

Dortmund Data Bank (DDB)

Retrieval, Display, Plot, and Calculation

Tutorial and Documentation

DDBSP – Dortmund Data Bank Software Package



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

2 Starting the Dortmund Data Bank Retrieval Program

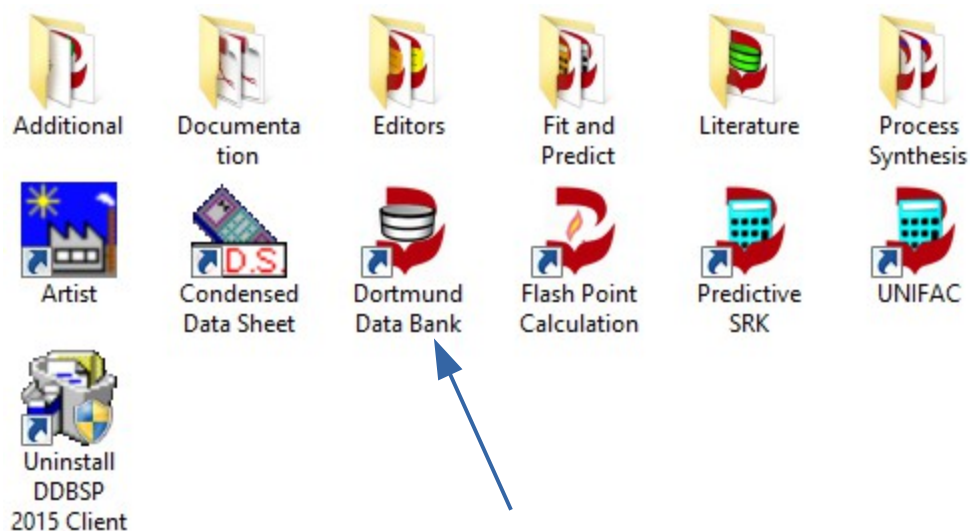


Figure 1

Figure 1 shows a typical program group for the DDB software package. This has become obsolete in Windows 8. The DDB software currently does not yet support the new graphical user interface well. We recommend to use tools like Classic Shell to return to Windows 7 behavior.

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

- Systems (build of components and of component lists)
- References (literature information)
- Single sets (data set numbers)
- Pure component properties
- A special query for selectivity searches (in the ACT database).

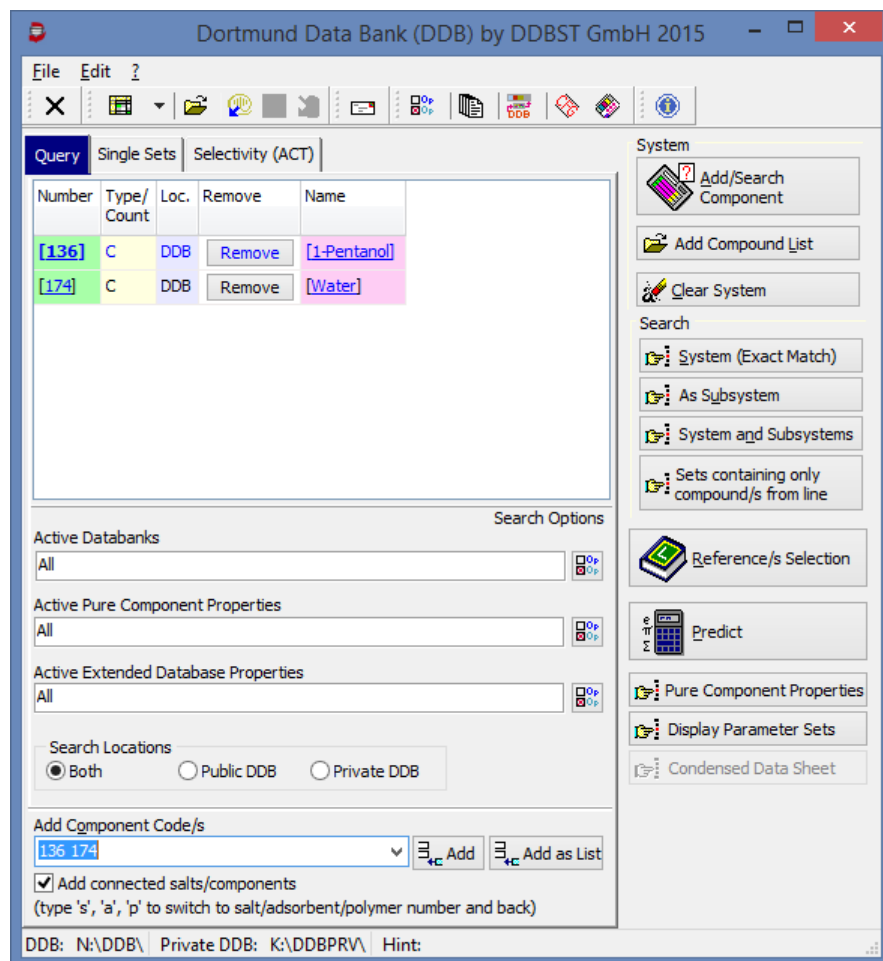


Figure 2 Dortmund Data Bank

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 the ComponentSelection program.

Press  and the ComponentSelection search dialog is displayed:

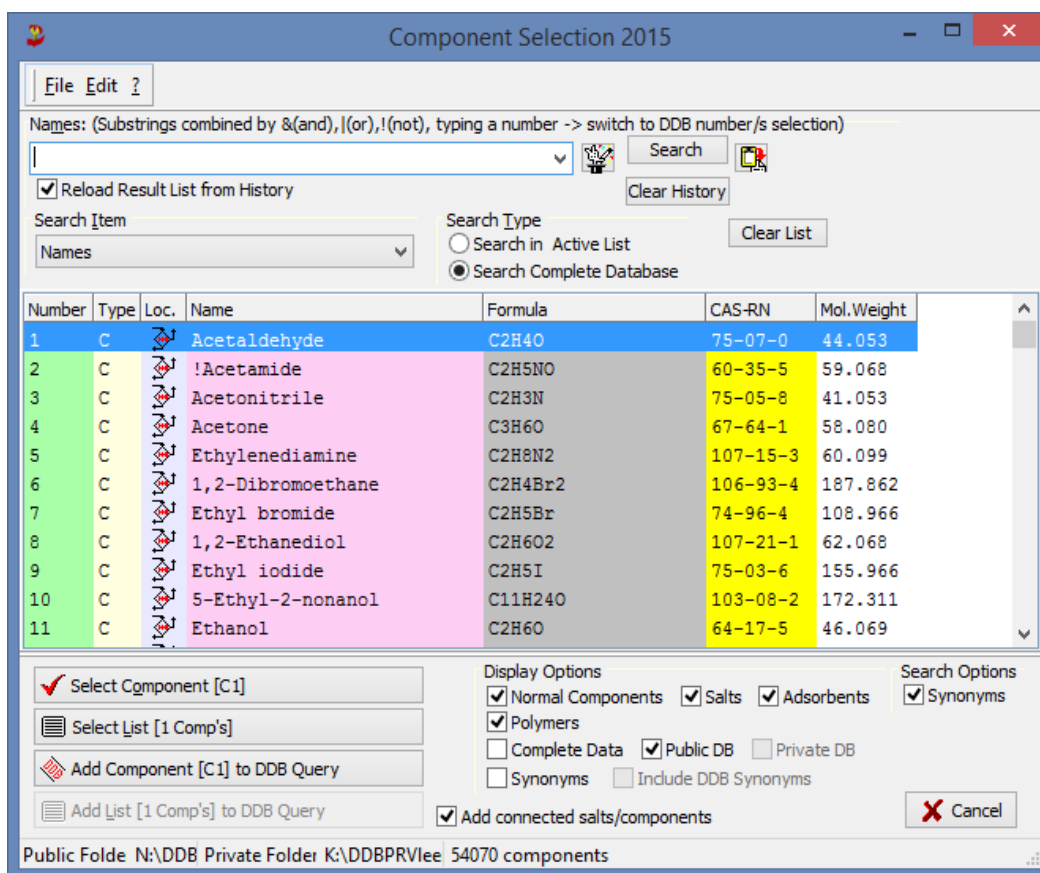



Figure 3 Component Selection

This program has a lot of different search modes which we will not cover here in depth. For the purposes of this tutorial it is sufficient to take a rather quick look at the program.

Component Selection displays the list of components with their

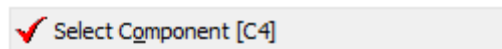
- DDB internal number,

- their type (normal → 'C', salt → 'S', adsorbent → 'A', polymer → 'P'),
- their location ( for the public – DDBST – component list, and PRV for private, customer defined components),
- the empirical formula,
- the CAS registry number,
- and the molecular weight.

3	C	DDB	Acetonitrile	C2H3N	75-05-8	41,05
4	C	DDB	Acetone	C3H6O	67-64-1	58,08
5	C	DDB	Ethylenediamine	C2H8N2	107-15-3	60,10

A component can be selected by a double-click

or by checking its line and pressing the



button.

Nonane has to be searched since it isn't displayed under the first twelve components which are initially shown. The search string “nonane” (cases are ignored) has to be typed in the search field.

Names: (Substrings combined by &(and),!(or),!(not), typing a number -> switch to DDB number/s selection)

nonane












☒ Reload Result List from History

Search

Clear History

After pressing the search button or by pressing the return/enter key the search is performed. ComponentSelection displays all components which names contain “nonane”. The single exact matching name is the first of the list.


Note: Dibutyl sulfide has been found because of the also stored synonym Thianonane.


Number	Type	Loc.	Name	Formula	CAS-RN	Mol.Weight
398	C		Nonane	C9H20	111-84-2	128,26
301	C		2-Hydroxy-2-methyl-propionic	C8H16O3	816-50-2	160,21
397	C		Perfluorooxacyclononane	C8F16O	1978-24-1	416,09
547	C		Nonanedioic acid dibutyl este	C17H32O4	2917-73-9	300,44
548	C		Nonylbenzene	C15H24	1081-77-2	204,35
725	C		2-Methyloctane	C9H20	3221-61-2	128,26
835	C		Diethylene glycol dimethyl et	C6H14O3	111-96-6	134,18
1119	C		2,2,4,4,6,8,8-Heptamethylnona	C16H34	4390-04-9	226,44
1255	C		Dibutylsulfide	C8H18S	544-40-1	146,29
1284	C		1,3-Nonanediol	C9H20O2	23433-07-0	160,26
1289	C		2,4-Dimethyl-2,4-nonanediol	C11H24O2	69201-96-3	188,31


After double-clicking the Nonane line the component is added to the query list. The third component shall be CH₄O – Methanol. The query result window now contains three components and the search buttons are all enabled now.


Number	Type/Count	Loc.	Remove	Name
[4]	C	DDB	<input type="button" value="Remove"/>	[Acetone]
[110]	C	DDB	<input type="button" value="Remove"/>	[Methanol]
[398]	C	DDB	<input type="button" value="Remove"/>	[Nonane]

Search





 System (Exact Match)

 As Subsystem

 System and Subsystems

 Sets containing only compound/s from line

The single buttons perform different type of searches:

<i>Button</i>	<i>Function</i>
 System (Exact Match)	An 'Exact Search' finds only data sets build of the three collected components.
 As Subsystem	An 'As Subsystem' search find all data sets build of the three collected components plus all data sets with these components and any other (quaternary and higher systems).
 System and Subsystems	A 'System and Subsystem' search finds all data sets build of the three components plus all data sets build by the binary (Acetone/Nonane, Acetone/Methanol, Nonane/Methanol) subsystems and data sets for the pure components.
 Sets containing only compound/s from line	This button is only enabled if a single line in the query result window is selected. This search only find sets for the components in that marked line. If this line only contains a single components, only pure component data sets will be found.


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	Ref.No.	Reference
[14163 0 0]	DDB	13	3	[C4 Acetone] [C110 Methanol] [C398 Nonane]	278 (const.)		n.a.		13 tie lines, 2 Ph.		2003	2225	[53809] Tc
[14164 0 0]	DDB	10	3	[C4 Acetone] [C110 Methanol] [C398 Nonane]	288 (const.)		n.a.		10 tie lines, 2 Ph.		2003	2225	[53809] Tc
[14165 0 0]	DDB	8	3	[C4 Acetone] [C110 Methanol] [C398 Nonane]	298 (const.)		n.a.		8 tie lines, 2 Ph.		2003	2225	[53809] Tc

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 build in ComponentSelection by selecting multiple components

and press the

 Select List [3 Comp's]

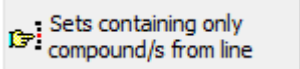
button. The resulting query window is

Number	Type	Loc.	Name	Formula	CAS-RN	Mol.Weight
3	C	DDB	Acetonitrile	C2H3N	75-05-8	41,05
4	C	DDB	Acetone	C3H6O	67-64-1	58,08
5	C	DDB	Ethylenediamine	C2H8N2	107-15-3	60,10
6	C	DDB	1,2-Dibromoethane	C2H4Br2	106-93-4	187,87
7	C	DDB	Ethyl bromide	C2H5Br	74-96-4	108,97
8	C	DDB	1,2-Ethanediol	C2H6O2	107-21-1	62,07
9	C	DDB	Ethyl iodide	C2H5I	78-03-6	155,97
10	C	DDB	5-Ethyl-2-nonanol	C11H24O	103-08-2	172,31
11	C	DDB	Ethanol	C2H6O	64-17-5	46,07
12	C	DDB	Diethyl ether	C4H10O	60-29-7	74,12
13	C	DDB	Ethylene oxide	C2H4O	75-21-8	44,05
14	C	DDB	2-Propanol-1-ol	C3H8O	107-18-6	58,08

Number	Type/ Count	Loc.	Remove	Name
[398]	C	DDB	Remove	[Nonane]
[110]	C	DDB	Remove	[Methanol]
[List]	3	-	Remove	Component List


If a component list is available on disk (".STL" or ".STX" files, can be stored within ComponentSelection) it is also possible to load these files by the  button.

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

The search mode  now has the effect that data sets are found (pure, binary, and ternary) which are only containing one, two, or three of the list's components.

3.3 Examining Further Query List Functionality

The component list contains three active areas.

1. The 'Number' column contains hyper links which allow to display the content of the line in ComponentSelection. This allows 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  button removes the component or list.
3. The 'Name' column contains hyper links which allow to display component details in the component editor.

Number				
[List]				
Number	Type/ Count	Loc.	Remove	Name
[4]	C	DDB	Remove	[Acetone]
[110]	C	DDB	Remove	[Methanol]
[398]	C	DDB	Remove	[Nonane]
[List]	3	-	Remove	Component List

File ?

Exit DDB PCP PSE Independent Window

Components Salts Adsorbents Ions Groups Polymers Flash Points Heats and

More Save Find New Clear App.Priv. Export Artist Print Stat. Search

Specification

Component number: 136 45867 components

English name: 1-Pentanol

Alternative name: n-Amyl alcohol

Formula: C5H12O CAS-No.: 71-41-0

Antoine constants T [°C] P [mmHg]

Low pressure:	7.44287	1439.27	177.758	Range:	20	138	°C	Tb=410.88 K
High pressure:	6.88703	1113.61	139.919		137	193	°C	Tb=411.20 K

Values

Crit. pressure:	3850.350	kPa	Heat of fusion:	9822.4	J/mol
Crit. temperature:	586.00	K	Melting point:	194.25	K
Crit. volume:	326.0	cm³/mol	Dipole moment:	1.70000	Debye
Acentric factor:	0.58000		Molecular weight:	88.150	g/mol

Density: 811.50 kg/m³ at 298.15 K

UNIFAC groups and UNIQUAC parameters



UNIFAC groups:	3	1001	4002	1014	0	0	0	0
mod. UNIFAC groups:	3	1001	4002	1014	0	0	0	0
UNIQUAC r-value:	4.12870	UNIQUAC q-value:	3.59200					

☒ Overwrite values by PRIVATE.PCP entries

License server state: Success.

Figure 5 Component Editor

The component list also has a context menu with some repeated and few new functions.

- “Main” resp. “Alternative” Names allows to switch between the two main synonyms stored in the component basic file.
- 'Add Component' and 'Add Compound List' are calling the same functions as the  Add/Search Component and  Add Compound List buttons.

- 'Display/Edit Compound List Entries' displays the current line in ComponentSelection (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.

- 'Display Structure' allows to take a look at the structure of the selected component.

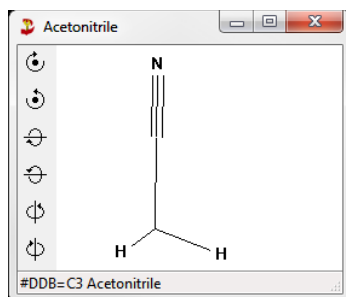


Figure 7: Display Structure

- 'Remove

Component/List' removes the selected component or list (same as pressing the 'Remove' button).

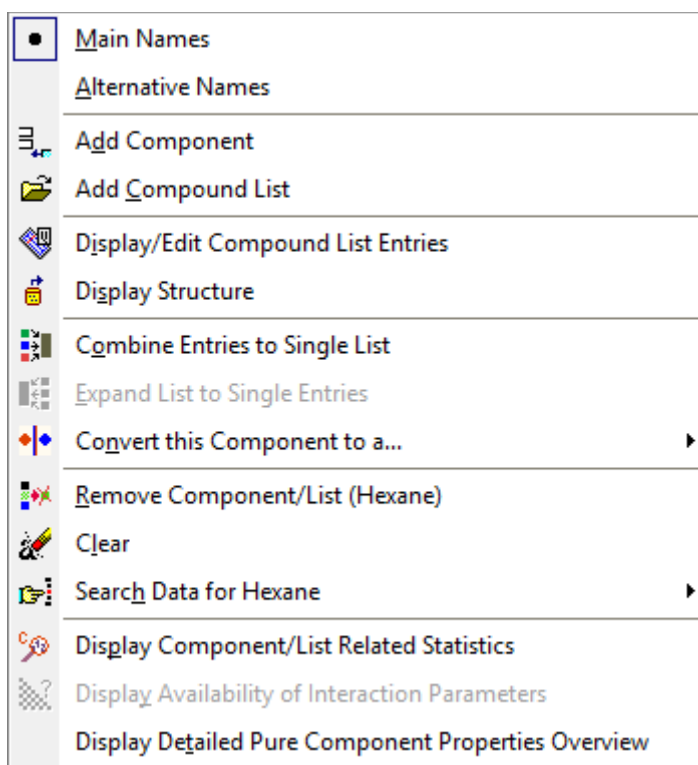
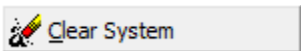
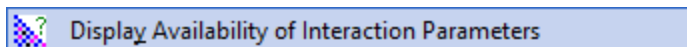
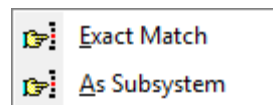
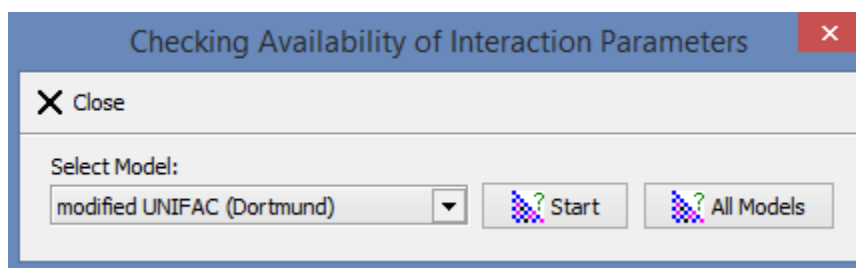


Figure 6: Context Menu - Query Window

- 'Clear' remove all components and lists and does the same as pressing the  button.
- "Search Data for Component List" or "Search Data for Component" allow the "Exact Match" or "As Subsystem" search for components or lists from a single selected line in the Query table without having to remove all other entries first.
- '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. An example is given in the appendix: Example for "Display Component or List Related Statistics" on page 143.
- 'Display Availability of Interaction Parameters'



starts a search for the availability of parameters for some group contribution models used in the Dortmund Data Bank software package:



This function searches for the parameters for all binary pairs from a list. Currently the models UNIFAC, modified UNIFAC(Dortmund), modified UNIFAC (Lyngby), ASOG, PSRK, VTPR, COSMO-RS(OI), COSMO-SAC, MOSCED, and NIST-modified UNIFAC are supported. See chapter 18.15 (Checking Availability of Model Parameters) for more information.

- 'Display Detailed Pure Component Properties Overview' show a detailed statistic over the available data for a component. An example is given in appendix: Example for “Display Detailed Pure Component Properties Overview” on page 144.

The edit field below the list allows to enter DDB component numbers directly 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, which are stored in separate definition files) have to be typed the data type can be switched to salts, adsorbents or polymers by pressing the 's', 'p', or 'a' 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:

11 1000011 2000011 3000011

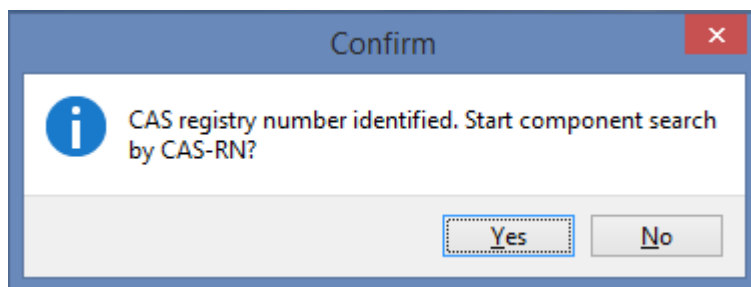
After adding the line the query list looks like

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]

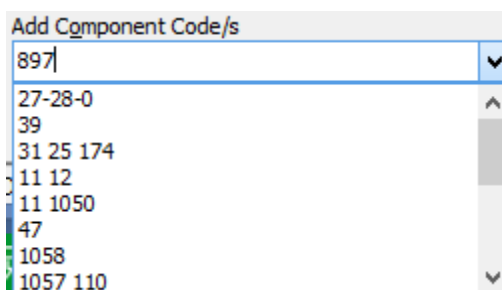
The “Add connected salts/components” check box is useful for adding components which are stored as normal components as well as salts. The DDB maintains currently four component lists (normal components, salts, adsorbents, polymers) and almost all salts are having entries also in the normal component 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 and polymers because these type of components don't have duplicate entries in two lists.

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

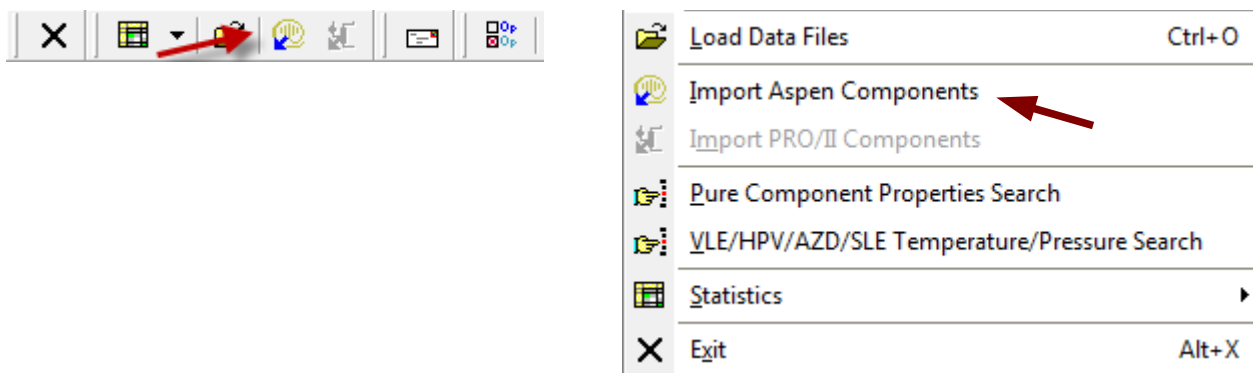


The text field has a history function where the last sixteen entries are stored.



3.4 Import Aspen Components

The Dortmund Data Bank program can read component information from Aspen projects and files.



The import can be done by

- using native internal routines inside the Dortmund Data Bank program. This is the quick and recommended way and supports the Aspen file types ".inp", ".bkp", and ".apt".
- using Aspen directly via an OLE access. This is only working if Aspen is installed on the same workstation where the Dortmund Data Bank program is running. This procedure is rather slow because Aspen has to be started in the background including a license request. The only advantage is that beside the three file types ".inp", ".bkp" and ".apt" also ".apw" files can be opened.

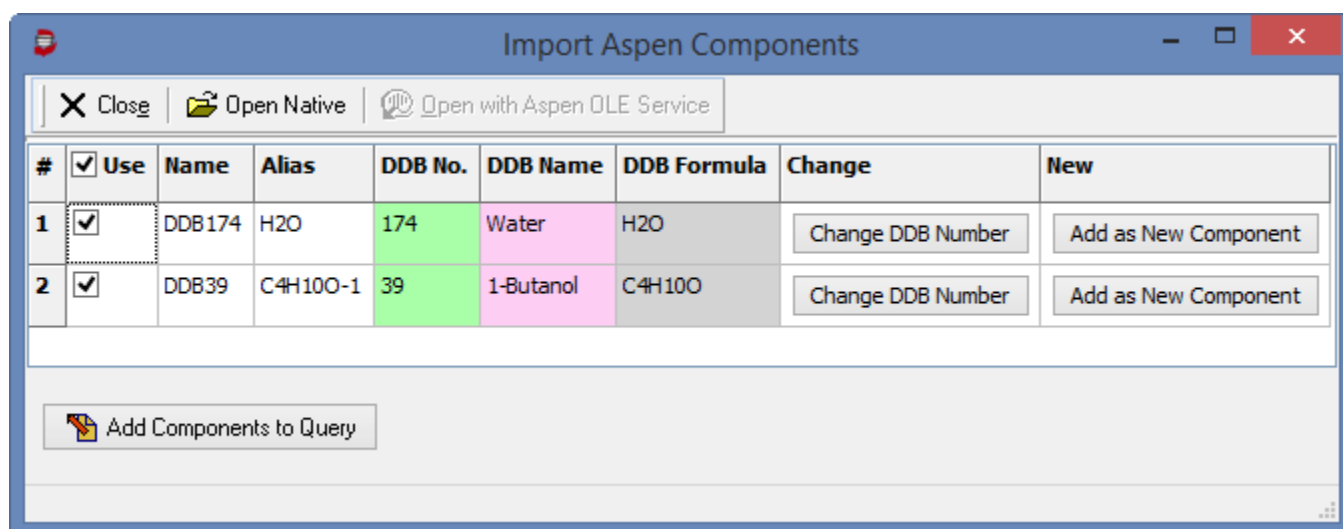


Figure 9: Importing Aspen Components

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 there are two possibilities:

- “Change the DDB Number”: This allows to search an already existing DDB component and use its number.

Figure 10: Adding a New Component

- “Add as New Component”: This opens a “New Component” dialog where the component can be added to the DDB component list (a private component number is preferred).

The component identification is done by a list of Aspen aliases, IDs, and names stored in the synonyms data base of the Dortmund Data Bank. This list has been created from Aspen's version 11.

3.5 Import Pro/II Components

The Dortmund Data Bank program can import components from PRO/II project files (".prz" files).

The component selection is almost the same dialog than the Aspen import dialog and lists all components found in the PRO/II project files and displays the found matching DDB components by their IPS codes which are stored and distributed in the DDB synonyms file.

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

If a component could not be identified it is possible to add a PRO/II component as a new component to the DDB system (private or customer's data bank, "Add as New Component" button).

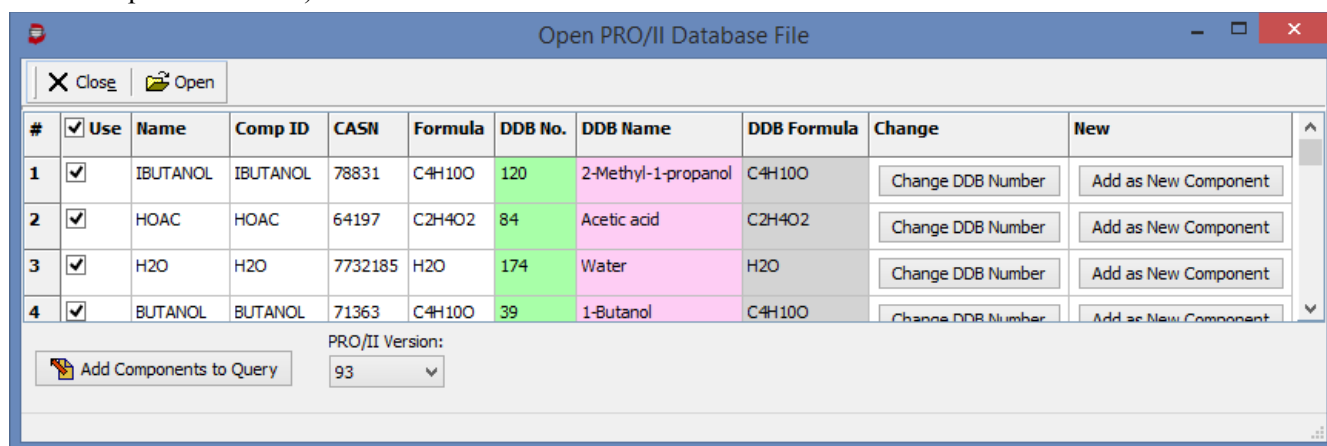
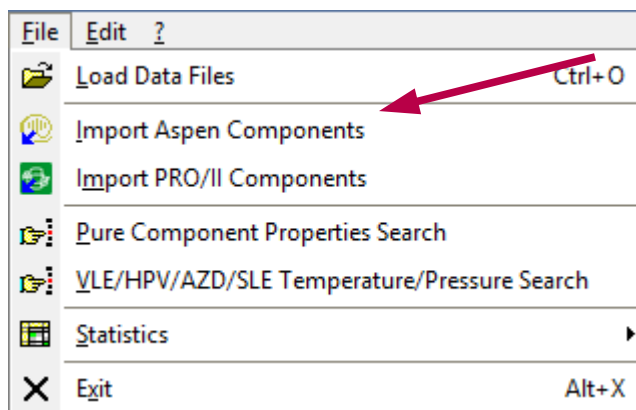
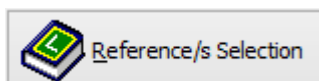


Figure 11: PRO/II Component Import

3.6 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 (LEAR) is a separate program but the dialogs are incorporated seamlessly. The literature search is started by pressing the



Search Query

Quick Search | Advanced Search

Authors*: cordes substring (separated by spaces)

Years*: 2003 (number range)

First Page: exact string

Journals*: Select (numbers, separated by spaces)

Volume: substring

Title: substring (separated by spaces)

Numbers: (number range, positive numbers only)

*) indexed entries Clear Copy to Adv. Search

Libraries to be Searched:

☒ DDBST/p

☒ DDBST

☐ Keep selection until next program start

Search Cancel


Figure 12 Search for References

button. LEAR provides two search modes, one for experienced users with many possible search items and possible combinations and one easier quick search mode which we'll 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
[30608]	An Automated Apparatus for Equilibrium Phase Compositions, Densities, and Interfacial Tensions: Data for Carbon Dioxide + Decane	Shaver R.D.; Robinson R.L.; Gasem K.A.M.	
[30613]	Infinite-dilution activity coefficients for several solutes in hexadecane and in n-methyl-2-pyrrolidone (NMP): experimental measurements and UNIFAC predictions	Schult C.J.; Neely B.J.; Robinson R.L.; Gasem K.A.M.; Todd B.A.	
[30620]	Improved correlations for heavy n-paraffin physical properties	Gao W.; Robinson R.L.; Gasem K.A.M.	

Datasets: 6

Figure 13 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 14: Data Sets from Specified Literature” show 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	Publ.Year	Ref.No.	Reference
[22766 0 0]	DDB	30	2	[C292 Methyl formate] [C174 Water]	298 (const.)		3	78	Px(T)		2001	5322	[48664] Wittig R., Lo
[22767 0 0]	DDB	34	2	[C16 Formic acid ethyl ester] [C174 Water]	298 (const.)		3	34	Px(T)		2001	5322	[48664] Wittig R., Lo
[22768 0 0]	DDB	52	2	[C174 Water] [C288 Formic acid butyl ester]	298 (const.)		3	7	Px(T)		2001	5322	[48664] Wittig R., Lo
[22769 0 0]	DDB	61	2	[C161 Toluene] [C8 1,2-Ethenediol]	323 (const.)		<1	13	Px(T)		2001	5322	[48664] Wittig R., Lo



Figure 14: Data Sets from Specified Literature

3.7 Search Data Sets by Data Set or Reference Numbers



Query **Single Sets** Selectivity (ACT)

Databank
ELE - Vapor-liquid equilibria for systems containing solved salts

Number/s Type
☒ Dataset Numbers ☐ Link Numbers

Input
1088  Show  Open Numbers File

9945 public and 0 private sets available. (Type negative data set numbers for private databanks)

Literature Numbers
131042  Show  Open Numbers File

146744 public and 27 private references available. (Type negative data set numbers for private databanks)

(Use "1/34;-56/-123" for ranges)

Figure 15 Search by Data Set Numbers

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

The reference numbers are actually coming in two flavors. The literature database contains special sub list numbers valid only for single data banks. There are references numbers 1,2,3,4 etc. for the VLE database, and reference numbers 1,2,3,4 etc. for the SLE database and for almost any other database. These sub numbers are called “REF Numbers” or “Link Numbers” whereas the numbers from the complete list are denoted LEAR numbers (the program's name).

“Data set Numbers” and “REF numbers”/“Link Numbers” are database specific and if either a data set number or a Link number shall be searched the database has to selected from the drop-down menu. In case of a search for LEAR number this data bank menu is deactivated.

The input edit fields allow to enter multiple numbers 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.

3.8 Searching Data Sets With Specified Pure Component Properties

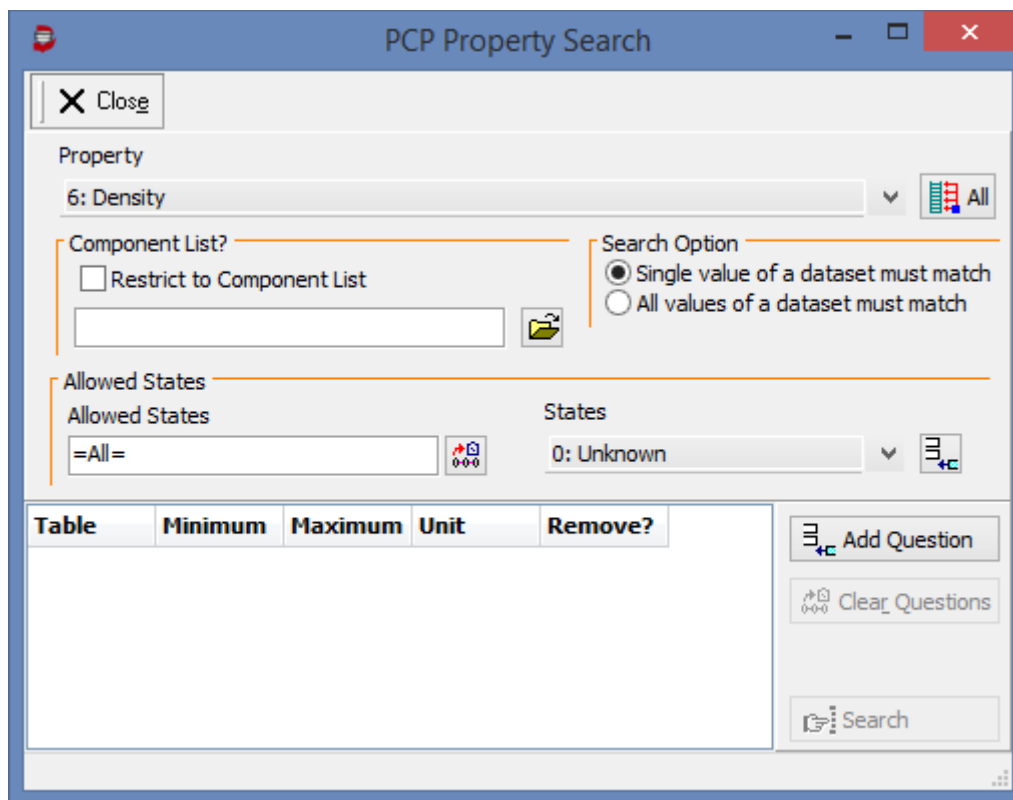

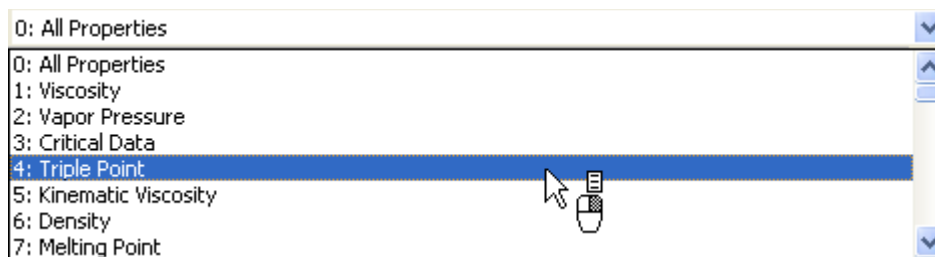


Figure 16: Pure Component Properties Search

The property search dialog can be displayed by pressing the  Pure Component Properties button.

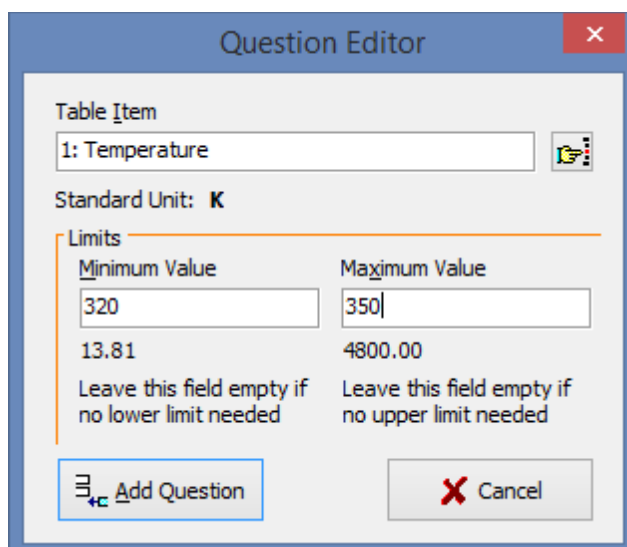
The property search dialog allows to specify the property, to restrict the search to a list of components and states, and allows to specify if a wanted value only needs to be present in a data set or if all data points of a set must meet the given criteria.



The questions (criteria) are simply upper and lower limits for a specific table item

Table Item	Minimum Value	Maximum Value	Unit	Remove?
1 T	320	350	K	<button>Remove</button>
7 VSK	0.5	6.0	m2/s	<button>Remove</button>

and are entered through a simple dialog.



Question Editor



Table Item
1: Temperature

Standard Unit: K

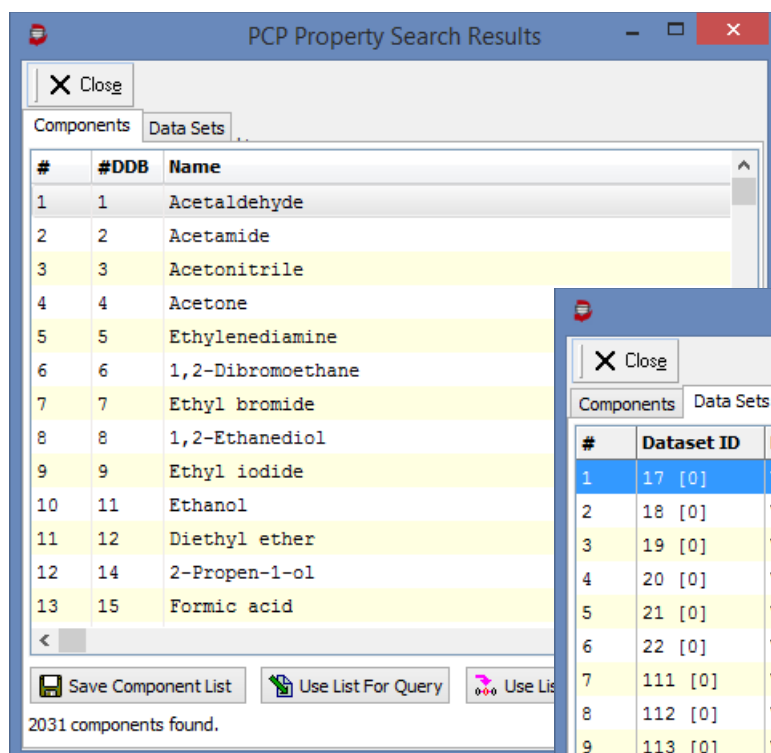
Limits

Minimum Value	Maximum Value
320	350
13.81	4800.00

Leave this field empty if no lower limit needed Leave this field empty if no upper limit needed

 Add Question  Cancel

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



PCP Property Search Results

Close

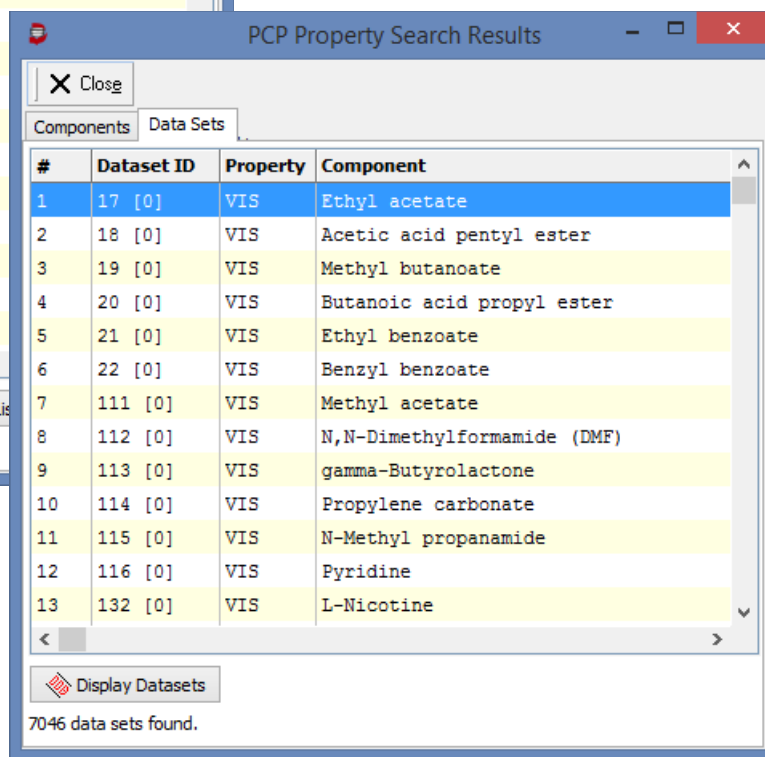
Components Data Sets

#	#DDB	Name
1	1	Acetaldehyde
2	2	Acetamide
3	3	Acetonitrile
4	4	Acetone
5	5	Ethylenediamine
6	6	1,2-Dibromoethane
7	7	Ethyl bromide
8	8	1,2-Ethanediol
9	9	Ethyl iodide
10	11	Ethanol
11	12	Diethyl ether
12	14	2-Propen-1-ol
13	15	Formic acid

Save Component List Use List For Query Use List For Query

2031 components found.

Figure 17: Property Search - Component List



PCP Property Search Results

Close

Components Data Sets

#	Dataset ID	Property	Component
1	17 [0]	VIS	Ethyl acetate
2	18 [0]	VIS	Acetic acid pentyl ester
3	19 [0]	VIS	Methyl butanoate
4	20 [0]	VIS	Butanoic acid propyl ester
5	21 [0]	VIS	Ethyl benzoate
6	22 [0]	VIS	Benzyl benzoate
7	111 [0]	VIS	Methyl acetate
8	112 [0]	VIS	N,N-Dimethylformamide (DMF)
9	113 [0]	VIS	gamma-Butyrolactone
10	114 [0]	VIS	Propylene carbonate
11	115 [0]	VIS	N-Methyl propanamide
12	116 [0]	VIS	Pyridine
13	132 [0]	VIS	L-Nicotine

Display Datasets

7046 data sets found.

Figure 18: Property Search - Data Set List

The component list can be saved (as a “.STL” 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.

3.9 Searching Vapor-Liquid and Solid-Liquid Equilibria with Specified Temperatures and Pressures

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

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.

Figure 20: VLE/AZD/SLE Temperature/Pressure Search Criteria

The search result are two different kind of windows.

