

# Dortmund Data Bank DDB Software Package

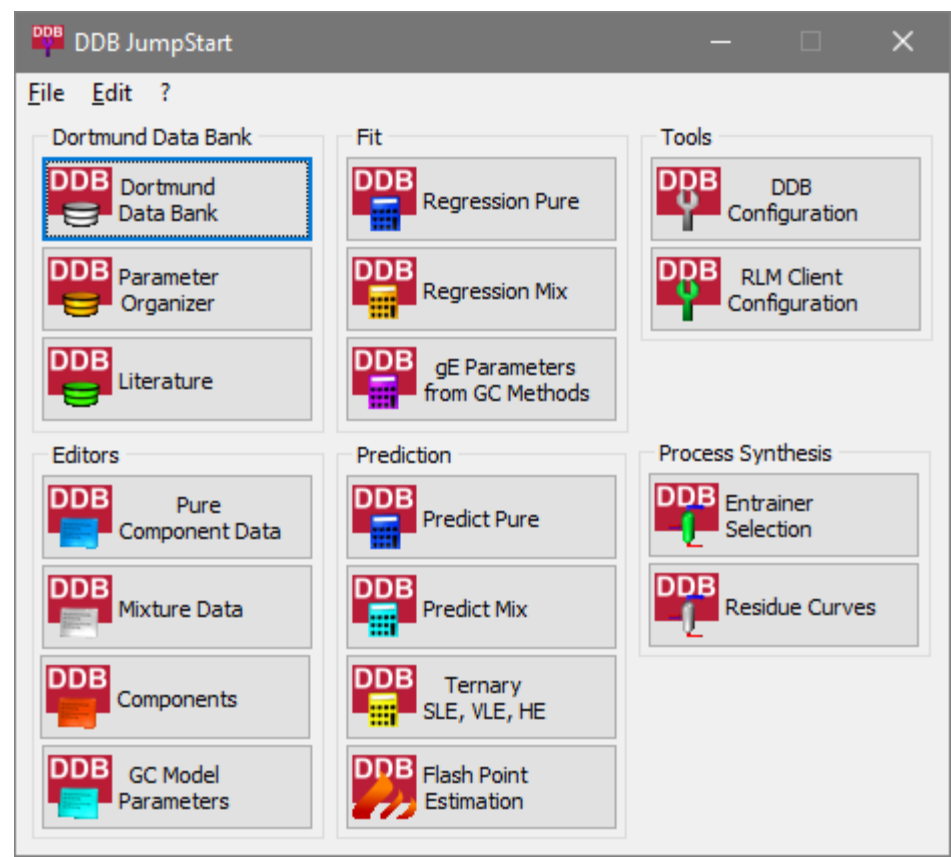
Chemical Thermodynamics and Physical Properties with DDB

- Parts of DDB
- Components and Component Lists in DDB
- DDB Literature Management
- Pure Component Data Estimation
- Pure Component and Mixture Data - Retrieval and Output
- Pure Component Data Regression
- Mixture Data Regression
- Simultaneous Mixture Data Regression
- Mixture Data Estimation
- Check Parameters Prior to Process Simulation
- DDB Parameter Data Bank
- Process Synthesis
- Data Input
- Data Import and Export

# Parts of DDB

## Lesson Objectives

- become familiar with how to start DDB
- some data in DDB (exp. and basic data)
- component types in DDB
- ways to select components and component lists
- store, retrieve and edit component lists
- component lists by substructure



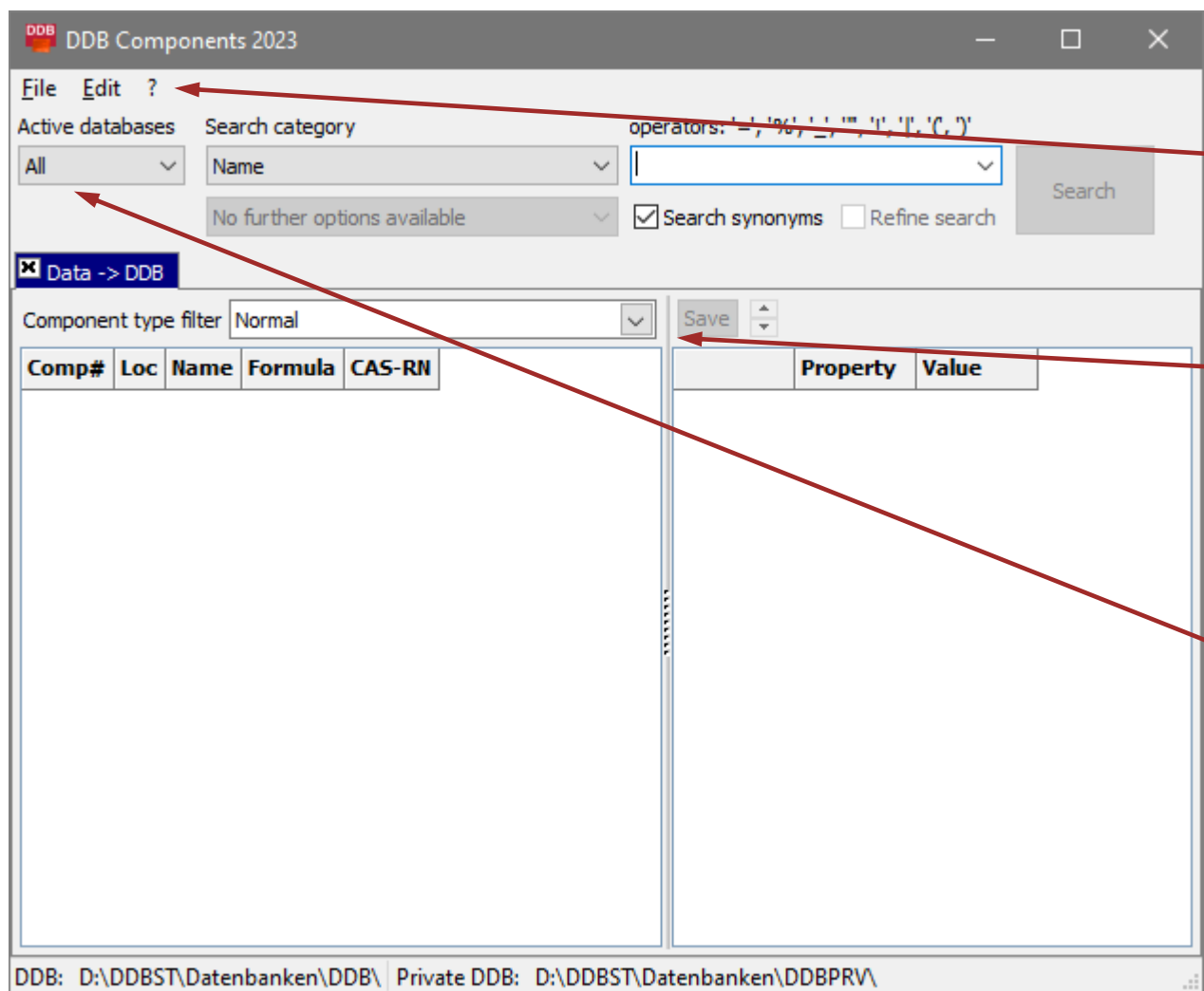
if not available here:



start via  
*Start – Programs –  
DDB 202x Client*

- normal components (organic and inorganic)
  - name, emp. formula, CAS#
  - Antoine constants, critical data, acentric factor, ...
  - melting point, heat of fusion
  - molecular weight, dipole moment
  - density (Wilson), R and Q values, ....
- salts
  - thermodynamic data, heat capacity
  - dielectric constant, ions, ...
- polymers
  - further specifications together with exp. data
- adsorbents
  - further specifications together with exp. data
- ions
- ....

