted

Figure 78: Data Points Export - Data Set List

### 22.3.2 Export Pure Component Properties

The pure component exports the data sets immediately without a possibility to collect them in a separate form. This export creates separate export dialogs for all properties found in the marked data sets. For example, if data sets with surface tensions, thermal conductivities, and vapor pressures have been selected three result windows will be created, for each property one window.

The result window and its functions are the same as for the mixture data.



## 23 Appendix – GLE Conversion

### 23.1 Overview

The following coefficients are supported.

- *Mole fraction Gas* (“x gas \*10<sup>4</sup>”, “x gas”)
 

The coefficient “x gas \*10<sup>4</sup>” is converted to mol(Gas)/mol(System).
- *Molar ratio / Loading* (“mole gas/mole solvent”, “mole gas/mole solv.1”, “mole gas/mole amine”)
 

The coefficient “mole gas/mole solvent” is converted to mol(Gas)/mol(Solvent).
- *Henry 1 – P<sub>gas</sub>/x<sub>gas</sub>* (“Henry co. (P)”, “Henry co. (f)”, “Henry co. (P)/1000”)
 

The coefficient “Henry co. (P)/1000” is converted to P(Gas)/(mol(Gas)/mol(System)).
- *Henry 2 – P<sub>gas</sub>/C<sub>gas</sub>*

The coefficient “P<sub>gas</sub>/(mol/dm<sup>3</sup>)” is converted to P(gas)/(mol(gas)/cm<sup>3</sup>(Solvent)).
- *Ostwald*

The coefficient “Ostwald co.\*1000” is converted to cm<sup>3</sup>(Gas)/cm<sup>3</sup>(Solvent).
- *Kuenen*

The coefficient “Kuenen co.\*1000” is converted to Ncm<sup>3</sup>(Gas)/g(Solvent).
- *V<sub>gas</sub>/ML* (“gas volume/g solvent”)
 

The coefficient is given in cm<sup>3</sup>(Gas)/g(Solvent).
- *Bunsen*

The coefficients “Bunsen co.\*100”, “Bunsen co.\*1000” are converted to Ncm<sup>3</sup>(Gas)/cm<sup>3</sup>(Solvent).
- *Molality* (“mole gas/g solvent”, “mole gas/g solv.\*10<sup>7</sup>”, “mole gas/1000 g solv.”)
 

The coefficients “mole gas/g solv.\*10<sup>7</sup>”, “mole gas/1000 g solv.” are converted to mol(Gas)/g(Solvent).
- *Molarity* (“mole gas/dm<sup>3</sup> solvent”, “mole gas/m<sup>3</sup> solvent”)
 

The coefficients are converted to mol(Gas)/cm<sup>3</sup>(Solvent).
- *Weight ratio* (“mg gas/kg solvent”)
 

The coefficient is converted to g(Gas)/g(Solvent).
- *Technical Coefficient* (“lambda”)
 

The coefficient is given in Ncm<sup>3</sup>(Gas)/g(Solvent)/at.

#### 23.1.1 Ostwald Special Treatment

The Ostwald coefficient  $c_o$  is converted first to a *Bunsen* coefficient  $c_b$  before further conversion steps are performed. The initial conversion assumes the rule for ideal gases applies. Given is  $c_o$  [cm<sup>3</sup>/cm<sup>3</sup>],  $P_{\text{gas}}$  [Pa],  $T$  [K]. Needed is  $c_b$  [cm<sup>3</sup>/cm<sup>3</sup>] with  $P_{\text{gas}} = 101325$  Pa and  $T = 273.15$  K.

So,  $c_b = c_o * 273.15 * P / (101325 * T)$ .

In case  $P_{\text{total}}$  instead of  $P_{\text{gas}}$  is given, then  $P_{\text{total}}$  is taken as pressure value (simplification!).

## 23.2 Conversion to Henry

The conversion is possible for binary systems (1 gas, 1 solvent) only.

For the coefficients *Henry 1*, *Henry 2* the pressure part is converted to Pa.

For the coefficient *Henry 1* the resulting value is now directly taken as Henry [Pa].

### 23.2.1 Mole of Gas Calculation

For the coefficient *Henry 2* – in case the total pressure is given – it is assumed  $C_{\text{gas}} = 1.0\text{E}^{-10} \text{ mol/cm}^3$ . So,  $P_{\text{gas}} [\text{Pa}] = \text{coeff\_value} * 1.0\text{E}^{-10}$  (simplification!). Now the *molality* =  $P_{\text{gas}}/\text{coeff\_value}$  is calculated. Which means the molality is always  $1.0\text{E}^{-10} \text{ mol(Gas)/cm}^3(\text{Solvent})$ .

For the coefficients *Kuenen*, *Bunsen*, *Technical Coefficient* the  $\text{Ncm3(Gas)}$  is converted by

$$\text{mol}_{\text{gas}} = \frac{c * D_{\text{norm}}}{M_{\text{gas}}},$$

where  $c$  is the given coefficient,  $D_{\text{norm}}$  is the norm density of the gas and  $M_{\text{gas}}$  is the gas molecular weight. The norm density [ $\text{g/cm}^3$ ] is taken from the file NormDensity.txt (unit=[ $\text{g/dm}^3$ ]). In case there is no stored norm density, then the norm density is calculated from the molecular weight:

$$D_{\text{norm}} = \frac{M_{\text{gas}}}{0.044615311}.$$

For the coefficient *Weight ratio* the mole of the gas is calculated from the weight of the gas by

$$\text{mol}_{\text{gas}} = \frac{c}{M_{\text{gas}}},$$

where  $c$  is the given coefficient.