1. A standard query result window showing all the found data sets
2. A table output with all matching data points

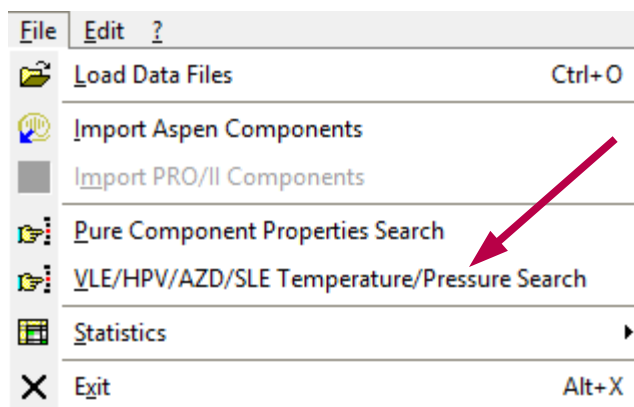


Figure 19: VLE/AZD/SLE Temperature/Pressure Search Menu Entry

Query Result [1] <AZD,CRI,GLE,HE,HPV,MPVT,SLE,VIS,X>

File Edit

AZD CRI GLE HE HPV MPVT SLE VIS X

All Sets All Points All Refs Sets Points Refs

54 54 5 54 54 5

=AZD= Azeotropic/zeotropic information

All References
 All Systems
 Binary
 All Components
 All Sources
 All Counters
 All Data Types

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]
[28777 0 0]	DDB	1	2	[C1051 Methane] [C134 Pentane]	186 (const.)		n.a.	
[28778 0 0]	DDB	1	2	[C1051 Methane] [C134 Pentane]	178 (const.)		n.a.	
[35063 0 0]	DDB	1	2	[C1051 Methane] [C134 Pentane]	278 (const.)		n.a.	
[35064 0 0]	DDB	1	2	[C1051 Methane] [C134 Pentane]	283 (const.)		n.a.	

[6813] Berry V.M., Sage B.H., Nat.Stand.Ref.Data Ser.NBS, 1-66, 1970

1 dataset/s marked.

Figure 21: Search Result in Standard Query Window

Grid Output

Close Print Copy Copy HTML Save Mail

Grid Output

Data bank	#Dataset	T [K]	P [kPa]	x1	x2	x3	y1	y2	y3	#DDB1	#DDB2
HPV	85	305.37	137.9000	0.00200			0.30200			1051 Methane	134 Pentane
HPV	86	310.93	137.9000	0.00120			0.16810			1051 Methane	134 Pentane
HPV	87	316.48	137.9000	0.00040			0.05030			1051 Methane	134 Pentane
HPV	114	310.93	108.2500	0.00000			0.00000			1051 Methane	134 Pentane
HPV	114	310.93	137.9000	0.00150			0.20900			1051 Methane	134 Pentane
HPV	144	348.15	122.7300	0.00000			0.00000			1051 Methane	89 Hexane
HPV	168	377.59	120.5200	0.00000			0.00000			1051 Methane	91 Heptane
HPV	193	310.93	137.9000	0.00705			0.99608			1051 Methane	60 Decane
HPV	194	344.26	137.9000	0.00617			0.97919			1051 Methane	60 Decane
HPV	195	377.59	137.9000	0.00521			0.91722			1051 Methane	60 Decane
HPV	227	310.93	108.2500	0.00000			0.00000			1054 Ethane	134 Pentane

Figure 22: Search Result as Data Point Table

3.10 Selectivity Search

The screenshot shows the 'Selectivity (ACT)' tab of a software interface. At the top, there are three tabs: 'Query', 'Single Sets', and 'Selectivity (ACT)'. Below the tabs, there are three input sections. The first section is for 'Solute 1', with a button labeled 'Solute 1' and an 'All Sets' button. The second section is for 'Solute 2', with a button labeled 'Solute 2' and an 'All Sets' button. The third section is for 'Single Solvent', with a checked checkbox, a button labeled 'Solvent', and an 'All Sets' button. At the bottom, there are two buttons: 'Search' and 'Predict'.

Figure 23: Selectivity Search

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

This dialog allows to perform three different tasks:

1. Specification of two solutes and a single solvent. The resulting query result and plot 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.
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.

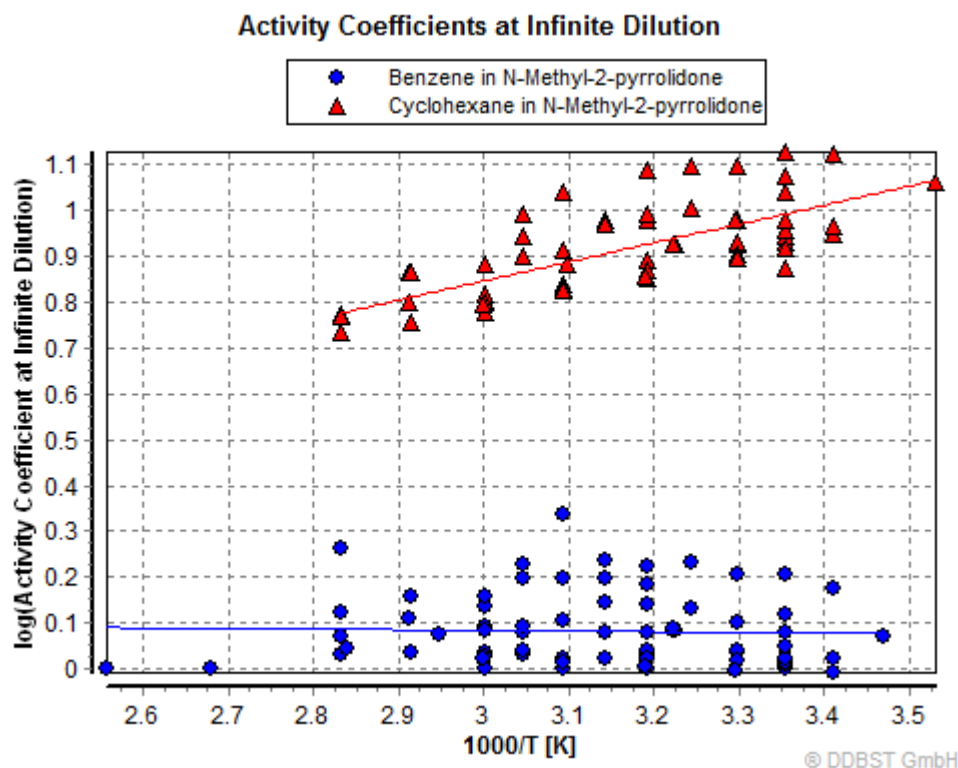


Figure 24: Selectivity Diagram

- Predicting selectivity. The prediction calculates activity coefficients at infinite dilution for both solvents in a single solvent and displays the result either as a table or as a query result in the Dortmund Data Bank program. The resulting plot is the same as for the data set search with the exception that only predicted data are displayed.

3.11 Search Options

3.11.1 Data Banks Preselection

Search Options

Active Databanks	<input type="text" value="All"/>	<input type="checkbox"/> 0p <input checked="" type="checkbox"/> 0p
Active Pure Component Properties	<input type="text" value="All"/>	<input type="checkbox"/> 0p <input checked="" type="checkbox"/> 0p
Active Extended Database Properties	<input type="text" value="All"/>	<input type="checkbox"/> 0p <input checked="" type="checkbox"/> 0p

Figure 25: Data Banks and Pure Component Property Preselection

The search can be restricted to specified data banks.

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.

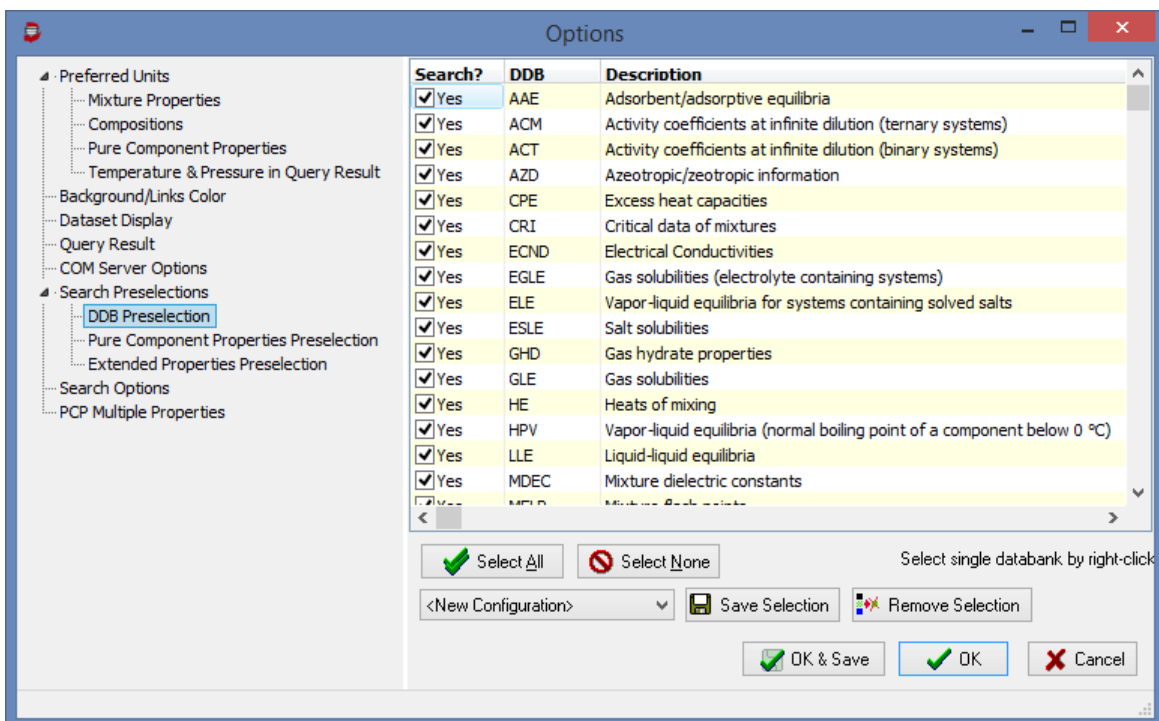


Figure 26: Data Bank Preselection

3.11.2 Pure Component Properties Preselection

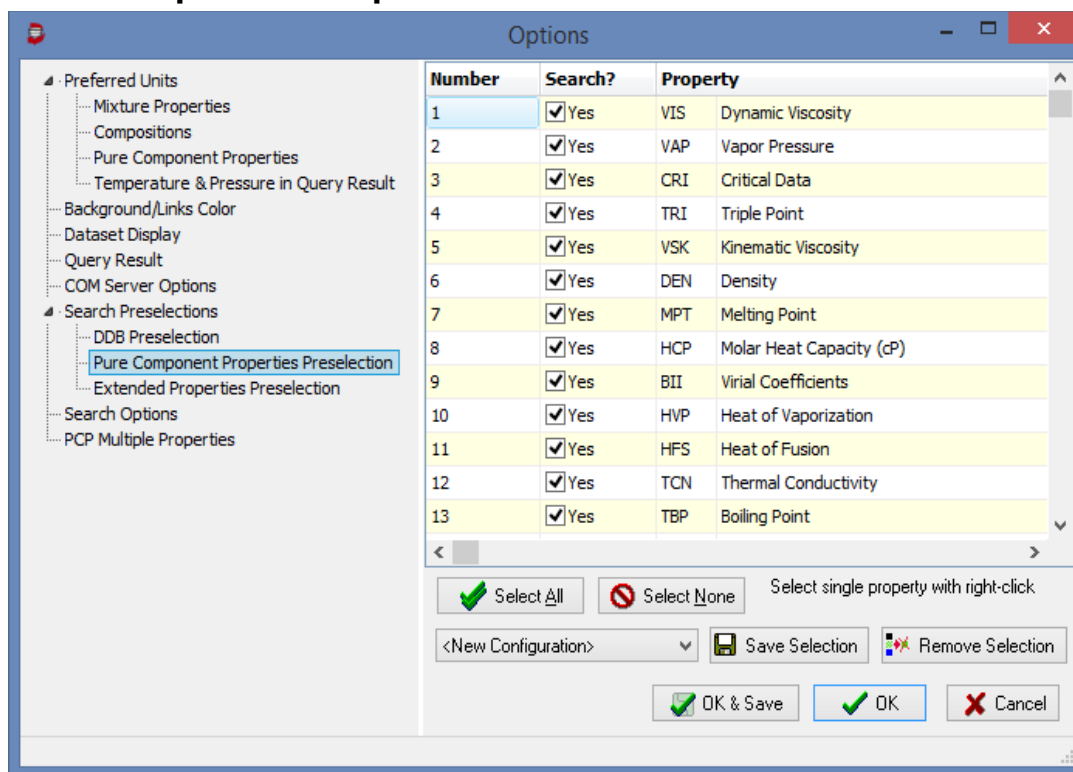


Figure 27: Pure Component Properties - Property Preselection

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

3.11.3 Extended Database Properties

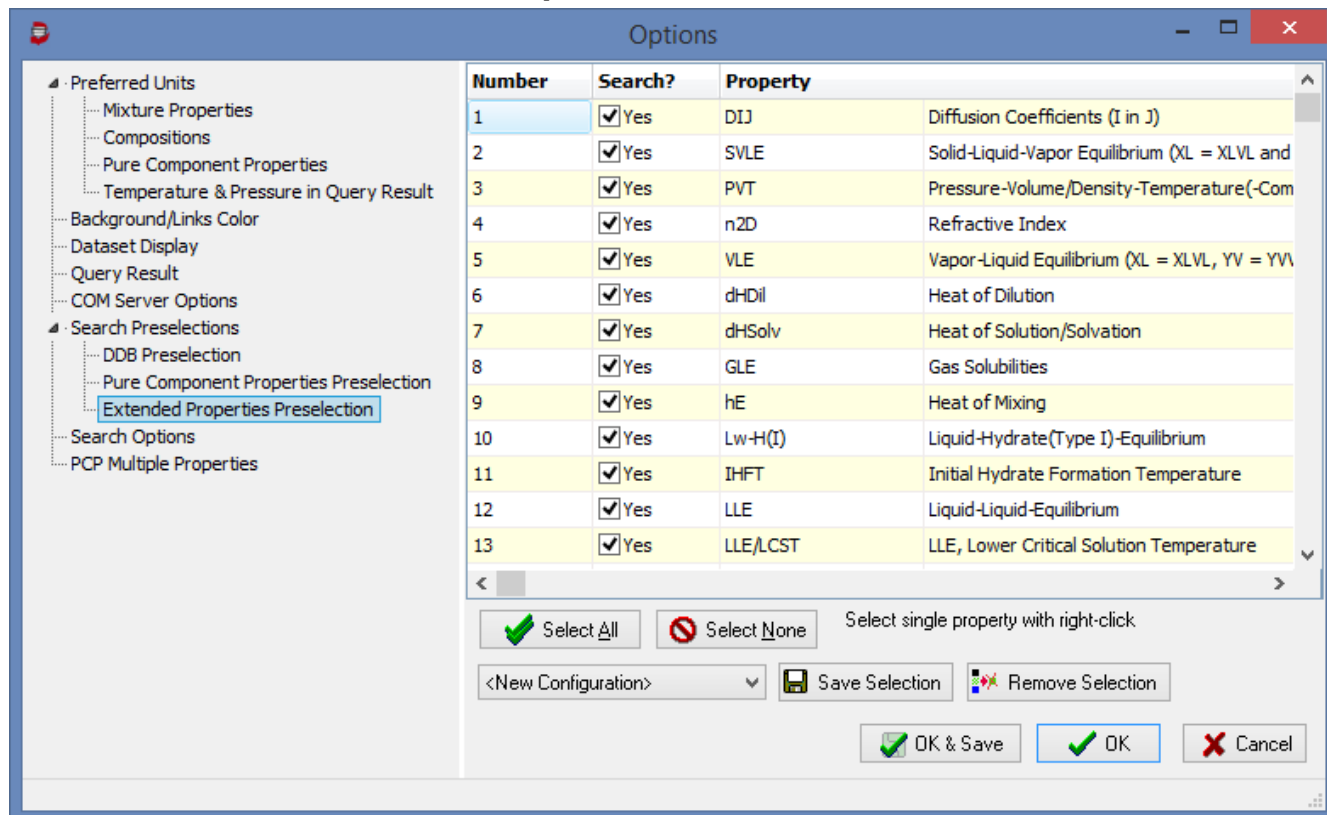
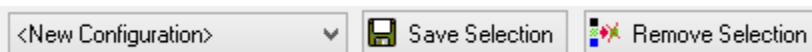


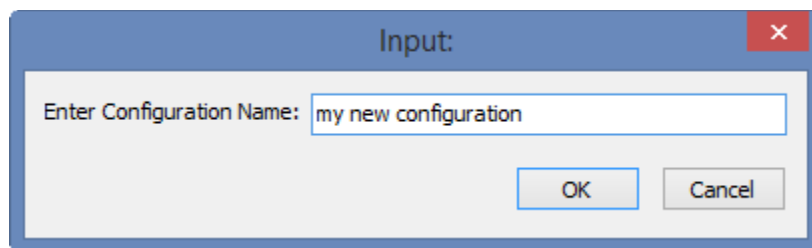
Figure 28: Extended Database - Property Preselection

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.

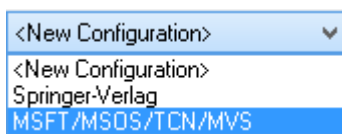
3.11.4 Configurations



Search options can be stored and restored through configuration files. If such a configuration hasn't been stored yet a "New Configuration" can be saved.



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



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

3.11.5 Other Search Options

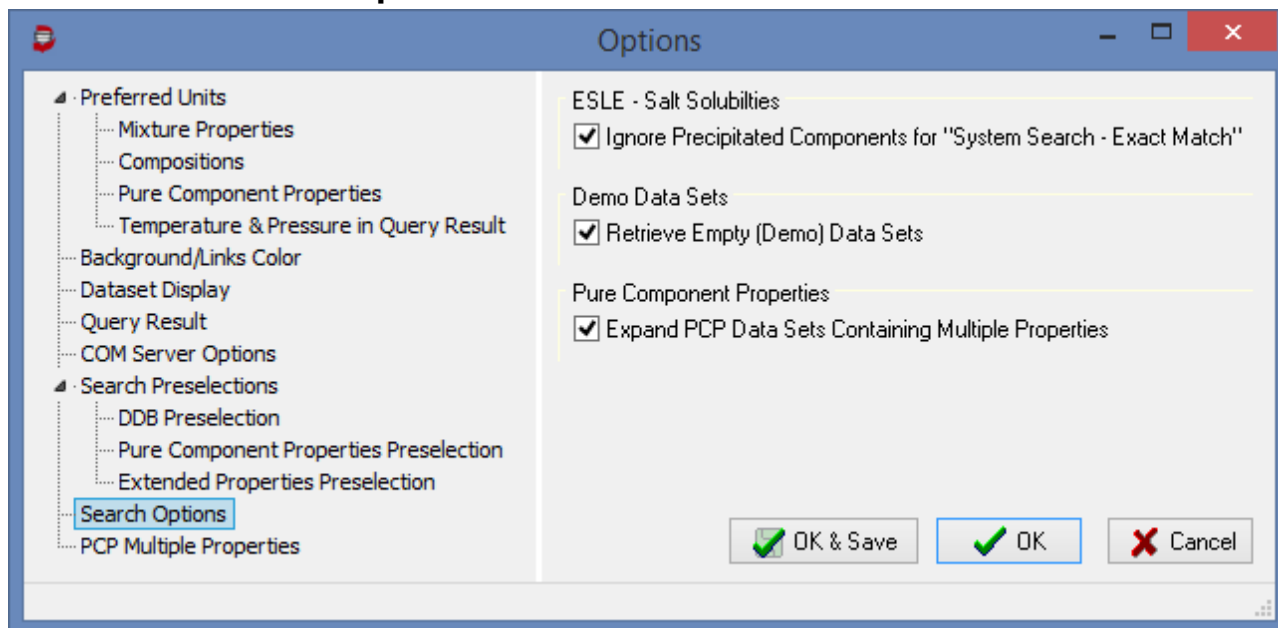


Figure 29: Other Search Options

3.11.5.1 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.

3.11.5.2 Demo Data Sets

The DDB is delivered with empty sets if a specific data base is not licensed. These data sets only contain only 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 to avoid the retrieval of demo data sets during initial search.

3.11.5.3 Expand PCP Data Sets Containing Multiple Properties

A pure component property data set can contain several properties like densities and heat capacities in the data table. These data sets are normally displayed either as a density or as a heat capacity data set. Switching on this option allows to duplicate the **display** of these data sets and the single data set will be displayed as a density data set and as a heat capacity data set as well.

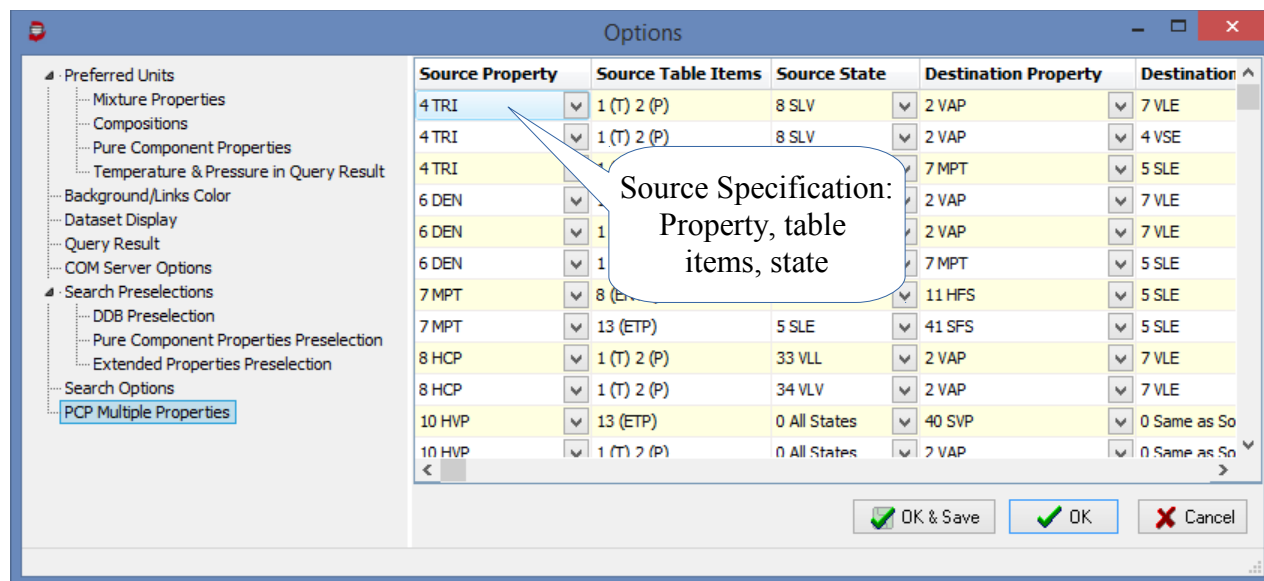
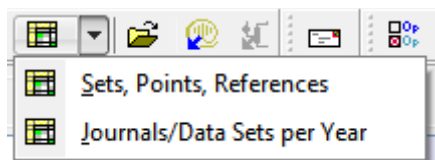


Figure 30: Multiple Properties PCP Data Set Expansion

4 Exploring the Data Bank – Statistics



4.1 DDB Statistics

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.

The sum of references is shown twice. The value in brackets is the sum of the reference counts shown above for the single data banks. But because many references are used in more than one database the real number of references is lower and shown separately.

Databank	Sets	Points	References	Sets (priv.)	Points (priv.)	References (priv.)	
AAE	4359	54006	263	0	0	0	Adsorbent/adsorpti
ACM	1592	9955	71	0	0	0	Activity coefficie
ACT	84904	84904	1346	0	0	0	Activity coefficie
AZD	56137	56125	8410	0	0	0	Azeotropic/zeotrop
CPE	6025	68664	748	0	0	0	Excess heat capac
CRI	3197	21868	998	0	0	0	Critical data of r
ECND	7251	74541	604	0	0	0	Electrical Conduct
EGLE	2575	14856	195	0	0	0	Gas solubilities
ELE	10872	134613	1537	0	0	0	Vapor-liquid equi
ESLE	38749	268734	7267	0	0	0	Salt solubilities
GHD	3383	25741	598	0	0	0	Gas hydrate proper
GLE	22365	105994	2136	0	0	0	Gas solubilities
HE	22471	332609	3267	0	0	0	Heats of mixing
HPV	38219	326229	4370	0	0	0	Vapor-liquid equi
LLE	29538	258452	4632	0	0	0	Liquid-liquid equi
MDEC	5162	50357	649	0	0	0	Mixture dielectric
MFLP	439	4201	73	0	0	0	Mixture flash poin
MPVT	10175	178974	694	0	0	0	Mixture P-v-T Data
MSFT	3641	45252	477	0	0	0	Mixture surface te
MSOS	8891	128834	1079	0	0	0	Mixture speeds of
MTCN	4014	34244	294	0	0	0	Mixture thermal co
PCP	272933	1755870	35950	0	0	0	Pure component pro
POLYMER	20021	203942	1661	0	0	0	Thermodynamic data
POW	14047	14047	563	0	0	0	Octanol-Water part
SLE	52761	435350	7548	0	0	0	Solid-liquid equi
VE	67549	762839	7175	0	0	0	Densities and (ex
VIS	25309	287332	2829	0	0	0	Mixture viscositie
VLE	36456	532921	7657	0	0	0	Vapor-liquid equi
X	107454	1208453	9595	0	0	0	Different thermody
Sum	960489	7479907	(112686) 70136	0	0	(0) 0	

Figure 31 Data Bank Statistics

The second and third pages are more detailed statistics. They display the number of different systems in the data banks separated in a summary, 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.

DDB	Components	Systems summary	Unary systems	Binary systems	Ternary systems	Quaternary systems	Higher systems
=All=	47268	177152 systems 960477 sets 7479907 points	36801 systems 290596 sets 1850391 points	93771 systems 517295 sets 4049998 points	29155 systems 116894 sets 1242725 points	6580 systems 16611 sets 150606 points	10845 systems 19081 sets 186187 points
AAE	141	601 systems 4359 sets 54006 points		409 systems 3444 sets 47621 points	155 systems 772 sets 5361 points	31 systems 123 sets 847 points	6 systems 20 sets 177 points
ACM	208	879 systems 1592 sets			879 systems 1592 sets		

Figure 32 Statistics on Systems

The compounds columns shows the number of components for which the DDB contains data.

The pure component properties grid has a context menu

Property	Compounds	References	Sets	Points
Dynamic Viscosity	3733	4825	25122	153585
Vapor Pressure	16141	11643	52611	299985
Critical Data	1235	1147	4377	4396
Triple Point	462	358	690	725
Kinematic Viscosity	1060	385	2290	10813
Density	12439	13021	72585	514315
Melting Point	15162	7352	35055	28380

Figure 33 Statistics on Pure Component Properties

#1 #2 #3	Save List of Components
#1 #2 #3	Save List of References
#1 #2 #3	Save List of Datasets
#1 #2 #3	Save List of All Components
#1 #2 #3	Save List of All References
	Save List of Deleted Sets
	Show Data Sets

that contains commands to save list of components, references, and data sets

for single properties. “Save List of Deleted Sets” is a special feature of the pure component data base. Sets aren't deleted but only marked as deleted by removing the reference information. These sets can still be shown through their data set numbers. “Show Data Sets” display all data sets of the property of a marked line.

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

4.2 Journals and Data Sets per Year

4.2.1 Data Sets per Year

This statistics show the distribution of data sets publication years. It is possible to either select a single data bank or a statistics for all data banks together. Besides a diagram the data are also available as data table and, additionally, a list for single year can be displayed.

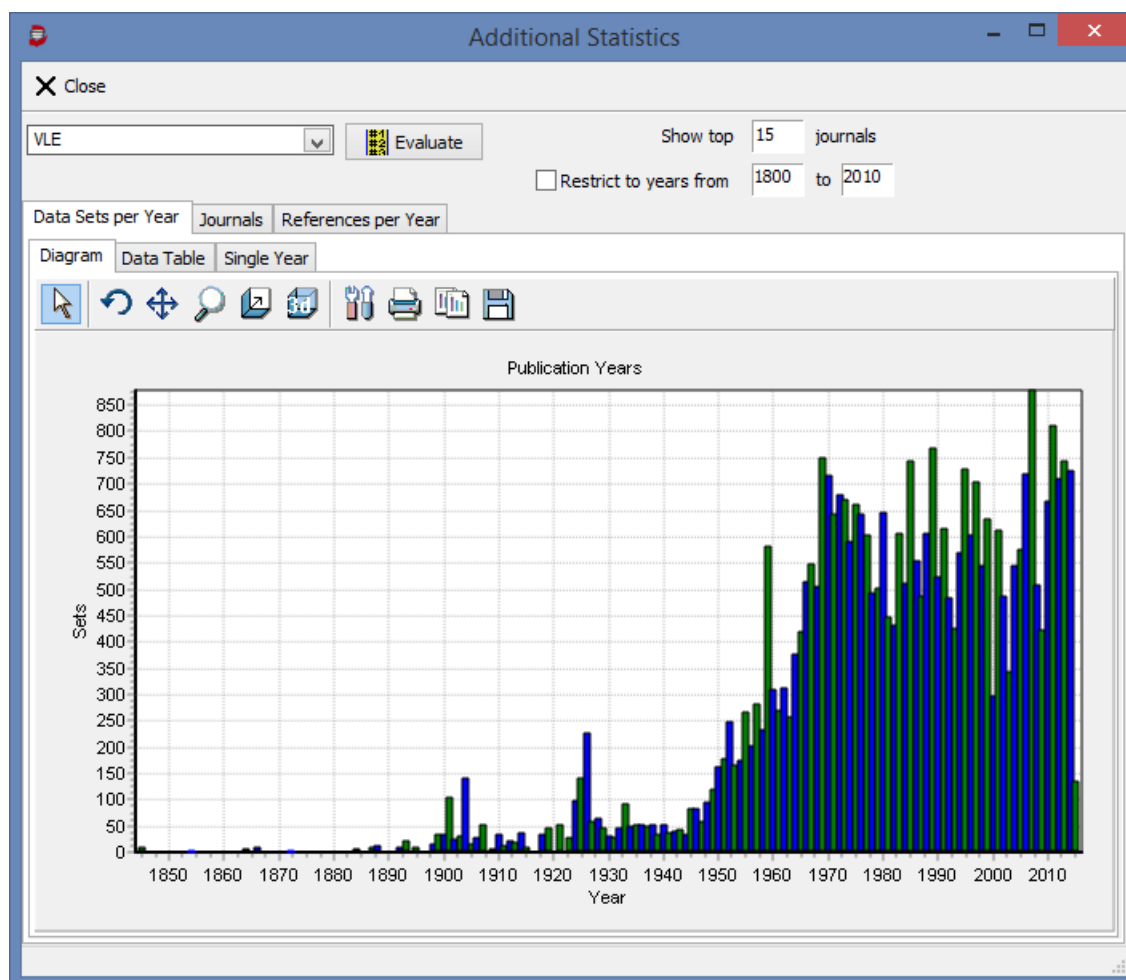


Figure 34: Additional Statistics

4.2.2 Journals

The journals statistics show the top journals a pie diagram and a data table with all journals. Additionally, a diagram for single journals can be displayed.

The number of journals displayed in the diagram can be set by “Show top ?? journal”. Other than the top journals are show together as “Other Journals” in the diagram.

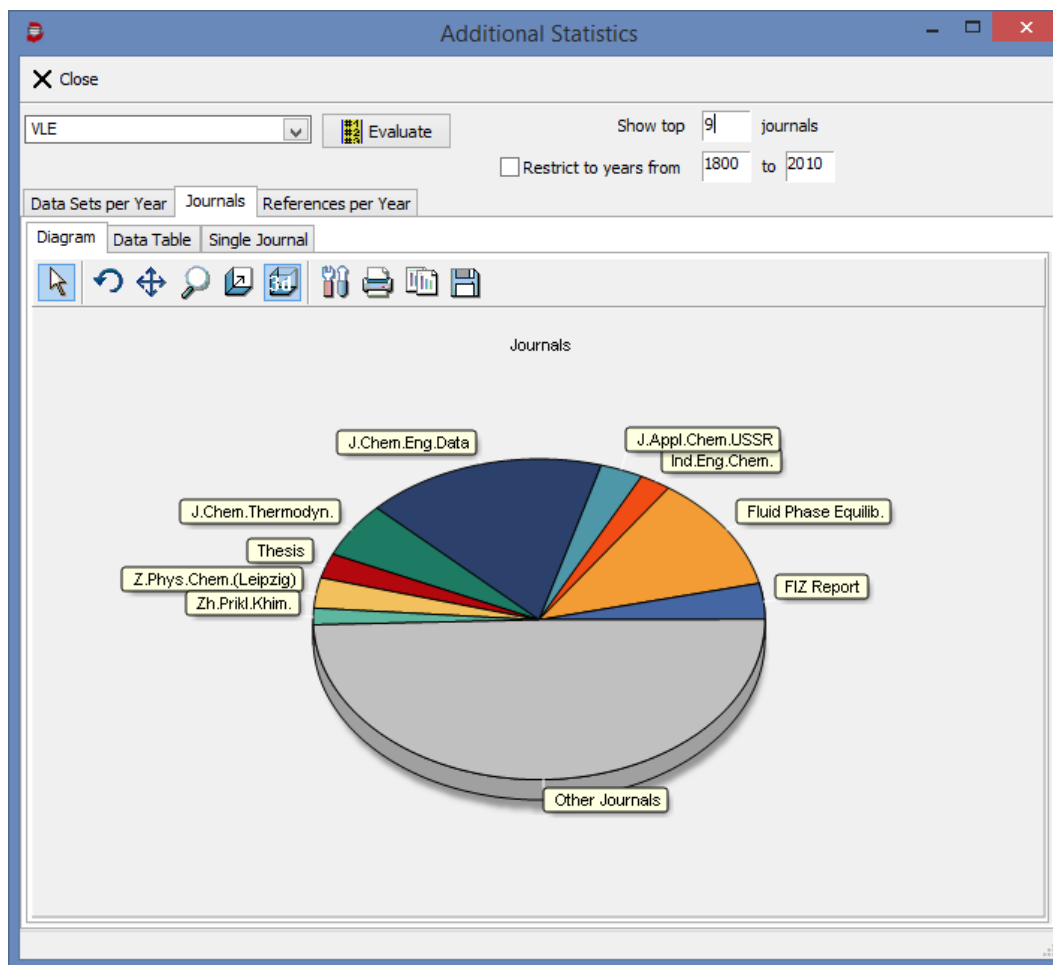


Figure 35: Journals

4.2.3 References per Year

This statistics shows a similar diagram than the “Data Sets per Year” diagram. The difference between these both diagrams give an insight how many publications have been evaluated and an estimation about the amount of data per published paper.

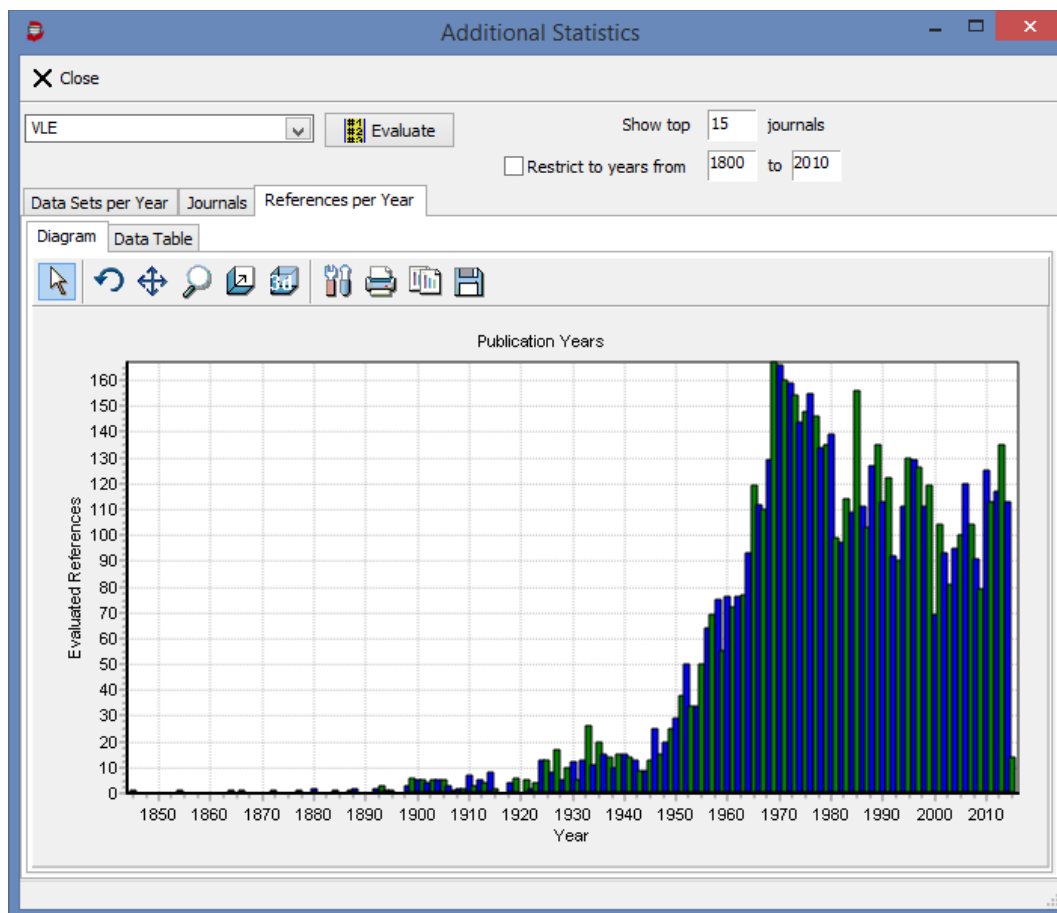
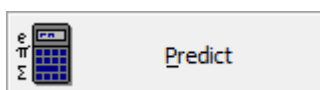


Figure 36: References per Year

5 A First Look at Predictions

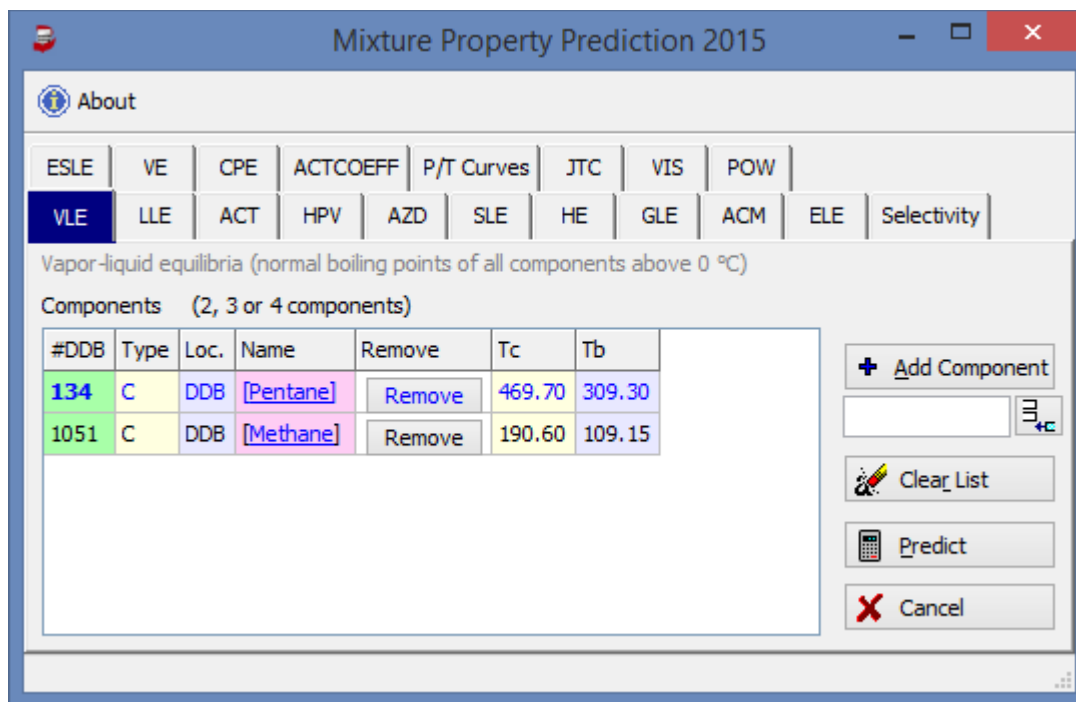


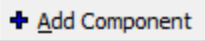

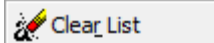
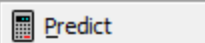
This part of the DDB software package contains a lot of dialogs for the different data banks and is explained in other chapters in more details. In this step we'll focus on some common features.

Predicting from the main window has been introduced for obtaining 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.

After pressing the 'Predict' button a dialog is displayed where a system of components has to be specified.

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, LLE, ACT, HPV, AZD, SLE, HE, GLE, ACM, ELE, and POW. A special calculation for selectivities completes the list.

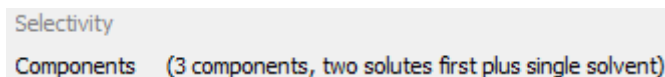


New components can be added () by the standard ComponentSelection dialog or, if the DDB component numbers are known, typed in directly ().  clears the entire list,  shows the prediction dialog for the current data bank.

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 displays 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	Name ▾	Remove	Tc	Tb
C11	Ethanol		516.20	351.45
C12	Diethyl ether		466.70	307.65

A repeated click in the sort row reverses the sort order. Sorting is possible by DDB number, name, T_c, and P_c. The single dialogs for the single data banks are described in chapters below.

#DDB	Name	Remove	Tc	Tb
C11	Ethanol	Remove	516.20	351.45
C12	Diethyl ether	Remove	466.70	307.65

6 Using and Understanding the Query Result Window

Query Result [2] <ACM,ACT,AZD,CRI,ECND,ELE,ESLE,GLE,HE,HPV,LLE,MDEC,MFLP,MPVT,MSFT,MSOS,MTCN,POLYMER,SLE,VE,VIS,VLE,X>

File Edit

ACM ACT **AZD** CRI ECND ELE ESLE GLE HE HPV LLE MDEC MFLP MPVT MSFT MSOS MTCN POLYMER SLE VE VIS VLE X

All Sets All Points All Refs Sets Points Refs

242 242 106 90 90 37

=AZD=
Azeotropic/zeotropic information

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]
[278 0 0]	DDB	1	3	[C4 Acetone] [C110 Methanol] [C174 Water]	n.a.		101 (co)
[416 0 0]	DDB	1	3	[C4 Acetone] [C47 Chloroform] [C110 Methanol]	331 (const.)		101 (co)
[4882 0 0]	DDB	1	3	[C70 Dichloromethane] [C4 Acetone] [C110 Methanol]	n.a.		101 (co)
[4883 0 0]	DDB	1	3	[C4 Acetone] [C47 Chloroform] [C110 Methanol]	331 (const.)		n.a.
[11487 0 0]	DDB	1	3	[C4 Acetone] [C110 Methanol] [C50 Cyclohexane]	298 (const.)		n.a.
[18525 0 0]	DDB	1	3	[C134 Pentane] [C4 Acetone] [C110 Methanol]	373 (const.)		n.a.
[19294 0 0]	DDB	1	3	[C4 Acetone] [C47 Chloroform] [C110 Methanol]	323 (const.)		76 (con)
[19295 0 0]	DDB	1	3	[C4 Acetone] [C47 Chloroform] [C110 Methanol]	313 (const.)		50 (con)
[20468 0 0]	DDB	1	3	[C4 Acetone] [C367 2,3-Dimethylbutane]	n.a.		101 (co)

20 Ternary Systems

Copy Save

#	System	
All		
<input type="checkbox"/> 1	C4 C9 C110	1 set/s
<input type="checkbox"/> 2	C4 C11 C110	1 set/s
<input type="checkbox"/> 3	C4 C31 C110	2 set/s
<input type="checkbox"/> 4	C4 C40 C110	2 set/s
<input type="checkbox"/> 5	C4 C44 C110	1 set/s
<input type="checkbox"/> 6	C4 C47 C110	8 set/s
<input type="checkbox"/> 7	C4 C50 C110	14 set/s
<input type="checkbox"/> 8	C4 C70 C110	1 set/s
<input type="checkbox"/> 9	C4 C82 C110	21 set/s

Acetone
2-Butanone
Methanol

1 dataset/s marked.