Start *Dortmund Data Bank* and select *Add/Search Component* to display the following Dialog:



Please look at the menu for further options!

- Component types:
- Normal Components
  - Salts
  - Adsorbents
  - Polymers

- Data banks
- Public DB (DDB)
  - Private DB

Same component may be **normal component** or **salt**.

## Sodium Chloride

- as a normal component  
density, vapor pressure, heat of vaporization, melting point, surface tension, viscosity, thermal conductivity  
VLE, AZD, LLE, SLE, ...

- as a salt  
electrolyte VLE  
electrolyte SLE  
...

Search criteria: Active databases: All, Search category: Formula, operators: '=', '%', '\_', '!', '|', '(', ')', Search: =NaCl

Component type filter: Normal,Salts

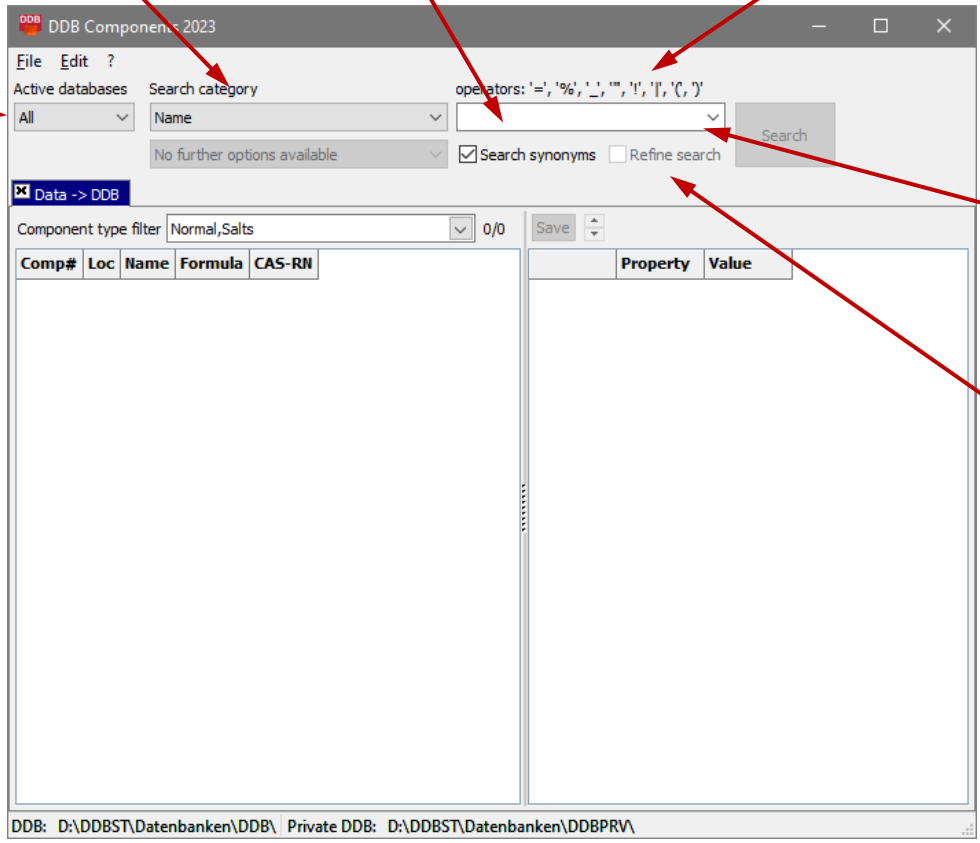
Comp#	Loc	Name	Formula	CAS-RN
4911	0	Sodium chloride	ClNa	7647-14-5

Property list for Sodium chloride:

Property	Value
Identification	
Name	Sodium chloride
Alternative name	Table salt
Formula	ClNa
CAS registry number	76-7-14-5
Location	0
Component number	4911
Additional component numbers	
Salt number	104
Adsorbent number	
Polymer number	
Ion number	
Monomer number	
Synonyms	
Component classes	
Atomic	
Molecular weight [g/mol]	58.4425

what to search for    query expression    query syntax

active data bank



Select previous query from history

search in all components or only those found in the active search

Search for „name“ searches also the alternative name.  
Search for „formula“ allows any order of the elements (H2SO4, SH2O4, ...).

.....



Comp#	Loc	Name	Formula	CAS-RN	Salt#
1	0	Acetaldehyde	C2H4O	75-07-0	
2	0	Acetamide	C2H5NO	60-35-5	6588
3	0	Acetonitrile	C2H3N	75-05-8	
4	0	Acetone	C3H6O	67-64-1	
5	0	Ethylenediamine	C2H8N2	107-15-3	
6	0	1,2-Dibromoethane	C2H4Br2	106-93-4	
7	0	Ethyl bromide	C2H5Br	74-96-4	
8	0	1,2-Ethanediol	C2H6O2	107-21-1	10331
9	0	Ethyl iodide	C2H5I	75-03-6	
10	0	5-Ethyl-2-nonanol	C11H24O	103-08-2	
11	0	Ethanol	C2H6O	64-17-5	
12	0	Diethyl ether	C4H10O	60-29-7	
13	0	Ethylene oxide	C2H4O	75-21-8	
14	0	2-Propen-1-ol	C3H6O	107-18-6	
15	0	Formic acid	CH2O2	64-18-6	7334
16	0	Formic acid ethyl ester	C3H6O2	109-94-4	
17	0	Aniline	C6H7N	62-53-3	
18	0	Methoxybenzene	C7H8O	100-66-3	
19	0	2-Methylpyridine	C6H7N	109-06-8	

As in the Windows Explorer:

- select or unselect components by mouse-click while pressing ctrl
- select from ... to by pressing shift when selecting the second item
- ctrl-a to select all components
- remove selected component(s) from the list: *del* button

Clicking on table header will sort for this item.

location (DDB 0, private 1)  
component code number

## Search for synonyms

Component type filter: Normal,Salts 18/18 Save Acetaldehyde

Comp#	Loc	Name	Formula	CAS-RN	Salt#
1	0	Acetaldehyde	C2H4O	75-07-0	
2	0	Acetamide	C2H5NO	60-35-5	6588
3	0	Acetonitrile	C2H3N	75-05-8	
4	0	Acetone	C3H6O	67-64-1	
5	0	Ethylenediamine	C2H8N2	107-15-3	
6	0	1,2-Dibromoethane	C2H4Br2	106-93-4	
7	0	Ethyl bromide	C2H5Br	74-96-4	
8	0	1,2-Ethanediol	C2H6O2	107-21-1	10331
1	1	OXAZOLNITRIL	C5H4N2O	1003-52-7	
2	1	CYANODIEMTHYLOXAZOL	C6H6N2O	59720-59-1	
3	1	Hydrogen sulfide	H2S	7783-06-4	
4	1	PYP-2-3			
5	1	CCU-3-F			
6	1	Acetaldehyde	C2H4O	75-07-0	
7	1				
8	1	alpha-Methyl styrene	C9H10	98-83-9	
9	1	New Name			
10	1	1-Butanol	C4H10O	71-36-3	

Property	Value
<b>Identification</b>	
Name	Acetaldehyde
Alternative name	Ethanal
Formula	C2H4O
CAS registry number	75-07-0
Location	0
Component number	1
<b>Additional component numbers</b>	
Salt number	
Adsorbent number	
Polymer number	
Ion number	
Monomer number	
<b>Synonyms</b>	
<b>Component classes</b>	
<b>Atomic</b>	
Molecular weight [g/mol]	44.053
Dipole momentum [Debye]	2.69
Van der Waals volume (UNIQAC-r)	1.8991

- synonyms
- component names and identifiers from Aspen Tech
- ...