In all equations above,  $M_{\text{gas}}$  is the molecular weight of the gas.

For the coefficient *Vgas/ML* the mole of the gas is calculated from the volume using the ideal gas law:

$$\text{mol}_{\text{gas}} = \frac{c * P_{\text{gas}}}{273.15 * 10^6 * 8.31433},$$

where  $c$  is the given coefficient and  $P_{\text{gas}}$  is the given gas partial pressure. If  $P_{\text{total}}$  is given, then the approximation  $P_{\text{gas}} \approx P_{\text{total}} - P_{\text{solv}}^S$  is used, where  $P_{\text{solv}}^S$  is the solvent vapor pressure.

### 23.2.2 Solvents Weight Calculation

For the coefficients *Henry 2*, *Bunsen*, *Molarity* the *molality* is calculated from the *molarity* by

$$\text{Molality} = \text{molarity} / \text{Density}_T(\text{Solvent}) [\text{mol(Gas)/g(Solvent)}].$$

For each solvent component, the density [ $\text{g/cm}^3$ ] is calculated at the given temperature using the DIPPR 105 equation. In case no equation parameters are available, the density value from the components database is taken (simplification!).

### 23.2.3 Mole Fraction of Gas Calculation

For the coefficient *Mole fraction Gas* the concentration value  $x_{\text{gas}} = \text{coeff\_value}$ .

For the coefficient “mole gas/mole solvent” the concentration value  $x_{\text{gas}} = \text{coeff\_value}/(1 + \text{coeff\_value})$ .

For the coefficient “mole gas/mole solv.1” (Systems with two or three solvents) the concentration value is calculated by

$$x_{\text{gas}} = \frac{c}{S+c},$$

where  $c$  is the given coefficient and  $S$  is the sum of moles of the solvents in solvent mixture (must be calculated assuming 1 mol of solvent 1 is present).

If given or calculated, the mole fraction of the gas is calculated from the *molarity*  $m$  by

$$x_{\text{gas}} = \frac{m \cdot M_{\text{solv}}}{m \cdot M_{\text{solv}} + 1},$$

where  $M_{\text{solv}}$  = the molecular weight of the gas-free solvent.

### 23.2.4 Partial Pressure Calculation

If  $P_{\text{total}}$  is given and  $x_{\text{gas}}$  is given or calculated, then  $P_{\text{gas}} = P_{\text{total}} - P_{\text{solv}}$ . Where  $P_{\text{solv}}$  is the solvent(s) partial vapor pressure:  $P_{\text{gas}} = P_{\text{total}} - \sum_i x_i \cdot P_i^S$ . For each solvent component, the vapor pressure is calculated using the Antoine equation.

### 23.2.5 Henry Coefficient Calculation

If  $P_{\text{gas}}$  and  $x_{\text{gas}}$  are given or calculated, then Henry =  $\frac{P_{\text{gas}}}{x_{\text{gas}}}$ .

## 23.3 Conversion to TPxy

### 23.3.1 Converting Solvents Molarity

For two or more solvents, the solvents *molarity* values are converted to gas free mole fractions.

First of all, the molar volumes for the solvents are calculated:

$$V_m(\text{solv}_i) = \frac{M(\text{solv}_i)}{D_{25}(\text{solv}_i)}$$

where  $M(\text{solv}_i)$  is the molecular weight of solvent  $i$  and  $D_{25}(\text{solv}_i)$  is the density of solvent  $i$ , calculated at 298.15 K as described in section 23.2.2.

Now the missing molarity of the last solvent is calculated:

$$M(\text{solv}_n) = \frac{1.0 - \sum_{i=1}^{n-1} M(\text{solv}_i) \cdot V_m(\text{solv}_i)}{V_m(\text{solv}_n)}$$

where  $n$  is the number of solvents.

Finally, the gas free mole fractions of the solvents are calculated by

$$x_{\text{gf}}(\text{solv}_i) = \frac{M(\text{solv}_i)}{\sum_{j=1}^n M(\text{solv}_j)}$$

### 23.3.2 Converting Solvents Weight Percent

For two or more solvents, the solvents *weight percent* values are converted to gas free mole fractions.

First of all, the total mole of the solvents is calculated

$$\text{mol}_{\text{solv}} = \sum_{i=1}^{n-1} \frac{w\%(\text{solv}_i)}{M_{\text{solv}_i}} + \frac{100.0 - \sum_{i=1}^{n-1} w\%(\text{solv}_i)}{M_{\text{solv}_n}}$$

where  $n$  is the number of solvents.

Now, the gas free mole fractions for  $n - 1$  solvents are

$$x_{\text{gf}}(\text{solv}_i) = \frac{w\%(\text{solv}_i)}{M_{\text{solv}_i} \cdot \text{mol}_{\text{solv}}}$$

and the gas free mole fraction of solvent  $n$  is

$$x_{\text{gf}}(\text{solv}_n) = 1.0 - \sum_{i=1}^{n-1} x_{\text{gf}}(\text{solv}_i)$$

### 23.3.3 Total Mole Fractions Calculation

When the gas free (or total) mole fractions of the solvent are given or calculated, then a missing  $x_{\text{gas}}$  is calculated as described in section 23.2.

Now  $x(\text{solv}_i) = x_{\text{gf}}(\text{solv}_i) * (1.0 - x_{\text{gas}})$ .

### 23.3.4 Total Pressure Calculation

If only  $P_{\text{gas}}$  is given, then  $P_{\text{total}} = P_{\text{gas}} - P_{\text{solv}}$ , where  $P_{\text{solv}}$  is calculated as described in section 23.2.4.