Figure 37: Query Result

6.1 File Menu

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

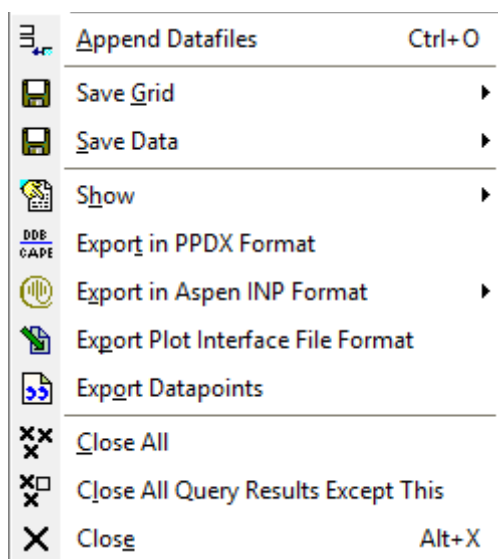
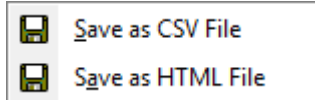


Figure 38: File Main Menu

'Append Data' resp. the 'Save Data' menu entries allows to load and save data in different formats – but all only in DDB specific formats. The single formats are described in the next steps (see chapter “Saving and Loading Data Files”).

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



'Show' allows to display 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 '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. This functions make most sense when an experimental and a predicted set is 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.

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

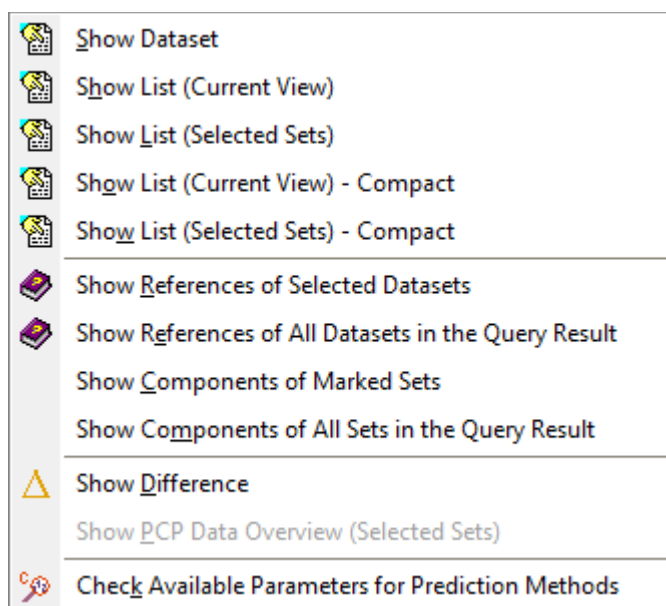
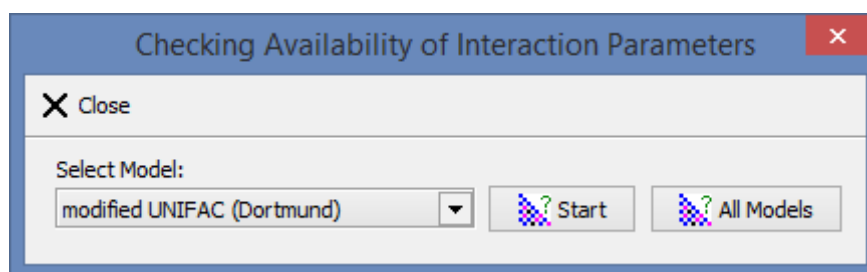


Figure 39: Show Sub Menu



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.

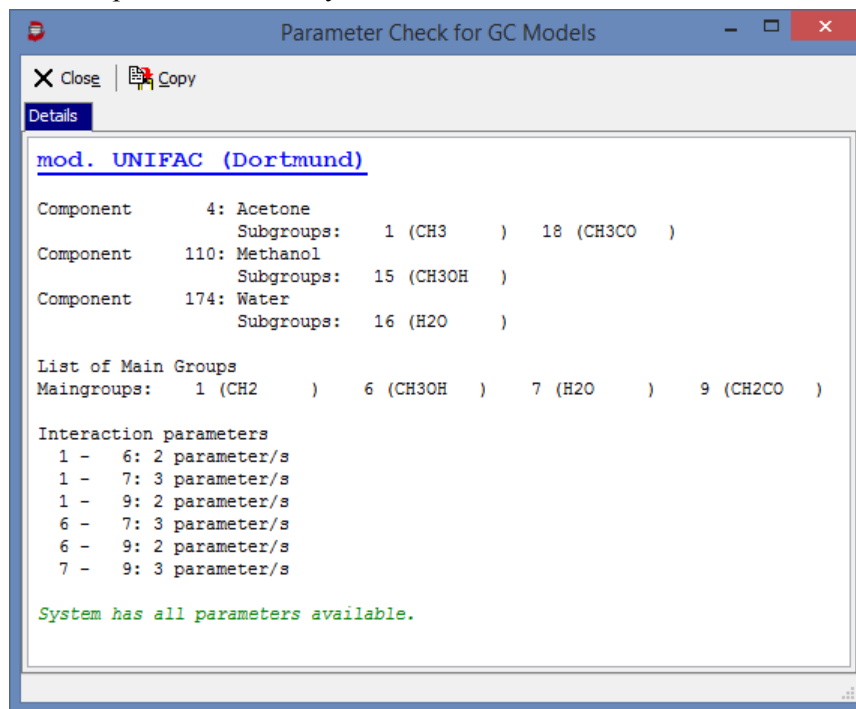


Figure 40: Parameter Availability Check for modified UNIFAC (Dortmund)

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

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

'Export Plot Interface File Format' writes a file for the plot program (MixPlot) which when can be loaded in the plot program.

'Export Datapoints' allows to write a table containing all data points

'Close All' closes all query result window

'Close All Query Results Except This' close 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.

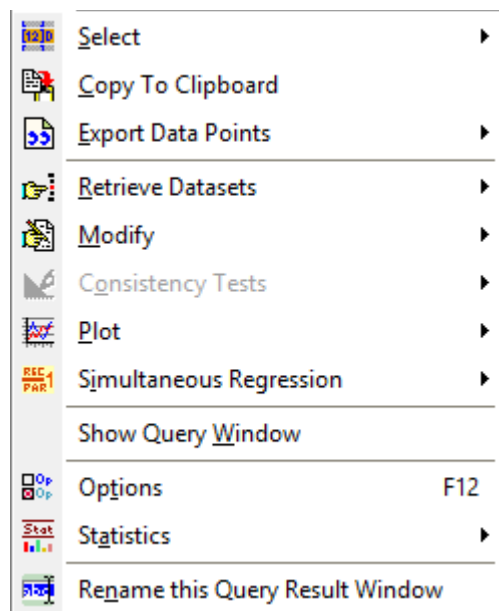


Figure 41: Edit Main Menu

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

'**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 to write experimental data to files in text and Excel format.

Please see chapter 22.3 on page 142 ("Data Points Export") for more information.

'**Consistency Tests**'

allows to call consistency tests for VLE data. See chapter 14 ("Consistency Tests") on page 61f for detailed information.

'**Plot**' shows diagrams of the selected data sets. See chapter 21 ("Plot") on page 134 for more information.

'**Simultaneous Regression**' is described in chapter 20 ("Simultaneous Fit – RecPar") on page 133f.

'**Modify**' allows to change data sets. This is explained in chapter 15 ("Modifying and Editing Datasets") on page 67f.

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

'**Options**' are explained in chapter 11 ("Data Set Display Options") on page 51f.

'**Statistics**' entries are display in chapter 17 ("Query Result Statistics") on page 78f.

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

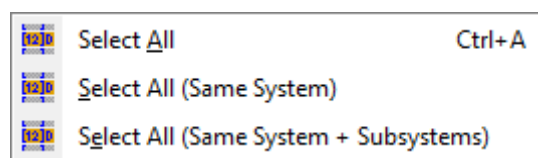


Figure 42: Select Sub Menu

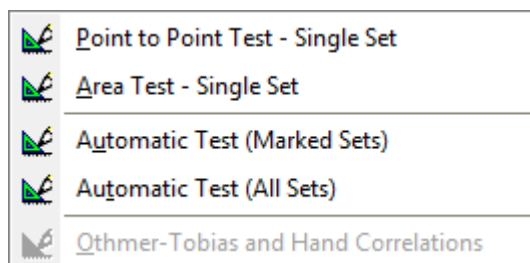


Figure 43: Consistency Sub Menu

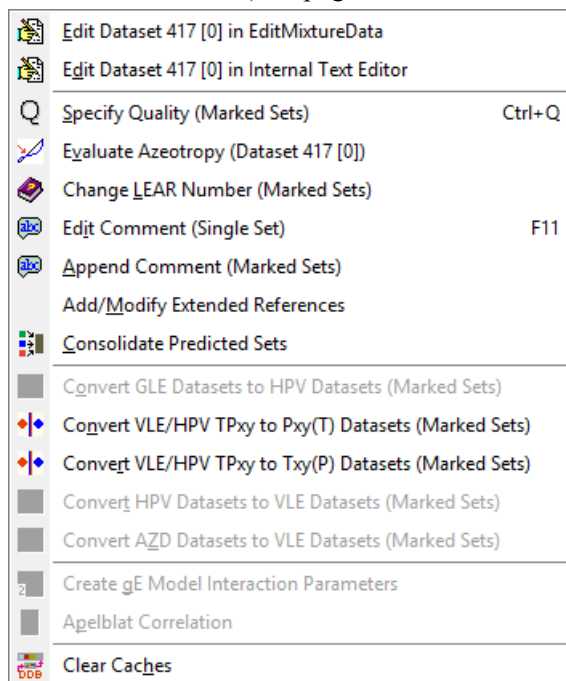
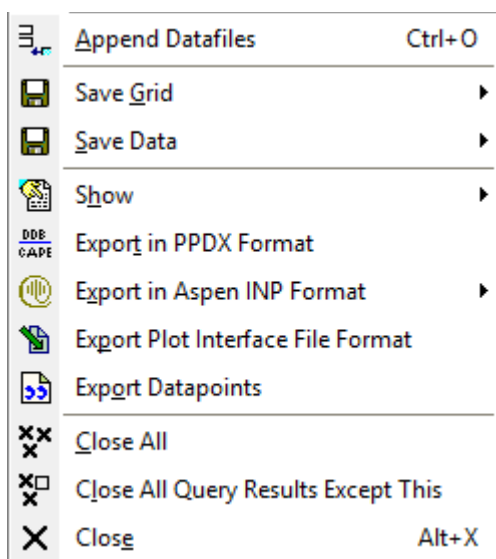


Figure 44: Modification Sub Menu

7 Saving and Loading Data Files

7.1 Open Files

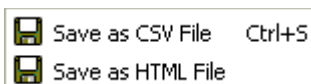
Data sets can be loaded in the query result window and in the query definition window. Loading multiple files in the main window will open multiple query result files, loading multiple files in a query result windows allow collecting all the data in that window.



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

MixView Query Result (*.qr)
 DDB Free Formatted Interface File (*.txt)
 DDB Binary Interface File (*.VLS;*.SLS;*.GLS;*.HES;*.
 DDB F77 Formatted Interface File (*.*)
 Data Handling File (*.dhp)
 Dataset Identifiers (*.txt)
 Raw Dataset Numbers (*.stx)
 Raw Dataset Numbers (*.txt)

'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. It's extension is “.qr”. It stores all data sets from all databases in the current query result (and allows to restore it). We now use it as standard exchange format.
- “**Save Single Set**”: This function stores a single data sets in the “.qr” format
- “**Save All Sets – All Databanks**”: The format is also the “.qr” format but allows storing the entire query result in one file.
- “**Binary Data/Interface File**”. This format contains a list of data sets in a FORTRAN binary format. The files can contain only data sets from a single database and have database specific extensions.



Figure 45: Save Sub Menu

- **VLS** → VLE and HPV database
- **SLS** → SLE database
- **GLS** → GLE database
- **HES** → HE database
- **ALS** → ACT database
- **AMS** → ACM database
- For the data banks ESLE, POW, MSFT, MSOS, MTCN, ECND, GHD, and CRI a binary format is not supported
- **Free Formatted Data/Interface File**. This format contains a list of data sets in text format. The extension of the files is '.TXT'. This file only contains data sets from a single database. This format is defined for all data banks.
- **Dataset Identifiers**. This format only stores the database name and data set identifiers (data set numbers, data bank location).
- **Raw Dataset Numbers**. This format (extension **.STX**) only stores the data set numbers Data bank information and location ids are lost.
- **Literature Numbers**. This file (also **.STX**) stores the literature numbers of the data sets. This file can be loaded in the literature management program (LEAR).
- **Component Numbers**. This file (also **.STX**) 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 (binary, free and F77 formatted, Query Result data sets).
2. File containing only data descriptors (Data set identifiers, literature numbers, raw data set numbers, component numbers).

The files containing only descriptors are damageable by data bank changes because the descriptor might point to a replaced data sets. 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	Ref.No.	Reference
[1632 0 0]	DDB	1	2	[C12 Diethyl ether] [C11 Ethanol]	n.a.		101 (const.)		none		1899	39	[5716] Haywood
[8082 0 0]	DDB	1	2	[C12 Diethyl ether] [C11 Ethanol]	273 (const.)		n.a.		none		1935	7555	[114495] Nagai
[8083 0 0]	DDB	1	2	[C12 Diethyl ether] [C11 Ethanol]	283 (const.)		n.a.		none		1935	7555	[114495] Nagai
[8084 0 0]	DDB	1	2	[C12 Diethyl ether]	293 (const.)		n.a.		none		1935	7555	[114495] Nagai

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 hyper links. A single-click opens the single-dataset display window (see next steps). The 'Links Details' window below the grid displays the dataset id details when the mouse cursor hovers above a link.
- **“Pts.”:** Number of points in the dataset.
- **“#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 (PDI).
- **“Pmin [kPa]” and “Pmax [kPa]”:** Pressure range of the data set.
- **“Comment”:** Further database-dependent details for the data set.
- **“Ref.No.”:** Reference number. This is a number specific for the current database.
- **“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 hyper links and allow displaying a special literature detail dialog that has functions to
 - search for all data sets for the current reference. The result will be displayed in a new query result window.

The screenshot shows a window titled "LEAR Dataset" with a close button (X) in the top right corner. Below the title bar is a navigation bar with four tabs: "Close", "Search Datasets", "Further Details", and "Linked Info". The "Search Datasets" tab is active, and the dataset number "5851" is entered in the "Dataset Number" field. The "Title" field displays "Rectification in Ternary Systems Containing Binary Azeotropes". The "Authors" field lists "Ewell R.H." and "Welch L.M.". The "Journal" field shows "Ind.Eng.Chem.". The "Pages" field indicates "1224 to 1231" and the "Publishing Years" field shows "1945". The "Volume" field is "37" and the "Issue" field is "12". The "Reference" field displays "[5851] Ewell R.H., Welch L.M., Ind.Eng.Chem., 37(12), 1224-1231, 1945".

Figure 46: Reference Details

- display a dialog in LEAR with all available details for the current reference (“Further Details”).
- display linked files (“Linked Info” button, see “Literature Management” manual for more details)

The data set grid allows to sort the data sets by clicking in the first – fixed – row.

A repeated click reverses the 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 function from the main menu, and from tool bars. Some features are unique.


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

Figure 47: Sort Order

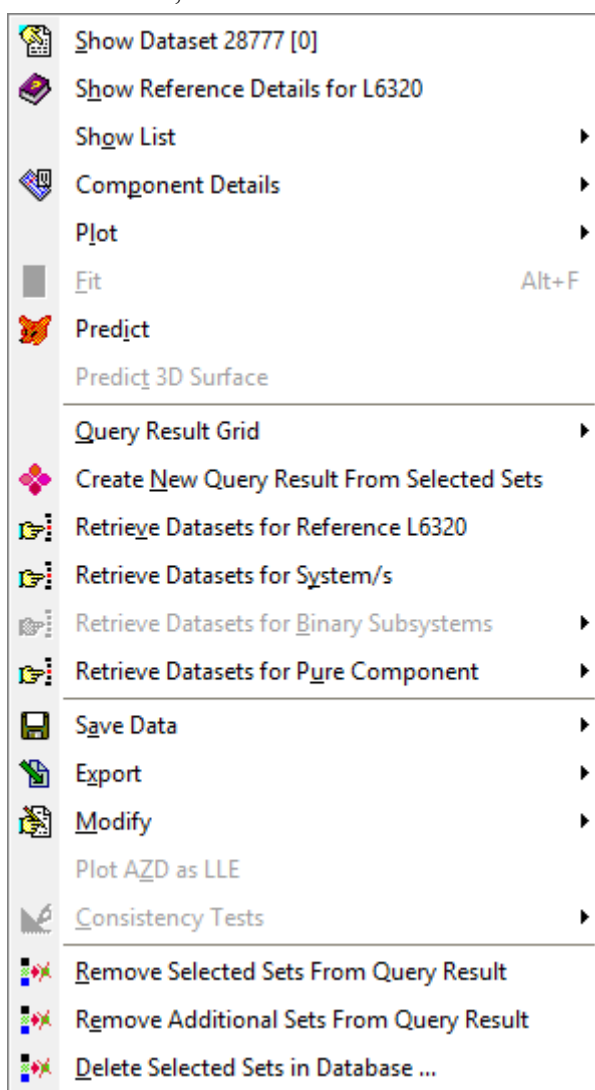


Figure 48: Query Result Context Menu

“Show Dataset” display the set in the single data set display.

“Show Reference Details” shows the complete reference information.

“Show List” display a list of sets in the single data set or in a compact format.

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

“Plot Selected Sets” plots the marked data sets. Details can be

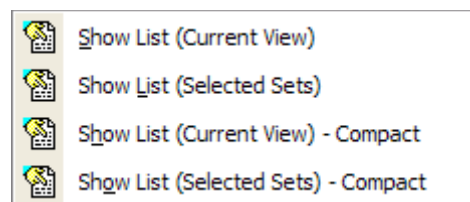


Figure 49: Show List Sub Menu

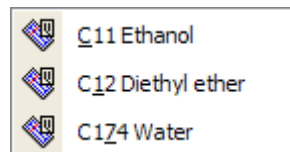


Figure 50: Component Details Sub Menu

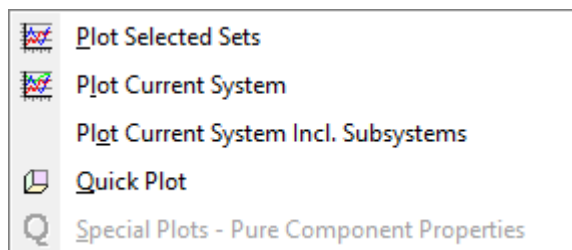


Figure 51: Plot Sub Menu

found in another step.

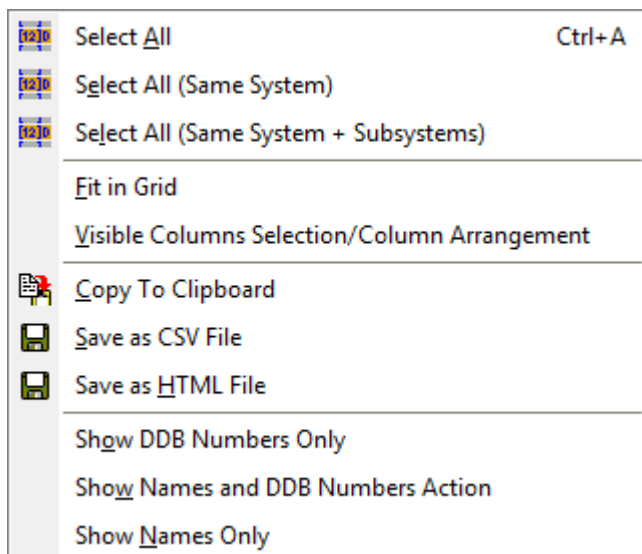
“Plot Current System” marks automatically all data sets build of the same components and plots them together.

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

“**Fit**” calls the fit routines, “**Predict**” the prediction routines. Both function are 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.

Figure 52: Query Result Grid Sub Menu

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

“**Retrieve Datasets for Reference**” performs a new search for the current reference. This allows to collect all data sets for a specific article.

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

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

“**Retrieve Datasets 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.

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

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

“**Delete Selected Sets in Database**” opens a dialog inside EditMixtureData (Editor) with the marked sets and allows to remove these data sets from the database (Figure 53). In this single case EditMixtureData is also used for pure component property data sets.

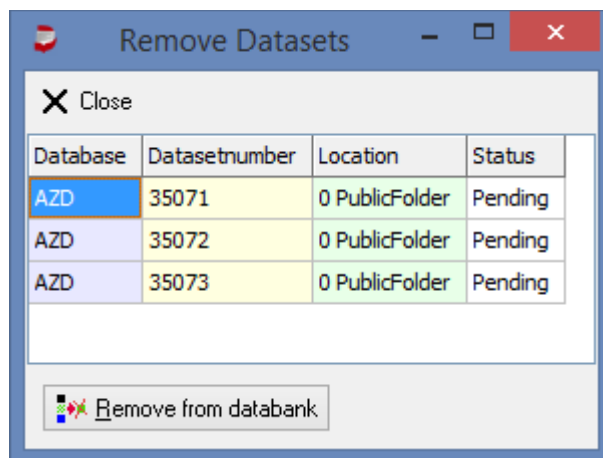


Figure 53 Remove Data Sets Dialog

9 Displaying Sub Lists

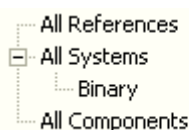


Figure 54 Sub List Overview

The complete list of data sets can be reduced by certain criteria.

- Display data set of single references.
- Display data sets for a single system.
- Display only binary, ternary, quaternary, quinary, or higher systems.
- Display data sets of single components.
- Display data sets for single solvents or solute (ACT and ACM data banks)
- Display data sets from single sources. Sources are private or public DDB or data sets predicted by different models.
- Display data sets with special counters. The counter is normally zero, only if multiple data sets with the same data set number and source are available the counter will be 1 or higher.

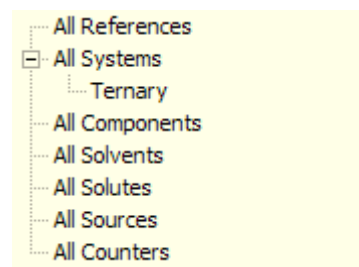


Figure 55 Overview for ACT, ACM

LEAR#	Reference
All	
<input type="checkbox"/> 4990	Thomas E.R., Newman B.A., Nicola
<input type="checkbox"/> 5180	Park J.H., Hussam A., Couasnon P
<input type="checkbox"/> 5269	Yang Y., Wu H., Xie S., Chengdu-K
<input type="checkbox"/> 5270	Yang Y., Xiao S., Li H., Fu Y., Cher
<input type="checkbox"/> 5282	Landau I., Belfer A.J., Locke D.C.,
<input type="checkbox"/> 5422	Wang S., Wang W., Feng X., Wu Y
<input type="checkbox"/> 5449	Scott L., Bush D., Brantley N.H., E

Figure 56 References

Comp#	Component
All	
<input type="checkbox"/> C3	Acetonitrile
<input type="checkbox"/> C4	Acetone
<input type="checkbox"/> C11	Ethanol
<input type="checkbox"/> C31	Benzene
<input type="checkbox"/> C47	Chloroform
<input type="checkbox"/> C75	1,4-Dioxane
<input type="checkbox"/> C80	Havana

Figure 58 Components

#	System	
All		
<input type="checkbox"/> 1	C3 C11 C47	1 set
<input type="checkbox"/> 2	C4 C11 C47	3 set
<input type="checkbox"/> 3	C4 C11 C47 C89	3 set
<input type="checkbox"/> 4	C4 C11 C47 C110	1 set
<input type="checkbox"/> 5	C4 C11 C47 C140	1 set
<input type="checkbox"/> 6	C11 C31 C47	6 set

Figure 57 Systems

The query result window displays separate statistics on the entire list currently loaded and the currently active sub list in its overview grid.

All Sets	All Points	All Ref's	Sets	Points	Ref's
8	79	4	1	13	1

The check boxes can be used to select single or multiple references (for example). A left-mouse-button-click in column two checks single lines.

10 Single Data Set Display

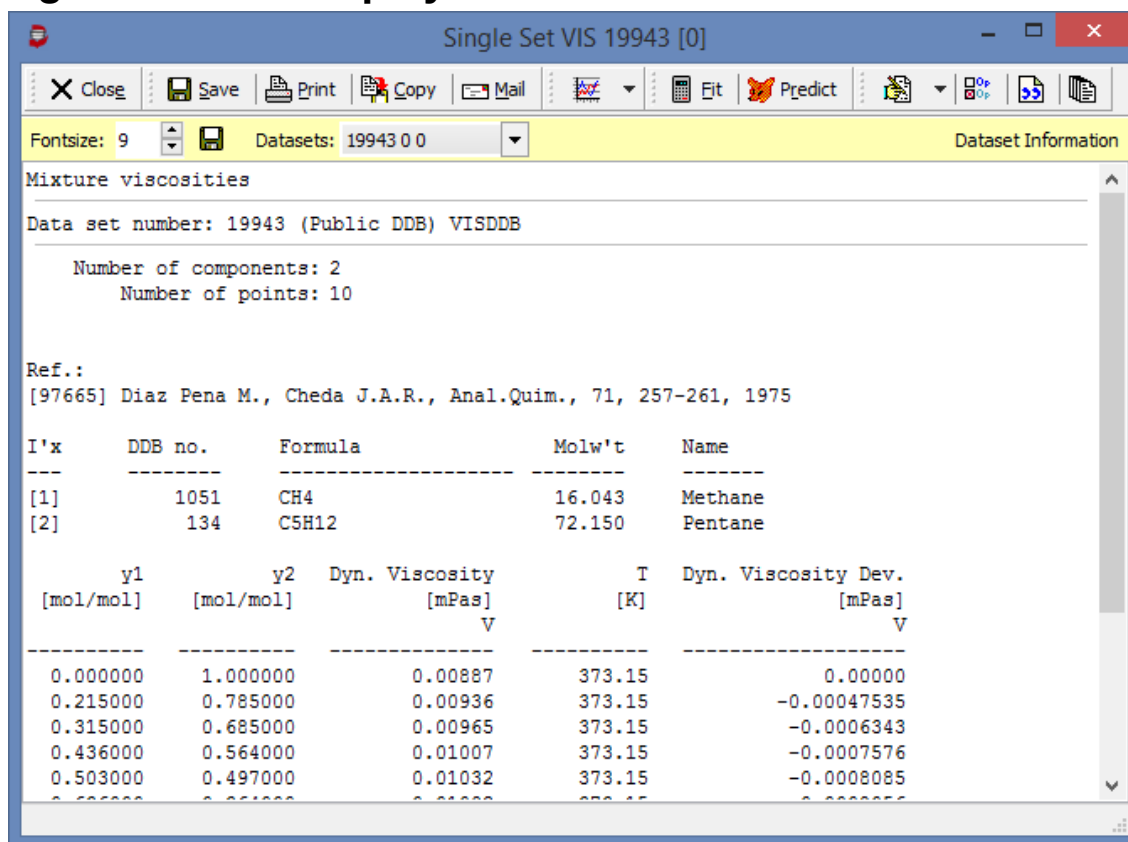






Figure 59: Single Data Set

The tool bar functions are

- **“Close”**: Closes the display window (the window can be closed also by pressing the Esc key).
- **“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.
- **“Mail”**: Saves the current window content to a temporary file, calls the standard mail program with an empty new mail window with the temporary file appended.
- **“Plot”**: Plot the current dataset (details in another chapter).
- **“Fit”**: Fits the current dataset (details in another chapter).
- **“Predict”**: Predicts the current dataset (details in another chapter).

-  **“Edit”**: Allows to modify the current dataset (but will not alter the database).
-  **“Options”**: Calls the options dialog (details in another chapter).
-  **“Export”**: Creates a data point table
-  **“Reference”**: Display reference details
- **“Edit in EditMixtureData”** uses the standard editor, the text editors entries allow to edit the data sets in a normal editor – displaying the rather cryptic free formatted format.

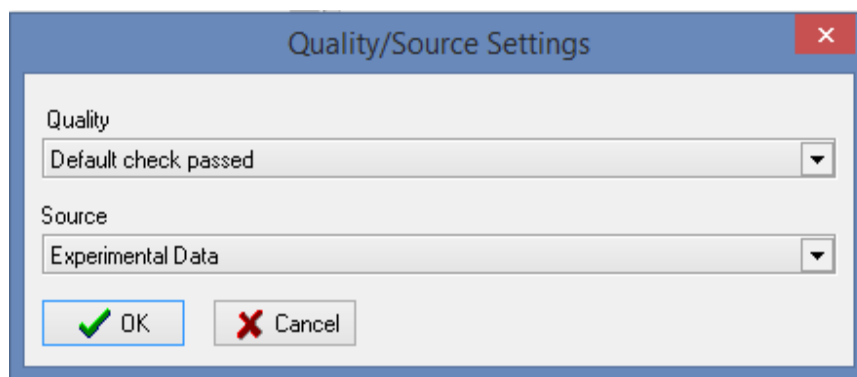
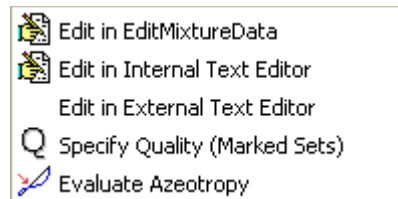
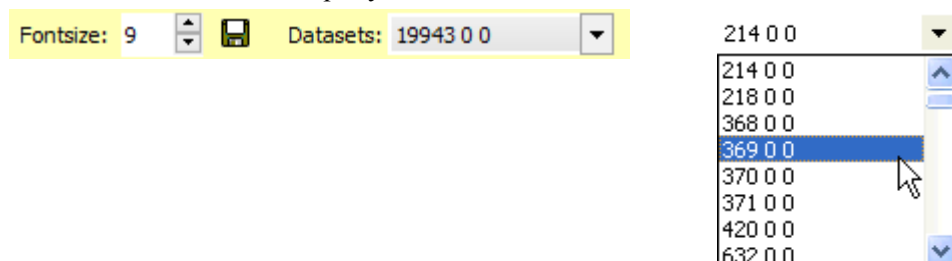


Figure 60 Quality and Source Settings

- **“Specify Quality”** allows to specify the quality and the source of the data, and
- **“Evaluate Azeotropy”** allows testing a VLE or HPV data set for an azeotrope.

The “Font size” control allows to change the size of the font, and the “Datasets” drop down-menu contains the entire list of data sets in the query results.



The data set display is slightly different for the different data banks. A typical output for VLE is

Data set number: 579 (Public DDB) VLEDDB x y T P = constant

```

number of components: 2
  number of points: 11
    quality check: 1 (Default check passed)
      data source: 0 (Experimental Data)
        reference number: 4
  
```

ref.:

[308] Amer H.H., Paxton R.R., van Winkle M., Ind.Eng.Chem., 48(1), p142-146, 1956

code no.	formula	molw't	name
----------	---------	--------	------

4	C3H6O	58.080	Acetone
11	C2H6O	46.069	Ethanol

Constant value/s:

P	101.325	[kPa]
---	---------	-------

T	x1	y1
[K]	[mol/mol]	[mol/mol]
351.45	0.000000	0.000000
349.55	0.033000	0.111000
347.15	0.078000	0.216000
343.95	0.149000	0.345000
342.25	0.195000	0.410000
338.75	0.316000	0.534000
336.55	0.414000	0.614000
334.45	0.532000	0.697000
332.15	0.691000	0.796000
330.45	0.852000	0.896000
329.25	1.000000	1.000000

The data set can be divided in four major parts.

1. Header information showing data point and component count, quality and data source.
2. Reference information
3. Component details
4. Data table

The four parts are always present for every database although the type of data will differ.

11 Data Set Display Options

11.1 Display Additional Information

The DDB retrieval program allow to add some calculated values to the data tables with experimental data sets.

The screenshot shows the 'Data Set Display Options' dialog box with the following sections and options:

- cpE Databank Options:**
 - ☒ Display excess cP values from cP datasets
- ESLE Databank Options:**
 - ☒ Always try to convert ESLE datasets for plots
- GLE Databank Options:**
 - ☒ Display converted GLE to T-Henry data
 - ☒ Display converted GLE to TPxy data
 - ☒ Ostwald conversion: Use given or calculated gas partial pressure
- vE Databank Options:**
 - ☒ Display converted densities from excess volume datasets
 - ☒ Display converted excess volumes from density datasets
- VLE/HPV Databank Options:**
 - ☒ Display relative volatility in VLE and HPV datasets
 - ☒ Display K factors
 - ☒ Display Activity Coefficients
- PCP Databank Options:**
 - ☐ Display molar densities
- PCP/POW Databank Options:**
 - ☒ Display structure in single set display
- LLE Databank Options:**
 - ☒ Display K factors
 - ☐ Sort Points by T
- Pure Constants:**
 - ☒ Add pure constants to diagrams
- VLE/HPV/SLE Databank Options:**
 - ☒ Display complete mole fractions
- Mixture Viscosity Databank Option:**
 - ☒ Display converted viscosity deviations from viscosities
- ☐ Display DCDS and AZDBook Information

A button labeled 'GLE Conversion Note' is located between the GLE and vE sections.

Figure 61: Data Set Display Options

These options are

1. Display excess c_p 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 to convert these multiple formats into two standard forms.

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

Ptot [mm Hg]	X gas *10 ⁴ [-]
248.300	50.8900
427.500	100.3000
579.800	143.4000
755.300	194.1000

Henry Recalculated Table

T [K]	Henry [bar]	Calculated [-]	Uncertain [-]
298.15	49.70088	Yes	No
298.15	49.07572	Yes	No
298.15	48.50892	Yes	No
298.15	47.91328	Yes	No

TPxy Recalculated Table

T [K]	P [kPa]	xgas [mol/mol]
298.15	33.104	0.005089
298.15	56.995	0.010030
298.15	77.300	0.014340
298.15	100.698	0.019410

3. "Ostwald Conversion: Use given or calculated gas partial pressure"

This option switches the conversion mode for data sets containing Ostwald coefficients. If this option is not set the conversion will take the given pressures disregarding the difference between total or partial pressure. If this option is set only partial pressures will be used. If only a total pressure is given the conversion tries to calculate the partial pressure and fails if this is not possible.

4. v^E-Data Bank Options

1. "Display converted density from excess volume data sets"
Densities will be calculated from excess volume data sets. Pure component densities are needed.
2. "Display v^E from densities"
If a density dataset contains pure component densities the programs calculates the excess density/volume.

5. VLE/HPV Data Bank Options

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

$$Rel. Vol. = \frac{\left(\frac{y_1}{x_1}\right)}{\left(\frac{y_2}{x_2}\right)}$$

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 $x_i y_i P_i^s = y_i P$. For some systems with associating carboxylic acids chemical theory is applied.

6. VLE/HPV/SLE Databank Options

1. Display Complete Mole Fractions

The data banks normally only contains mole fractions for n-1 components. For a binary systems only a single mole fraction is stored and displayed. This options allows to display the mole fraction of all components.

7. PCP Databank Options

1. Display Molar Densities

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

P [kPa]	DEN [kg/m3]	DEM [mol/l]
4910.000	588.200	7.936
9810.000	598.000	8.068
19620.000	611.300	8.247

8. PCP/POW Databank Options

1. Display Structure in Single Set Display

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

9. VIS Databank Options

1. Display converted viscosity deviations from viscosities

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

10. LLE Dabank Options

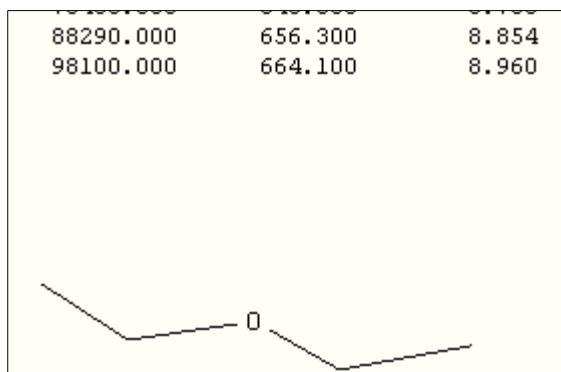


Figure 62 Structure append to Single Set Display

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. **Display DCDS and AZDBook Information**

Some parts of some data banks have been published in the DECHEMA Chemistry Data Series and the data bank about azeotropic and zeotropic data in a separate publication. Some information (volume, pages) are available in some data banks and can be displayed optionally.

11.2 Query Result Options

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

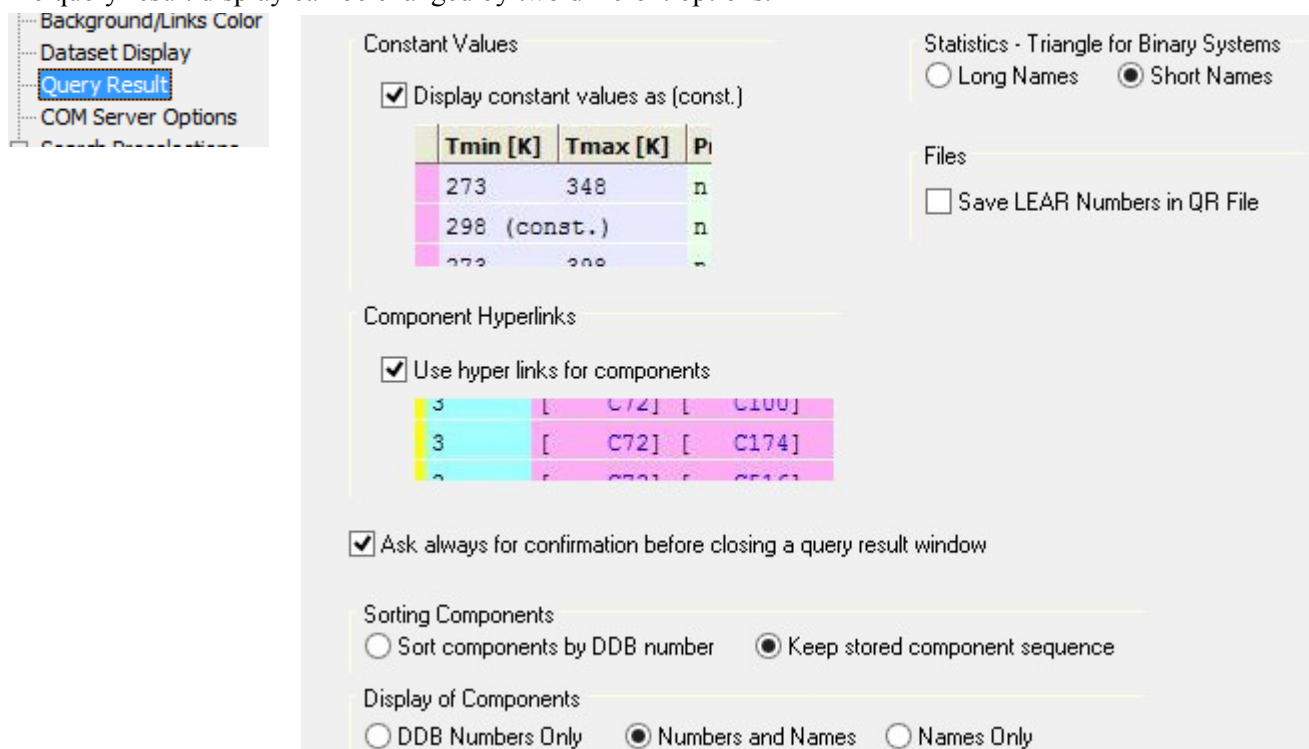


Figure 63: Query Result Display Options

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	308	n	273	308	n

2. Display of hyper links for components

The grid is able to display hyper links 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
3	[C72]	[C174]	2	C125	C284	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

Three options are 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 65: DDB Number Only

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

Figure 66: Names Only

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

Figure 64: Numbers and Names

7. Save LEAR Numbers in QR File

This options adds the standard literature number to all data sets written to a query result file (qr files) . This is useful for the older data banks still storing some separate reference numbers only. The written files are compatible with the qr files without the LEAR numbers.

12 Compact Data Display

The compact displays 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, dataset count, and value ranges. An exception is the output for pure component properties, see below.

A typical output for VLE is

VLEDDB - Vapor-Liquid Equilibrium Data

```
(1) 11      C2H6O          Ethanol
(2) 12      C4H10O        Diethyl ether
```

References:

- 1 [475] Gordon A.R., Hornibrook E.J., Can.J.Res., 24, p263-267, 1946
- 2 [476] Kireev V.A., Khachadurova E.M., Zh.Prikl.Khim. (Leningrad), 7(4), p495-496, 1934
- 3 [477] Nagai J., Ishii N., J.Soc.Chem.Ind.Jap. = Kogyo Kagakkai, 38(3), p86-95, 1935
- 4 [866] Moeller W.P., Englund S.W., Tsui T.K., Othmer D.F., Ind.Eng.Chem., 43(3), p711-717, 1951
- 5 [3229] Borisova I.A., Erlykina M.E., Sokolov N.M., Mikhailov V.A., Zakharov D.L., Gorbunov A.I., Deposited Doc., Code SPSTL 308 KHP-D 82, p1-13, 1982
- 6 [4581] Wuellner A., Poggendorff's Ann.Phys.Chem., 79(11), p353-366, 1866

no.	type	values	t[degC]	P[mmHg]	ref	data set
1	xyT (P)	10		2156.30	4	175 VLEDDB
2	xyT (P)	10		5414.30	4	176 VLEDDB
3	xyT (P)	10		3862.90	4	177 VLEDDB
4	xyT (P)	8		7224.40	4	178 VLEDDB
5	xyP (T)	19	25.00		1	636 VLEDDB
6	xyT (P)	27		760.00	2	637 VLEDDB
7	xyP (T)	19	0.00		3	638 VLEDDB
8	xyP (T)	19	10.00		3	639 VLEDDB
9	xyP (T)	19	20.00		3	640 VLEDDB
10	xyP (T)	19	30.00		3	641 VLEDDB
11	xyP (T)	19	40.00		3	642 VLEDDB
12	xyP (T)	19	50.00		3	643 VLEDDB
13	xyT (P)	20		760.00	5	11357 VLEDDB
14	xyPT (-)	8			6	20637 VLEDDB
15	xyPT (-)	10			6	20638 VLEDDB
16	xyPT (-)	10			6	20639 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.

PCPDDB - 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., Oniitekhim, Code 919 KHP - 87, 1-24, 1987

2 (31442) Grigorev B.A., Keramidi A.S., Prisyazhnyuk S.I., Oniitekhim, Code 217 KHP - 89, 1-25, 1989

T K	P kPa	VIS mPas	State	Prop:	Ref:
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]
(stripped some lines)					
398.15	882.000	0.00947	G	1	[31442]
398.15	971.000	0.00957	G	1	[31442]

13 Units

13.1 Mixture Data Banks – Compositions

Compositions can be displayed in mol/mol (mole fraction) or in g/g (mass fraction). LLE data sets are always displayed in percent (mass or molar).

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

VLE	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	HPV	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
LLE	<input checked="" type="radio"/> Mole Percent	<input type="radio"/> Mass Percent	SLE	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
VE	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	CPE	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
HE	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	ACM	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
AZD	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	ELE	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
CRI	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	VIS	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
MSFT	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	MSOS	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
MTCN	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	MDEC	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction
GHD	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction	ECND	<input checked="" type="radio"/> Mole Fraction	<input type="radio"/> Mass Fraction

Note: LLE-Plot always in Fractions

Overwrite Settings for Table Display:
☐ Show Both

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 to show the DDB data sets in original database specific units.

Act. Coeff. at Inf. Dilution 0: -

Temperature 1: K

Pressure 0: °C

Enthalpy 1: K

Excess Heat Capacity 2: °F

Density 3: °R

Excess Molar Volume 0: J/(mol*K)

☐ Disable Conversion (DDB Original Units)

Act. Coeff. at Inf. Dilution 0: -

Temperature 1: K

Pressure 5: kPa

Enthalpy 0: J/mol

Excess Heat Capacity 0: J/(mol*K)

Density 0: kg/m3

Excess Molar Volume 0: cm3/mol

Henry Coefficient 5: kPa

Molar Volume 0: cm3/mol

Dynamic Viscosity 1: mPas

Kinematic Viscosity 1: cSt

13.3 Pure Component Properties

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

Table Item	Unit	Unit of Errors	Precision
Temperature	1: K	1: K	2
Pressure	5: kPa	5: kPa	3
Molar Volume	0: cm3/mol	0: cm3/mol	2
Dynamic Viscosity	1: mPas	1: mPas	4
Density	1: g/cm3	0: kg/m3	3
Second Virial Coefficient	0: cm3/mol	0: cm3/mol	4
Kinematic Viscosity	0: m2/s	0: m2/s	2
Molar Enthalpy	0: J/mol	0: J/mol	2
Molar Heat Capacity (cP)	0: J/(mol*K)	0: J/(mol*K)	2
Thermal Conductivity	0: W/(m*K)	0: W/(m*K)	4
Surface Tension	1: mN/m	1: mN/m	4
Mass Heat Capacity	0: J/(g*K)	0: J/(g*K)	2
Molar Entropy	0: J/(mol*K)	0: J/(mol*K)	2

Figure 67 Pure Component Properties: Units

1: g/cm3

0: kg/m3

1: g/cm3

2: g/ml

3: kg/l


4: g/m3

5: kg/dm3

6: g/l

7: lb/ft3

Figure 68 Unit Drop-Down Menu

The button “  Standard ” resets all setting to DDB standard settings.