Companies can add special names and identifiers for their inhouse systems.

Searching synonyms is much slower .....

The screenshot shows the DDB Components 2023 software interface. The search criteria are set to 'Component number(s)' with the value '11'. The search results table shows one entry for Ethanol (Component number 11, Location 0, Formula C<sub>2</sub>H<sub>6</sub>O, CAS-RN 64-17-5). The right-hand pane displays the properties of Ethanol, categorized into Identification, Atomic, and Phase change.

Comp#	Loc	Name	Formula	CAS-RN	Salt#
11	0	Ethanol	C <sub>2</sub> H <sub>6</sub> O	64-17-5	

Property	Value
<b>Identification</b>	
Name	Ethanol
Alternative name	Ethyl alcohol
Formula	C <sub>2</sub> H <sub>6</sub> O
CAS registry number	64-17-5
Location	0
Component number	11
<b>Additional component numbers</b>	
<b>Synonyms</b>	
<b>Component classes</b>	
<b>Atomic</b>	
Molecular weight [g/mol]	46.069
Dipole momentum [Debye]	1.69
Van der Waals volume (UNIQAC-r)	2.1055
Van der Waals area (UNIQAC-q)	1.972
Dielectric constant	
Dielectric constant temperature [K]	
Dielectric constant frequency [Hz]	
Radius [Å]	
Charge	
<b>Phase change</b>	
Critical temperature [K]	516.2
Critical pressure [kPa]	6383.475
Critical volume [cm <sup>3</sup> /mol]	167
Acentric factor	0.635
Normal boiling point [K]	351.58
Melting point [K]	158.65
Enthalpy of fusion [J/mol]	5017.49

Molecular Structures (ChemDB)  
 Model Parameters (ParamDB)  
 Literature Sources,  
 Documents (LITERATURE)  
 COSMO  $\sigma$ -Profiles

...

## Different Sheets for Each Data Bank

The screenshot shows the DDBST software interface with a data table for activity coefficients at infinite dilution. A red arrow points to the 'ACT' tab in the top navigation bar. The table contains the following data:

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	Publ.Year	Reference
[763 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	297 (const.)		n.a.		Act.Inf.=5.4000		1985	[5375] * Cori L., Delogu P., Private
[764 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	298 (const.)		n.a.		Act.Inf.=4.2800		1980	[5318] Schmidt I.W., US-Patent, Pat.
[765 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	298 (const.)		n.a.		Act.Inf.=4.4400		1985	[5163] Endler I., Hradetzky G., Bitt
[766 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	298 (const.)		n.a.		Act.Inf.=5.2100		1988	[5270] Yang Y., Xiao S., Li H., Fu
[767 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	298 (const.)		n.a.		Act.Inf.=5.2100		1991	[5282] Landau I., Belfer A.J., Locke
[768 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	298 (const.)		n.a.		Act.Inf.=6.0000		1964	[5252] Deal C.H., Derr E.L., Ind.Eng
[769 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	313 (const.)		n.a.		Act.Inf.=4.2600		1985	[5163] Endler I., Hradetzky G., Bitt
[770 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	313 (const.)		n.a.		Act.Inf.=5.1800		1960	[5218] Hofstee M.T., Kwantes A., Ri
[771 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	318 (const.)		n.a.		Act.Inf.=4.6800		1983	[5269] Yang Y., Wu H., Xie S., Cheng
[772 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	319 (const.)		n.a.		Act.Inf.=5.1000		1985	[5375] * Cori L., Delogu P., Private
[773 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	323 (const.)		n.a.		Act.Inf.=4.6600		1983	[5269] Yang Y., Wu H., Xie S., Cheng
[774 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	333 (const.)		n.a.		Act.Inf.=5.5000		1964	[5252] Deal C.H., Derr E.L., Ind.Eng
[775 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	335 (const.)		n.a.		Act.Inf.=4.7000		1985	[5375] * Cori L., Delogu P., Private
[776 0 0]	DDB	1	2	C11 Ethanol C31 Benzene	346 (const.)		n.a.		Act.Inf.=4.4000		1982	[4990] Thomas E.R., Newman B.A., Nic

At the bottom of the window, a status bar indicates: [5163] Endler I., Hradetzky G., Bitttrich H.-J., J.Prakt.Chem., 327(4), 693-697, 1985. Below that, it says "1 data set/s marked."

- Workshop
  - bring up the Jumpstart menu
  - start "Dortmund Data Bank" under the "Dortmund Data Bank" header
  - in the dialog window, click "Add/Search Component"
  - de-select search option synonyms
  - search for component R134a
    - view/edit component data and explore the pure component basic data display
      - close the dialog "edit component data"
      - display structure
  - select component (via doubleclick or right mouse button)

### PredictPure

- search (full structure, sub-structure)
- display and structure input
- fragment molecules into structural groups for ≈ 100 methods
- estimate properties using ≈ 100 methods
- .....

```

...
...
#ATOMS
12
      35      81.08      0 C 0 0 * 1
      35      116.1      0 C 0 0 * 1
     65.33     133.6      0 N 0 0 * 1
     95.67     116.1      0 C 0 0 * 1
...

```

```

...
...
#BONDS
13
1 2 2 1 *
2 3 1 1 *
3 4 2 1 *
4 5 1 1 *
5 6 2 1 *
6 1 1 1 *
5 7 1 1 *
7 8 1 1 *
...

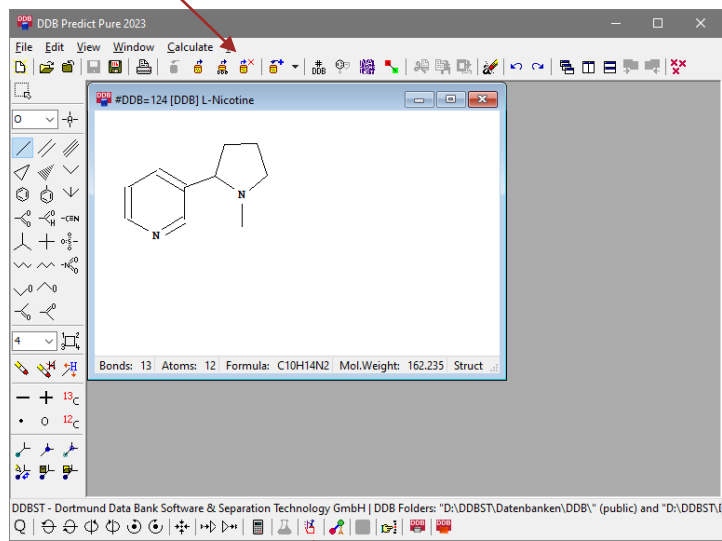
```

**Connection matrix example**

Basic Structures

Fragments

### Structure Database



3D-Rotation

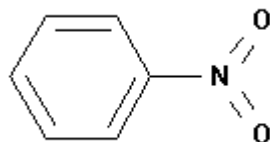
Group Assignment

## Demonstration

- Entering a structure in PredictPure.

## Workshop

- Start PredictPure and open a new structure document.
- Enter the following structure:



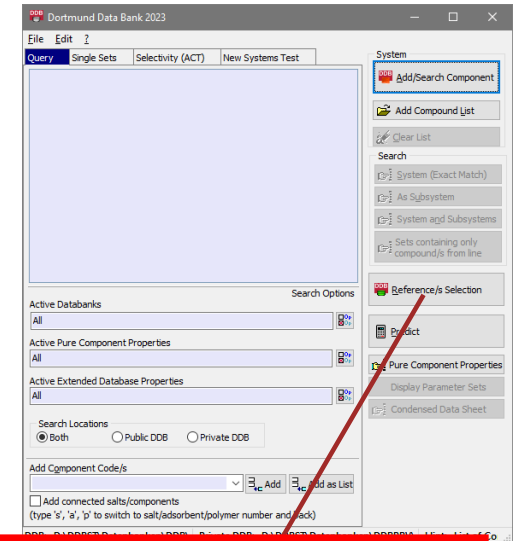
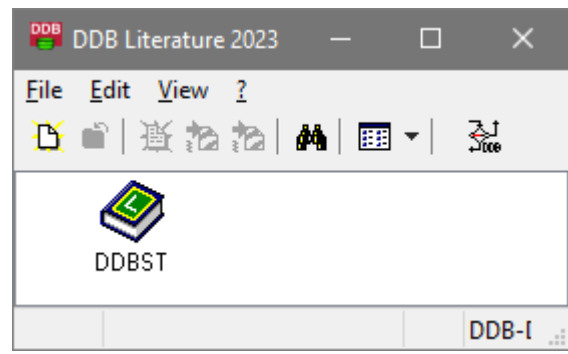
- Search as sub-structure. Stop the search after the first 2,000 components.
- Save the components matching the search structure as a list under the name "nitrobenzenes"

# DDB Literature Management

## Lesson Objectives

- Open and search Literature data banks
- Linked documents
- Links to data banks
- Find data from a reference





Complete Library [DDBST]

Results Edit Search View Options Windows

Number	Title	Authors	Pl
30608	An Automated Apparatus for ...	Shaver R.D.; Robinson R.L.; Gasem K.A...	
30609	Further evaluation of the Sha...	Shariati A.; Peters C.J.; Moshfeghian M.	
30610	Modeling Phase Behavior of M...	Hassan A.; Levien K.L.; Morrell J.J.	
30611	Measurement and Correlation...	Lee J.W.; Park M.W.; Bae H.K.	
30612	Thermodynamics of the nitro...	Cerdeirina C.A.; Tovar C.A.; Gonzales D...	

Datasets: 203453

Search Query

Quick Search | **Advanced Search**

Search for literature matching ALL of the following queries

Field	Mode	Operator	String Mode	Words
Title	must contain	any	substring	consistency

query dialog

quick and advanced search

Search Results [1]

Results Edit Search View Options Windows

Number	Title	Authors	Publication Year	Pages
419	Thermodynamic Consistency ...	Ramachandran K.; Laddha G.S.	1966	88 - 92
925	Consistency of Isobaric Binar ...	Naik K.A.; Husain A.; Chari K.S.	1964	255 - 258
		Kogan V.B.	1969	2403 - 24
		p H.	1980	2261 - 22
		nivasan D.; Laddha G.S.	1968	130 - 133
		nivasan D.; Laddha G.S.	1969	16 - 19

query result list

Edit Entry 6976 [DDBST]

Literature Kind: Article in Journal

Dataset Number: 6976

Title: Experimental Determination of Critical Data of Mixtures and their Relevance for the Development of Thermodynamic Models

Authors: Horstmann S., Fischer K., Gmehling J.

Pages: 6905 to 6913 Volume: 56

Year: to 2001 Journal: 4 Chem.Eng.

Keywords: critical data;

Comments:

URLs: 1

DOI:

Links: pcp[27413];

Save Close

query result data set

Display External Links

Found Files

List Grid

	Files
Open Folder	N:\DatenQuellenLear\bis09999\
Open File	L00419bk.xls
Open File	L00419ja.xls
Open Folder	S:\LEAR-Artikel\_\#000001-\
Open File	L000419.pdf

Linked document list  
(not in delivered Version)

## How are Documents linked to Literature References?

- Each user can individually specify a list of directories for each Literature data bank.
- Lear will search these directories for files or folders that start with “< Literature Number>” or “L< Literature number>”

Example: Valid links for Literature dataset 1234:

- 1234 calculation.xls
- L01234 FPE 1983 p 33.pdf
- .....

Links are public or limited to groups or individual users through the operating system folder access rights.

Linked files can easily be moved without generating broken link errors.

Document Linking can

- make original (scanned) reports for your own in-house data available to a specific set of users.
- make documents with calculations, notes etc. concerning a document easily available to a defined set of users.

## Workshop

- In the Mixture Properties Query dialog, select Reference/s Selection
- Search for papers where “Ihmels” is among the authors:

Search Query

Quick Search | Advanced Search

Authors: Ihmels whole word (separated by spaces)

Years: (number range)

First Page: exact string

Journals: Select (numbers, separated by spaces)

Volume: whole word

Title: substring (separated by spaces)

Numbers: (number range, positive numbers only)

\*) indexed entries Clear Copy to Adv. Search

Search

or

Search Query

Quick Search | Advanced Search

Search for literature matching ALL of the following queries

Field	Mode	Operator	String Mode	Words
Authors	must contain	any	substring	Ihmels

Insert Query Line

Remove Query Line

Clear All Lines

Load Query

Save Query

Search

(in Literature, complex queries can be entered, saved and loaded)

Select reference number 32869 and click 

A Mixture Properties query result dialog will show all the data from the references found. Select different data bank sheets and explore the tree-view for the system studied in the paper.

## Lesson Objectives

- Draw molecular structures
- Retrieve structures from the DDB
- Fragment structures for group contribution methods
- Estimate different properties
- Judge method quality
- Optimize the 3D-structure
- Prepare an input file for Gaussian ( $\sigma$ -Profile calculation)

# Molecular Structure Editor

structure database

component search

toolbar →

symbols →

basic structure fragments →

rings →

charges →

user fragments →

property estimation

reactions

fragmentation

all method qualities

3D-rotation,...

molecular modeling

mixture behavior (act. coeff.)

Calculation Methods Form - #DDB=24 Benzyl alcohol

Calculate | Temp. Range

Literature | Quality | Description | Selected Methods

**Additionally needed properties...**

Normal Boiling Point [K]  
478.74 K by DDB-PURE  Modifiable Group Assignment

Result - Text | Result - Grid

Save | Copy | Print | Clear | Remove Error Lines

Save in ParameterDB | Export to INP | Export to ProSim | Fit

Property	Method	Result	Unit	Export to Aspen?	Export to ProSim?	Used Data	Component	Additionally Calculated Data
----------	--------	--------	------	------------------	-------------------	-----------	-----------	------------------------------

Show Values from DDB Basic Parameters File

Further required input.

Selecting a property enables quality if available.

Calculation Methods Form - #DDB=24 Benzyl alcohol

Calculate | Temp. Range

Literature Quality Description **Rarey/Nannoolal (given Tb)**

Additionally needed properties...