14 Consistency Tests

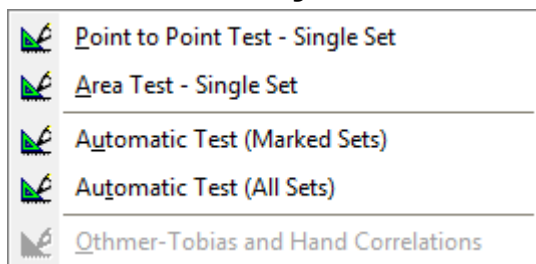


Figure 69: Consistency Test Menu

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 consistency test 1 offered is the so-called point-to-point test of van Ness et al.¹ in the version of Fredenslund et al.²

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, the data set is considered to be consistent.

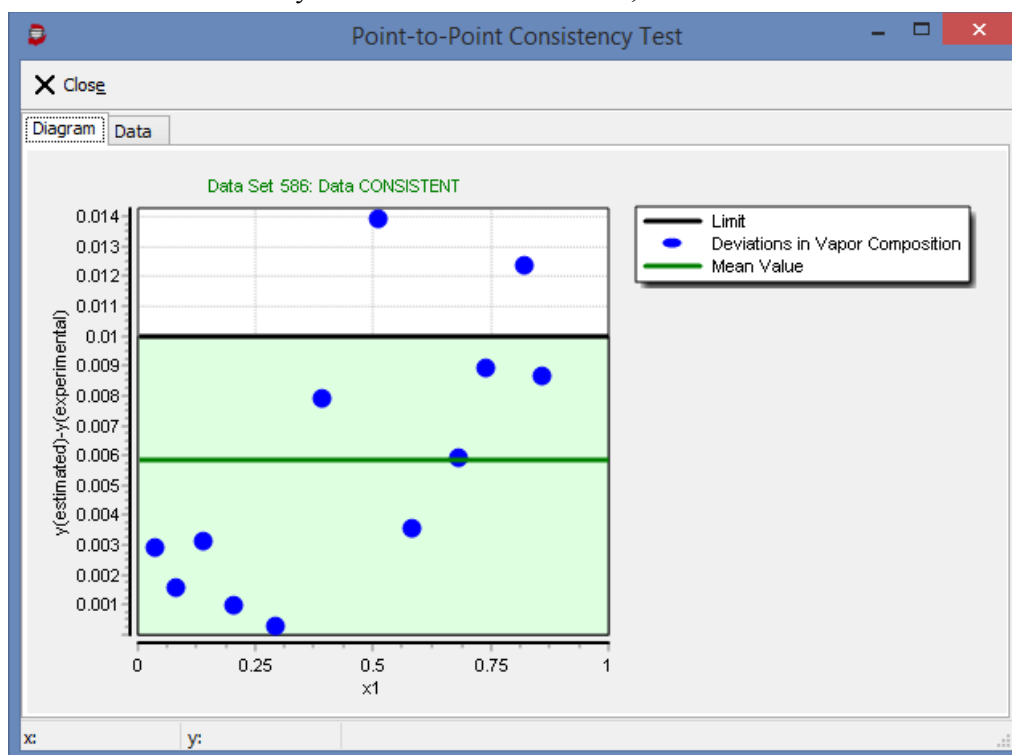


Figure 70: Point-to-Point Consistency Test

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

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

14.2 Area Test

The consistency test 2 is the so-called integral or area test using the method of Redlich-Kister³ and Herington⁴⁵. 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 degree 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:

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

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.

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

4 Herington E.F.G., Nature 160, 610 (1947)

5 Herington E.F.G., J. Inst. Petrol. 37, 457 (1951)

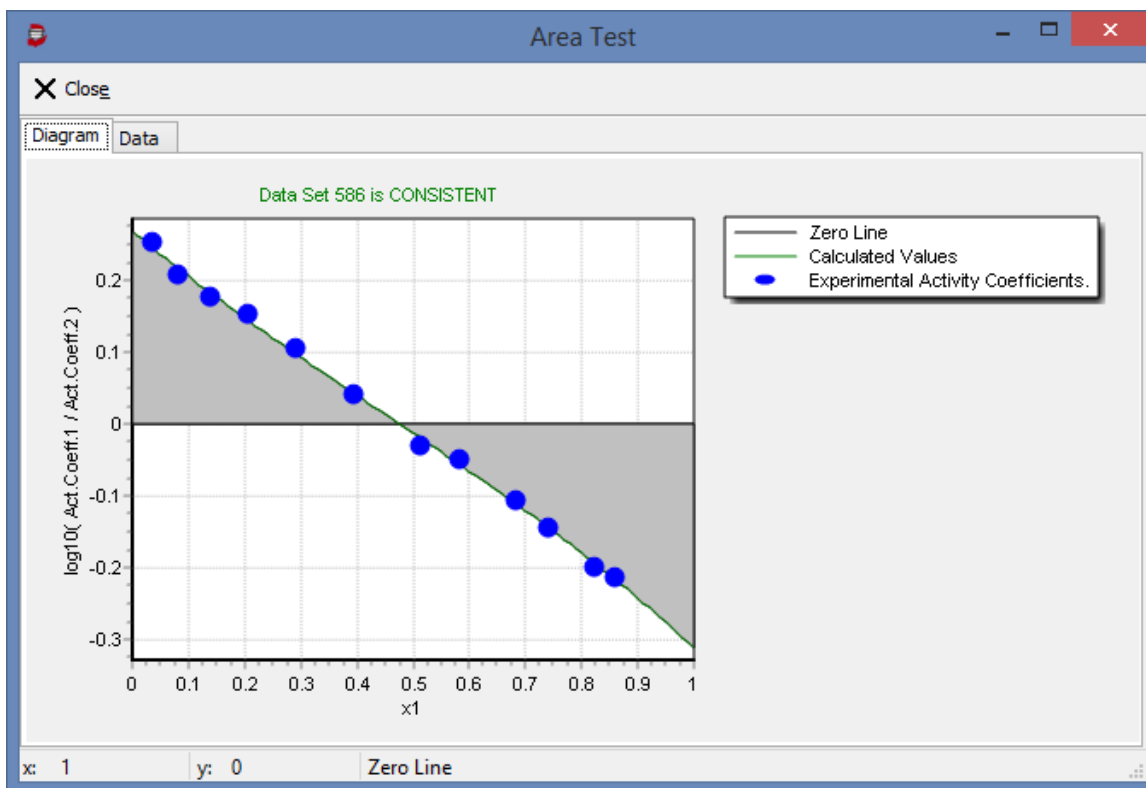


Figure 71: Area Test

14.3 Automatic Tests

“Automatic Tests” starts the consistency tests for all marked sets in the background and display their results in the “Comment” column of the data set grid.

“-” denotes an inconsistent data sets

“+” denotes an consistent set.

“?” denotes consistency test failure.

“*” shows that the consistency tests hasn't been performed.

Comment
{--} Txy(P)
{-?} Txy(P)
{--} Txy(P)
{-?} Txy(P)
{+-} Pxy(T)
{--} Txy(P)
{++} Pxy(T)
{++} Pxy(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 Tobias⁶ published a correlation which can be used to check tie lines in ternary mixture with two immiscible component and a single co-solvent for their consistency.

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

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_1 : Weight fraction of solvent a in the solvent a rich phase (typically Water)

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

n : Slope

S : Constant

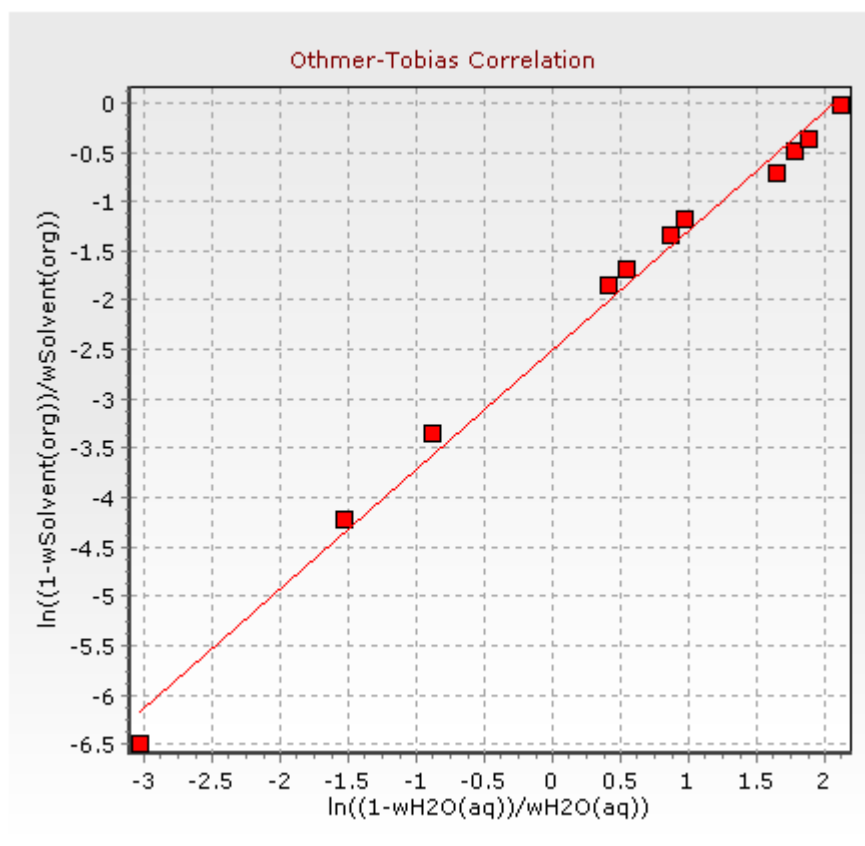


Figure 72: Othmer-Tobias Correlation

14.4.2 Hand Tie Line Correlation

Hand⁷ published a correlation which can be used to check tie lines in ternary mixture with two immiscible component and a single co-solvent for their consistency.

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

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

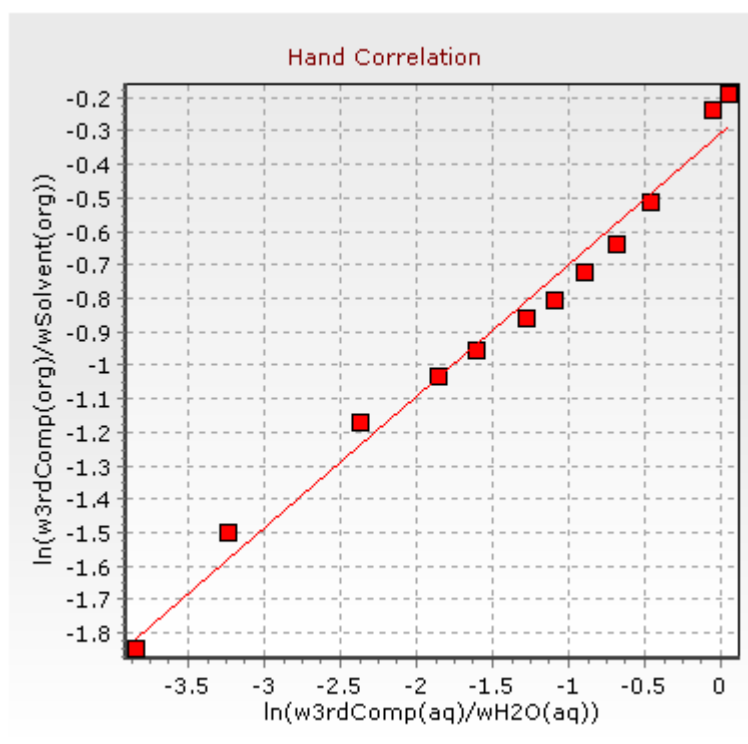


Figure 73: Hand Correlation

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 (cosolvent) is Acetic acid.

	<i>W't Fract. (Aq.) Water</i>	<i>W't Fract. (Aq.) Acetic Acid</i>	<i>W't Fract. (Aq.) Benzene</i>	<i>W't Fract. (Org.) Water</i>	<i>W't Fract. (Org.) Acetic Acid</i>	<i>W't Fract. (Org.) Benzene</i>
<i>Equation Terms</i>	<i>a₁</i>	<i>c₁</i>	<i>b₁</i>	<i>a₂</i>	<i>c₂</i>	<i>b₂</i>
	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

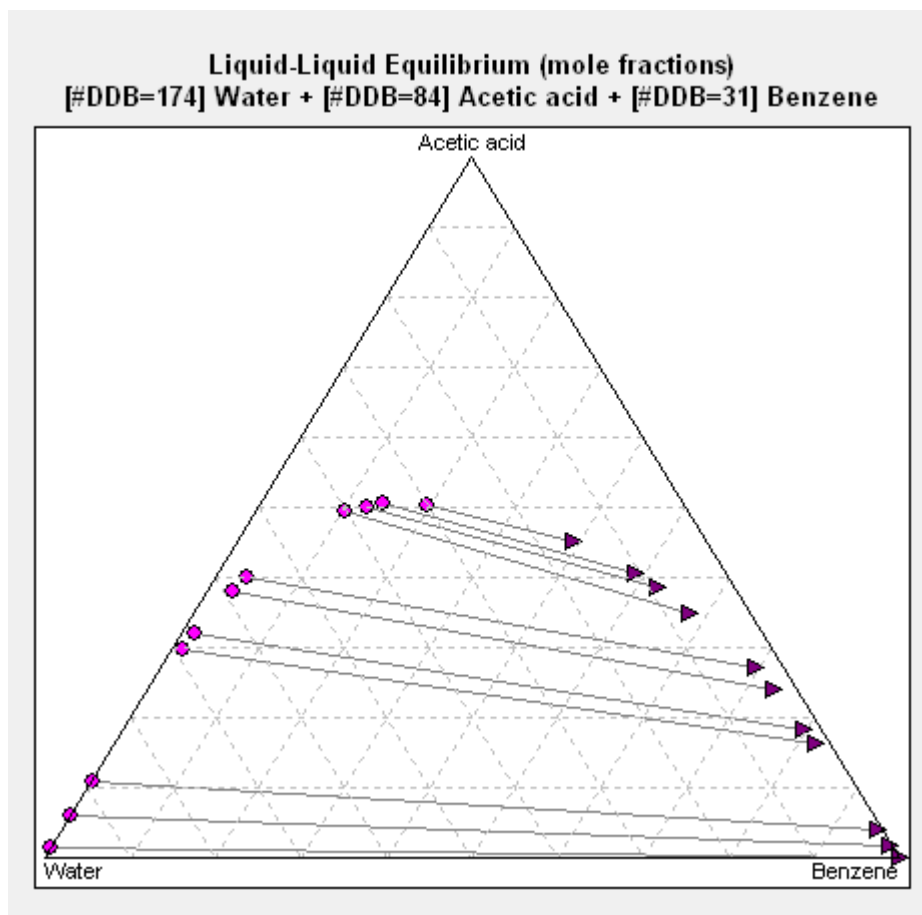


Figure 74: LLE Data Set No. 1367

15 Modifying and Editing Datasets

15.1 Editing Experimental Data

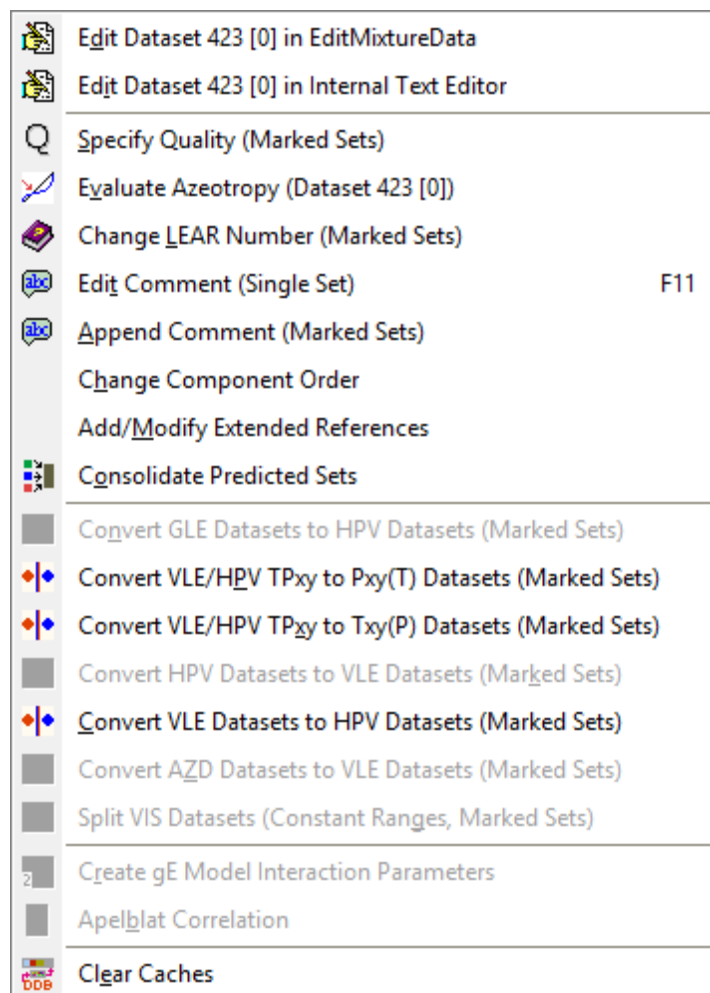


Figure 75 Sub Menu for Editing Functions

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

Modifications of data sets from the main retrieval program are not changing database content. It only allows to edit the currently loaded data set. 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 “Edit Pure Data” resp. “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 and Data Source

The quality settings are used to comment on special weaknesses. Almost 99 % of the data sets carry the comment “Default check passed” which means after the default check during the data input no further problem has been detected. The type of comment is rather widespread since further tests are mentioned, changes, problems with the references and so on.

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

The “Source” settings comment on the original data source. 99 % of the data sets in the DDB are original experimental data published in tables. Other comments are given if these data are smoothed or have been evaluated from diagrams.

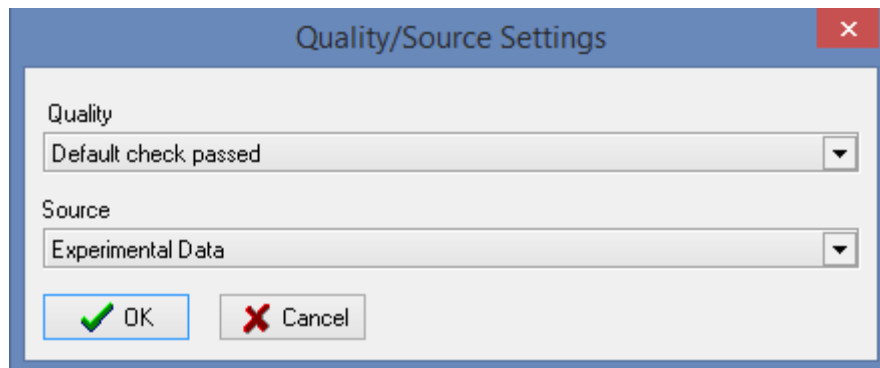


Figure 76: Quality/Source Settings

15.3 Evaluate Azeotropy

For binary VLE and HPV data sets it is possible to determine the azeotropic point or if the mixture is zeotropic.

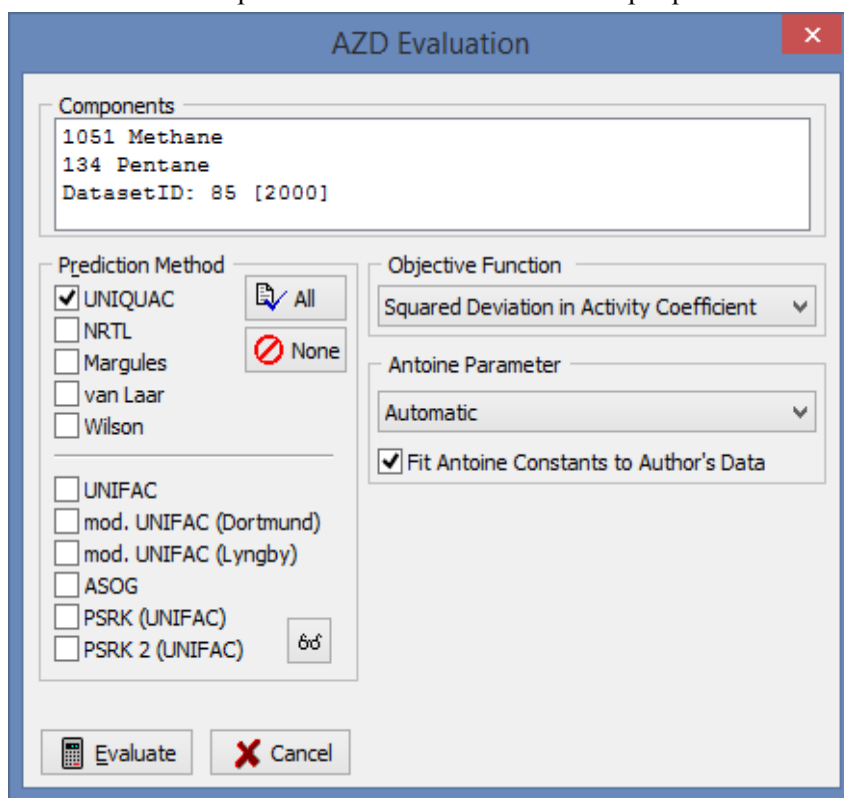
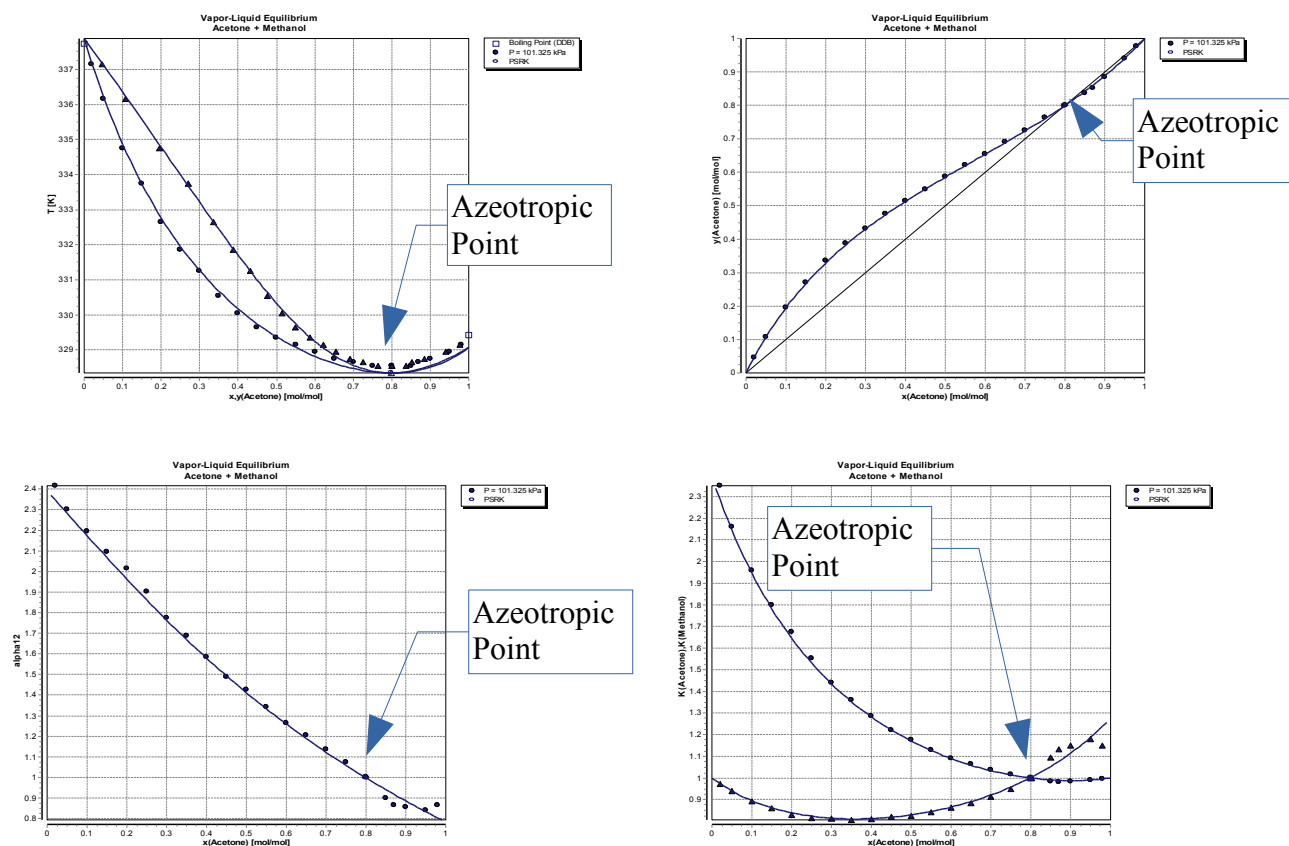


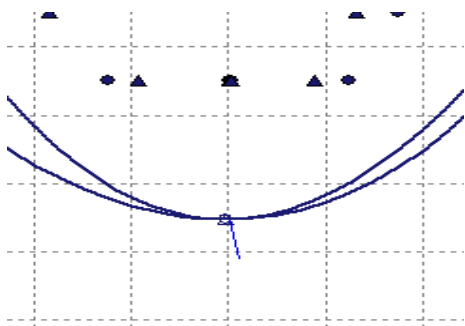
Figure 77 Evaluation of Azeotropy

The VLE data sets is displayed together with predicted data from activity coefficient models. In case of the g^E models UNIQUAC, NRTL, Margules, van Laar, and Wilson parameters are directly fitted with temperature-independent parameters. The program uses the predicted curves which contain 101 points from $x_1=0.$ to $x_1=1.$ in $x_d=0.01$ steps to determine the $x=y$ position by interpolating between the closest values.

The following diagrams are displayed:



The found azeotropic point is displayed as an uncolored hollow symbol.

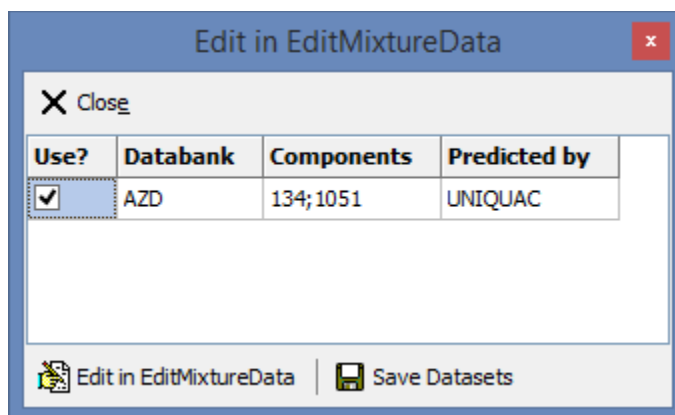


The additional text output gives the exact numerical value of the found temperature, pressure, composition, and type of azeotrope.

Azeotropic Point Prediction				
4:	Acetone	C3H6O	67-64-1	
110:	Methanol	CH4O	67-56-1	
Temperature	Pressure	y (Comp.1)	y (Comp.2)	Type

[K]	[kPa]				
328.35	101.33	0.7986	0.2014	homPmax	PSRK

If a azeotropic point has been found it is possible to save this point in the Dortmund Data Bank (via EditMixtureData) or in a data file (".qr" format).



15.4 Change LEAR Number

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

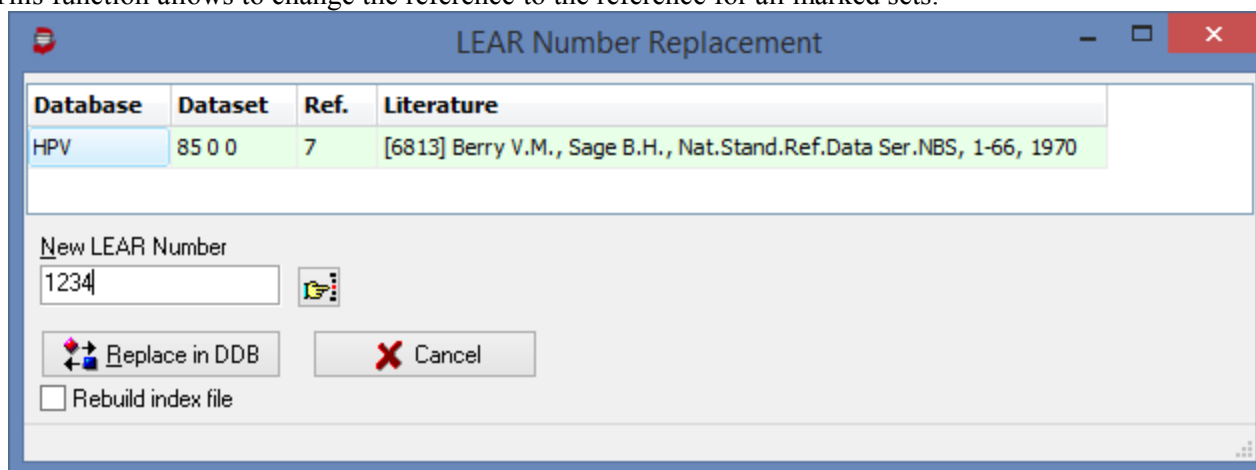


Figure 78 Changing Literature Number

The dialog list all marked data sets together with the references which will be exchanged. The "Rebuild index file" option allows to update the data bank index. Otherwise the index has to be updated separately later in the *IndexManager* program.

15.5 Edit Comment

This command allows to specify comments for single sets.

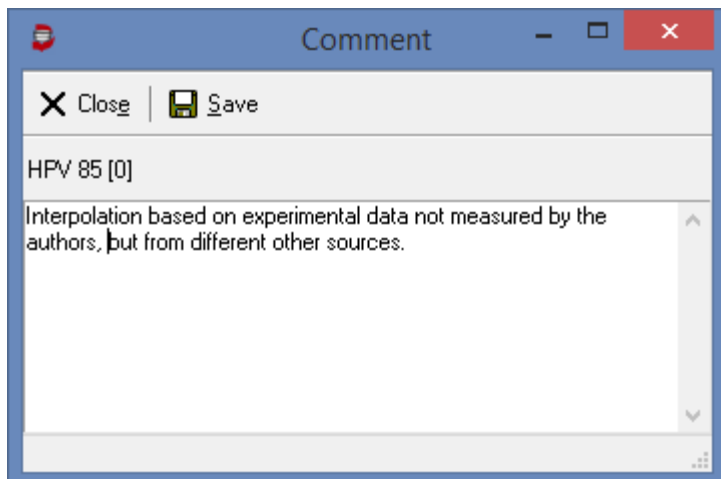


Figure 80 Comment Dialog

15.6 Append Comment

This command allows to enter a single comment 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.

15.7 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.

15.8 Add/Modify Extended References

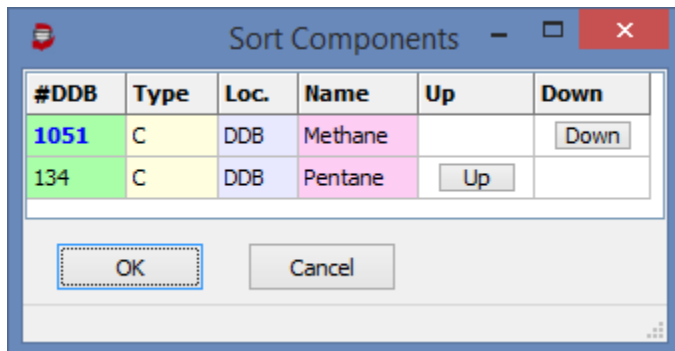


Figure 81: Change Component Order

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

15.9 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 to add convertible GLE data sets 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.

15.10 Convert HPV Data Sets to VLE Data Sets

HPV and VLE are both containing vapor-liquid equilibrium data sets. The only difference is that pressure and temperature are in different units. This function allows to alter temperature and pressure and use HPV data sets as VLE data sets. This conversion is useful or necessary if VLE and HPV data sets need to be plotted, printed, or exported together.

15.11 Convert VLE/HPV TPxy to Pxy(T) Datasets and Txy(P) Datasets

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

15.12 Split VIS Datasets (Isoplethic Ranges, Marked Sets)

The mixture viscosities data bank contain several very large data sets with multiple isothermal or isobaric regions or regions with constant compositions. This function allows to split these sets where one of these properties is constant. This make it much more readable and also improves some diagrams.

15.13 Create g^E Model Interaction Parameters

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

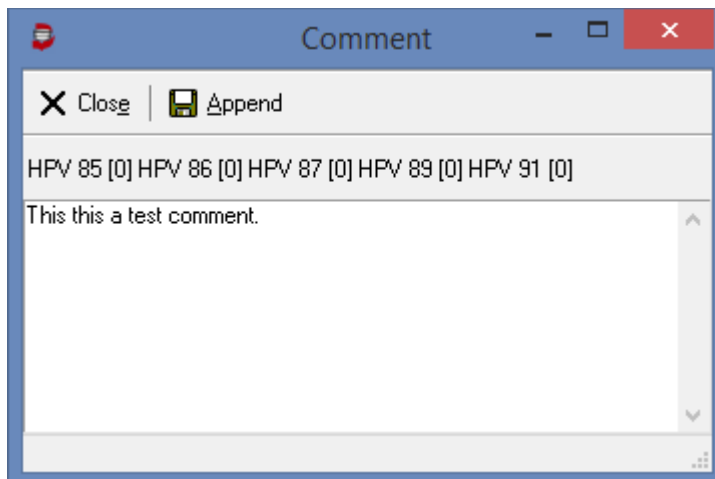


Figure 79: Comment Dialog (Multiple Sets)

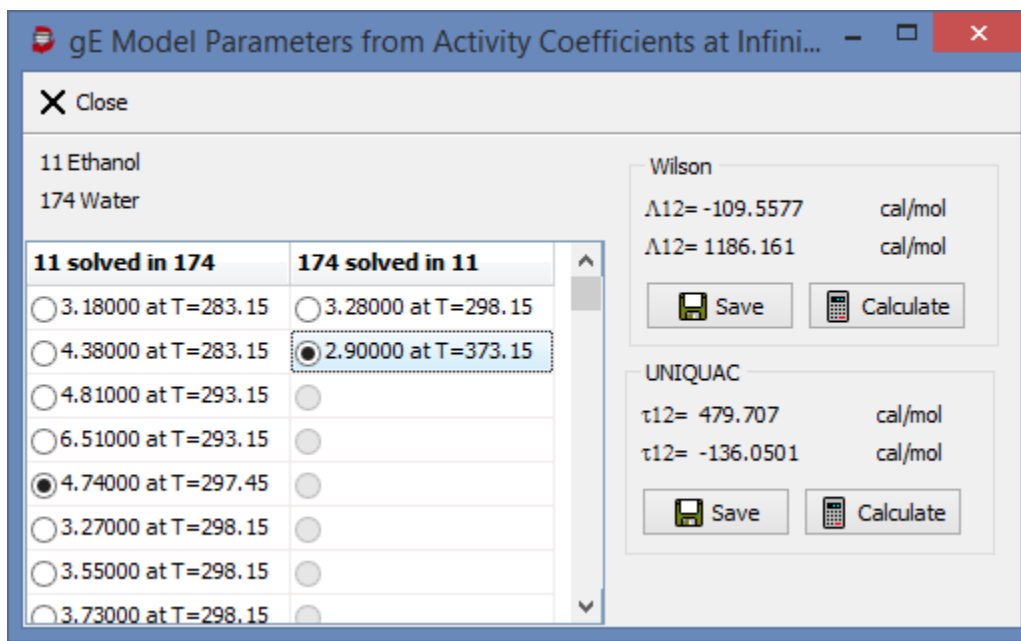


Figure 82: g^E Model Parameters from Activity Coefficients at Infinite Dilution

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 τ_{12}/τ_{21} for UNIQUAC are calculated immediately. The selected coefficients should be measured at similar temperatures.

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

15.14 Apelblat Correlation

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

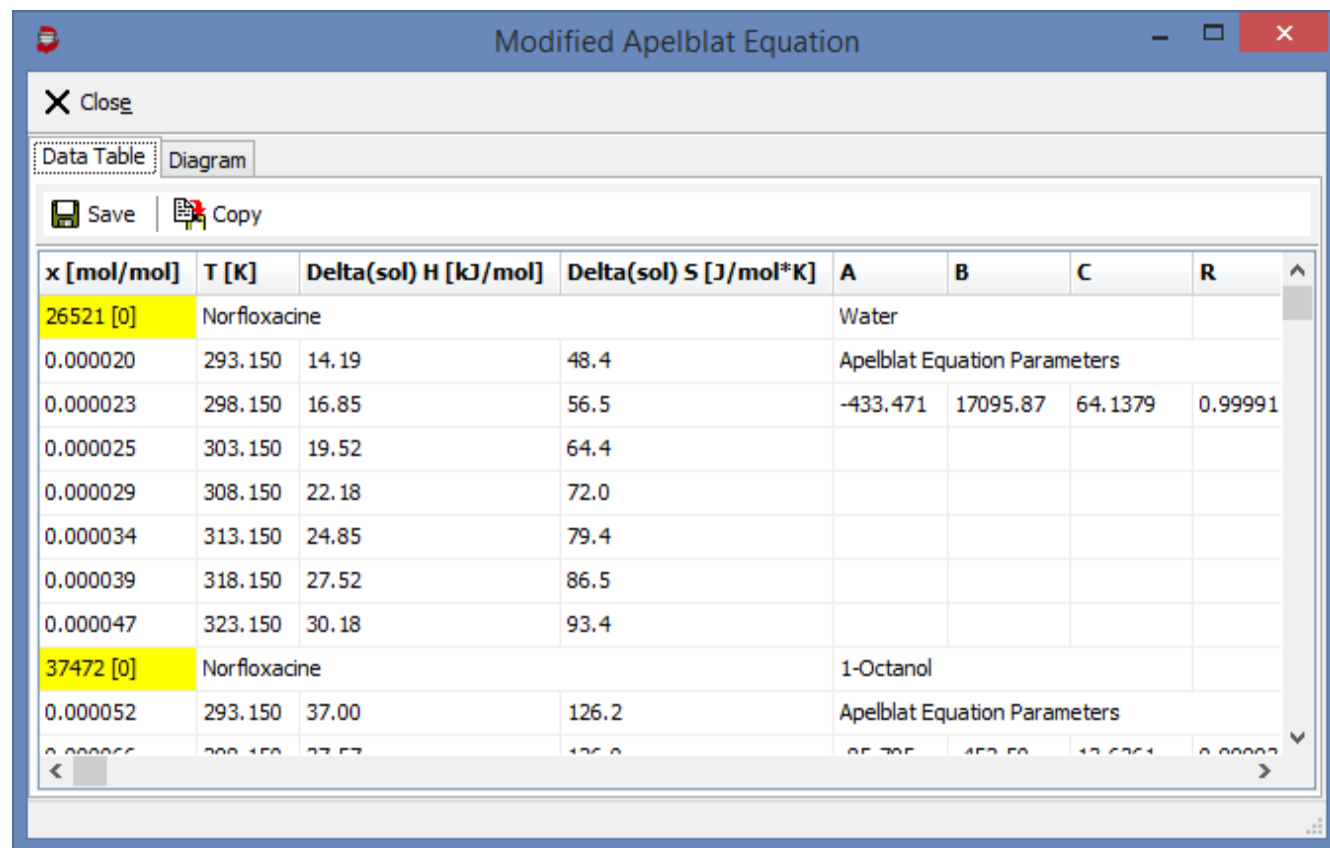
$$\ln x = A + \frac{B}{T} + C \ln T$$

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.

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

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

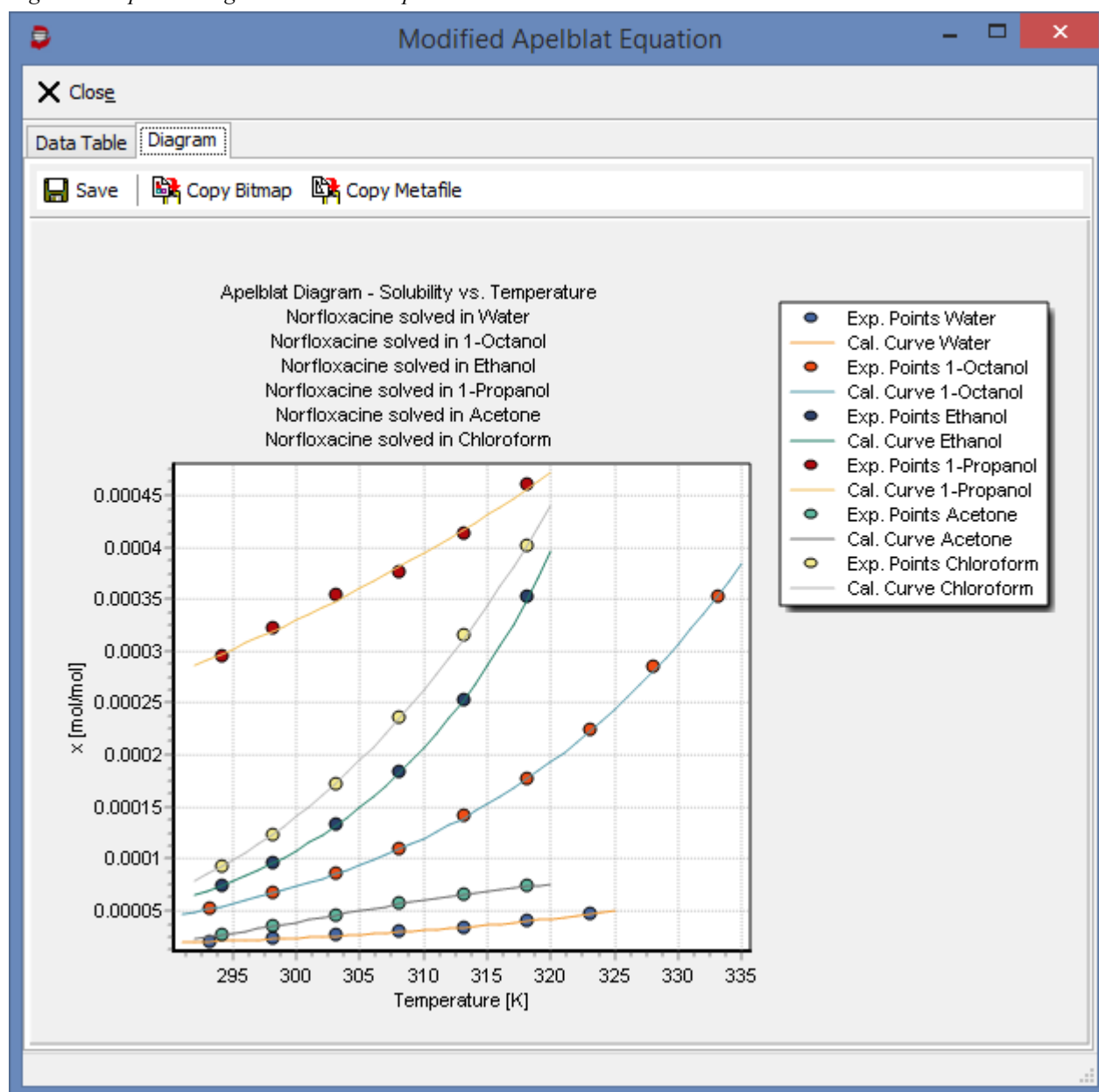
The Apelblat equation can only be used for small solubilities. An example is the solubility of Norfloxacin in some alcohols, Water and Acetone. The program shows a table and a diagram with the regression results.



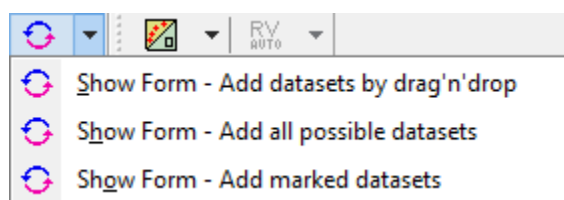
x [mol/mol]	T [K]	Delta(sol) H [kJ/mol]	Delta(sol) S [J/mol*K]	A	B	C	R
26521 [0]	Norfloxacin			Water			
0.000020	293.150	14.19	48.4	Apelblat Equation Parameters			
0.000023	298.150	16.85	56.5	-433.471	17095.87	64.1379	0.99991
0.000025	303.150	19.52	64.4				
0.000029	308.150	22.18	72.0				
0.000034	313.150	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			
0.000066	303.150	37.57	136.0	85.705	452.50	12.6261	0.99993

Figure 83: Apelblat Regression - Table Output

Figure 84: Apelblat Regression - Plot Output



16 Converting Data Sets to ELE Data Sets



This function can convert VLE, HPV, GLE, and EGLE data sets to ELE data sets. 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.