Normal Boiling Point [K] Temperature [K]

478.74 K by DDB-PURE   Modifiable Group Assignment

Result - Text Result - Grid

Save Copy Print Clear Remove Error Lines

Save in ParameterDB Export to INP Export to ProSim Fit

Property	Method	Result	Unit	Export to Aspen?	Export to ProSim?	Used Data	Component	Additionally Calculated Data
Selecting a single method for a T-dependent property allows to estimate over a range								

Show Values from DDB Basic Parameters File



Calculation Methods Form - #DDB=24 Benzyl alcohol

Calculate | Temp. Range

Literature | Quality | Description | **Rarey/Nannoolal (given Tb)**

**Additionally needed properties...**

Normal Boiling Point [K]: 478.74 K by DDB-PURE | Temperature [K]: 373.15 |  Modifiable Group Assignment

Result - Text | **Result - Grid**

Save | Copy | Print | Clear | Remove Error Lines

Save in ParameterDB | Export to INP | Export to ProSim | Fit



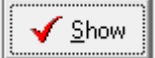
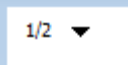
Property	Method	Result	Unit	Export to Aspen?	Export to ProSim?	Used Data
P	Rarey/Nannoolal (given Tb)	2.17641	kPa	No	No	T=373.15 K by Us BPT=478.74 K by

Show Values from DDB Basic Parameters File

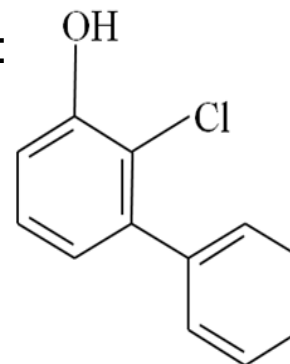
Short and detailed results

Save results or export to process simulators

## Workshop

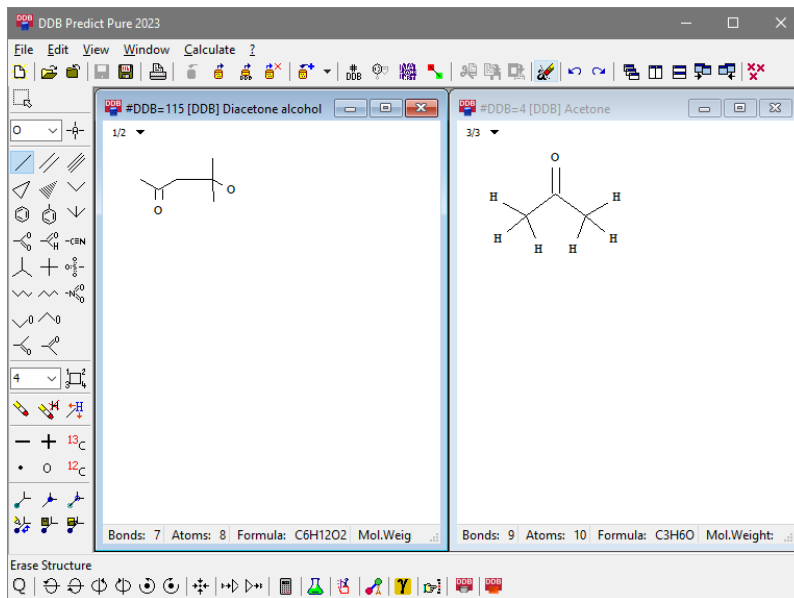
- Start PredictPure, open a new document window and draw the structure of 1,4-butanediol ( $\text{HO-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-OH}$ ) using .
- Use  to add and delete hydrogen atoms.
- Search the structure in the DDB (exact search).
- Accept the found component 614 . Now PredictPure has access to all properties stored in DDB for this component. 2 different structures are stored .
- Fragment the structure into the UNIFAC-groups (Calculate – Group Assignment, UNIFAC.ink).
- Go to Calculate – Calculate and mark the node Critical Temperature in the tree-view (Additional needed properties will offer the normal boiling point from the DDB).
- Compare the estimated values with the basic data value of 727 K.
- Retrieve the quality information for critical temperature estimation methods.
- Estimate the normal boiling point (experimental value approx. 503.15 K).
- Generate vapor pressure values between 273.15 and 393.15 K in 5 K steps (Rarey/Nannoolal with estimated  $T_b$ ) and regress Antoine constants.

- Enter the following Structure into PredictPure:
- Add and remove hydrogen atoms



- Search this structure in the DDB as substructure
- Estimate important properties like critical data, normal boiling temperature and vapor pressure curve using different methods. Compare the results. (the experimental normal boiling point is 590.15 K)
- Examine the method quality estimation for a method ranking.
- Select some estimation results and export these to an Aspen inp file.

- Load acetone and diacetone alcohol into 2 separate drawing windows in PredictPure.
- Calculate the heat of formation and reaction enthalpy using Domalski/Hearing.



Reaction Enthalpy Calculation

Calculate Heat of Formations by Domalski/Hearing  Modifiable Groups

Available Components Drag and drop components from one list to the other

Number	Description	Comment	Formula	Mol. Weight	Heat of Formation	State	Moles
1	#DDB=115 [DDB] Diacetone alcohol		C6H12O2	116.160	-465.5 kJ/mol	Gas	1
2	#DDB=4 [DDB] Acetone		C3H6O	58.080	-221.71 kJ/mol	Gas	2

Educts			Products		
Number	Description	Mol	Number	Description	Mol Count
2	#DDB=4 [DDB] Acetone	2	1	#DDB=115 [DDB] Diacetone alcohol	1

Heat of Form. (Educts) Heat of Form. (Products) Reaction Enthalpy

Calculate Reaction Enthalpy

Calculating heat of formation finished.

The DDB structure data bank can store any number of different structures for each component.

Typically a flat structure and a 3D-structure can be found.

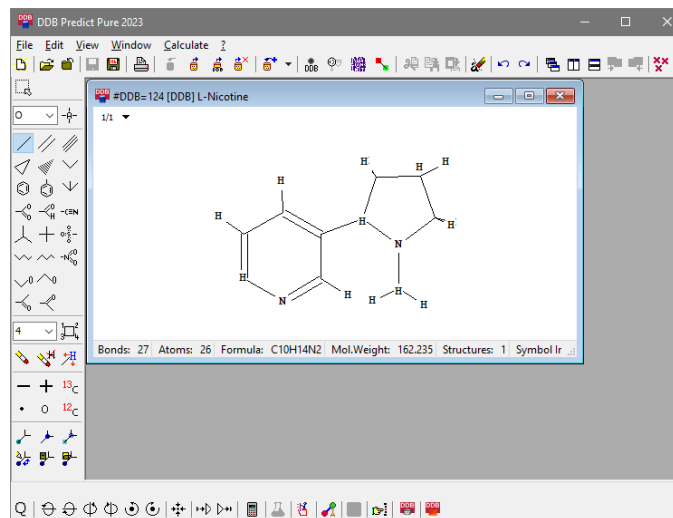
When adding hydrogen to a flat structure, a simple geometry optimization is performed automatically.

More rigorous structure optimization can be performed using the free packages MOPAC and Tinker.

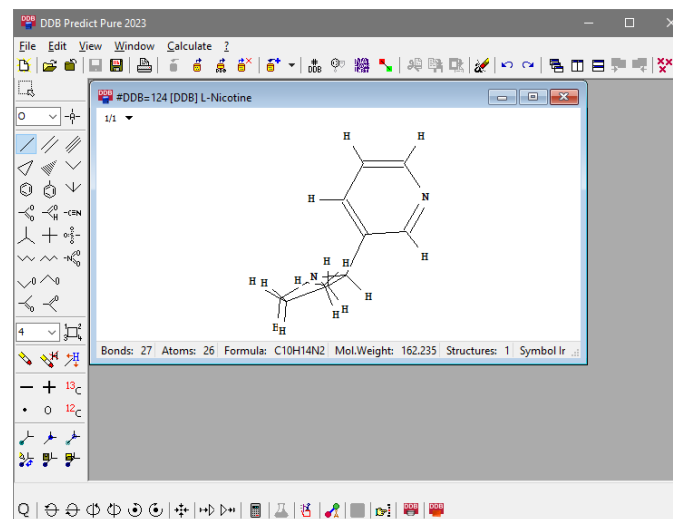
PredictPure allows to save the current structure as a Gaussian input file with the commands for a COSMO-calculation as required by COSMO-RS and COSMO-RS(OI).

3D display is available via the free tool RasWin.

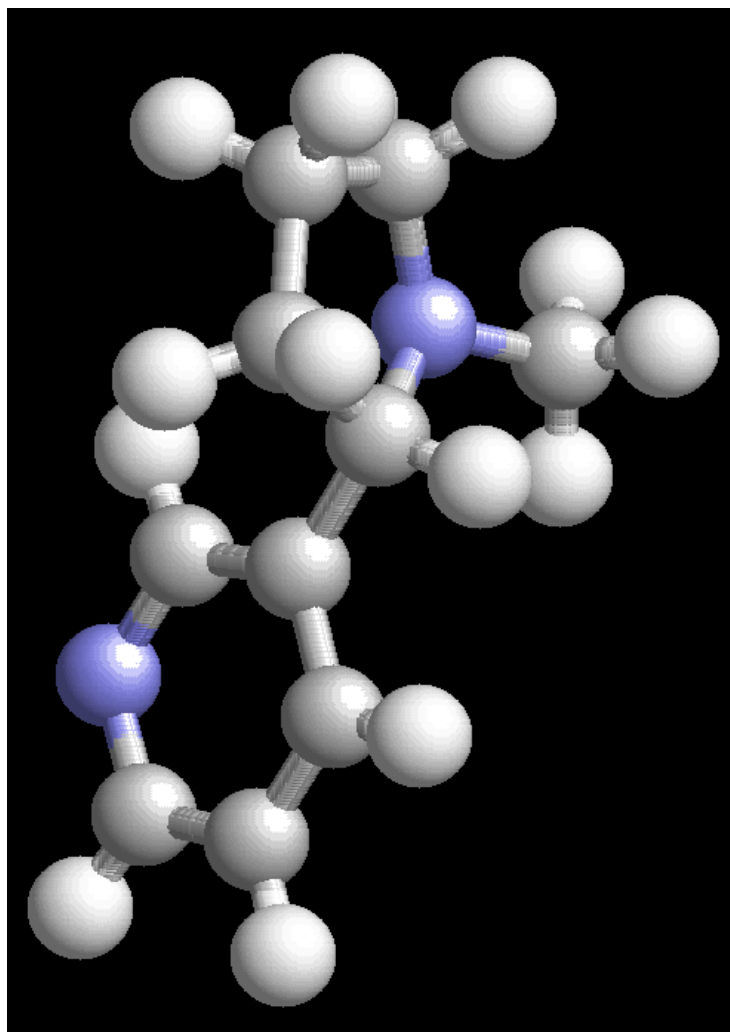
Load nicotine and add hydrogen atoms.



Calculate – MOPAC - run to optimize the molecular geometry, use coordinates.  
Rotate the structure.



Display the structure using RasWin:



```
%chk=E:\DDBMAIN\scr\GaussianCheckpointFile(#DDB=124).chk
%mem=20MW
%nproc=1
#P B3LYP/6-311G(d,p) opt=(MAXCYCLE=10) scf=tight geom=connectivity
```

```
B3LYP/6-311G(d,p) OPTIMIZATION GAS PHASE
ChemDB (#DDB=124)
```

```
0 1
C -2.8829 -1.6512 -0.5383
C -3.8184 -1.1358 0.4748
...
...
```

```
--Link1--
```

```
%chk=E:\DDBMAIN\scr\GaussianCheckpointFile(#DDB=124).chk
#P B3LYP/6-311G(d,p) opt=(MAXCYCLE=99) geom=checkpoint
scf=(tight,novaracc) SCRF=(CPCM,Read)
```

```
B3LYP/6-311G(d,p) OPTIMIZATION GAS PHASE
ChemDB (#DDB=124)
```

```
0 1
```

```
RADII=KLAMT
```

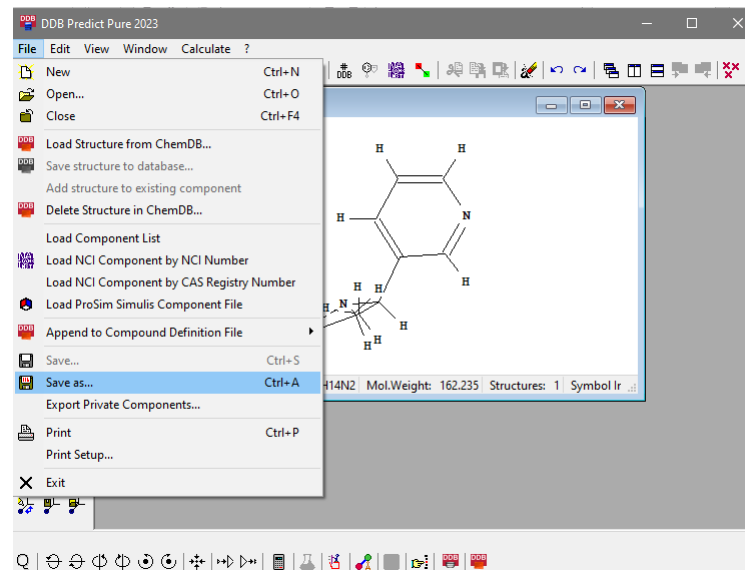
```
--Link1--
```

```
%chk=E:\DDBMAIN\scr\GaussianCheckpointFile(#DDB=124).chk
#P B3LYP/6-311G(d,p) scf=(tight,novaracc) SCRF=COSMORS guess=read geom=checkpoint
```

```
B3LYP/6-311G(d,p) COSMO SINGLE POINT
ChemDB (#DDB=124)
```

```
0 1
```

```
E:\DDBMAIN\scr\GaussianCosmoOutputFile(#DDB=124).cosmo
```





# Pure Component and Mixture Data: Retrieval and Output

## Lesson Objectives

- learn to retrieve data of interest
- study the different specific tabular and graphical output options



The largest data bank in DDB is PURE

Access via “Dortmund Data Bank”

The programs contain a multitude of options, please explore the menu items.

- Data can be stored to files and loaded, exported as CAPE-Open files or Aspen inp-files, csv-files for Excel, .....
- Different units can be selected for plots and tables
- Data can be shown graphically in 2D- or 3D-representations.
- Data can be shown together with the results from correlation equations or group contribution methods
- Data can be regressed using a multitude of equations.
- .....