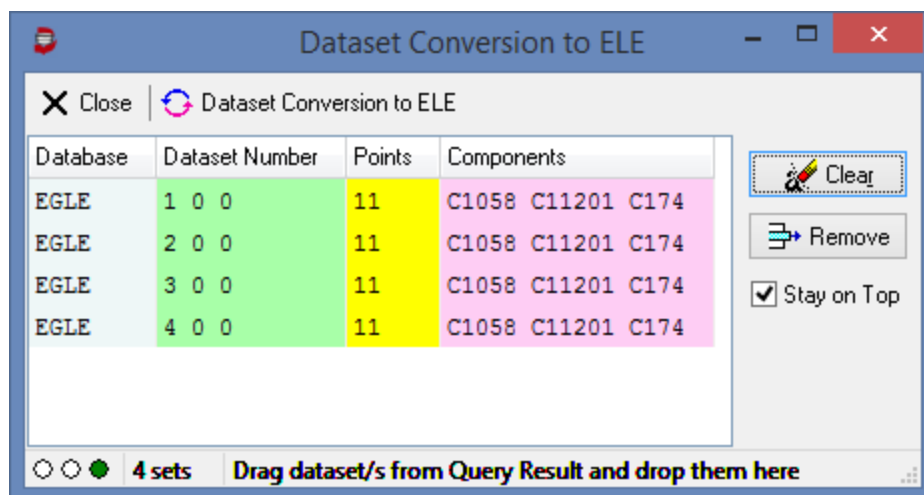


Figure 85: Data Set Conversion to ELE Format

The result is a list of ELE data sets (VLE data sets for electrolyte-containing mixtures) which can be plotted together or used in the prediction mainly by PSRK LIFAC.

17 Query Result Statistics

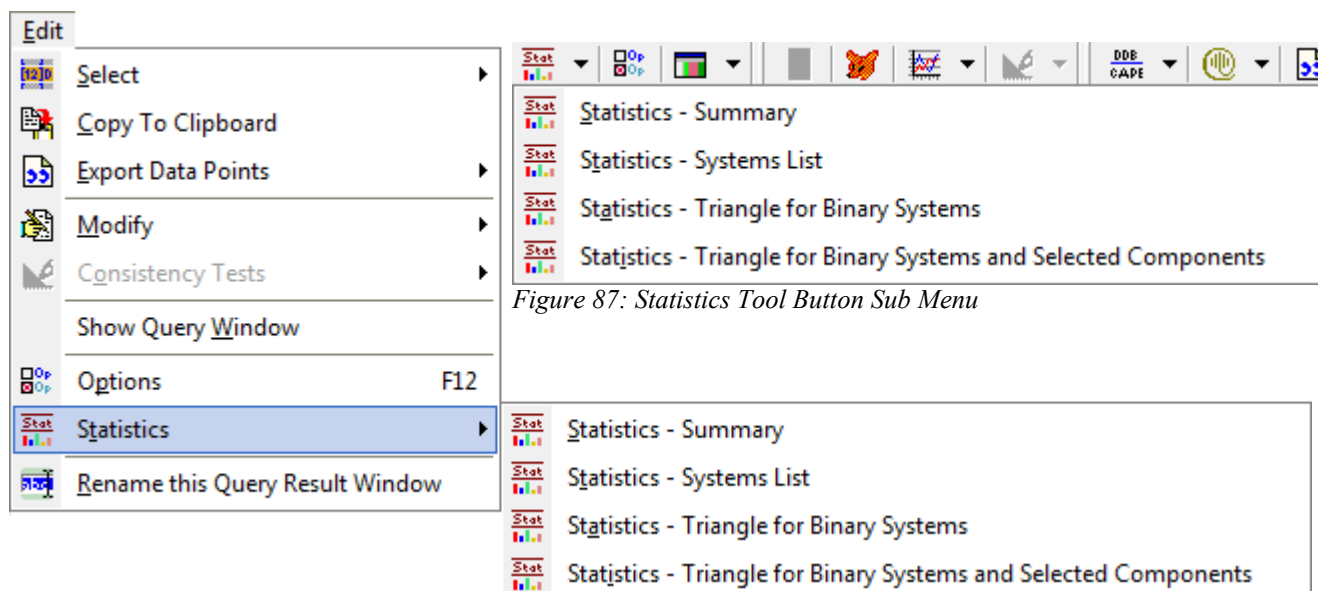


Figure 87: Statistics Tool Button Sub Menu

Figure 86: Statistics Sub Menu

17.1 Summary

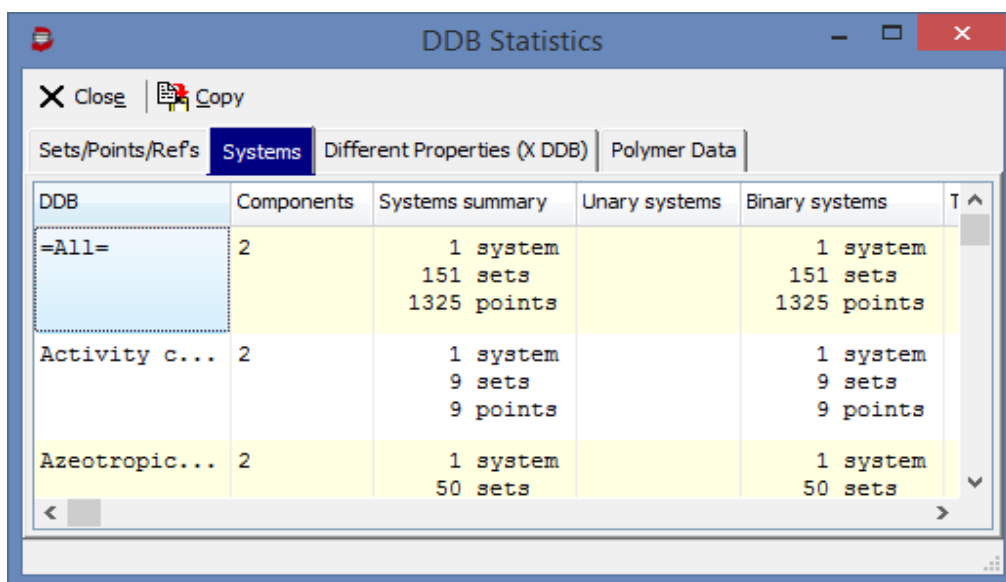
The “Statistics – Summary” for a query result grid shows approx. the same information as the statistics for the complete list of data banks..

1. Number of sets/points/references for every database

Databank	Sets	Points	References	DDB Description
ACT	9	9	4	Activity coefficients at infinite dilution
AZD	50	50	36	Azeotropic/zeotropic information
HE	7	98	7	Heats of mixing
MFLP	2	13	1	Mixture flash points
MPVT	1	1	1	Mixture P-v-T Data
MSFT	1	11	1	Mixture surface tensions
MSOS	3	43	2	Mixture speeds of sound
MTCH	1	10	1	Mixture thermal conductivities

Figure 88 Data Bank Statistics

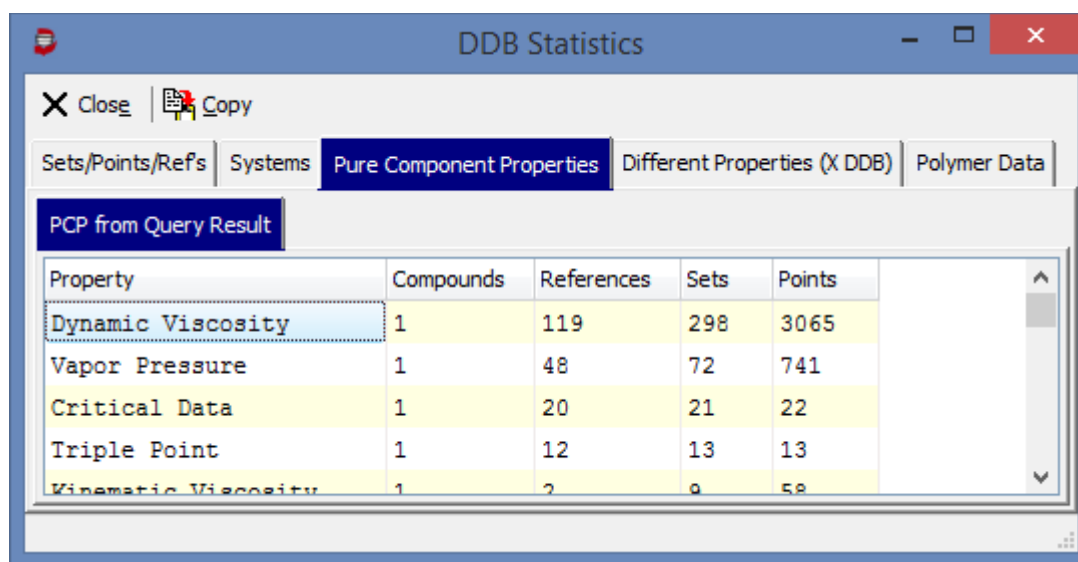
2. Overview over available systems



DDB	Components	Systems summary	Unary systems	Binary systems
=All=	2	1 system 151 sets 1325 points		1 system 151 sets 1325 points
Activity c...	2	1 system 9 sets 9 points		1 system 9 sets 9 points
Azeotropic...	2	1 system 50 sets		1 system 50 sets

Figure 89 Systems Statistics

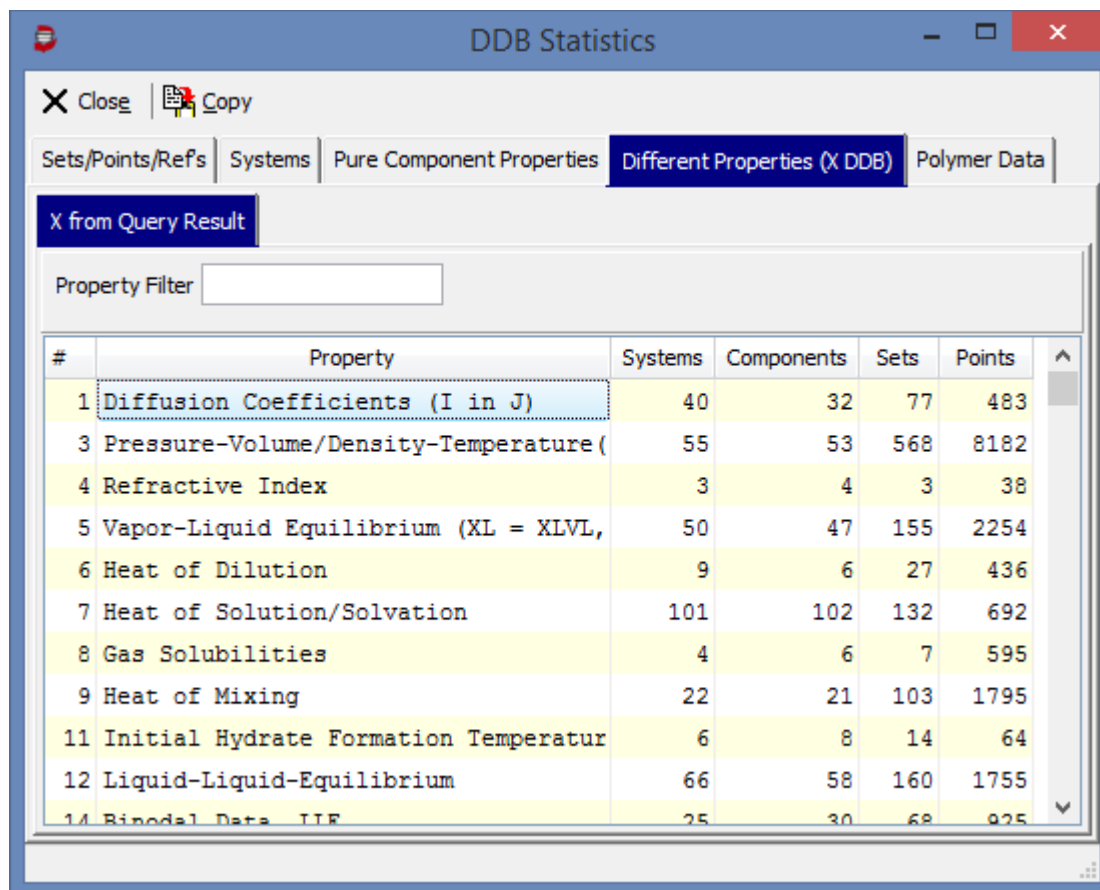
3. Number of sets/points/references for every property in the pure component properties database.



Property	Compounds	References	Sets	Points
Dynamic Viscosity	1	119	298	3065
Vapor Pressure	1	48	72	741
Critical Data	1	20	21	22
Triple Point	1	12	13	13
Kinematic Viscosity	1	2	9	58

Figure 90 Pure Component Properties Statistics

4. Details of the Data Sets of the Extended Data Bank ("X")



DDB Statistics

Close Copy

Sets/Points/Refs Systems Pure Component Properties Different Properties (X DDB) Polymer Data

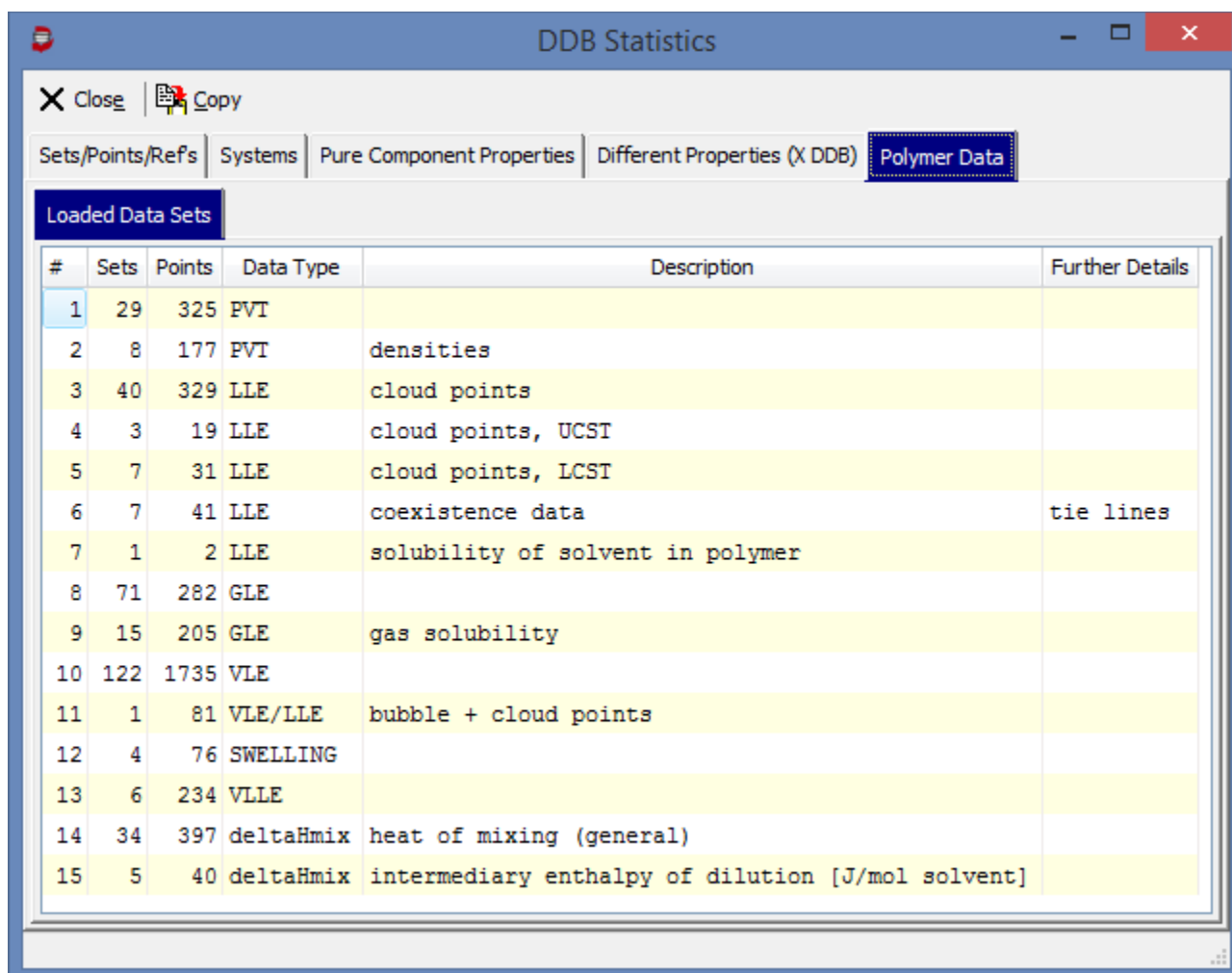
X from Query Result

Property Filter

#	Property	Systems	Components	Sets	Points
1	Diffusion Coefficients (I in J)	40	32	77	483
3	Pressure-Volume/Density-Temperature (55	53	568	8182
4	Refractive Index	3	4	3	38
5	Vapor-Liquid Equilibrium (XL = XLVL,	50	47	155	2254
6	Heat of Dilution	9	6	27	436
7	Heat of Solution/Solvation	101	102	132	692
8	Gas Solubilities	4	6	7	595
9	Heat of Mixing	22	21	103	1795
11	Initial Hydrate Formation Temperatur	6	8	14	64
12	Liquid-Liquid-Equilibrium	66	58	160	1755
14	Binodal Data - ILE	25	30	68	825

Figure 91: Details for "X" Data Bank

5. Details of the PolymerDDB properties



#	Sets	Points	Data Type	Description	Further Details
1	29	325	PVT		
2	8	177	PVT	densities	
3	40	329	LLE	cloud points	
4	3	19	LLE	cloud points, UCST	
5	7	31	LLE	cloud points, LCST	
6	7	41	LLE	coexistence data	tie lines
7	1	2	LLE	solubility of solvent in polymer	
8	71	282	GLE		
9	15	205	GLE	gas solubility	
10	122	1735	VLE		
11	1	81	VLE/LLE	bubble + cloud points	
12	4	76	SWELLING		
13	6	234	VLLE		
14	34	397	deltaHmix	heat of mixing (general)	
15	5	40	deltaHmix	intermediary enthalpy of dilution [J/mol solvent]	

Figure 92: 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.

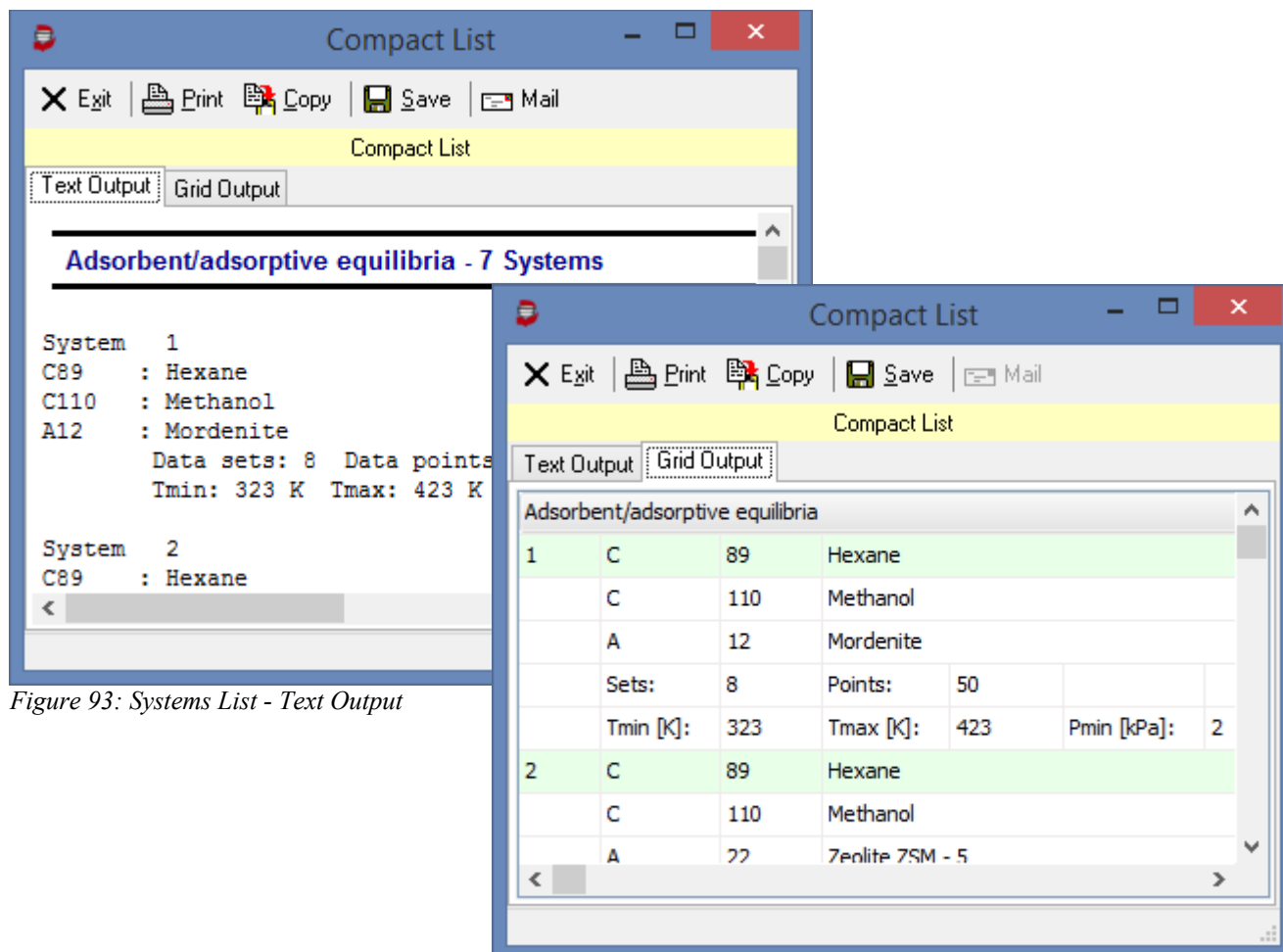


Figure 93: Systems List - Text Output

Figure 94: 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.

17.3.1 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.

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

DDB#	Component	Position
4	Acetone	<input type="radio"/> Left Side <input checked="" type="radio"/> Top Side
11	Ethanol	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side
47	Chloroform	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side
140	1-Propanol	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side
174	Water	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side
344	1-Octanol	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side
1050	Carbon dioxide	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side
17172	Polyethylene glycol 400	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side
22790	Norfloxacin	<input checked="" type="radio"/> Left Side <input type="radio"/> Top Side

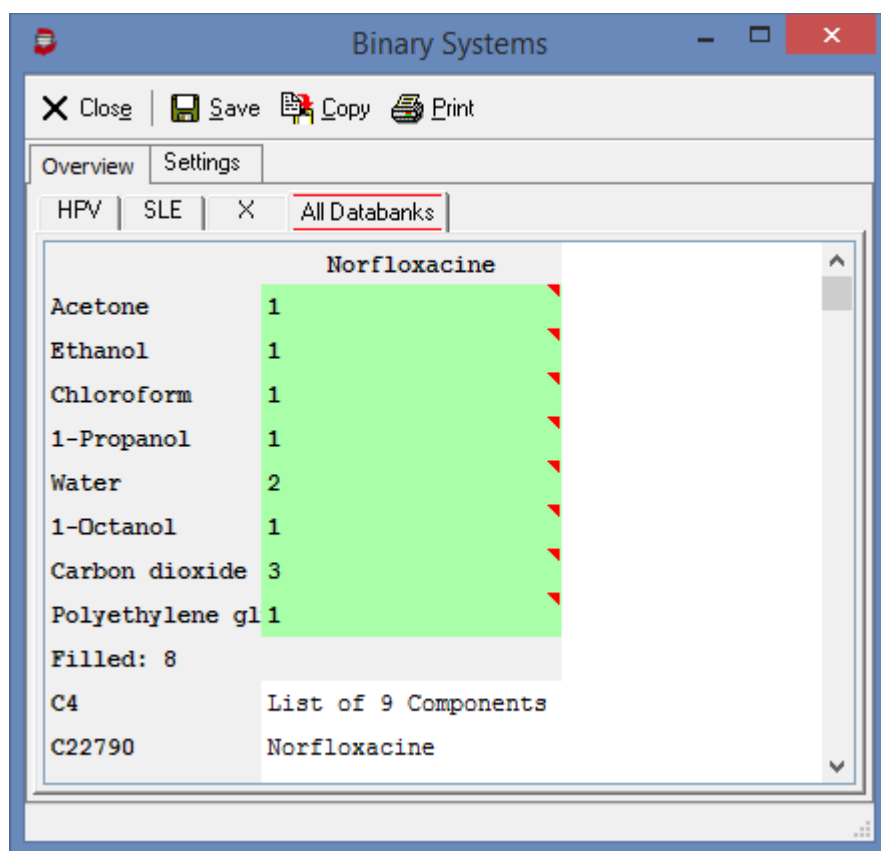


Figure 95: Binary Systems - Tabular Display

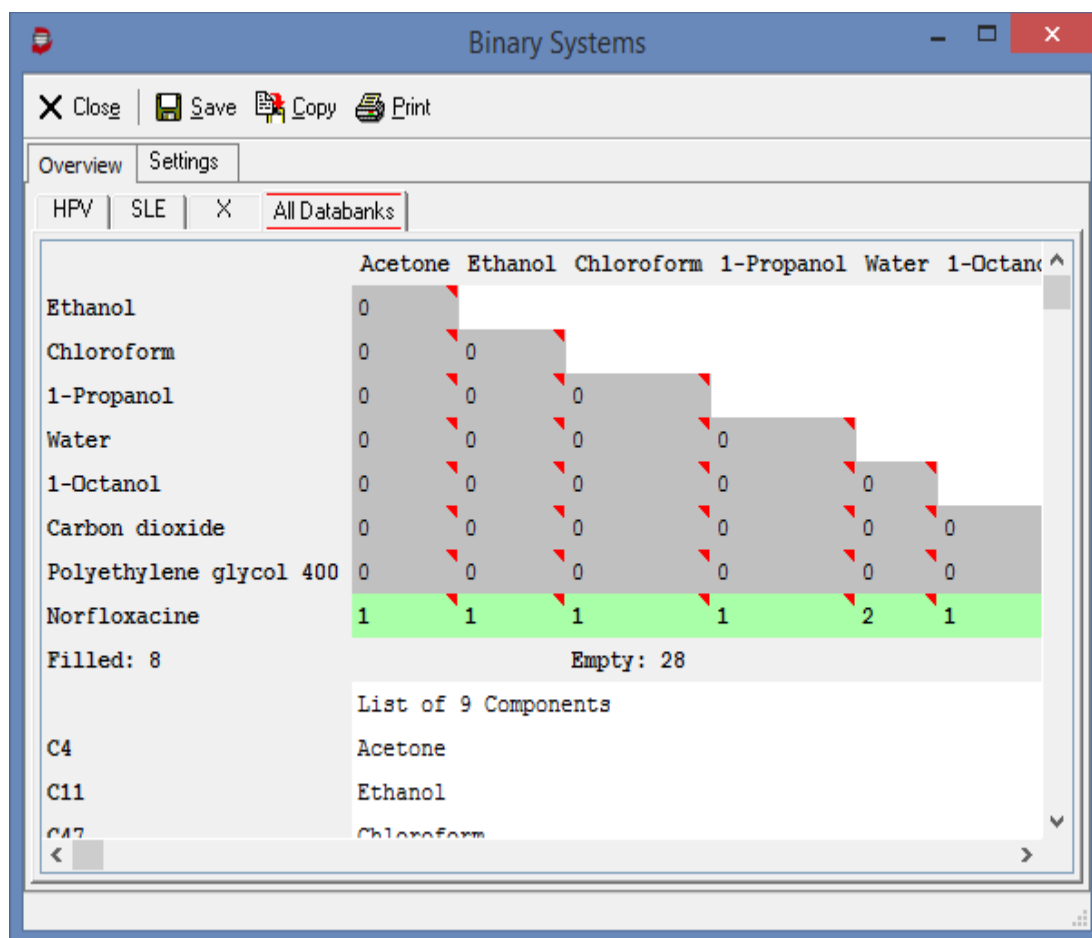



Figure 96: Triangle Diagram for Binary Systems

18 Predict

Prediction routines are available for many data banks and data types. If started from the query result window ( Predict) component are some data ranges are already set. Almost every prediction creates artificial data sets that are returned to the retrieval programs and displayed in a new data set grid together with the used data set.

18.1 ACM

Prediction of activity coefficients at infinite dilution of a single solute in a mixture of two solvents.

Figure 97: Prediction of Activity Coefficients at Infinite Dilution - Binary Solvents

The ACM prediction allows selecting between some g^E model, some group contribution models, the COSMO-SAC model, and with the thermodynamics engine of the Aspen simulator. 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

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 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.

ACT Prediction
✕

Components

11	Ethanol	Tc=516.20 K	Pc=6383.5 kPa	Tm=158.65 K	Hfus=1199.2 J/mol
89	Hexane	Tc=507.40 K	Pc=3014.4 kPa	Tm=177.85 K	Hfus=3123.6 J/mol

Prediction Method

All Models ▾

- NRTL
- UNIQUAC
- Wilson
- Margules
- van Laar
- UNIFAC
- Mod. UNIFAC (Ly)
- ASOG
- MOSCED 1984
- MOSCED 2005
- PSRK
- VTPR
- COSMO-RS(OI)

Active Models

Model	Options
Mod. UNIFAC (Do)	
NIST-mod. UNIFAC	

Calculation Mode

☒ Temperature Range

Start: °C

End: °C

Step Width: °C

☐ Experimental Temperatures

T=15.00°C A.C.=83.7000 ▾ °C

Predict (Table Output)

Predict (Plot Output)

Predict (Result => Query Result)

✕ Cancel

Figure 98: Prediction of Activity Coefficient at Infinite Dilution

18.2.1 Selectivity Calculation

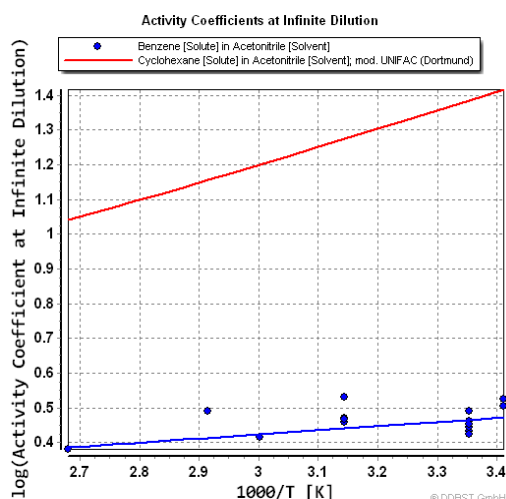


Figure 99: Activity Coefficient Diagram

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.

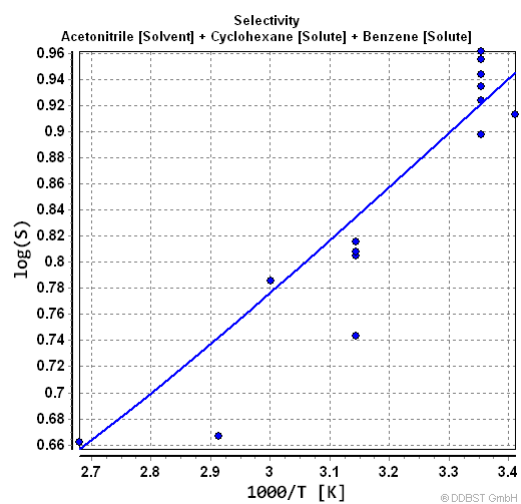


Figure 100: Selectivity Diagram

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

ACT Prediction

X

Components

3	Acetonitrile	Tc=548.00 K	Pc=4833.2 kPa	Tm=229.30 K	Hfus=2128.1 J/mol
31	Benzene	Tc=562.10 K	Pc=4894.0 kPa	Tm=278.68 K	Hfus=2376.7 J/mol

Prediction Method

All Models ▾

- NRTL
- UNIQUAC
- Wilson
- Margules
- van Laar
- UNIFAC
- Mod. UNIFAC (Ly)
- ASOG
- MOSCED 1984
- MOSCED 2005
- PSRK
- VTPR
- COSMO-RS(OI)

➡

⬅

↔

⊞

Active Models

Model	Options
Mod. UNIFAC (Do)	
NIST-mod. UNIFAC	

Calculation Mode

☒ Temperature Range

Start: °C

End: °C

Step Width: °C

☐ Experimental Temperatures

T=20.00 °C A.C. = 3.1900 ▾ °C

Predict (Table Output)

Predict (Plot Output)

Predict (Result => Query Result)

Cancel

Selectivity Calculation

Select 2 Solutes:

☒ 31: Benzene

☒ 50: Cyclohexane

Select Single Solvent:

☒ 3: Acetonitrile

Predict (Table Output)

⊞

Predict (Dataset/s => Query Result)

Predict (Plot Output)

Figure 101: Selectivity Prediction Dialog

18.3 AZD

Prediction of azeotropic points for binary 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 allows two main choices:

1. The “Antoine-Low” equation has by far the most parameters available but it not able to reproduce the entire vapor pressure curve from the triple to the critical point
2. The DIPPR 101 equation is able to reproduce the entire curve but there are parameter sets for much less components available.

The DIPPR 101 parameters can be obtained from two different sources. The ParameterDDB contains parameters made by DDBST. The other source is DIPPR but these parameters are not up-to-date anymore.

AZD Prediction

Components					
89	Hexane	Tc=507.40 K	Pc=3014.4 kPa	Tm=177.85 K	Hfus=3123.6 J/mol
11	Ethanol	Tc=516.20 K	Pc=6383.5 kPa	Tm=158.65 K	Hfus=1199.2 J/mol

Prediction Method

All Models

- NRTL
- UNIQUAC
- Wilson
- Margules
- van Laar
- UNIFAC
- NIST-mod. UNIFAC
- ASOG
- PSRK
- PSRK2
- VTPR
- COSMO-RS(OI)
- COSMO-SAC

Active Models

Model	Options
Mod. UNIFAC (Do)	
Mod. UNIFAC (Ly)	

Temperature Range

Start: 263.15 End: 483.15 Step Width: 5 K

Pressure Range

Start: 24.755 End: 4130.060 Step Width: 50 kPa

☐ Recalculate experimental P or T

Activity Coefficient Model Options

Vapor Pressure Equation: Antoine-Low

Vapor Phase Fugacity Model: Ideal

Poynting Correction: No Correction

(not for PSRK/VTPR)

Predict (Table Output) Predict and Plot Predict (Result => Query Result) Cancel

Figure 102 Prediction of Azeotropic Data

18.4 ELE

Prediction of vapor-liquid equilibria for electrolyte-containing systems.

The available ELE models are Sander, Electrolyte-NRTL, Macedo, UNIFAC (Kikič), LiQUAC, LiFAC (by Hans-Martin Polka), and modified LiQUAC, LiFAC (by Jörn Kiepe), PSRK LIFAC, and VTPR LiFAC. These models can also handle binary solvents.

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

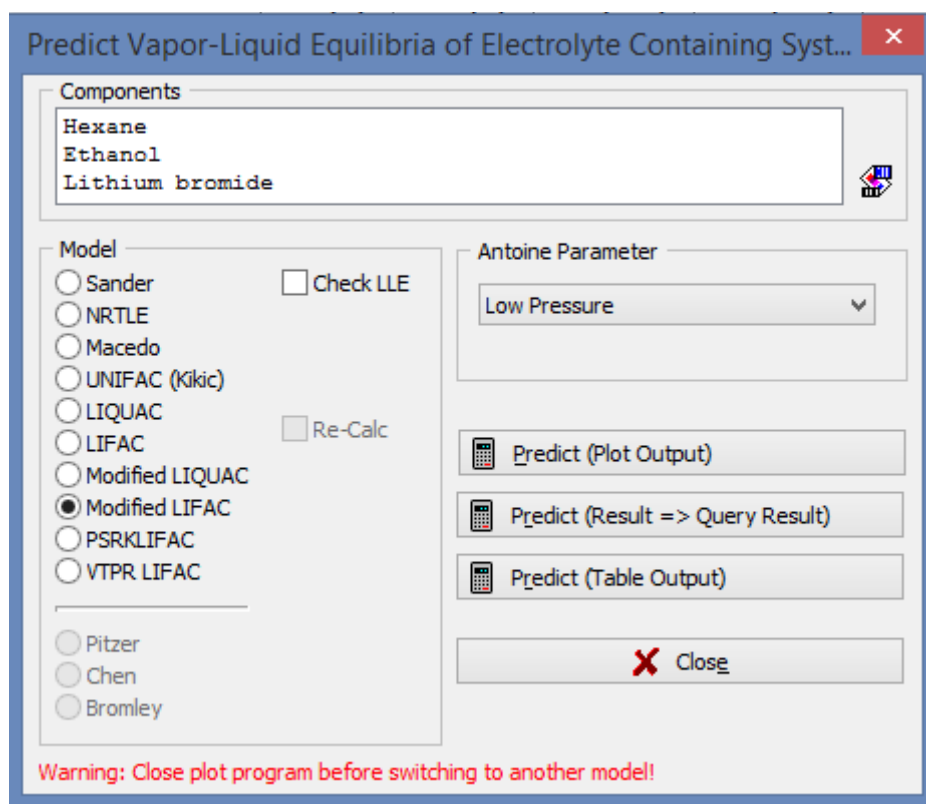


Figure 103 Prediction of Vapor-Liquid Equilibria of Electrolyte-Containing Systems

18.5 GLE

Prediction of gas solubilities.

GLE Prediction

Components

11	Ethanol	Tc=516.20 K	Pc=6383.5 kPa	Tm=158.65 K	Hfus=1199.2 J/mol
89	Hexane	Tc=507.40 K	Pc=3014.4 kPa	Tm=177.85 K	Hfus=3123.6 J/mol

Prediction Method

All Models

Active Models

Model	Options
Prausnitz-Shair	

Temperature

Temperature: 298.15 to 298.15 K

Step Width: 10 K

Buttons: Predict (Table Output), Predict and Plot, Predict (Result => Query Result), Cancel, VLE Prediction

No VLE sets created.

Figure 104: 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 93).

7 VLE sets created. Prediction of VLE is enabled.

VLE Prediction

18.6 HE

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 the equation of state based models PSRK and VTPR.

hE Prediction

Components

89	Hexane	Tc=507.40 K	Pc=3014.4 kPa	Tm=177.85 K	Hfus=3123.6 J/mol
11	Ethanol	Tc=516.20 K	Pc=6383.5 kPa	Tm=158.65 K	Hfus=1199.2 J/mol

Prediction Methods

All Models

- NRTL
- UNIQUAC
- Wilson
- UNIFAC
- Mod. UNIFAC (Ly)
- ASOG
- PSRK
- VTPR
- COSMO-RS(OI)
- COSMO-SAC
- Aspen Model

Active Models

Model	Options
Mod. UNIFAC (Do)	
NIST-mod. UNIFAC	

Conditions

T [°C]	P [bar]
25.00	2.16

Pressure is only used in PSRK and VTPR

Mole Fraction Range

Min. x	Max. x	Stepwidth
0.0	1.0	0.01

Create Data Points

Special Data Point Creation

0 Points

x [89] x [11]

Predict (Table Output) Predict and Plot

Predict (Result => Query Result) 3D Predict and Plot Cancel

Figure 105: Prediction of Excess Enthalpies

For more information about using Aspen projects, please see page 110, chapter “Using Aspen Projects“.

18.7 VLE/HPV

Prediction of vapor-liquid equilibria.

Figure 106 Prediction of Vapor-Liquid Equilibria

Vapor-liquid equilibria can be calculated by g^E models and by EOS based models.

Simple g^E equation based models are Wilson, UNIQUAC, NRTL, Margules, and van Laar. These equation need binary interaction parameters for all binary subsystems. These parameters can be fitted by RecPar.

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), modified UNIFAC (Dortmund), and ASOG. The UNIFAC models are based on UNIQUAC, and ASOG is based on Wilson.

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 equation parameters.

The PSRK and the VTPR models are based both on equations of state and a group contribution method and allow to predict VLE data sets even if components are super-critical. VTPR is a rather new prediction method. It currently has a limited number of parameters.

PSRK is under development for more than a decade now and has a much wider range of applicability.

COSMO-SAC is a method based on molecular structure and the charge distribution of the molecular surface. This model needs component specific “profile” files.

“Recalculate Data Points” allows the user to calculate the data points of given experimental data sets.

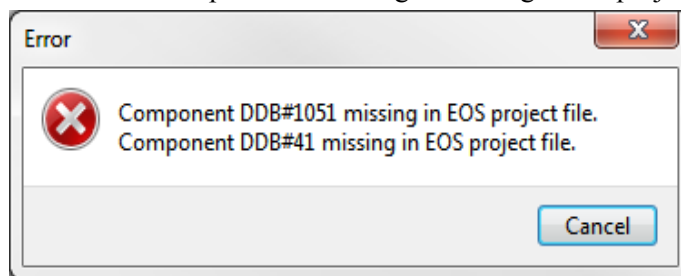
For the selection of the vapor pressure equation please refer to the description for the explanation above in the azeotropy prediction chapter.

The vapor phase description can be done by Raoult's Law (“Ideal”), or by equation of states, or by the Hayden-'O'Connell method.

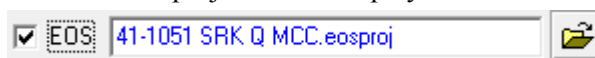
18.7.1 Predict with EOS

The prediction of VLE with EOS is based on EOS project files. The project files can be generated by the *Generate EOS Mixing Rule Parameters* program (short *GenPar*). A project file can contain interaction parameters for several binary component pairs.

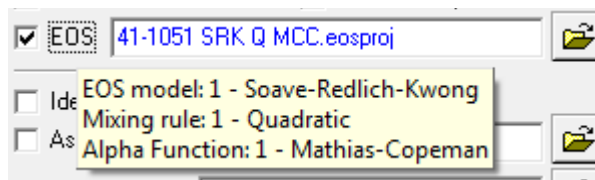
First of all a suitable EOS project file has to be selected using the EOS open button. An error message will appear if any of the components in the VLE prediction dialog is missing in the project.



After the project was loaded the name of the project file is displayed in the text field next to the EOS check box.



If the mouse is over the EOS check box and a project is loaded some details about the project are displayed as hint.



Now the EOS can be used like any other model.

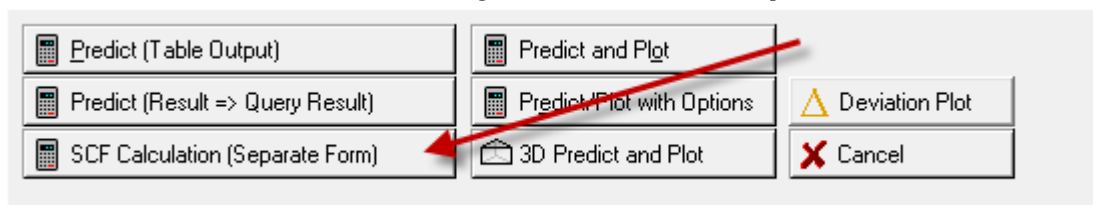
If the option “Recalculate Data Points” is activated the text out will contain the deviations for temperature, pressure and/or vapor composition (depending on the type of data set).

18.7.2 Prediction by Aspen or PRO/II Projects or by “Extension”

These predictions use the thermodynamic engines of the Aspen or Pro/II simulators. “Extension” is a customer-specific extension.

In all three cases a simulator-specific project file has to be loaded before starting the calculation. Details to these prediction types is available in the chapters “Using Aspen Projects” and “PRO/II Calculations” below.

18.7.3 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.

 A screenshot of the 'SCF Prediction' dialog box. The 'Components' section lists '925: Anthracene' and '1050: Carbon dioxide'. The 'Supercritical Gas (Solvent)' dropdown is set to '1050: Carbon dioxide'. The 'Temperature/s' is set to '308.00' K. The 'Solute (High Boiler)' dropdown is set to '925: Anthracene'. The 'Antoine Parameters' are '8.4004 2771.1 176.02'. The 'Solid Volume (Solute)' is '0.14259 dm³/mol at 2'. The 'Co-solvent' is set to '= None ='. The 'Sublimation Vapor Pressure Calculation' is set to 'Antoine'. On the right, there are buttons for 'PSRK', 'PSRK2', and 'VTPR'.