## Workshop

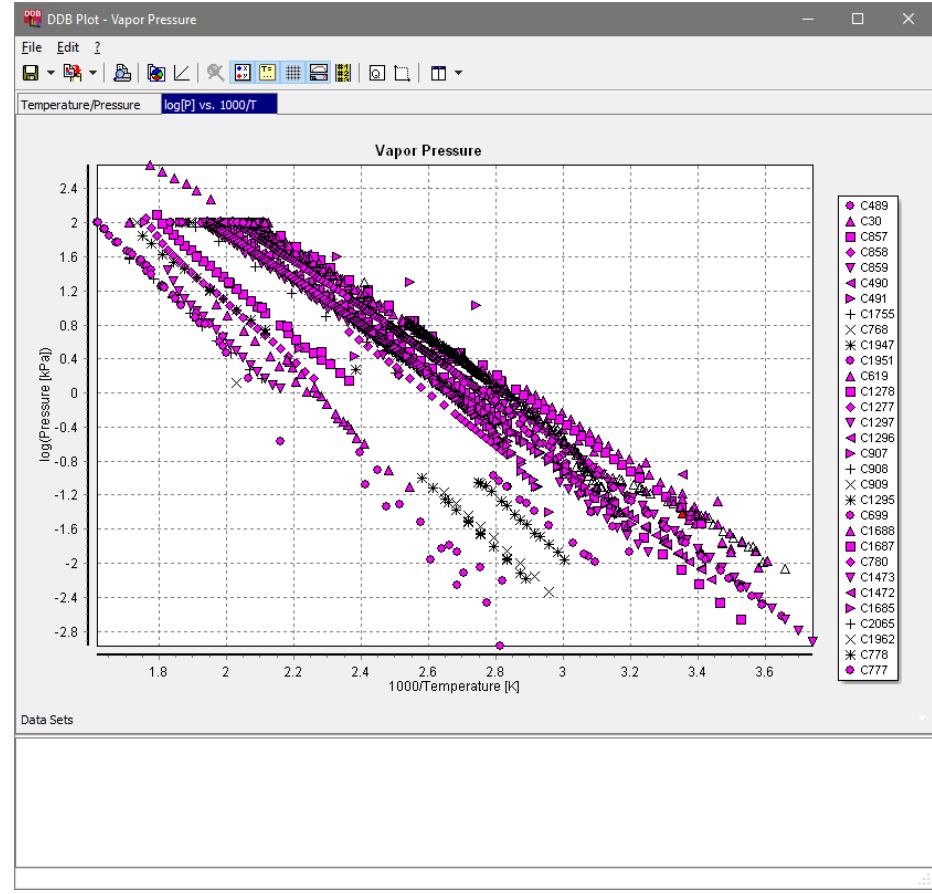
- Start „Dortmund Data Bank" and search for data for acetone (System (Exact Match))
- Select all vapor pressure data (use property list below tree on the left to display only vapor pressure data and then mark one set and enter ctrl-a to select all data points)
- Plot the vapor pressure data as  $\ln(P)$  vs.  $1/T$  using  .
- Zoom, move the mouse to see the values and sources of individual data points.
- Plot the thermal conductivity. Explain the data.
- Plot the 2<sup>nd</sup> virial coefficient together with predictions using the RK, SRK and PR equations of state using  .

It is also possible to select and view data for a group of components.

**Workshop**

- Plot the vapor pressure of nitrobenzenes as  $\log(P)$  vs.  $1000/T$ .

Use the component list file previously stored from PredictPure.



# Search for a system via components

The screenshot shows the Dortmund Data Bank 2023 software interface. The main window is titled 'Dortmund Data Bank 2023' and has a menu bar with 'File', 'Edit', and '?'. Below the menu bar are three tabs: 'Query', 'Single Sets', and 'Selectivity (ACT)'. The 'Query' tab is active, displaying a table with columns: 'Number', 'Type/Count', 'Loc.', 'Remove', and 'Name'. The table contains two rows: one with '11', 'C', 'DDB', 'Remove', and '[Ethanol]'; the other with '31', 'C', 'DDB', 'Remove', and '[Benzene]'. Below the table is a 'Search Options' section with three dropdown menus: 'Active Databanks' (set to 'All'), 'Active Pure Component Properties' (set to 'All'), and 'Active Extended Database Properties' (set to 'All'). There are also radio buttons for 'Search Locations' (Both, Public DDB, Private DDB). At the bottom, there is an 'Add Component Code/s' section with a dropdown menu showing '31', 'Add', and 'Add as List' buttons. The status bar at the bottom shows 'DDB: D:\DDBST\Datenbanken\DDB\ Private DDB: D:\DDBST\Datenbanken\DDBPRV\ Hint:'. On the right side of the interface, there is a 'System' panel with several buttons: 'Add/Search Component', 'Add Compound List', 'Clear List', 'System (Exact Match)', 'As Subsystem', 'System and Subsystems', 'Sets containing only compound/s from line', 'Reference/s Selection', 'Predict', 'Pure Component Properties', 'Display Parameter Sets', and 'Condensed Data Sheet'.

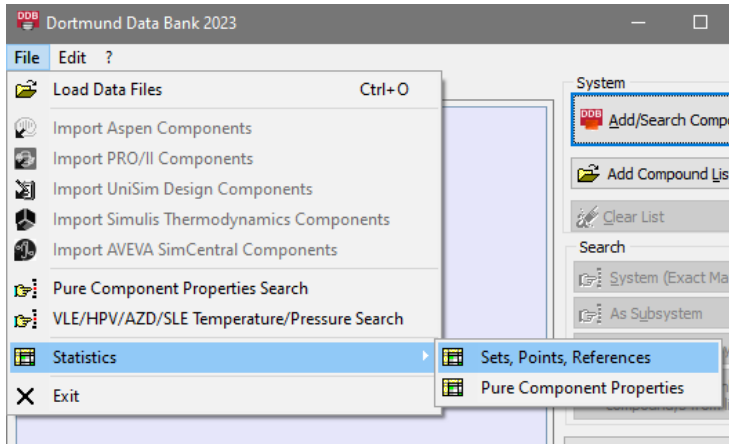
Special Selectivity Query

Add components via selection dialog, component lists via file open dialog

List of components or component lists

Select data banks to search (usually all)

Add components or component lists via code numbers



DDB Statistics

Copy

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

Databank	Sets	Points	References	Sets (priv.)	Points (priv.)	References (priv.)	
AAE	6239	86463	387				Adsorbent/adsorptive equilibria
ACM	2497	13499	107				Activity coefficients at infinite d
ACT	126812	126812	1564	574	574	3	Activity coefficients at infinite d
AZD	61313	61313	9515	59	59	3	Azeotropic/zeotropic information
CPE	7873	91794	972				Excess heat capacities
CRI	4311	25642	1203				Critical data of mixtures
DIF	3929	24028	601				Diffusion coefficients
ECND	17156	184571	1588				Electrical conductivities
EGLE	4929	30749	476				Gas solubilities (electrolyte conta
ELE	15149	191921	2165				Vapor-liquid equilibria for systems
ESLE	52154	356337	9840				Salt solubilities
GHD	6628	45813	1134				Gas hydrate properties
GLE	31332	153165	3149	10	75	1	Gas solubilities
HE	24986	365182	3648	947	16404	2	Heats of mixing
HPV	50285	421035	5702	27	188	1	Vapor-liquid equilibria (normal boi
LLE	41064	380887	6337	29	336	5	Liquid-liquid equilibria
MDEC	8673	79538	1093				Mixture dielectric constants
MFLP	1447	9742	235				Mixture flash points
MPVT	23190	391567	1775				Mixture P-v-T Data
MSFT	10893	112620	1237				Mixture surface tensions
MSOS	38767	440407	3139				Mixture speeds of sound
MTCN	6067	57642	555				Mixture thermal conductivities
NANO	475	9322	79				Nanofluids related Data
PCP	392322	2357853	51543	65	467	1	Pure component properties
POLYMER	23752	258331	2025				Thermodynamic data for polymer cont
POW	15354	15354	671				Octanol-Water partition coefficient
SLE	93091	806808	12464	130	1387	3	Solid-liquid equilibria (mainly org
VE	90302	1016505	9284				Densities and (excess) volumes of m
VIS	71538	740183	6110				Mixture viscosities
VLE	43883	633910	8937	550	17924	3	Vapor-liquid equilibria (normal boi
X	237662	2533281	20281				Different thermodynamic properties
Sum	1325310	9926841	100019	37414		14	

# Workshop

In the „Dortmund Data Bank“ query dialog, select edit-options and explore the different option screens