Figure 107: SCF Calculation

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. 2800 180

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 Volumes: 0.265

The “Cosolvent” combo box allows to specify a single additional solvent.

Cosolvent

89 Hexane

= None =

1050 Carbon dioxide

925 Anthracene

89 Hexane

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

The result of a SCF calculation are a data table and a diagram.

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
.....						

The table contains the solubilities of the high-boiling component in the “Y(2)” column as mole fractions. The calculation is automatically for a pressure range from 2 to 600 bar. “VV” is the vapor volume, “PHI” is the

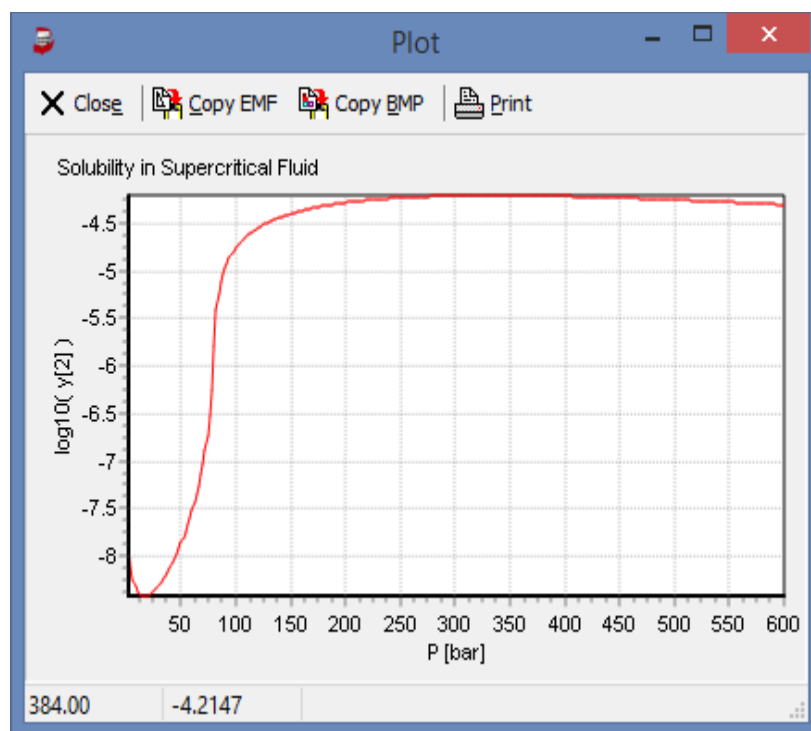


Figure 108: Solubility in a Supercritical Fluid

fugacity, and “POIN” the poynting factor.

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

18.7.4 Deviation Plot

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

18.7.5 Phase Envelope Calculation

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

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

These P/T curves can be calculated with PSRK and VTPR.

The buttons “PSRK (Return Result)” and “VTPR (Return Result)” will create a new Query Result window with the calculation results whereas the normal button only show the results in the current dialog.

Additional composition can be added manually into the data grid.

Mole Fraction	
0.887100	0.321
0.112900	0.679

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

The function “Check Interaction Parameter Availability” is described in the chapter 18.15 - “Checking Availability of Model Parameters”.

18.7.5.1 Options

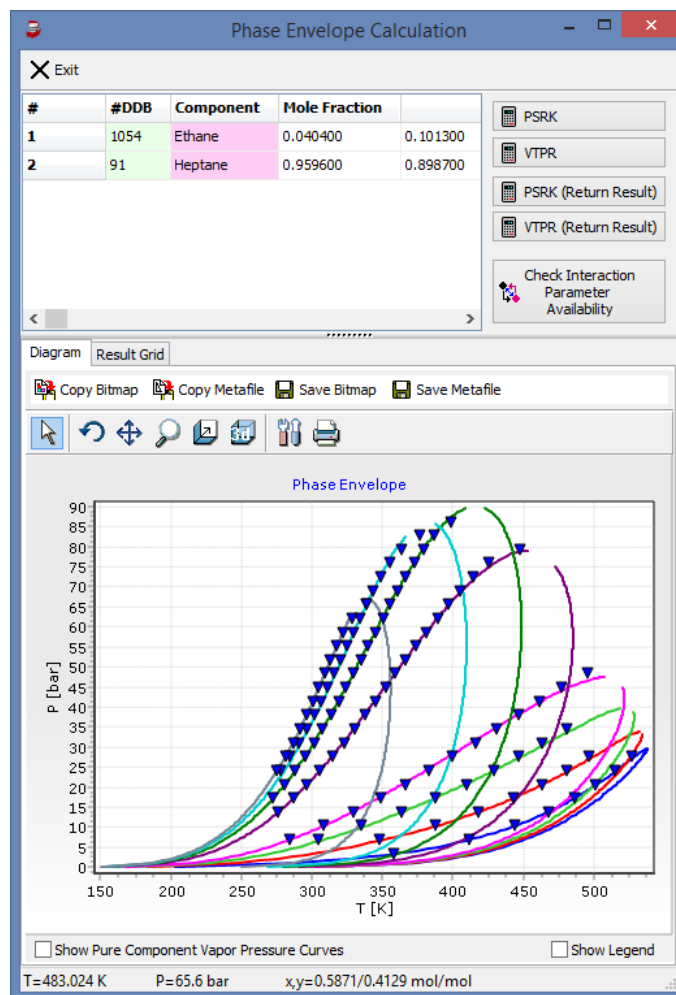


Figure 109: Phase Envelope Calculation

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

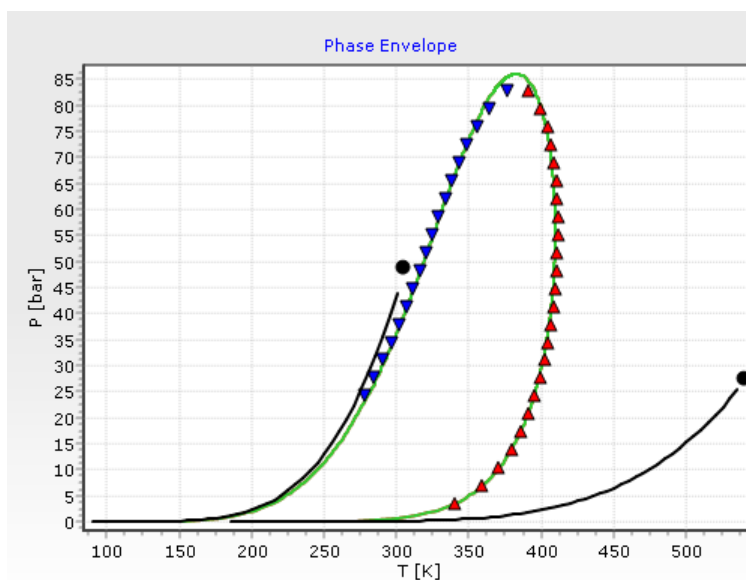


Figure 110: Phase Envelopes: Pure Component Vapor Pressures

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

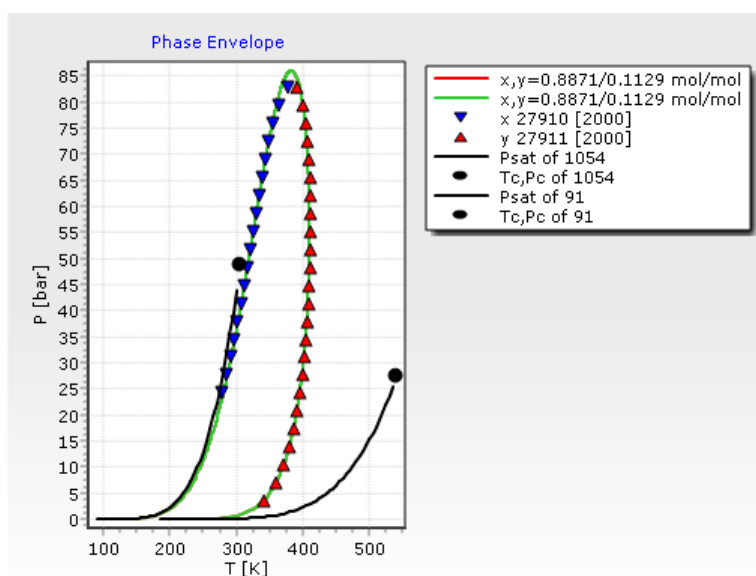


Figure 111: Phase Envelopes: Show Legend

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



18.8 LLE

Prediction of miscibility gaps.

Components

174	Water	Tc=647.30 K	Pc=22048.3 kPa	Tm=273.15 K	Hfus=1433.1 J/mol
47	Chloroform	Tc=536.40 K	Pc=5471.6 kPa	Tm=209.55 K	Hfus=2101.8 J/mol

Prediction Method

All Models

- NRTL
- UNIQUAC
- UNIFAC
- UNIFAC-LLE
- ASOG
- PSRK
- VTPR
- COSMO-RS(OI)
- COSMO-SAC
- Aspen Model

Active Models

Model	Options
Mod. UNIFAC (Do)	
NIST-mod. UNIFAC	
Mod. UNIFAC (Ly)	

Temperature Range

Lower Limit: 272.15 K

Lower Limit: 327.15 K

Steps: 20

Pressure: 1.00 bar
(Only EOS/Simulator)

☐ Recalculate Data Points

Figure 112 Prediction of Miscibility

Liquid-liquid equilibria are predicted with the g^E models UNIQUAC and NRTL – where component-specific interaction parameters are needed. These parameters can be obtained by RecPar. The other models (original UNIFAC, modified UNIFAC (Dortmund and Lyngby), and ASOG) are group contribution methods where the component specific parameters are replaced by group specific interaction parameters.

Newer additions to the LLE prediction are the EOS group-contribution methods PSRK and VTPR and the support for using the thermodynamic engine of the Aspen simulator.

In 2013 the COSMO based models have been introduced.

18.9 PCP

Prediction of pure component properties.

The PCP prediction works in quite different way. Since the PCP database contains multiple properties the program has to determine the property and the state (VLE for vapor pressures e. g.) 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. The other source are parametrized equations where the parameters have been fitted in advance ("PCP Equation Fit" and ParameterDDB).

Vapor pressures 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.

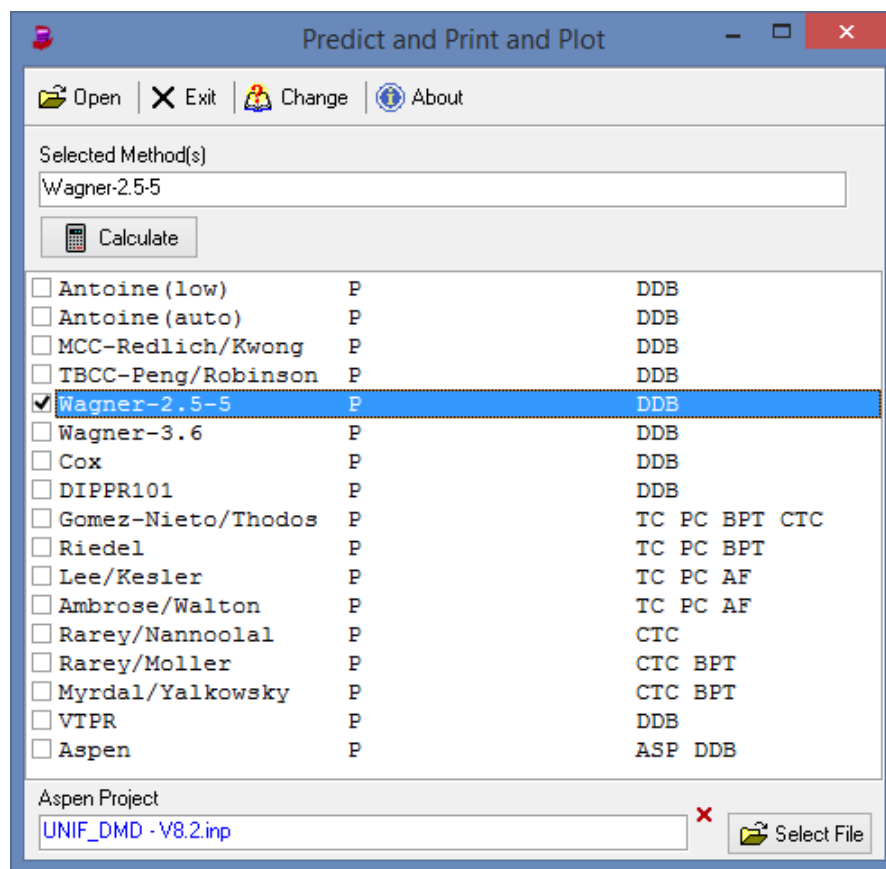


Figure 113 Prediction of Pure Component Properties

18.10 POW

Prediction of Octanol/Water partition coefficients.

For Octanol/Water partition coefficient the UNIFAC model developed by Wienke and Gmehling (1998)⁸ is implemented and additionally the "normal" activity coefficient models original, modified UNIFAC, and NIST-modified UNIFAC as well as COSMO-RS(OI), PSRK, and VTPR.

⁸ Wienke G., Gmehling J., "Prediction of Octanol-Water Partition Coefficients, Henry Coefficients and Water Solubilities Using Unifac", Toxicol. Environ. Chem., 65, 57-86, 1998

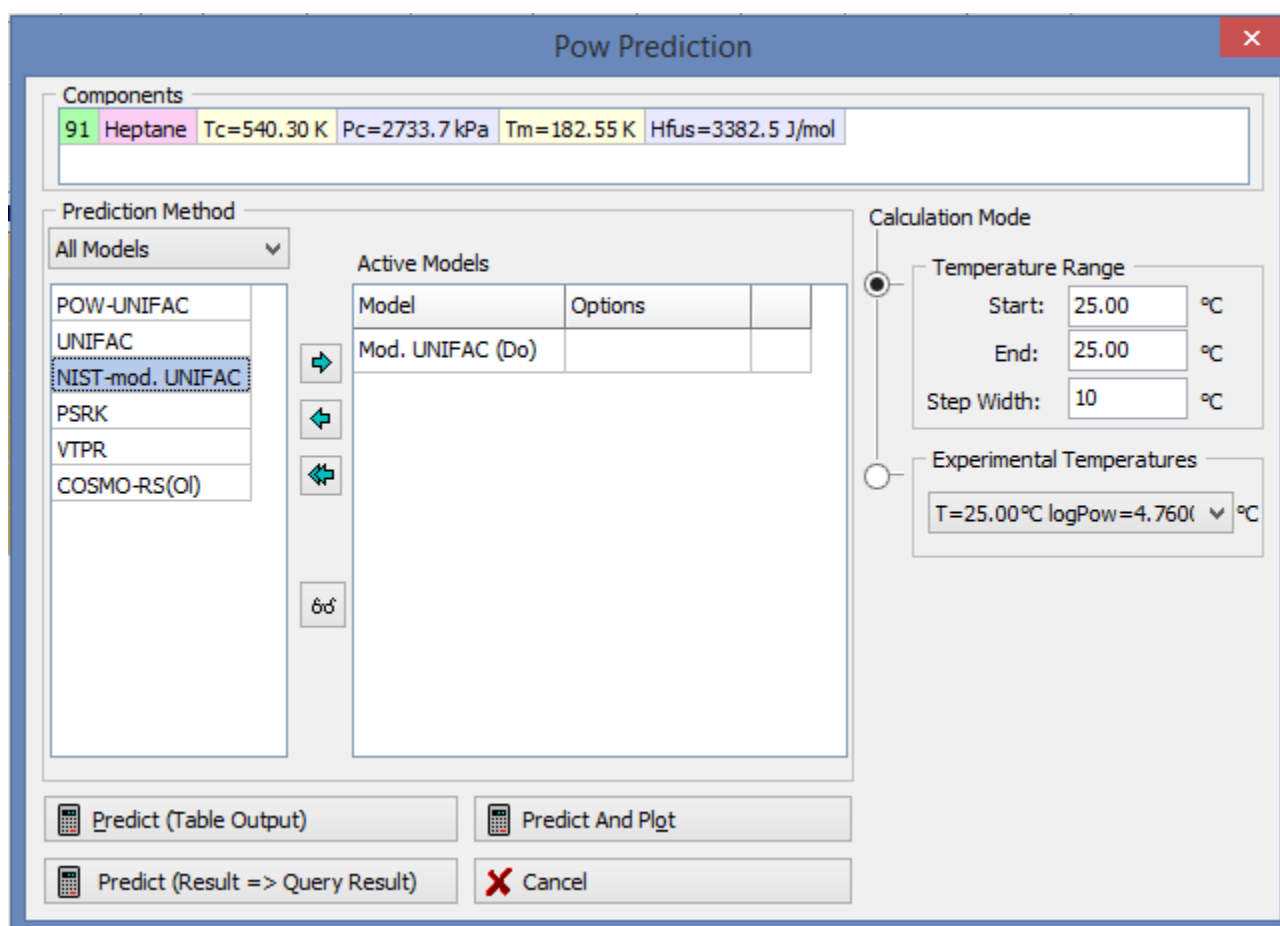


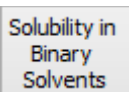
Figure 114: Prediction of Octanol-Water Partition Coefficients

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 show eutectic behavior.

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.

SLE Prediction

Components

128	Octane	Tc=568.80 K	Pc=2494.6 kPa	Tm=216.35 K	Hfus=4932.6
161	Toluene	Tc=591.70 K	Pc=4113.8 kPa	Tm=178.16 K	Hfus=1636.3

Prediction Method

All Models

NRTL
UNIQUAC
Wilson
Margules
van Laar
NIST-mod. UNIFAC
Mod. UNIFAC (Ly)
ASOG
VTPR
COSMO-RS(OI)
COSMO-SAC
Raoult's Law

Active Models

Model	Options
UNIFAC	
Mod. UNIFAC (Do)	
PSRK	

Mole Fraction Range

Min. x	Max. x	Stepwidth
0.0	1.0	0.1

x [128] x [161] x [925]

Predict (Table Output) **Predict (Result => Query Result)** **Cancel**

Figure 115: Prediction of Solid-Liquid Equilibrium

Solubility in Binary Solvent

Components

128: Octane
161: Toluene
925: Anthracene

Prediction Method

☐ UNIFAC ☒ mod. UNIFAC (Dortmund) ☐ mod. UNIFAC (Lyngby) ☐ NIST-mod. UNIFAC ☐ ASOG ☐ Ideal (Raoult's Law)

Check **All** **None**

Solute **Temperature [K]**

925: Anthracene 298.15

Mole Fraction Range

Min. x	Max. x	Stepwidth
0.0	1.0	0.01

Create Data Points **Special Data Point Creation**

x [128] x [161]

Predict (Table Output) **Predict (Result => Query Result)** **Predict and Plot** **Cancel**

Figure 116: 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.

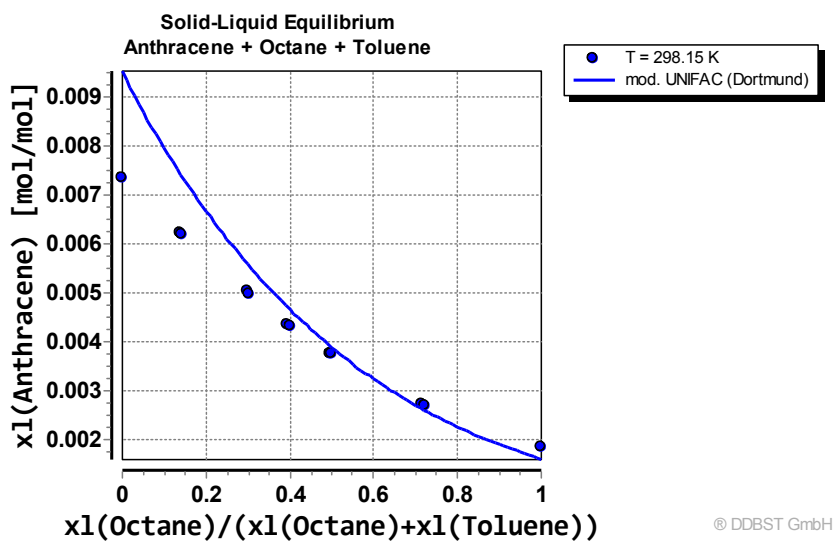


Figure 117: Solubility of a high-melting component in a binary solvent mixture (Example: Anthracene in Octane/Toluene)

18.12 VE

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 page 123, chapter “CPE, VE, HE, VIS”).

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

VE Prediction

Components

31	Benzene	Tc=562.10 K	Pc=4894.0 kPa	Tm=278.68 K	Hfus=2376.7 J/mol
50	Cyclohexane	Tc=553.80 K	Pc=4080.4 kPa	Tm=279.75 K	Hfus=628.2 J/mol

Prediction Methods

All Models ▼

- PSRK
- VTPR
- Sum of Symmetri...
- Aspen Model

→

←

↔

Active Models

Model	Options
Redlich-Kister	

Conditions

T [°C]	P [bar]
25	1

Pressure is only used in PSRK and VTPR

Recalculate

☐ Recalculate Data Points

☐ Use PSRK Volume Correction

📊

Predict (Table Output)

📊

Predict (Result => Query Result)

📊

Predict and Plot

✖

Cancel

⚠

Deviation Plot

Figure 118: Prediction of Excess Volumes

VE

Prediction of excess volumes and densities.

18.13 VIS

Prediction of Mixture Viscosities

Mixture viscosities can be predicted by the two methods Grunberg/Nissan/Isdale⁹ and UNIFAC-VISCO¹⁰ and the three simple mixing rules from Arrhenius and 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 PCPEquationFit 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.

Components	
4	Acetone Tc=508.10 K Pc=4701.5 kPa
11	Ethanol Tc=516.20 K Pc=6383.5 kPa

Pure Component Models	#4	#11
Andrade	<input checked="" type="radio"/>	<input checked="" type="radio"/>
Vogel	<input type="radio"/>	<input type="radio"/>
DIPPR101	<input type="radio"/>	<input type="radio"/>
PPDS9	<input type="radio"/>	<input type="radio"/>
ExtAndrade	<input type="radio"/>	<input type="radio"/>

Type: ☒ Isothermal 298.15 K

☐ Calculate all points (1 Sets)

Mixture Viscosity Model (Mixing Rule)

☐ Arrhenius ☒ Grunberg/Nissan/Isdale ☒ UNIFAC-VISCO ☐ Kendall ☐ Linear

Mole Fraction Range: Min. x: 0.0, Max. x: 1.0, Stepwidth: 0.01

x [4] x [11]

Figure 119: Mixture Viscosity Prediction

18.14 Entering g^E Model Parameters

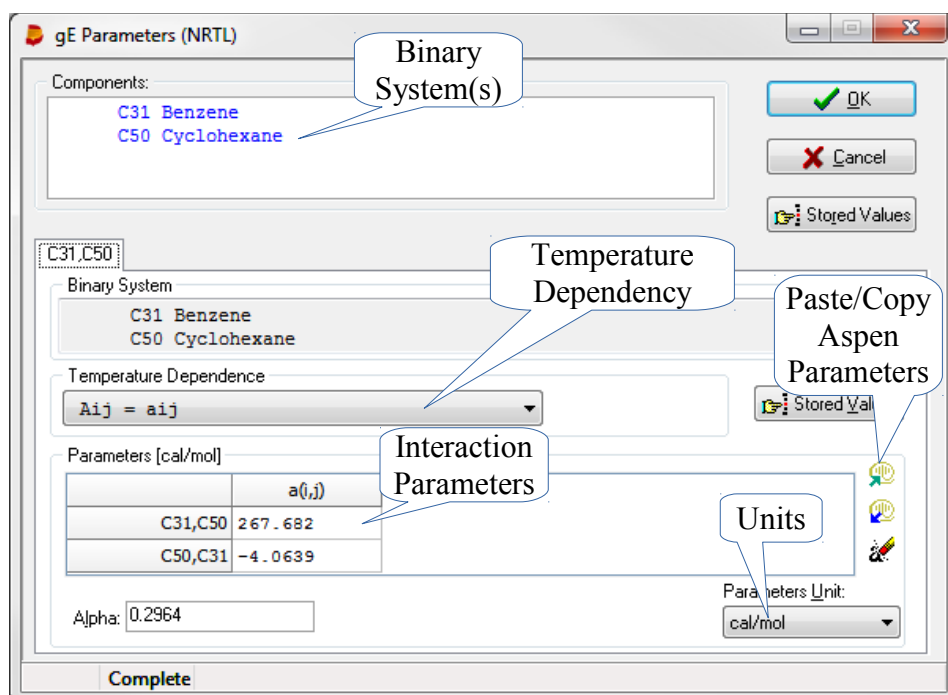
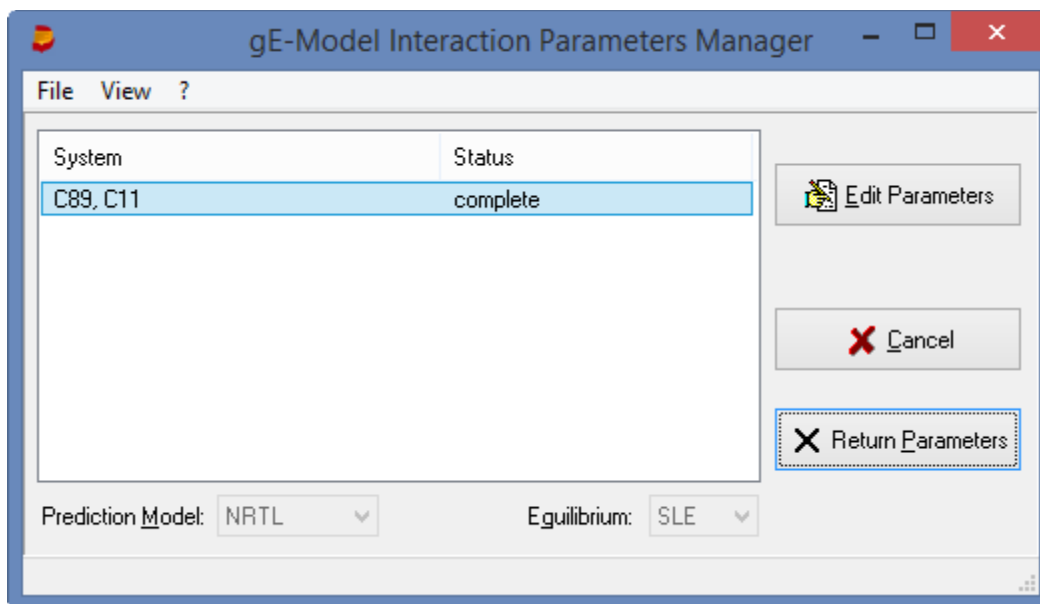
If a g^E model (NRTL, UNIQUAC, Wilson, van Laar, Margules, etc.) has been selected for the prediction parameters for the binary component pairs have to be entered

The starting dialog displays the system or systems for which the parameters are needed.

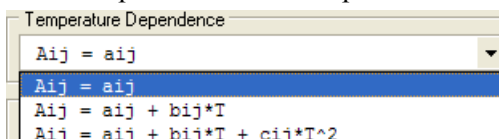
The "Edit Parameters" buttons opens a dialog where the single binary parameters can be edited.

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

10 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

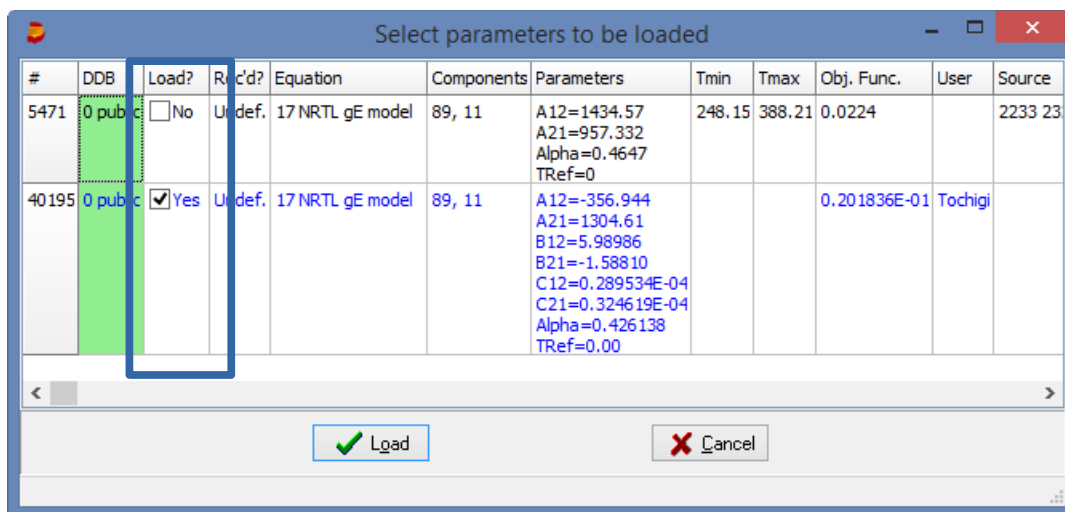



The dialog supports different temperature dependencies for the parameters



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

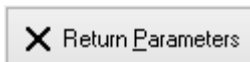
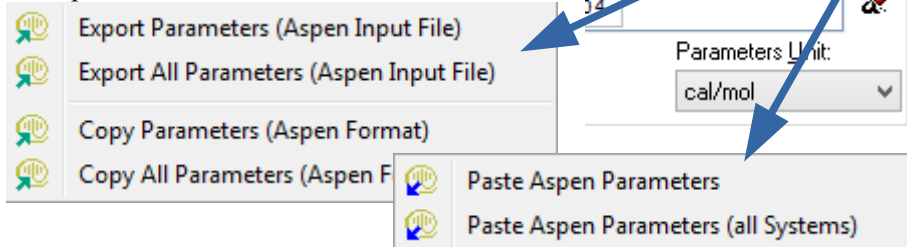
The dialog has a “Load?” column where the wanted parameter set has to be checked.



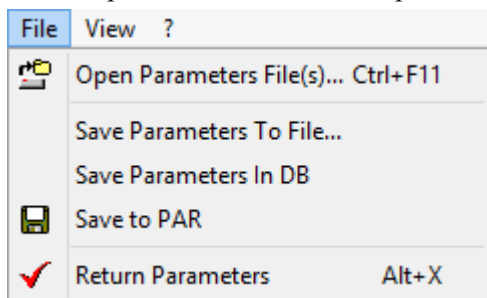
The button with the AspenTech icon  allows to export the entered parameters to a Aspen INP (“.inp”) file. This file can be loaded in the Aspen simulator. If Aspen compatible data are available in the Windows clipboard (copied from inside Aspen) it is also possible to insert these parameters.

Parameters can be entered either in [cal/mol], [J/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 a parameter file (“.gpf”) or to the ParameterDDB.



The “.gpf” files can also be loaded (“Open Parameters File(s)”). Additionally it is possible to import data from “.rvo” files generated from RecPar, the simultaneous fit tool.

18.15 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.

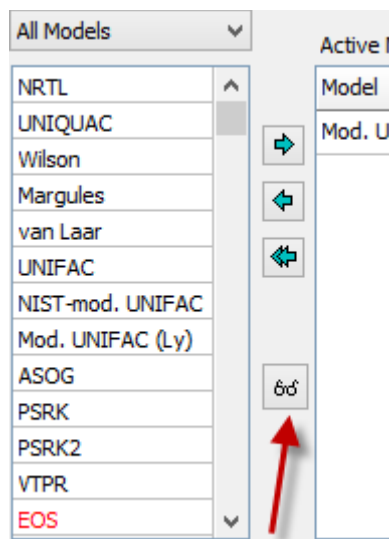


Figure 120: Checking Availability of Parameters

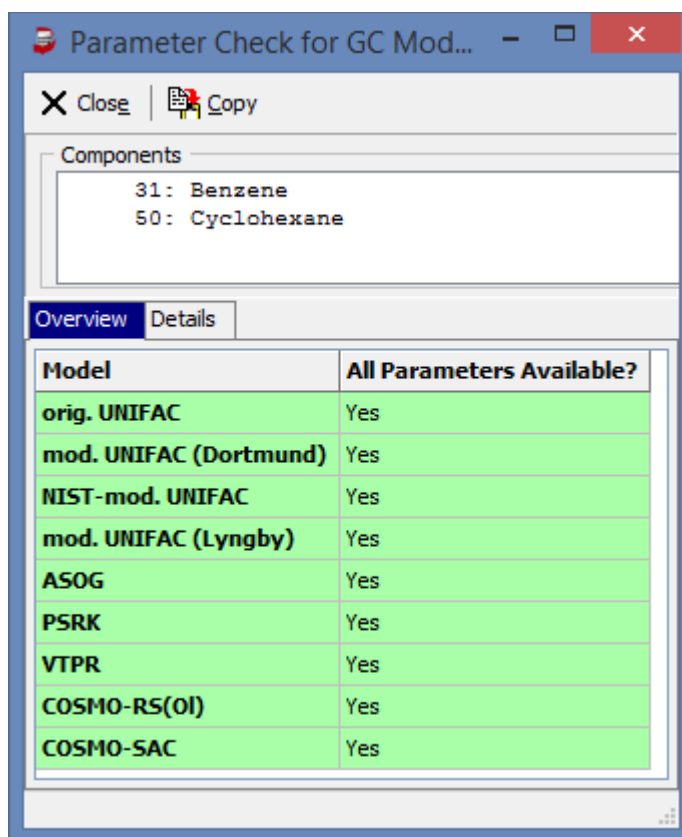


Figure 121: Checking Availability of Parameters of Group Contribution Methods

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			

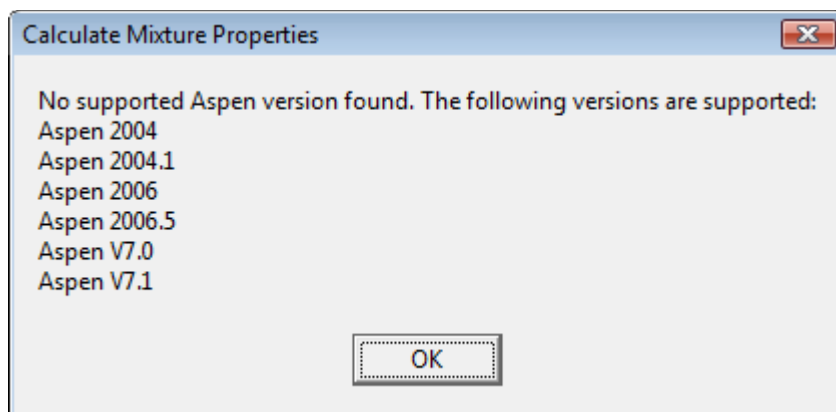
Subgroups: none given

18.16 Using Aspen Projects

In some prediction dialogs it is possible to select an Aspen simulator project.



If no Aspen simulator software is installed an error message is shown with the supported Aspen software versions:

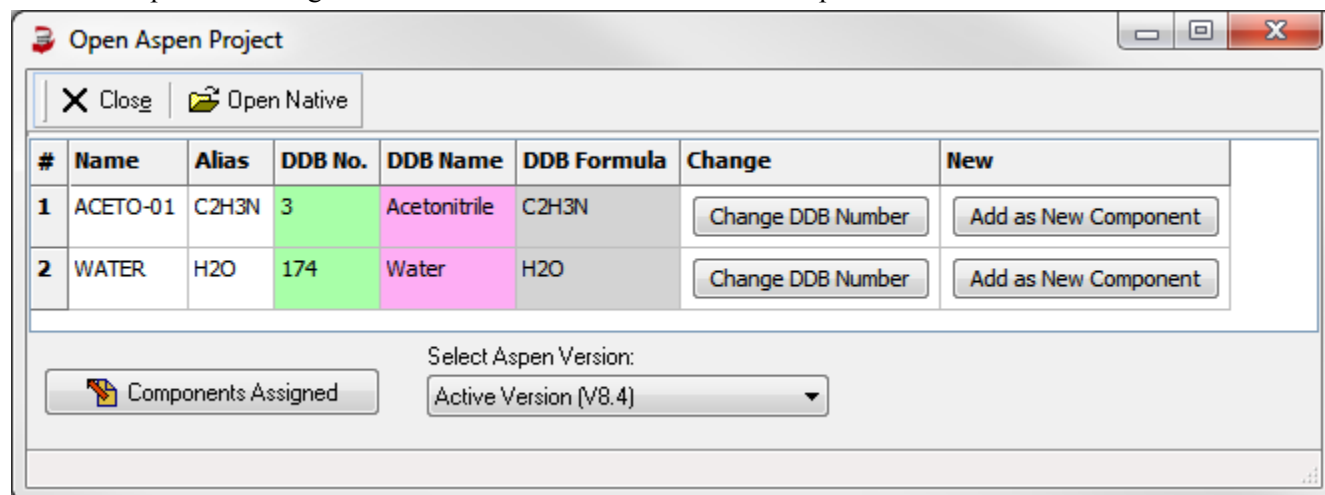


If Aspen is installed and an Aspen project is selected the prediction will use the Aspen internal thermodynamic calculation functions to calculate the respective property and create DDB standard diagrams and table outputs.

Aspen Projects (“inp”, “bkp” and “apt” files) can be loaded and the information about the components can be extracted.



The first step after loading such a file is the identification of the components.



The Dortmund Data Bank knows already many of the Aspen internal component codes and is able to identify several hundred of the components directly. If a component has not been identified it is either necessary to find the component in the DDB or add the component to the DDB component list.

If multiple Aspen simulator versions are installed it is possible to select one of them through a drop-down menu.

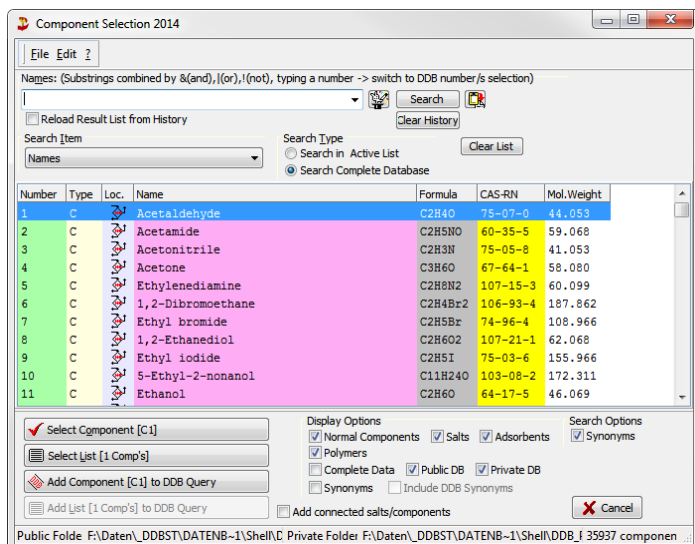


Figure 122: Change Component Number

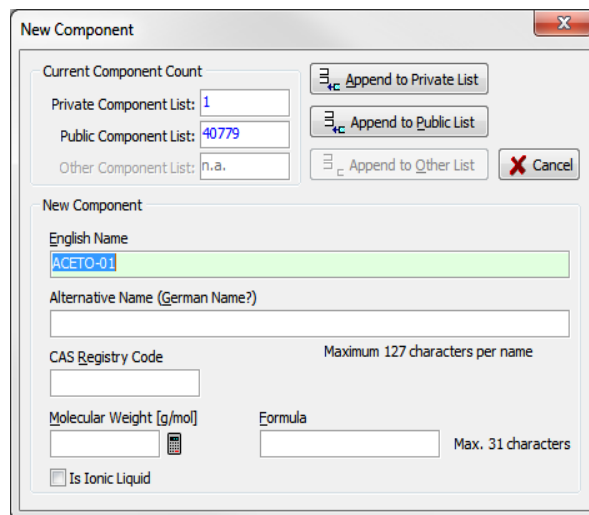


Figure 123: Add as New Component

The components in the loaded Aspen file must match the currently selected component list.

Components			
3	Acetonitrile	Tc=548.00 K	Pc=4833.2 kPa
174	Water	Tc=647.30 K	Pc=22048.3 kPa

If the component lists don't match an error message is displayed and a prediction will fail.

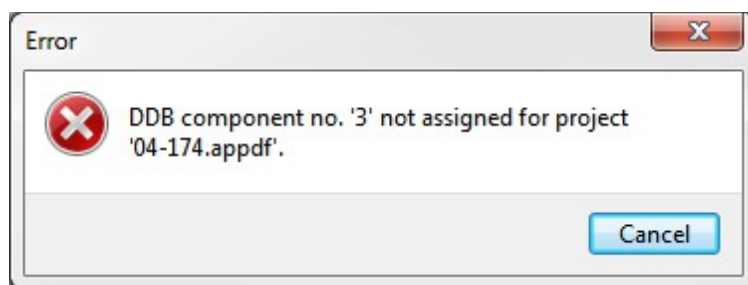


Figure 124: Error Message for Non-matching Components

This allows on the one hand the comparison of the calculation results of the Aspen engine with experimental data from the Dortmund Data Bank and on the other hand the comparison of the Aspen models and parameter with DDB models and parameters.

18.17 PRO/II Calculations

18.17.1 Introduction

This chapter describes briefly in a step-by-step tutorial how to use the PRO/II thermodynamics in the DDB software.

The connection between DDBSP and PRO/II is using a COM interface.

The supported features are:

- Reading components from a PRO/II database file (*.prz)
- Calculation of V(L)LE using the thermodynamics defined in a PRO/II database file

18.17.2 Step 1: Read Components from a PRO/II Database File

In order to compare the experimental data stored in the DDB with a PRO/II model the components in a PRO/II database file must be identified and assigned to DDB components.

To identify the components in a database file start the *Dortmund Data Bank* program.

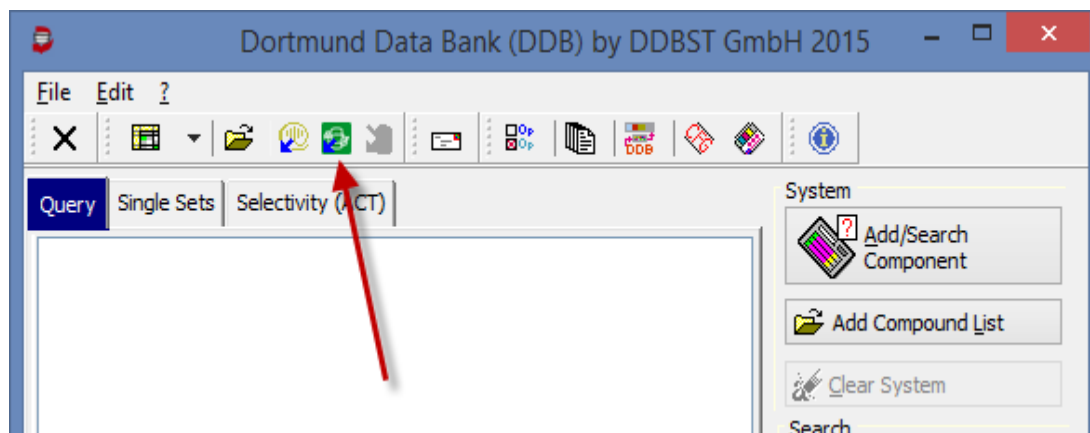


Figure 125: The Dortmund Data Bank Program

Click on the *Import PRO/II Components* button to open a PRO/II database file. After opening the file a component assignment dialog is displayed.

The system tries to assign the components automatically. This is done by the *ChemAbsNum* stored in the PRO/II database.

If a component could not be identified or the identification is wrong the user can select a component from the DDB component list using the *Change DDB Number* button. If the component is not found in the DDB a new component can be defined using the *Add as New Component* button.

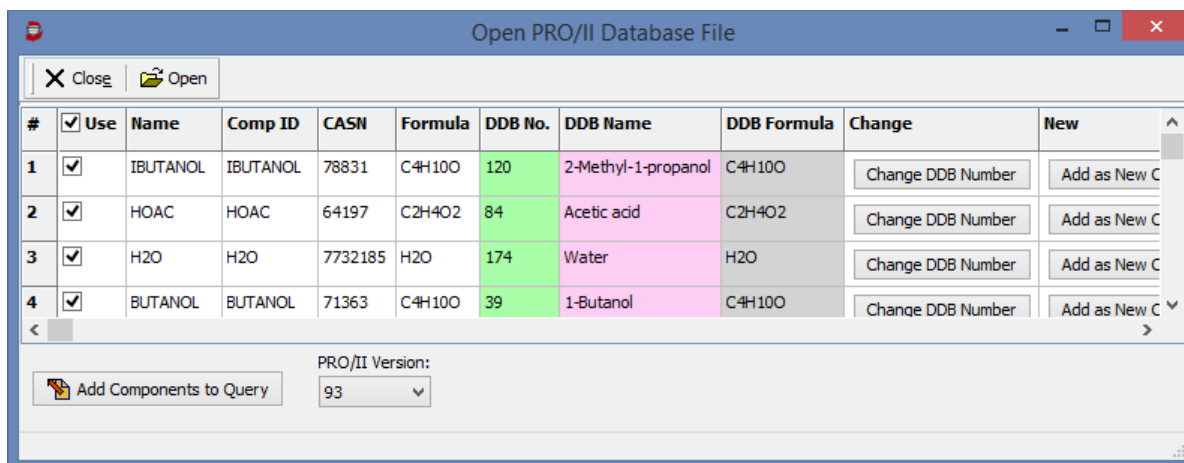


Figure 126: Open PRO/II Database File Dialog

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

Number	Type/Count	Loc.	Remove	Name
[174]	C	DDB	Remove	[Water]
[95]	C	DDB	Remove	[2-Propanol]
[50]	C	DDB	Remove	[Cyclohexane]
[31]	C	DDB	Remove	[Benzene]

Figure 127: Query Component List

Unwanted components can be removed from the list using the *Remove* button.

18.17.3 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 to find experimental data. In order to search for data for the system Cyclohexane + 2-Propanol the components with the DDB number 50 and 95 have to be added to the query. Click on the button *System (Exact Match)* in the *Search* area to find data for the binary system.

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	Publ.Year	Ref.No.	Reference
[699 0 0]	DDB	11	2	C50 Cyclohexane C95 2-Propanol	343	353	101 (const.)		Txy(P)		1963	335	[439] Nagata I., Mem.Fac.Technol.Kanazawa
[700 0 0]	DDB	13	2	C50 Cyclohexane C95 2-Propanol	331	340	67 (const.)		Txy(P)		1965	84	[388] Nagata I., J.Chem.Eng.Data, 10(2),
[1712 0 0]	DDB	11	2	C50 Cyclohexane C95 2-Propanol	342	350	101 (const.)		Txy(P)		1968	642	[946] Verhoeve L.A.J., J.Chem.Eng.Data,

Figure 128: Query Result for Binary System

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

18.17.4 Step 3: Calculate VLE Using the PRO/II Thermodynamics

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

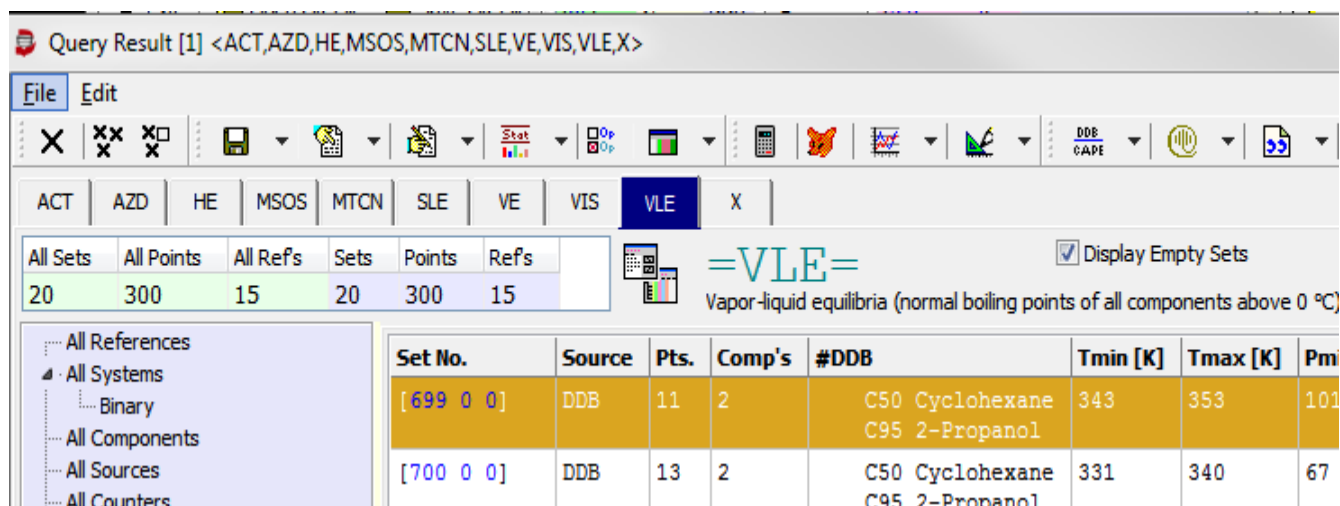


Figure 129: Query Result with VLE Predict Button

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

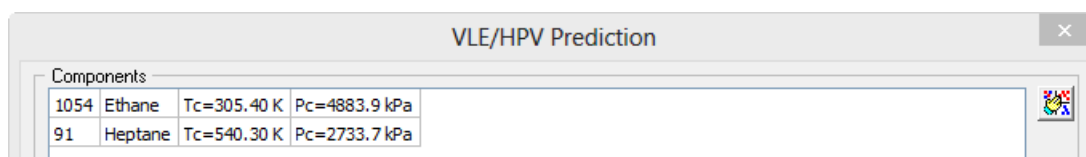



Figure 130: VLE Prediction Components

The PRO/II database file which has been opened most recently within the DDB software is selected as default file to be used for a calculation with PRO/II. If Pro/II isn't part of the "Active Models" list double-click on "Pro/II Model" in the "All Models" list or used the arrow button  to activate Pro/II.

Use the "Edit" button next to the displayed file name to select a different file for the calculation. Then a dialog similar to Figure 126 on page 113 will be displayed. In addition to the dialog in step 1 the thermo set can be selected.

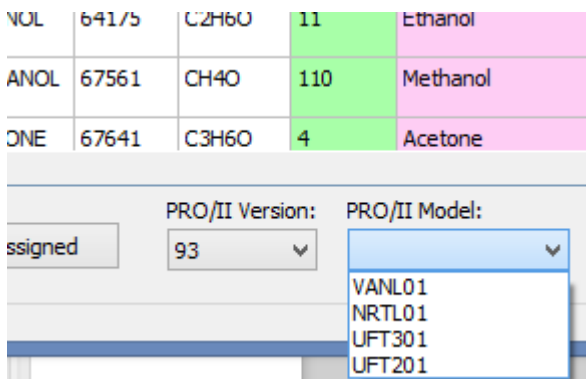


Figure 131: Thermo Set

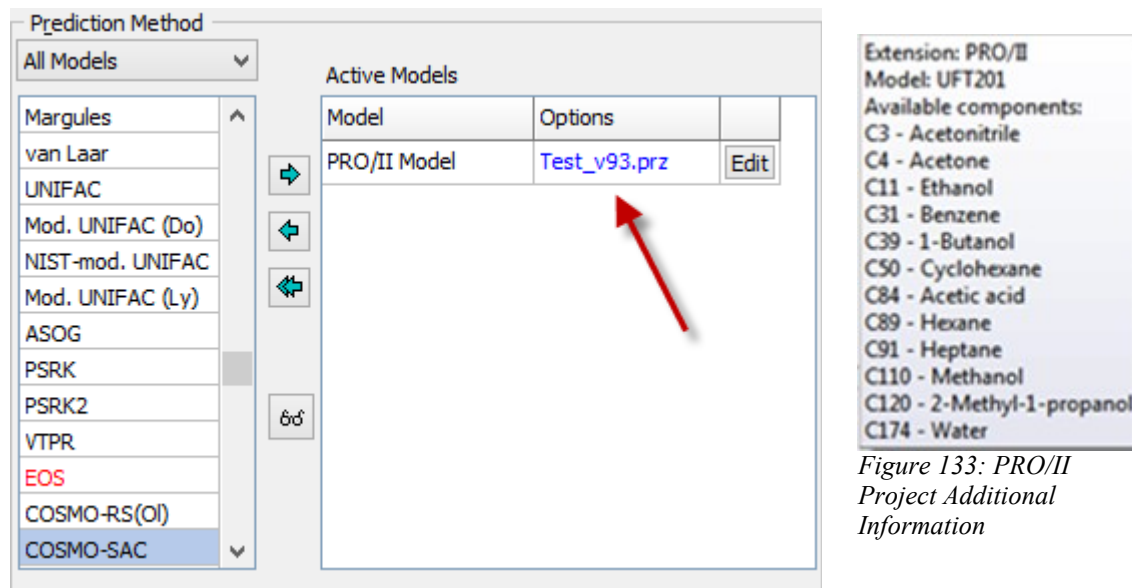


Figure 133: PRO/II
Project Additional
Information

Figure 132 Activated PRO/II Model; PRO/II Project File

If the mouse is over the *PRO/II Model* name some additional information is displayed.

To calculate with PRO/II only all models in the Prediction Method area have to be deselected, just the PRO/II model must be active. All selected models will be used in a calculation.

If several data sets have been selected it is possible to calculate all temperatures (for isothermal calculation), all pressures (for isobaric calculation), or all points.

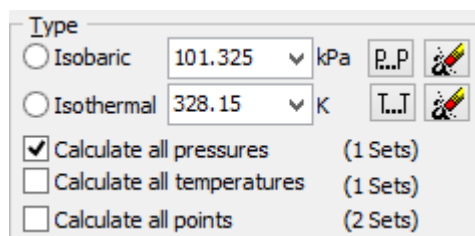


Figure 134: Calculate All Pressures

For a quick comparison between the experimental data and the model(s) the *Predict and Plot* button can be used.

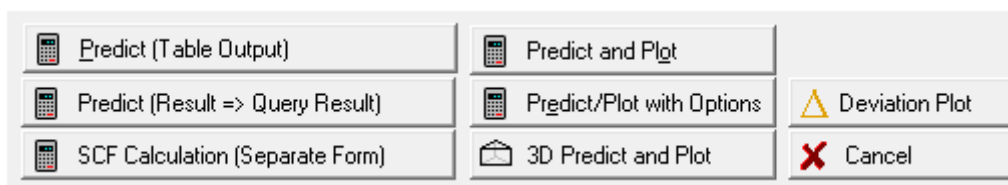


Figure 135: Predict Buttons

The experimental data together with the calculated results will be displayed 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.

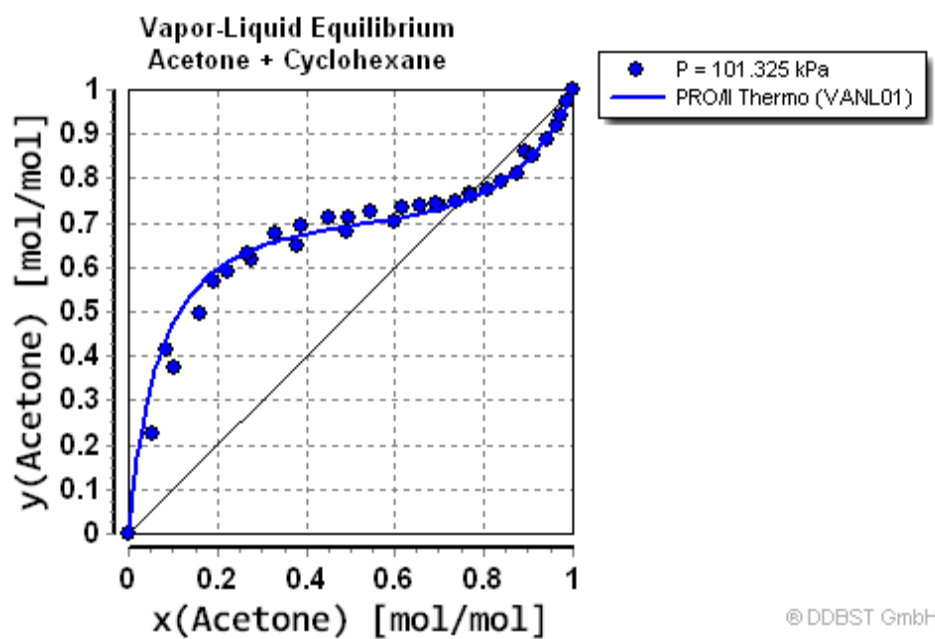


Figure 136: VLE x/y Diagram

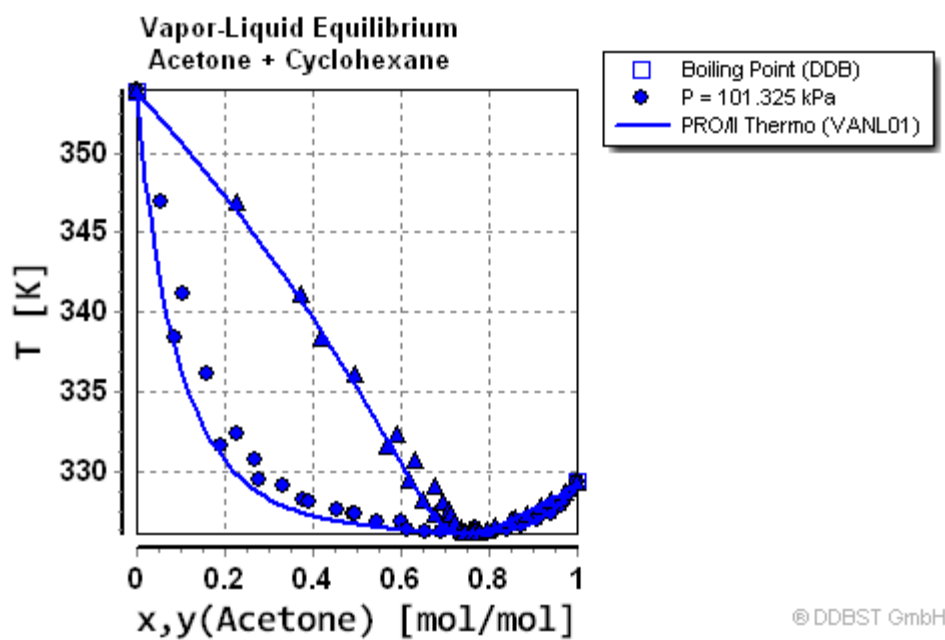


Figure 137: VLE T/x,y Diagram

18.18 UniSim Calculations

18.18.1 Introduction

This document describes briefly in a step-by-step tutorial how to use the UniSim Design thermodynamics in the DDB software. The connection between DDBSP and UniSim Design is using a COM interface.

The supported features are:

- Reading components from a UniSim Design case file (*.usc)
- Calculation of V(L)LE using the thermodynamics defined in a UniSim Design case file

18.18.2 Step 1: Read Components From a UniSim Design Case File

In order to compare the experimental data stored in the DDB with a UniSim Design model the components in a UniSim Design case file must be identified and assigned to DDB components.

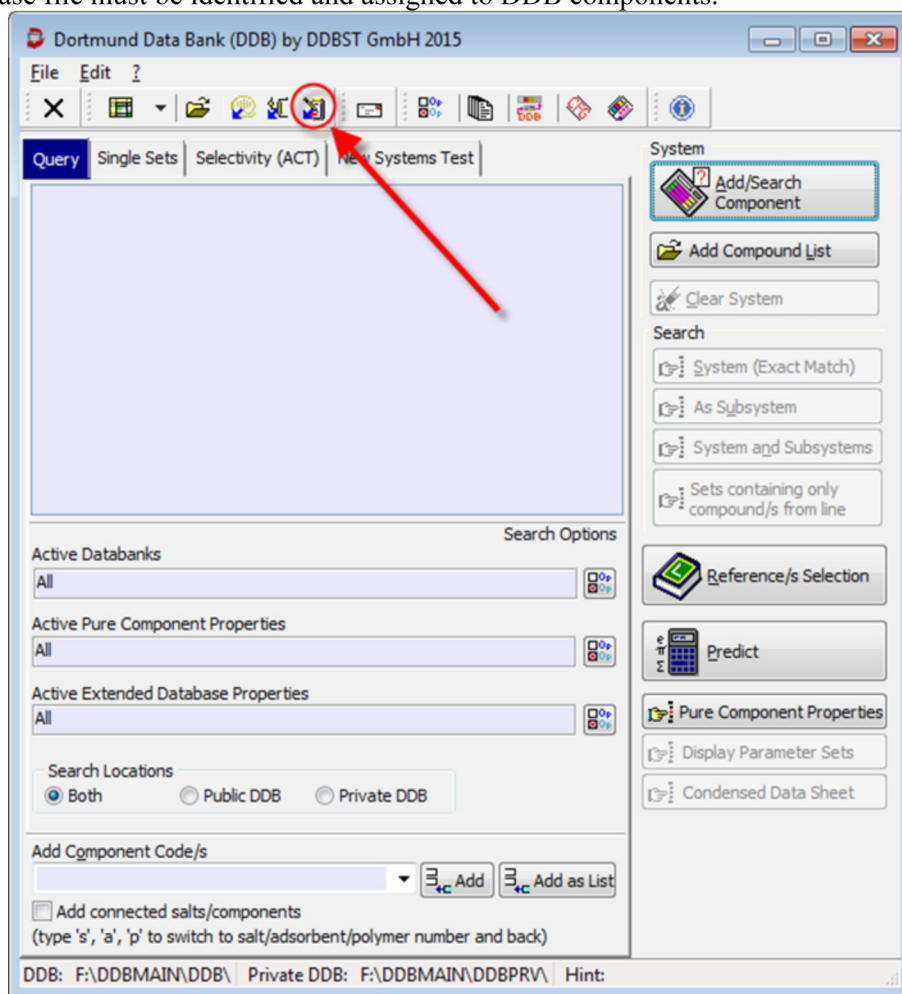


Figure 138: The Dortmund Data Bank Program

Click on the *Import UniSim Design Components* button to open a UniSim Design simulation case. After opening the file a component assignment dialog is displayed.

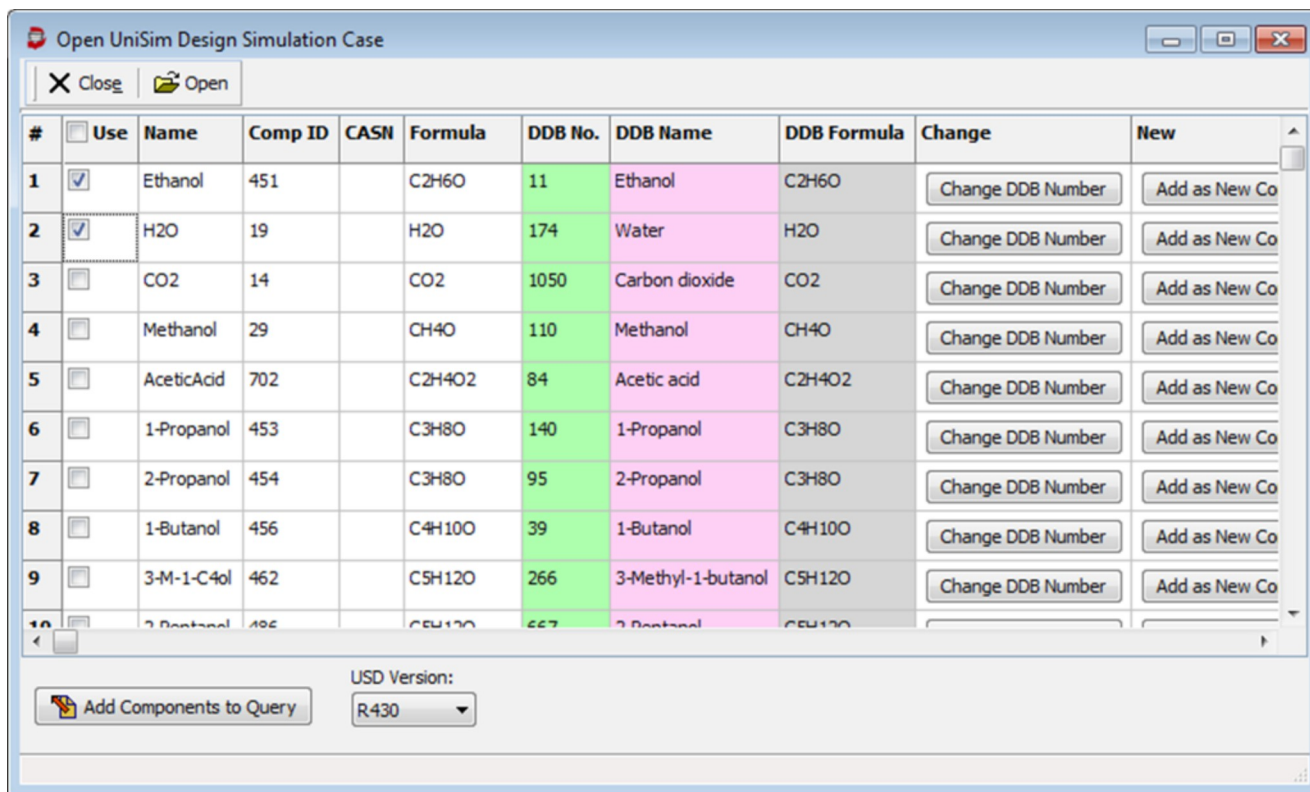


Figure 139: Open UniSim Design Simulation Case Dialog

The system tries to assign the components automatically. This is done by a predefined mapping between the UniSim Design component ID and the DDB component number.

If a component could not be identified or the identification is wrong the user can select a component from the DDB component list using the *Change DDB Number* button. If the component is not found in the DDB a new component can be defined using the *Add as New Component* button. Only assigned components can be used.

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

Number	Type/ Count	Loc.	Remove	Name
[11]	C	DDB	Remove	[Ethanol]
[174]	C	DDB	Remove	[Water]

Figure 140: Query Component List

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. In order to search for data for the system Ethanol + Water, the components with the DDB number 11 and 174 have to be added to the query. Click on the button *System (Exact Match)* in the *Search* area to find data for the binary system.

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]
[547 0 0]	DDB	25	2	[C11 Ethanol] [C174 Water]	n.a.		13 (const.)	
[548 0 0]	DDB	22	2	[C11 Ethanol] [C174 Water]	n.a.		25 (const.)	
[549 0 0]	DDB	20	2	[C11 Ethanol] [C174 Water]	n.a.		51 (const.)	
[550 0 0]	DDB	14	2	[C11 Ethanol]	n.a.		101 (const.)	

[5052] Shaffer D.L., Daubert T.E., Anal.Chem., 41(12), 1585-1589, 1969

1 dataset/s marked.

Figure 141: Query Result for Binary Systems

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 the UniSim Design Thermodynamics

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

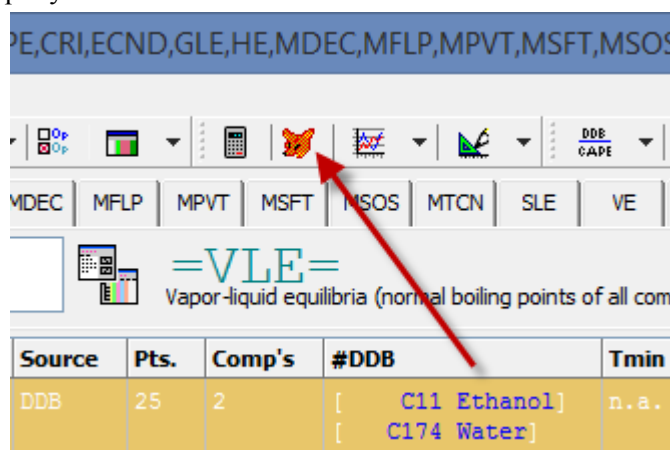


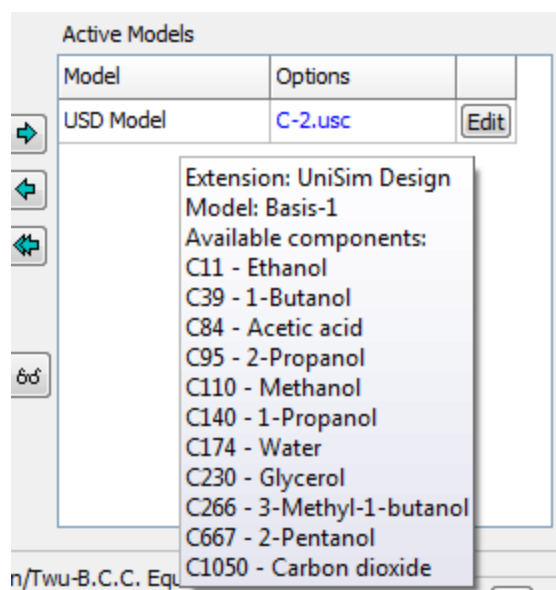
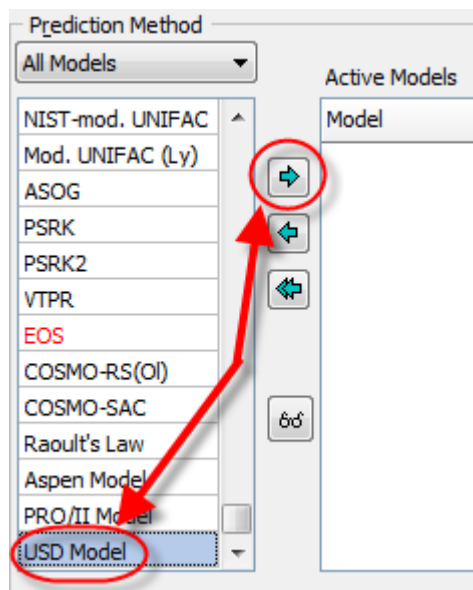
Figure 142: VLE Prediction Button

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

VLE/HPV Prediction			
Components			
11	Ethanol	Tc=516.20 K	Pc=6383.5 kPa
174	Water	Tc=647.30 K	Pc=22048.3 kPa

Figure 143: Components (VLE Prediction)

Scroll down the list of available models, select “USD model” and use the right arrow button to make the model active.



The UniSim Design simulation case file which has been opened most recently within the DDB software is selected as default file to be used for a calculation with UniSim Design.

If the mouse is over the *USD 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 dialog similar to Figure 2 on page 4 will be displayed. In addition to the dialog in step 1 the fluid package can be selected.

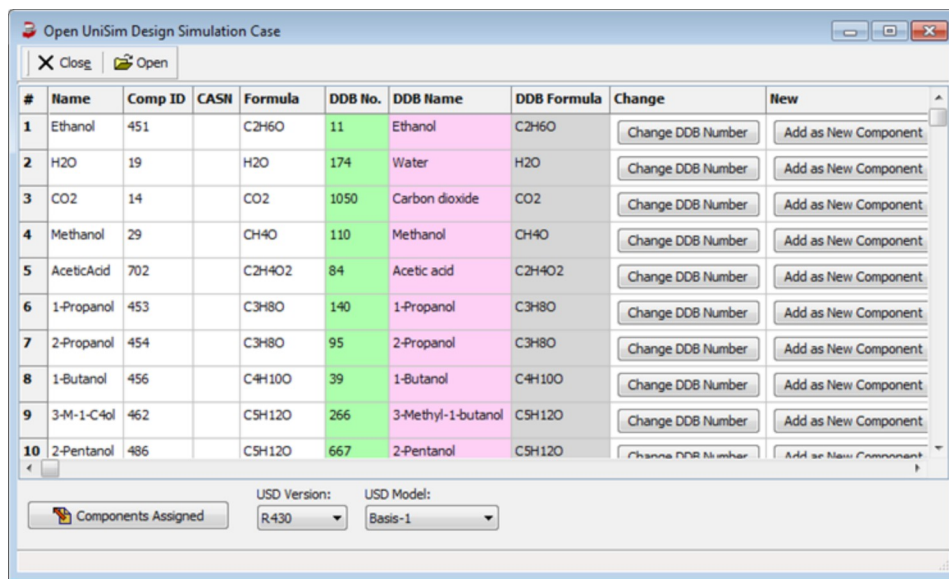


Figure 144: USD Calculation Settings

To calculate with UniSim Design only make sure *USD Model* is the only model in the *Active Models* list. All active models will be used in a calculation.

If several datasets have been selected it is possible to calculate all temperatures (for isothermal calculation) or all pressures (for isobaric calculation).

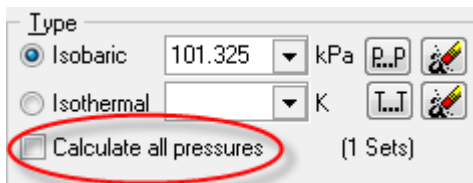
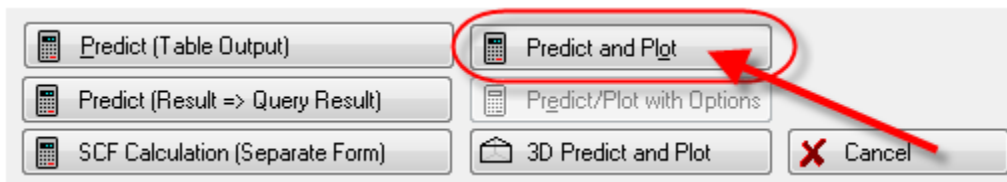


Figure 145: Calculate All Pressures

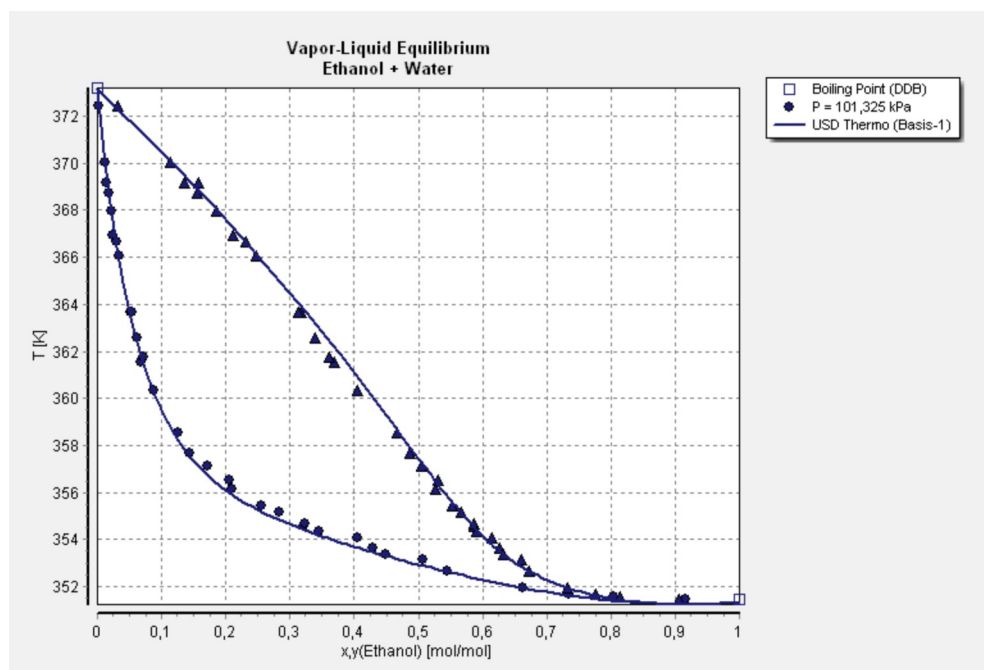
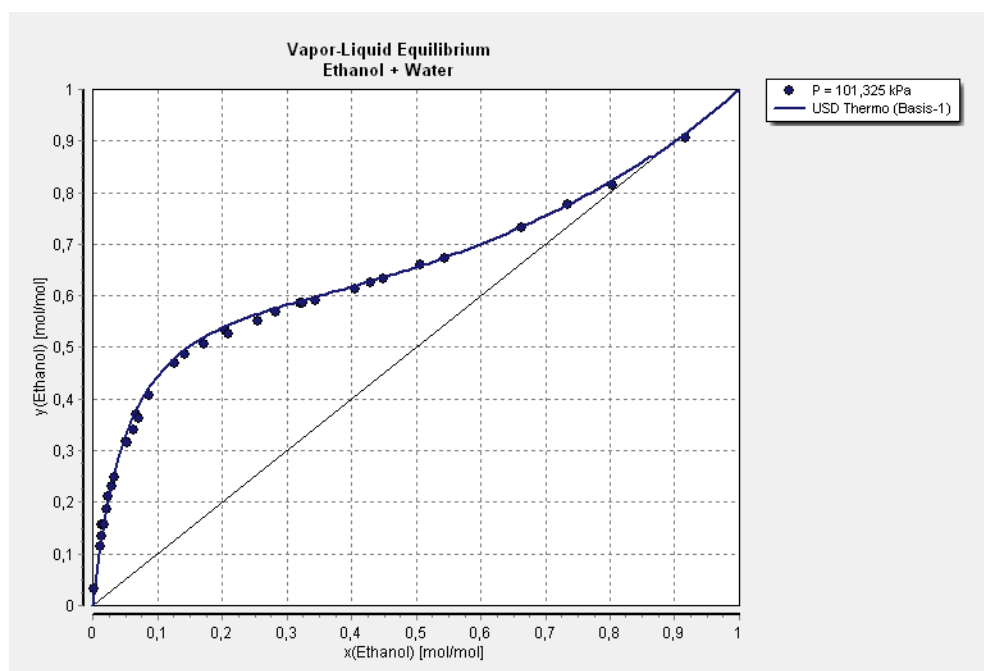
For a quick comparison between the experimental data and the model(s) the *Predict and Plot* button can be used.




The experimental data together with the calculated results will be displayed 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.

The next two diagrams show example results for the calculation of VLE for the Ethanol+Water mixture at normal pressure.

Figure 146: VLE $T/x,y$ DiagramFigure 147: VLE x/y Diagram

19 Fit Equation Parameters

Fit programs are available for some data banks. The fit routine ( Fit) always uses the list of marked sets, if the fit routine can handle multiple sets or the currently sets, if only single sets can be used.

19.1 AAE

Adsorbent-adsorptive equilibria data sets with isothermal and single adsorptive data sets can be fitted.

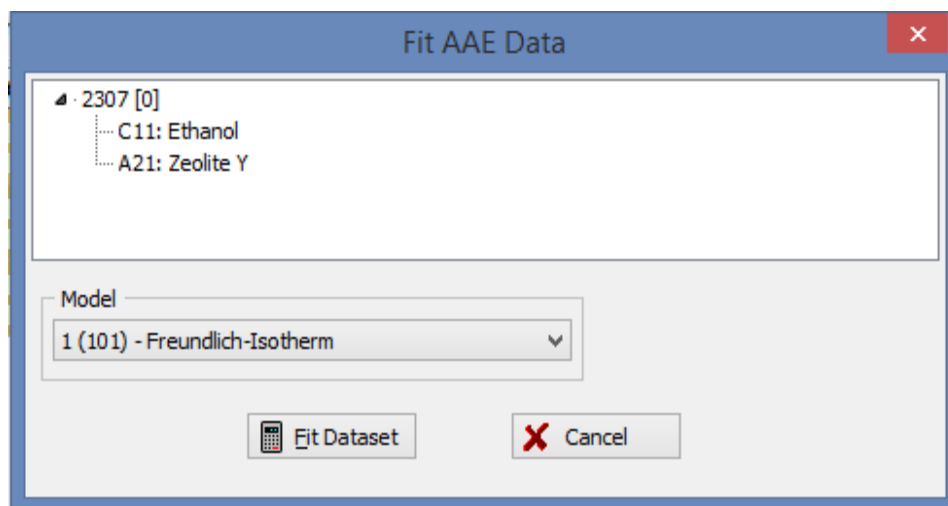


Figure 148 Fit of Adsorbent-Adsorptive Equilibria

19.2 CPE, VE, HE, VIS

The four data banks contain excess data or data that be converted to an excess property (excess heat capacities, excess volumes, excess enthalpies, 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

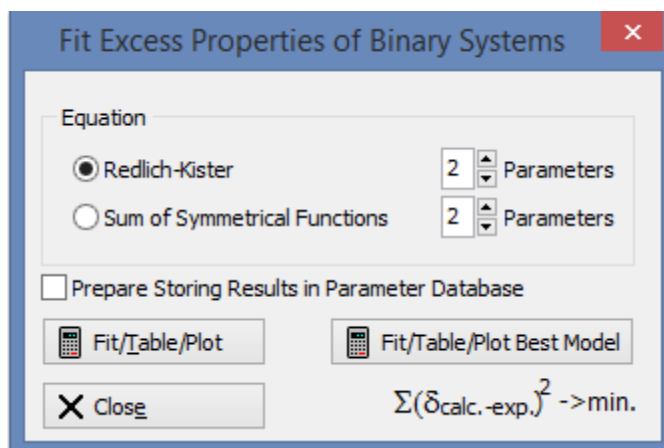


Figure 149 Fit of Excess Properties

19.2.2 Sum of Symmetrical Functions

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

m=1..3

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

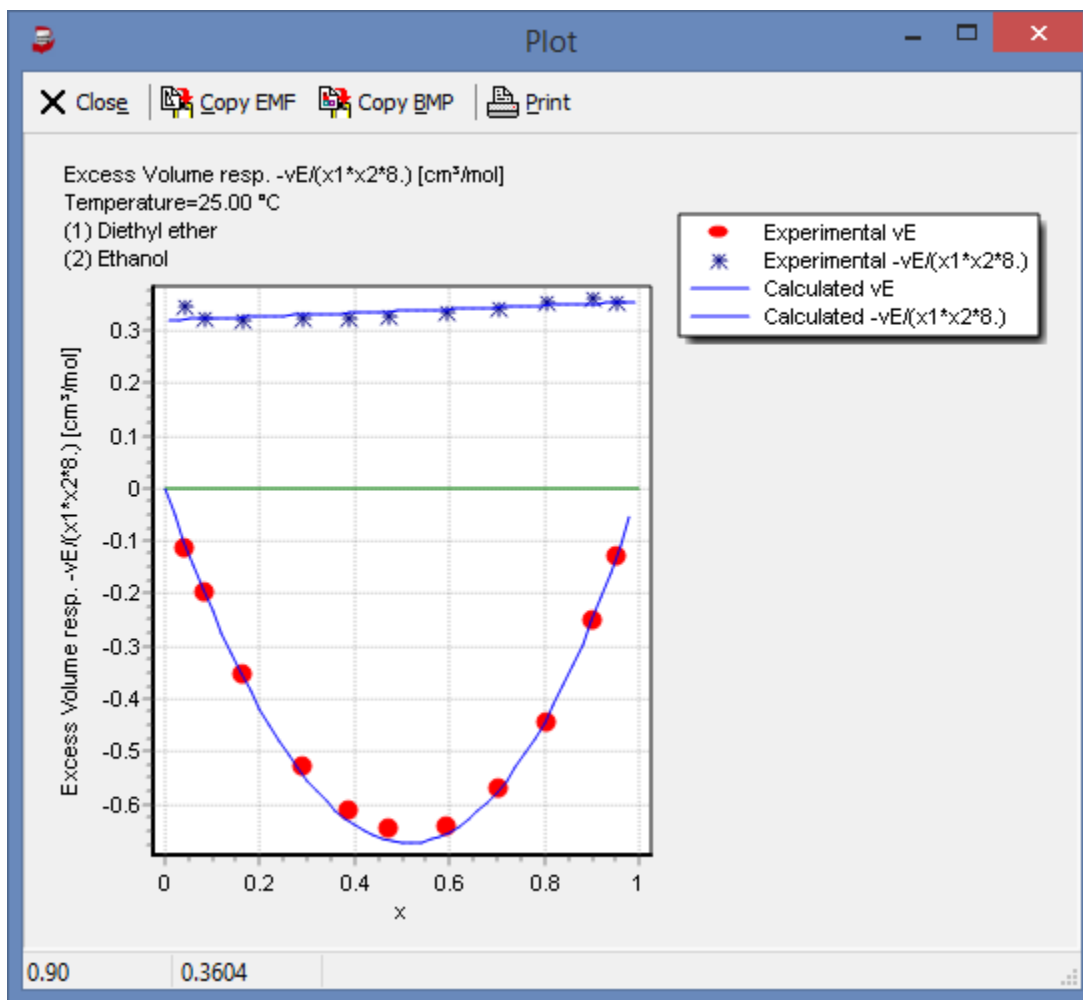


Figure 150 Plot Result for Excess Properties' Fit (Volume)

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.

What?	Value
C1	12
C2	11
COUNT	2
Comment	Redlich-Kister Parameters. Use for vE
DateD	15
DateM	4
DateY	2015
EQID	78
ObjectiveFunction	0.00183305
ParameterA	-2.61497
ParameterB	-0.104129
ParameterC	-0.199988

Store Data Set

Public DDB Private DDB Cancel

Figure 151: Excess Properties Fit: Store Parameters

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		SSF	
vE cm ³ /mol	x1 Diff	vE cm ³ /mol	vE Calc'ed cm ³ /mol
-0.1138	0.0432	-0.0119	-0.1019
-0.1981	0.0839	-0.0074	-0.1906

19.3 GLE

Only binary gas-solubility data – which are also convertible to T/Henry data – can be fitted.

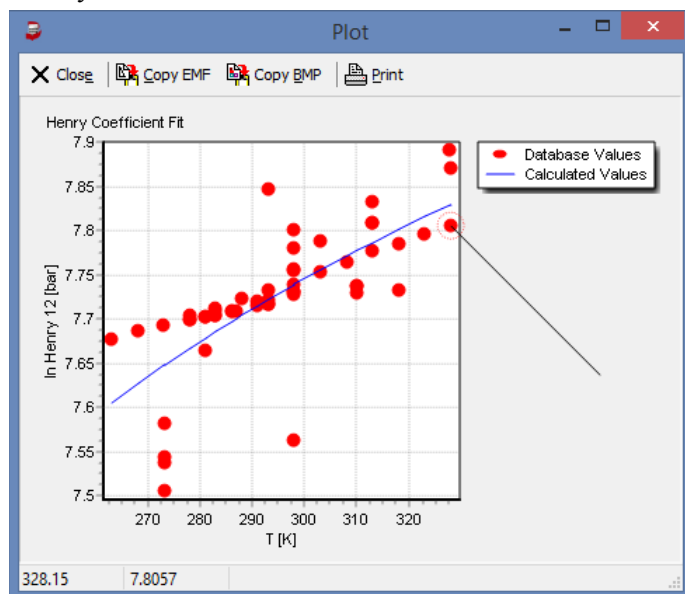


Figure 152: Result of Henry Coefficients Fit

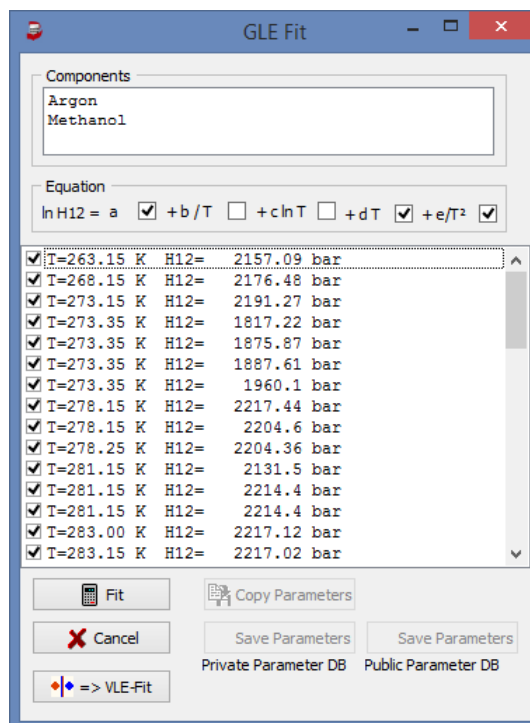
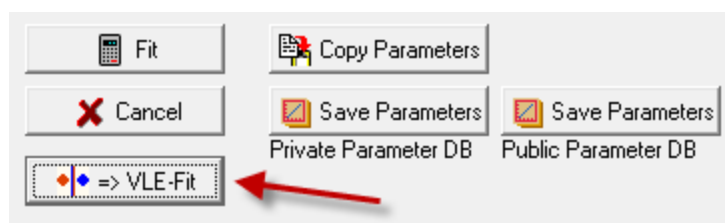


Figure 153: Gas Solubilities: Fit of Henry Coefficients

a=	7.82574	b=	0	c=	0	d=0.000918465	e=	-32019.5

T=263.15 K	H12exp=	2157.09 bar	H12calc=	2008.31 bar	Rel.Diff. [%]=	-6.90		
T=268.15 K	H12exp=	2176.48 bar	H12calc=	2052.31 bar	Rel.Diff. [%]=	-5.70		

The obtained parameters can be saved in the ParameterDDB



If the GLE data set can be converted to TPxy data it is possible to transfer the set to the VLE/HPV fit. This VLE fit then allows the regression of g^E model parameters.

19.4 LLE

Liquid-liquid equilibrium data can be fitted by NRTL and UNIQUAC. If binary sets are selected it is possible to select temperature-dependent equation for the interaction parameters.

In case of ternary data sets only temperature independent parameters can be fitted.

Binary LLE data sets must contain at least two tie-lines, ternary data sets must have three.

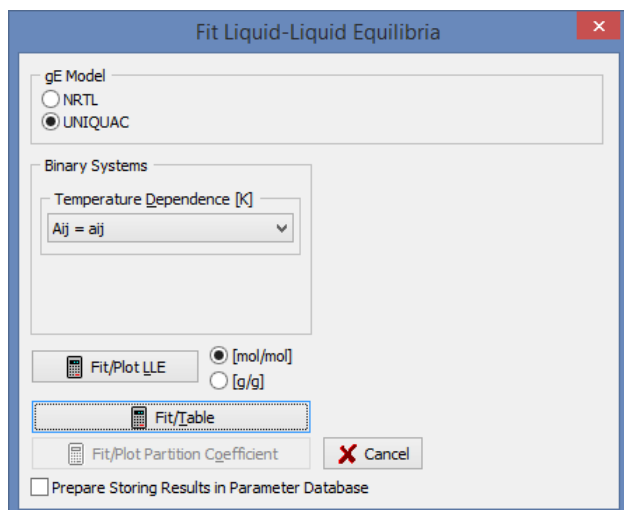


Figure 154 Fitting Binary LLE Datasets

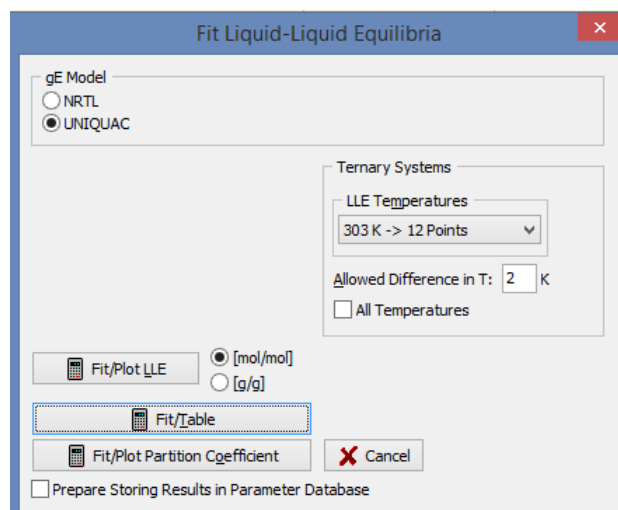


Figure 155 Fitting Ternary LLE Datasets

If the option

☐ Prepare Storing Results in Parameter Database

is checked it is possible to save the fitted parameters in the private ParameterDB.

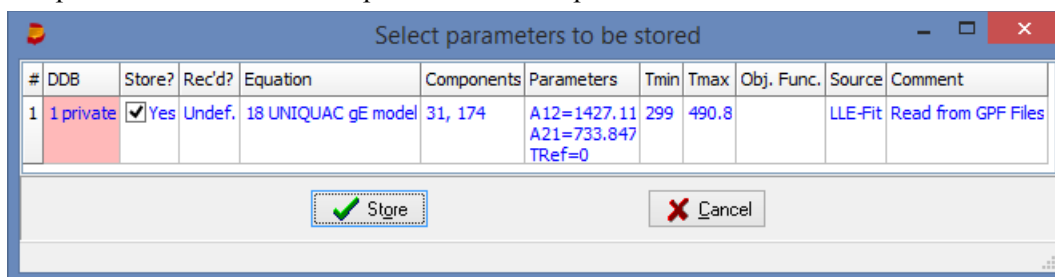


Figure 156 Storing Fitted LLE Parameters

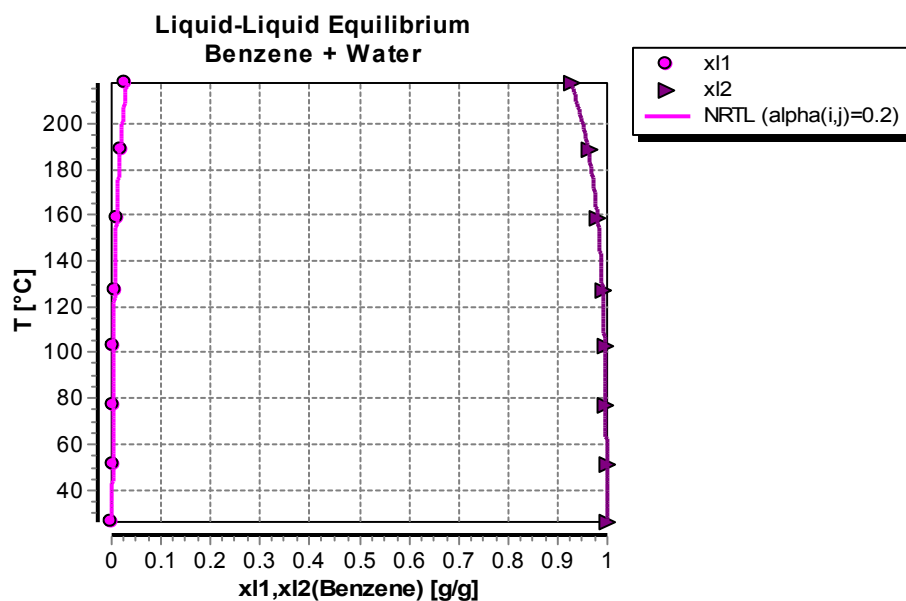


Figure 157: LLE Fit Result

Only the first three temperature dependencies (constant, linear, quadratic) are supported.

19.5 PCP

For pure component data the external program “PCPEquationFit” is started.

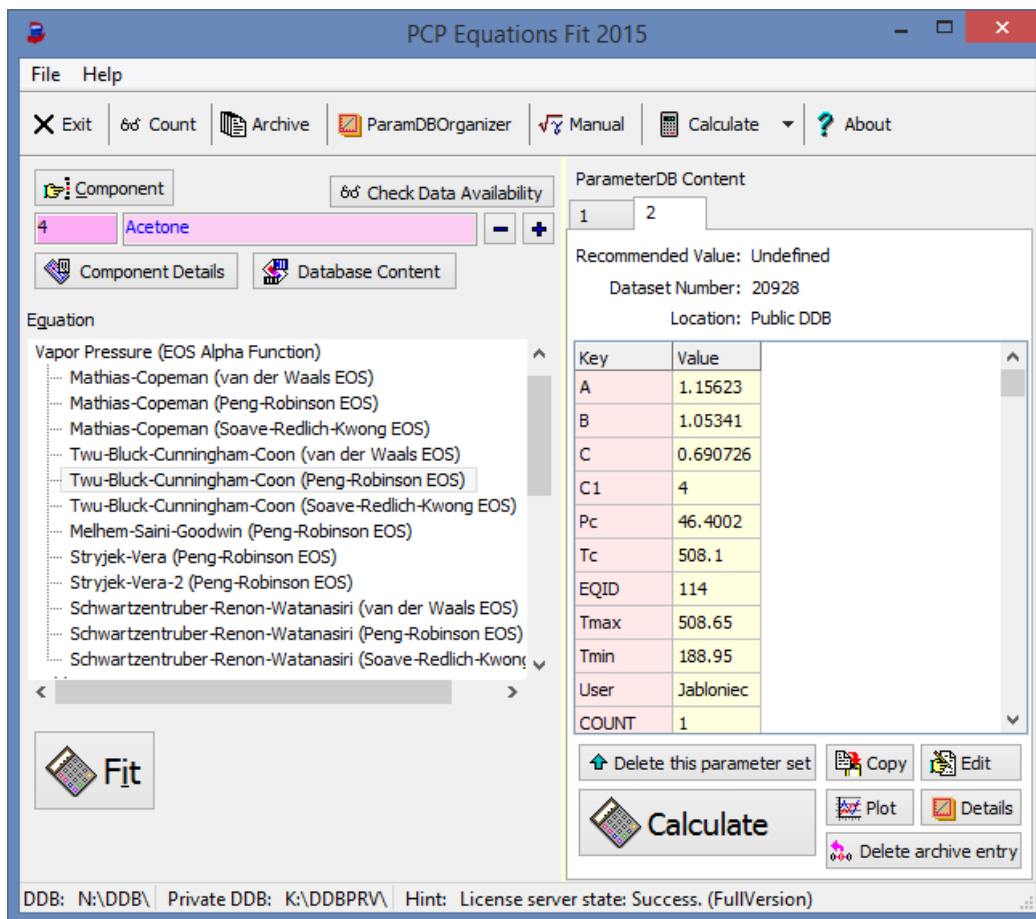


Figure 158 Fitting Pure Component Properties

This program is described in a separate manual.

19.6 SLE

Solid-liquid equilibrium data can be fitted by g^E models.

If “Prepare Storing Results...” is checked the program allows to store the fitted parameters to the ParameterDDB.

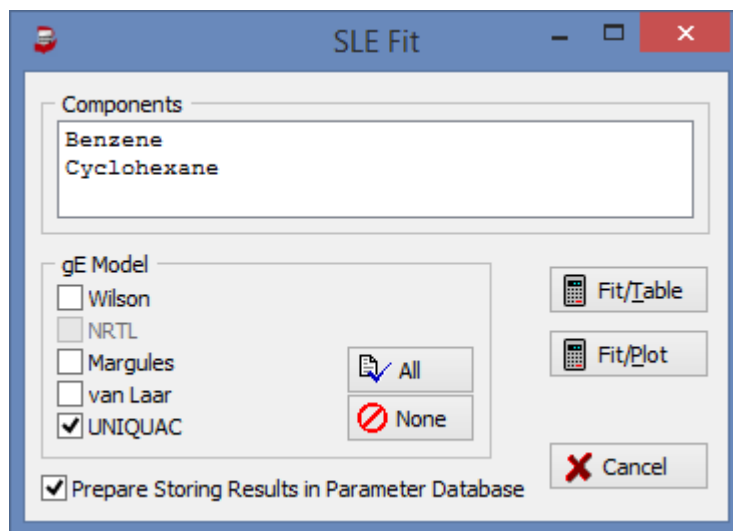


Figure 159 Fitting SLE Datasets

Only binary eutectic systems can be fitted.

Plot Result

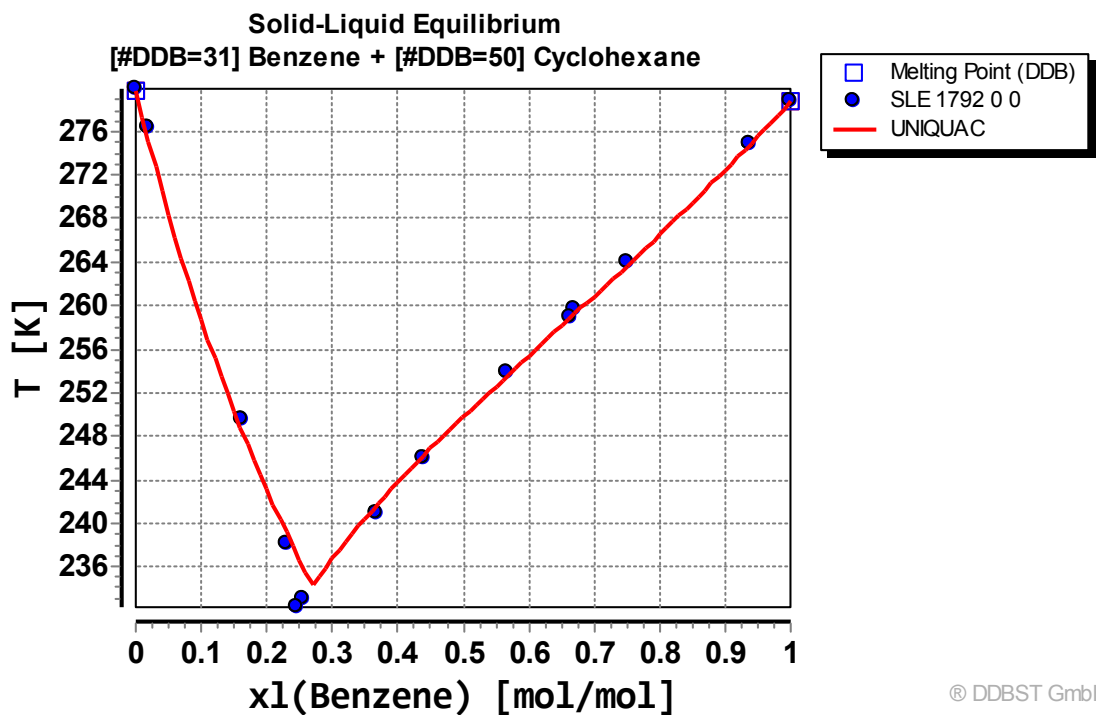


Figure 160: SLE Fit Result

Text Result

DDB#		formula	name			
(1)	31	C6H6	Benzene			
(2)	50	C6H12	Cyclohexane			
Tmelt [K]		Hf [J/mol]				
(1)	278.68	9944.101				
(2)	279.75	2628.400				
=====						
Jackowski A.W., Rocz.Chem. 48(9),1517(1974).						
T [K]		x1	exp.gam1	exp.gam2	calc.gam1	calc.gam2
278.69	1.00000					
274.85	0.93800	1.0041			1.0025	2.0314
263.95	0.75200	1.0464			1.0432	1.6561
259.58	0.67000	1.0882			1.0810	1.5237
259.00	0.66300	1.0884			1.0850	1.5135
253.80	0.56700	1.1578			1.1522	1.3820
246.08	0.43900	1.2899			1.2933	1.2390
241.02	0.36800	1.3895			1.4093	1.1744
233.17	0.25400	1.7034			1.6881	1.0898
232.33	0.24700	1.7195	1.0540			
238.04	0.23000		1.0649		1.7555	1.0727
249.57	0.16200		1.0404		1.9767	1.0351
276.30	0.02000		1.0056		2.5674	1.0005
279.87	0.00000					

Jackowski A.W.,
Rocz.Chem. 48 (9), 1517 (1974).

```
=====
UNIQUAC
parameters [cal/mol] : -153.540      404.965
objective function (sum of gam(rel)**2):  0.48554E-03
```

19.7 VLE/HPV

Vapor-liquid equilibrium data sets can be fitted by g^E models (Margules, van Laar, Wilson, NRTL, UNIQUAC).

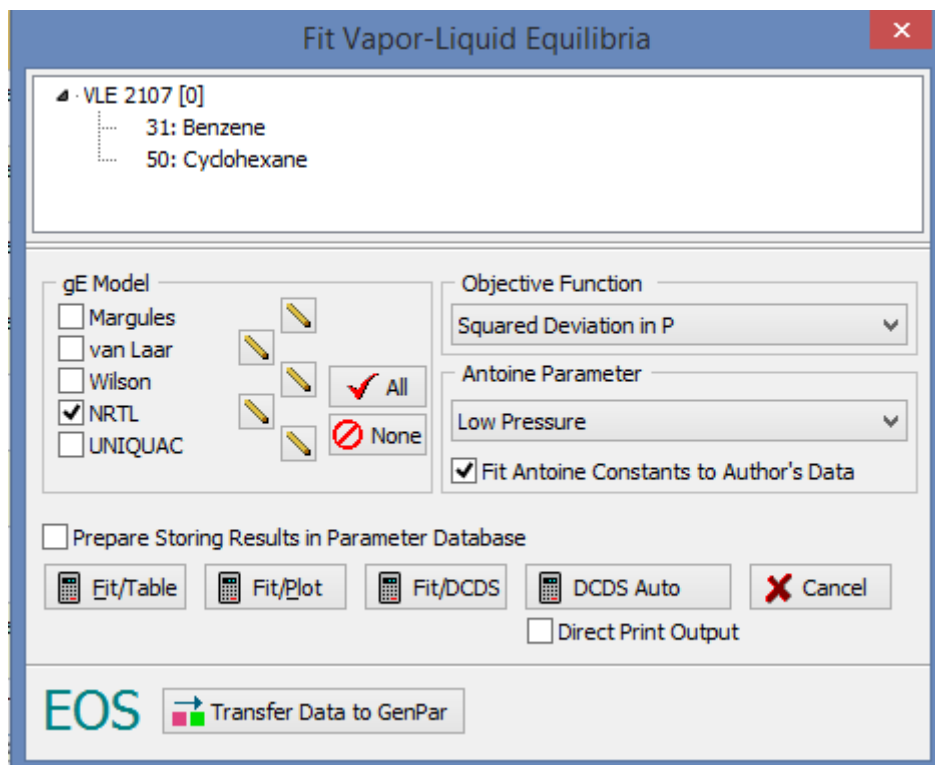



Figure 162 Fitting VLE Datasets

For fitting EOS mixing rule parameters it is necessary to transfer the data to “GenPar”, out fitting tools for such parameters. GenPar is described in a separate manual.

The buttons  allow to enter starting values for the fit.

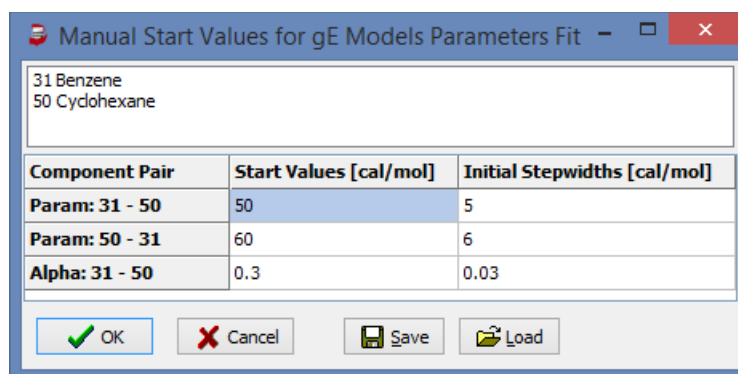


Figure 163 Manual Exchange of Start Values

The option ☒ **Fit Antoine Constants to Author's Data** should be used if the VLE data sets seem to use a different pure component pressure than the normal Antoine constants are calculating. Since the g^E models only fit the difference between the real and the ideal vapor pressure curve (activity) a larger gap would result in wrong fits. “Fit/Table” and “Fit/Plot” do what they are expected to do. “Fit DCDS” creates a data page for the **DECHEMA Chemistry Data Series**.

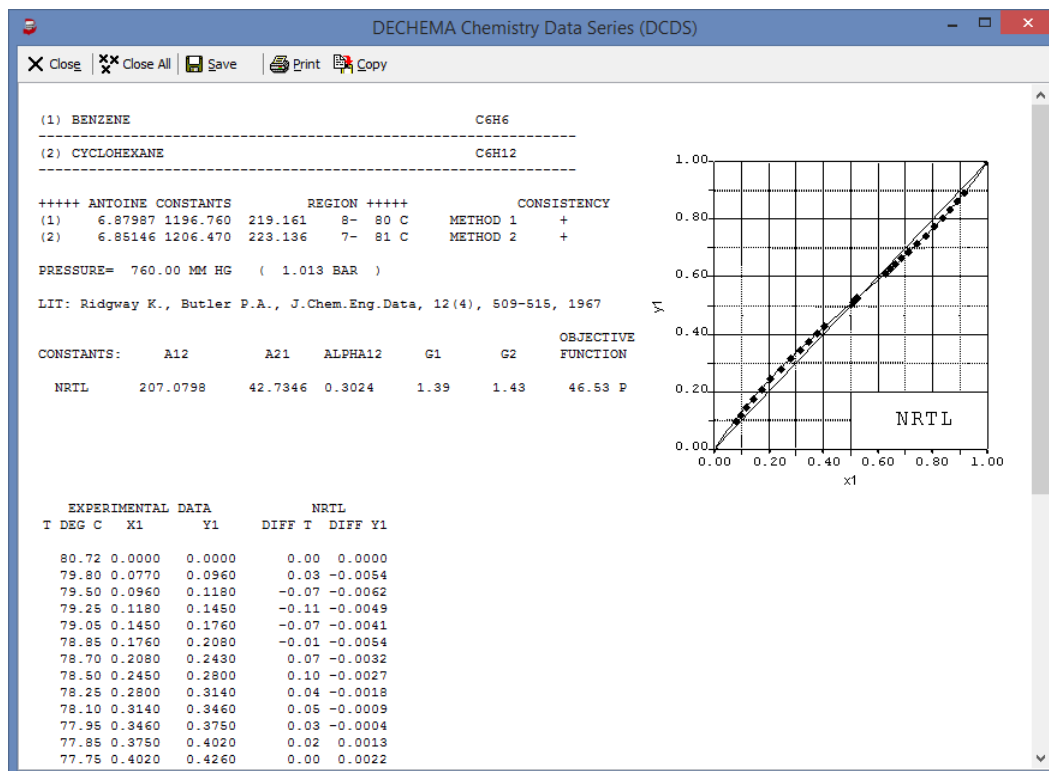
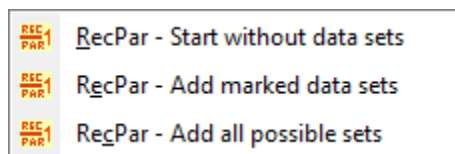


Figure 164 DCDS Compatible Output

20 Simultaneous Fit – RecPar

RecPar performs the fit of parameters to different properties simultaneously. Invoking RecPar is slightly different from invoking RecVal because it is an internal dialog within Dortmund Data Bank software – so no data have to be transferred.



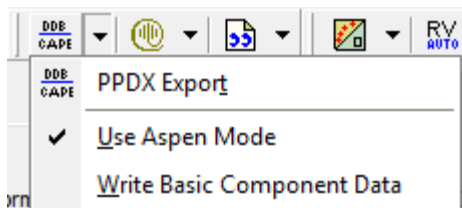
A full description is available in a separate PDF.

21 Plot

The plot functions are explained in a separate document.

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 [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.

A typical output is

```
! PHYSICAL-PROPERTY-DATA-EXCHANGE
! DDBST-PPDX-INTERFACE, Rel. 1.1.0.2
! -----
! 29.04.2004 10:22:47
! Copyright: DDBST GmbH (2000-2002)
! -----

VERSION      IKC-PPDX      1.6

INITIALIZE
END INITIALIZE

PRIVATE
END PRIVATE

IGNORE
END IGNORE

SOURCE
  KEY Lit-477
  AUTHOR "Nagai J.,Ishii N."
  TITLE "Studies on Volatility of Fuels Containing Ethyl Alcohol. II-IV.
& Calculation of Starting Temperatures of an Engine when using Ethyl
& Alcohol-Ethyl Ether Mixtures as its Fuel"
  JOURNAL "J.Soc.Chem.Ind.Jap. = Kogyo Kagakkai"
  YEAR 1935
  PAGE 86-95
```

```
VOLUME 38
ISSUE 3
END KEY Lit-477

KEY Lit-0
AUTHOR "Gmehling et al."
TITLE "Dortmund Databank - Pure Component Basic File"
JOURNAL "Electronic Databank"
YEAR 1973-2004
END KEY Lit-0
END SOURCE

COMP-DEF
CID DDB11
NAME Ethanol
CAS-NO 64-17-5
FORMULA C2H6O-2
END CID DDB11

CID DDB12
NAME Diethyl ether
CAS-NO 60-29-7
FORMULA C4H10O-5
END CID DDB12

END COMP-DEF

PURE-COMP-DATA
PROPERTIES
MW $ DDB11 46.069 kg/kmol $ $ $ Lit-0
TC $ DDB11 516.20 K $ $ $ Lit-0
PC $ DDB11 63.0 atm $ $ $ Lit-0
VC $ DDB11 167.00 cm^3/mol $ $ $ Lit-0
OMEGA $ DDB11 0.63 - $ $ $ Lit-0
TMP $ DDB11 -114.50 C $ $ $ Lit-0
HLSM $ DDB11 1199.2 J/mol $ $ $ Lit-0
MW $ DDB12 74.122 kg/kmol $ $ $ Lit-0
TC $ DDB12 466.70 K $ $ $ Lit-0
PC $ DDB12 35.9 atm $ $ $ Lit-0
VC $ DDB12 280.00 cm^3/mol $ $ $ Lit-0
OMEGA $ DDB12 0.28 - $ $ $ Lit-0
TMP $ DDB12 -116.30 C $ $ $ Lit-0
HLSM $ DDB12 1736.9 J/mol $ $ $ Lit-0
END PROPERTIES

PARAMETERS
UNIQVAC r $ DDB11 2.1055
UNIQVAC q $ DDB11 1.9720
UNIQVAC r $ DDB12 3.3949
UNIQVAC q $ DDB12 3.0160
END PARAMETERS

FUNCTION vapor-pressure
NAME ANTOINE
COMPONENT DDB11
PROPERTY PVL T
UNIT mmHg C
LOWER-BOUND -57
UPPER-BOUND 80
COEFFICIENTS 8.2042 1642.9 230.30
END FUNCTION vapor-pressure
FUNCTION vapor-pressure
NAME EXANTOINE
COMPONENT DDB11
```



```

PROPERTY      PVL  T
UNIT           mmHg C
LOWER-BOUND   -57
UPPER-BOUND    80
COEFFICIENTS  21.0157  3782.9  -42.85
END FUNCTION vapor-pressure
FUNCTION vapor-pressure
NAME          ANTOINE
COMPONENT     DDB12
PROPERTY      PVL  T
UNIT           mmHg C
LOWER-BOUND   -101
UPPER-BOUND    35
COEFFICIENTS   7.1263  1151.8  236.99
END FUNCTION vapor-pressure
FUNCTION vapor-pressure
NAME          EXANTOINE
COMPONENT     DDB12
PROPERTY      PVL  T
UNIT           mmHg C
LOWER-BOUND   -101
UPPER-BOUND    35
COEFFICIENTS  18.5337  2652.0  -36.16
END FUNCTION vapor-pressure
END PURE-COMP-DATA

MIXTURE-DATA
TABLE VLE641
SOURCE-KEY      Lit-477
COMPONENTS      DDB12 DDB11
PROPERTY        P      x      y      T
STATE VLE
UNIT            "kPa"      "mol/mol" "mol/mol" "K"
DATA            20.526      0.05      0.5092      303.150
DATA            29.731      0.1       0.6771      303.150
DATA            37.197      0.15      0.7538      303.150
DATA            43.323      0.2       0.7977      303.150
DATA            48.657      0.25      0.8278      303.150
DATA            51.926      0.3       0.8455      303.150
DATA            57.201      0.35      0.8656      303.150
DATA            60.595      0.4       0.8785      303.150
DATA            63.731      0.45      0.8897      303.150
DATA            66.493      0.5       0.8993      303.150
DATA            68.96       0.55      0.9077      303.150
DATA            71.141      0.6       0.9153      303.150
DATA            73.101      0.65      0.9223      303.150
DATA            76.26       0.7       0.9305      303.150
DATA            76.996      0.75      0.9371      303.150
DATA            78.794      0.8       0.9451      303.150
DATA            80.633      0.85      0.954       303.150
DATA            82.473      0.9       0.9651      303.150
DATA            84.333      0.95      0.9789      303.150
END TABLE VLE641
END MIXTURE-DATA

```

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

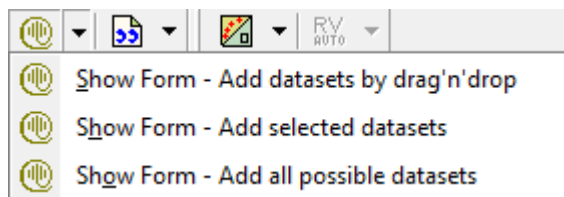
- HE – mixing enthalpies
- GLE – gas solubilities
- VE – (excess) volumes and densities
- PCP – pure component properties
- ACT – activity coefficients at infinite dilution
- AZD – azeotropic information
- SLE – solid-liquid equilibria
- CPE – (excess) heat capacities

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 databanks 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 can't 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.

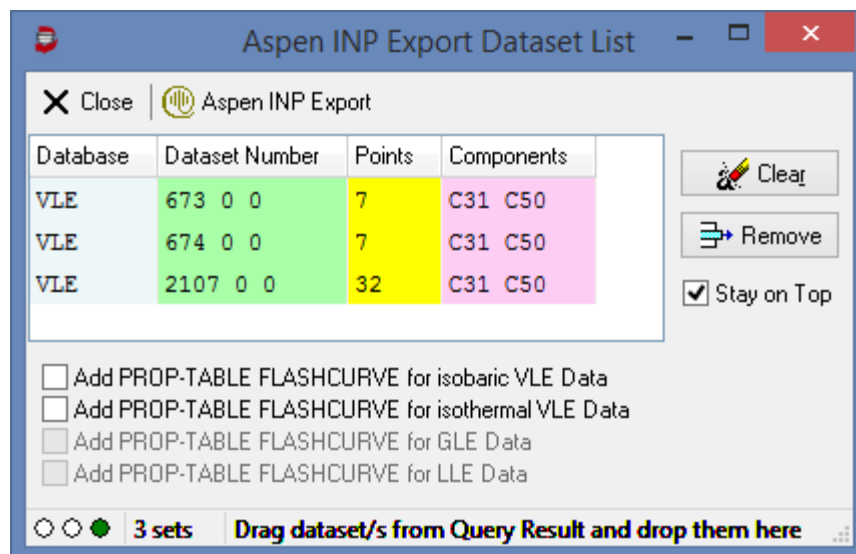


Figure 165: Aspen INP Export - Data Set List – Mixture Data Banks

- “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 have the extension “.INP” but can also have the extension “.APRINP”.

A typical output is

```
;
; INP file generated by DDBSP 2014/Mixture Properties
; 07.03.2014 10:22:27
; Copyright: DDBST GmbH, Marie-Curie Str. 10, D-26129 Oldenburg
;
; Filename: C:\Scratch\test.inp
;
; NOTE (GLE Conversion)
;
; The GLE conversion makes the following assumptions and usage of equations:
;
; The gas partial pressure calculation from total pressure or vice versa
; assumes that Raoult's Law and Dalton's Law are valid. Furthermore the
; vapor pressure of the solvent is calculated using the Antoine equation.
;
; If necessary for the calculation of the amount of substance a liquid density
; equation, a fixed Normdensity table (Bunsen, Kuenen) or the Ideal Gas Law
; is used. It is furthermore assumed that mixing effects are irrelevant for the
; liquid density.
;
DRS

TITLE 'Export of DDB Datasets'
```

```
IN-UNITS SI TEMP=C PRES=MMHG

DATABANKS 'APV84 PURE28' / 'APV84 INORGANIC' / 'APV84 AQUEOUS' / NOASPENPCD
PROP-SOURCES 'APV84 PURE28' / 'APV84 INORGANIC' / 'APV84 AQUEOUS'

; cid cname outid
; cid is always DDB????? with ????? as DDB component number
; cname is Aspen component id, if available or * if not
; outid is empty.

COMPONENTS
  DDB11 C2H6O-2 /
  DDB12 C4H10O-5

PROPERTIES IDEAL

CASE R-1
  DATA-GROUPS VLE175 / VLE176 / VLE177
  REPORT KVL GAMMA PBUB ALPHA
  CASE-OPTION REGRESSION=NO

DATA-GROUP VLE175
  DESCRIPTION "[866] Moeller 1951, VLE175"
  IN-UNITS PRESSURE=KPA TEMPERATURE=K
  SYSTEM-DEF TPXY DDB12 DDB11 COMPOSITION=MOLE-FRAC
  PHASE-EQ VL DDB12 DDB11
    DATA 1 377.65 287.483 0.007 0.16 /
    2 376.75 287.483 0.009 0.129 /
    3 373.15 287.483 0.025 0.248 /
    4 365.45 287.483 0.08 0.426 /
    5 359.65 287.483 0.132 0.527 /
    6 355.45 287.483 0.205 0.641 /
    7 348.15 287.483 0.405 0.779 /
    8 346.95 287.483 0.454 0.786 /
    9 343.65 287.483 0.64 0.877 /
    10 342.15 287.483 0.863 0.96
  STD-DEV 1 0.1 -0.1 -1 -1

DATA-GROUP VLE176
  DESCRIPTION "[866] Moeller 1951, VLE176"
  IN-UNITS PRESSURE=KPA TEMPERATURE=K
  SYSTEM-DEF TPXY DDB12 DDB11 COMPOSITION=MOLE-FRAC
  PHASE-EQ VL DDB12 DDB11
    DATA 1 400.15 721.847 0.065 0.251 /
    2 396.35 721.847 0.119 0.36 /
    3 395.65 721.847 0.127 0.359 /
    4 386.15 721.847 0.303 0.555 /
    5 384.65 721.847 0.323 0.575 /
    6 383.15 721.847 0.363 0.602 /
    7 381.05 721.847 0.447 0.664 /
    8 380.15 721.847 0.565 0.759 /
    9 379.15 721.847 0.723 0.842 /
    10 378.15 721.847 0.933 0.967
  STD-DEV 1 0.1 -0.1 -1 -1

DATA-GROUP VLE177
  DESCRIPTION "[866] Moeller 1951, VLE177"
  IN-UNITS PRESSURE=KPA TEMPERATURE=K
  SYSTEM-DEF TPXY DDB12 DDB11 COMPOSITION=MOLE-FRAC
  PHASE-EQ VL DDB12 DDB11
    DATA 1 382.55 515.011 0.039 0.217 /
    2 379.15 515.011 0.105 0.382 /
    3 377.65 515.011 0.192 0.523 /
```

```

4 376.65 515.011 0.207 0.528 /
5 374.15 515.011 0.259 0.573 /
6 371.05 515.011 0.314 0.635 /
7 367.05 515.011 0.44 0.721 /
8 366.85 515.011 0.513 0.761 /
9 364.15 515.011 0.812 0.913 /
10 363.15 515.011 0.943 0.984
STD-DEV 1 0.1 -0.1 -1 -1

```

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 to specify data sets.

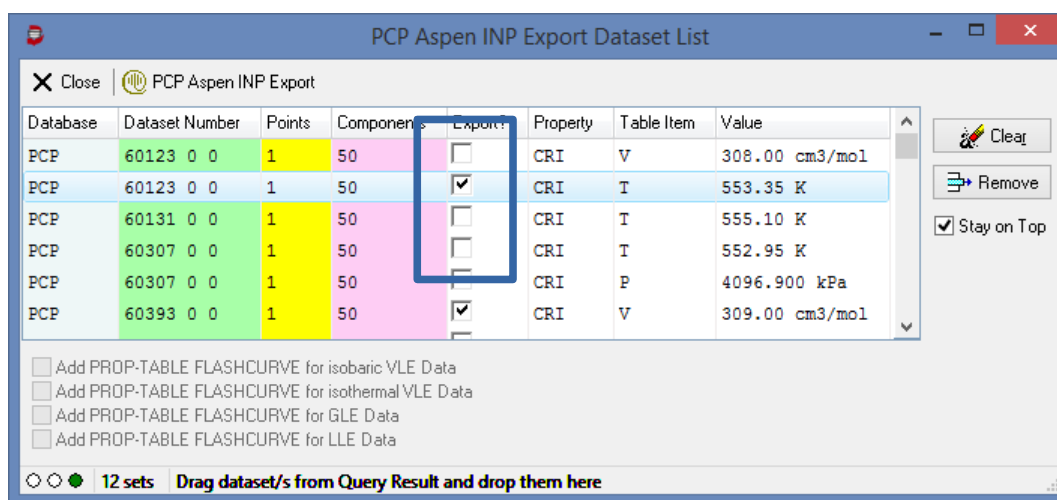


Figure 166: Aspen INP Export - Data Set List – Pure Component Properties Data Bank

22.3 Data Points Export

22.3.1 Export Mixture Data

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.

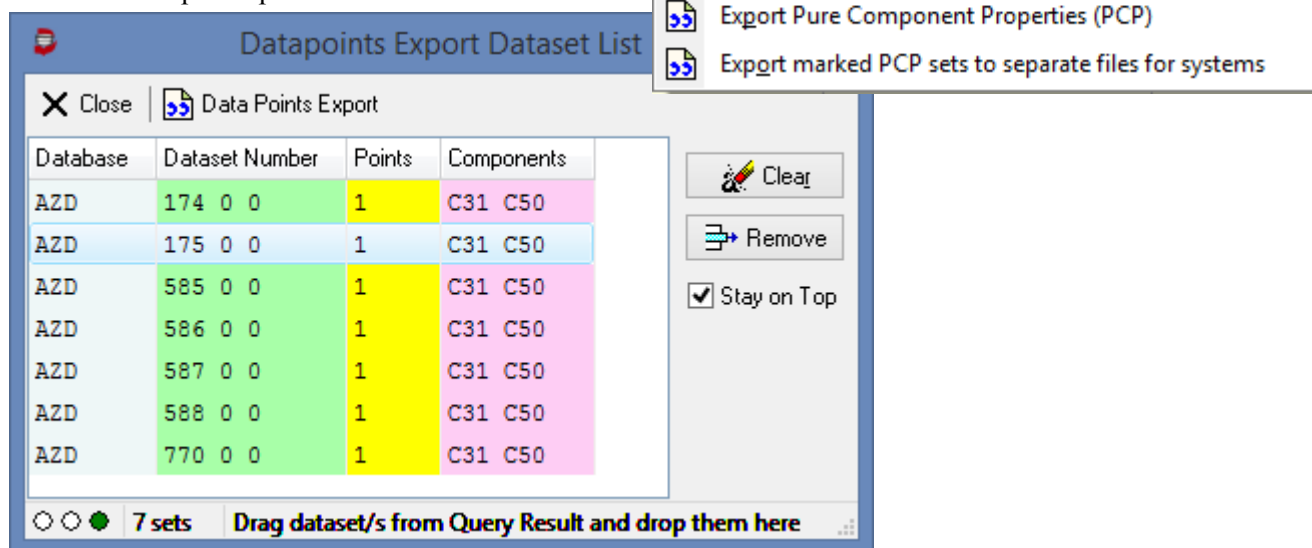


Figure 167: Data Points Export - Data Set List

The Data Points Export creates a table (see Figure 168) 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 spread sheet (like Microsoft Excel) compatible format. Supported file formats are the “.csv” format (comma separated values) and the “.xls” format of Microsoft Excel.

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 (see Figure 168).

#	#DDB1	#DDB2	#Dataset	#Ref.Number	Comment	Database	P	T	vE	x1		
[#]	[#]	[#]	[#]	[#]	[-]	[-]	[kPa]	[K]	[cm3/mol]	[mol/mol]		
1	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.15455	0.046200	12: Diethyl ether	110: Methano
2	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.24680	0.082500	12: Diethyl ether	110: Methano
3	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.49007	0.198400	12: Diethyl ether	110: Methano
4	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.59875	0.284300	12: Diethyl ether	110: Methano
5	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.69619	0.385800	12: Diethyl ether	110: Methano
6	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.73084	0.509200	12: Diethyl ether	110: Methano
7	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.71815	0.603400	12: Diethyl ether	110: Methano
8	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.67453	0.679800	12: Diethyl ether	110: Methano
9	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.55692	0.783000	12: Diethyl ether	110: Methano
10	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.35300	0.882400	12: Diethyl ether	110: Methano
11	12	110	13483	1907	vE [LL]	VE	101.320	288.15	-0.30167	0.913300	12: Diethyl ether	110: Methano
1907 [13146] Canosa J., Rodriguez A., Tojo J., Fluid Phase Equilib., 156, 57-71, 1999												

Figure 168: Data Points Export - Result Table

23 Appendix

23.1 Example for "Display Component or List Related Statistics"

In this example diethyl ether has been selected. This overview show some component details and a overview on available data sets in all data banks.

Diethyl ether

```

Alternative Name:      3-Oxapentane
Empirical Formula:    C4H10O
CAS Registry Number:  60-29-7
269 sets Activity coefficients at infinite dilution (binary systems)
  8 sets Activity coefficients at infinite dilution (ternary systems)
299 sets Azeotropic/zeotropic information
 18 sets Critical data of mixtures
 88 sets Densities and volumes of mixtures
 52 sets Gas solubilities
116 sets Heats of mixing
 86 sets Liquid-liquid equilibria
  6 sets Octanol-Water partition coefficients
459 sets Pure component properties
      46 sets Viscosity
      73 sets Vapor Pressure
      28 sets Critical Data
      10 sets Kinematic Viscosity
147 sets Density
      20 sets Melting Point
      31 sets Molar Heat Capacity (cP)
      18 sets Virial Coefficients
      10 sets Heat of Vaporization
       8 sets Heat of Fusion
      22 sets Thermal Conductivity
  
```

18 sets	Surface Tension
2 sets	Entropy
2 sets	Std. Heat of Formation
1 set	G-function (G-G0)/T
1 set	Transition Temperature
4 sets	Ideal Gas Heat Capacity
8 sets	Dielectric Constant
9 sets	Speed of Sound
1 set	Virial Coefficients (Berlinform)
44 sets	Salt solubilities
173 sets	Solid-liquid equilibria for systems without salts
17 sets	Thermodynamic data for polymer containing systems
283 sets	Vapor-liquid equilibria
4 sets	Vapor-liquid equilibria for systems containing solved salts

23.2 Example for “Display Detailed Pure Component Properties Overview”

The overview is a table which can be printed, copied, saved, and mailed.

Grid Output						
<div> Close Print Copy Copy HTML Save Mail </div>						
PCP Statistics						
Property	Points	Sets	Temperature Range	Pressure Range	States	Sets
Boiling Point	1	1	(-)	(-)	Vapor-Liquid	1
Compressibility (isentropic)	11	8	293-333 K	(-)	Liquid	8
Compressibility (isothermal)	5	2	293-318 K	(-)	Liquid	2
Compressibility Factor (isothermal)	45	3	523-573 K	1520-10133 kPa	Vapor	3
Critical Data	72	71	(-)	(-)	Critical Point	71
Density	4945	820	178-623 K	0-1078830 kPa	Liquid	751
					Vapor	24
					Supercritical	17
					Liquid Phase of VLE	12
					Vapor Phase of VLE	9
					Superheated Liquid	4
					Critical Point	3
Dielectric Constant	292	63	182-473 K	98-400000 kPa	Liquid	63
Diffusion Coefficient	25	6	193-348 K	100-24300 kPa	Liquid	6
Dynamic Viscosity	1881	264	175-631 K	0-1176798 kPa	Liquid	223

23.2.1 Example Output for n-Hexane

Property	Points	Sets	Temperature Range	Pressure Range	States	Sets
Boiling Point	1	1	(-)	(-)	Vapor-Liquid	1
Compressibility (isentropic)	11	8	293-333 K	(-)	Liquid	8
Compressibility (isothermal)	5	2	293-318 K	(-)	Liquid	2
Compressibility Factor (isothermal)	45	3	523-573 K	1520-10133 kPa	Vapor	3
Critical Data	72	71	(-)	(-)	Critical Point	71
Density	4945	820	178-623 K	0-1078830 kPa	Liquid	751
					Vapor	24
					Supercritical	17
					Liquid Phase of VLE	12
					Vapor Phase of VLE	9
					Superheated Liquid	4
					Critical Point	3
Dielectric Constant	292	63	182-473 K	98-400000 kPa	Liquid	63
Diffusion Coefficient	25	6	193-348 K	100-24300 kPa	Liquid	6
Dynamic Viscosity	1881	264	175-631 K	0-1176798 kPa	Liquid	223
					Vapor	23
					Superheated Liquid	12
					Vapor Phase of VLE	2
					Vapor-Liquid	1
					Supercooled Liquid	1
					Supercritical	1

					Liquid Phase of VLE 1	
Entropy	3	3	298-298 K	(-)	Vapor	3
Flash Point	4	4	247-262 K	(-)	Liquid	4
G-function (G-G0)/T	35	3	298-1500 K	(-)	Vapor	3
Heat of Fusion	7	7	176-178 K	101-101 kPa	Solid-Liquid	7
Heat of Vaporization	66	14	298-508 K	(-)	Vapor-Liquid	14
Ideal Gas Heat Capacity	42	5	298-1500 K	(-)	Ideal Gas	5
Kinematic Viscosity	55	18	178-423 K	(-)	Liquid	18
Melting Point	39	33	(-)	(-)	Solid-Liquid	33
Molar Heat Capacity (cP)	1101	125	13-624 K	98-863800 kPa	Liquid	94
					Vapor	20
					Critical Point	6
					Solid	4
					Liquid Phase of VLE 1	
Molar Heat Capacity (cV)	803	31	243-653 K	5000-700000 kPa	Vapor	16
					Liquid	14
					Liquid Phase of VLE 1	
Molar Saturation Heat Capacity	15	2	278-348 K	(-)	Liquid	2
Speed of Sound	1297	180	183-521 K	0-980665 kPa	Liquid	166
					Superheated Liquid	5
					Vapor	4
					Liquid Phase of VLE 4	
					Supercritical	1
Std. Heat of Combustion	4	4	291-298 K	(-)	Liquid	4
Std. Heat of Formation	5	5	291-298 K	(-)	Liquid	3
					Vapor	2
Surface Tension	258	58	173-507 K	101-101 kPa	Liquid	56
					Liquid Phase of VLE 2	
Thermal Conductivity	786	93	183-729 K	0-643700 kPa	Liquid	62
					Vapor	23
					Supercritical	6
					Superheated Liquid	2
Thermal Expansion Coefficient	66	2	303-503 K	500-35290 kPa	Liquid	2
Triple Point	1	1	(-)	(-)	Solid-Liquid-Vapor	1
Vapor Pressure	1703	383	174-508 K	0-3058 kPa	Vapor-Liquid	383
Virial Coefficients	85	20	298-663 K	(-)	Vapor	20