The screenshot shows the 'Options' dialog box with the 'Preferred Units' section expanded. The 'Pure Component Properties' option is highlighted in the left sidebar. The main table displays the following data:

Table Item	Unit	Unit of Errors	Precisio
Temperature	1: K	1: K	
Pressure	5: kPa	5: kPa	
Molar Volume	0: cm <sup>3</sup> /mol	0: cm <sup>3</sup> /mol	
Dynamic Viscosity	1: mPas	1: mPas	
Density	0: kg/m <sup>3</sup>	0: kg/m <sup>3</sup>	
Second Virial Coefficient	0: cm <sup>3</sup> /mol	0: cm <sup>3</sup> /mol	
Kinematic Viscosity	0: m <sup>2</sup> /s	0: m <sup>2</sup> /s	
Molar Enthalpy	0: J/mol	0: J/mol	
Molar Heat Capacity (c <sub>P</sub> )	0: J/(mol*K)	0: J/(mol*K)	
Thermal Conductivity	0: W/(m*K)	0: W/(m*K)	
Surface Tension	1: mN/m	1: mN/m	
Mass Heat Capacity	0: J/(g*K)	0: J/(g*K)	
Molar Entropy	0: J/(mol*K)	0: J/(mol*K)	
Enthalpy (H-H <sub>0</sub> )/T	0: J/(K*mol)	0: J/(K*mol)	
Enthalpy (H-H <sub>0</sub> )	0: J/mol	0: J/mol	

At the bottom right of the dialog, there are two buttons: 'OK & Save' and 'OK'.

The screenshot shows the Dortmund Data Bank 2023 software interface. The main window is titled "Dortmund Data Bank 2023" and has a menu bar with "File", "Edit", and "?". Below the menu bar are three tabs: "Query", "Single Sets", and "Selectivity (ACT)". The "Query" tab is active, displaying a table with the following data:

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

Below the table are "Search Options" for "Active Databanks", "Active Pure Component Properties", and "Active Extended Database Properties", all set to "All". There are also "Search Locations" options: "Both" (selected), "Public DDB", and "Private DDB". At the bottom, there is an "Add Component Code/s" field containing "11 50 174" and buttons for "Add" and "Add as List".

On the right side of the interface, there is a "System" panel with several buttons: "Add/Search Component", "Add Compound List", "Clear List", "System (Exact Match)", "As Subsystem", "System and Subsystems", "Sets containing only compound/s from line", "Reference/s Selection", "Predict", "Pure Component Properties", "Display Parameter Sets", and "Condensed Data Sheet". A red arrow points to the "System (Exact Match)" button.

Search for a system

Once a list of components or component lists was entered, different search options are available.

It is possible to go back to the search dialog with or without closing the result dialog.

Data sets can be moved between the search result dialogs by drag'n drop.

Salts like sodium chloride appear both as normal components and as salts.



## Search for a system

### **System (exact match)**

Search for all data sets for the given system. If a list item is a component list, any one component in the list matches the query

#### Example:

Component: ethanol

Component: water

List: benzene, cyclohexane

All data for the systems ethanol-water-benzene and ethanol-water-cyclohexane will be found.

#### Example:

Component: benzene

List: nitrobenzenes.stl

All binary mixtures of benzene with a nitrobenzene will be found.

## Search for a system

### As Subsystem

Search for all data sets for the given system and higher systems where this system is a subsystem.

#### Example:

Component: ethanol

Component: water

List: benzene, cyclohexane

All data for the systems ethanol-water-benzene and ethanol-water-cyclohexane will be found as well as quaternary and quinary systems with additional components, e.g.

ethanol – water – benzene - ethyl-3-methyl butyrate

ethanol – water – cyclohexane - i-octane - xylene

## Search for a system

### **System and Subsystems**

Search the system of the components specified plus all subsystems. This is the typical search when compiling the available data for the description of a multicomponent mixture. Instead of single components also lists of components can be included.

Instead of only including m-xylene, it is a good idea to include a list of the 3 isomers plus "xylene (isomer not specified)". There is practically no difference in the activity coefficients when exchanging the isomers in a mixture.

### **Example:**

Specifying the components ethanol – water – cyclohexane will retrieve data for the systems

- ethanol – water
- water – cyclohexane
- ethanol – cyclohexane
- ethanol – water - cyclohexane

- **Data Bank Pages:**

show data sets of only one data bank. Switch between the data banks by a single-click on the data bank pages.

- **Overview Line:**

shows number of references, data points and sets found in the selected data bank for the current view of the 'Dataset List'.

- **Tree View with Info Field:**

shows list of references, systems, components, properties (only PCP), solutes and solvents (only ACT, ACM)

- **Dataset List:**

shows the data sets for the current data bank with some elementary information

- **Extended Hint Field:**

shows background information when moving the mouse cursor over the Tree View, Info Field and Data Set List

Query Result [1] <ACT,AZD,CPE,CRI,DIF,ECND,CHD,GLE,HE,MDEC,MFLP,MPVT,MSFT,MSOS,MTCN,SLE,VE,VIS,VLE,X>

File Edit

ACT AZD CPE CRI DIF ECND GHD GLE HE MDEC MFLP MPVT MSFT MSOS MTCN SLE VE VIS VLE X

All Sets 76 All Points 32 All Refs 1 All Sys. 76 Sets 76 Points 28 Refs 1 Systems 1

**=ACT=**  
Activity coefficients at infinite dilution (binary systems)

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	Publ.Year	Reference
[917 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=3.2800		1900	[5318] Schmidt T.W., US-Patent, Pat.
[5526 0 0]	DDB	1	2	C11 Ethanol C174 Water	283 (const.)	n.a.			Act.Inf.=3.1800		1980	[5318] Schmidt T.W., US-Patent, Pat.
[5527 0 0]	DDB	1	2	C11 Ethanol C174 Water	283 (const.)	n.a.			Act.Inf.=4.3800		1992	[5338] Pividal K.A., Birtigh A., Sar
[5528 0 0]	DDB	1	2	C11 Ethanol C174 Water	283 (const.)	n.a.			Act.Inf.=4.8100		1992	[5338] Pividal K.A., Birtigh A., Sar
[5529 0 0]	DDB	1	2	C11 Ethanol C174 Water	293 (const.)	n.a.			Act.Inf.=6.5100		1966	[5009] Pecsar R.E., Martin J.J., Am
[5530 0 0]	DDB	1	2	C11 Ethanol C174 Water	297 (const.)	n.a.			Act.Inf.=4.7400		1969	[5052] Shaffer D.L., Daubert T.E., J
[5531 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=3.2700		1984	[5114] Lebert A., Richon D., J.Agric
[5532 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=3.5500		1985	[5193] Richon D., Sorrentino F., Voi
[5533 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=3.7300		1978	[5323] Rytting J.H., Huston L.P., Hi
[5534 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=3.7600		1987	[5180] Park J.H., Hussam A., Couanc
[5535 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=3.9100		1973	[5217] Larkin J.A., Pemberton R.C.,
[5536 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=3.9200		1980	[5212] Mash C.J., Pemberton R.C., Ne
[5537 0 0]	DDB	1	2	C11 Ethanol C174 Water	298 (const.)	n.a.			Act.Inf.=4.0300		1991	[5282] Landau I., Belfer A.J., Locke
[5538 0 0]	DDB	1	2	C11 Ethanol C174 Water	299 (const.)	n.a.			Act.Inf.=4.2850		1988	[5259] Kohn J., Master's Thesis, Uni

Copy Save

1 data set/s marked.

# Workshop

In the query dialog, search for data for the system ethanol – water – acetone and its subsystems

In the query result dialog, select VLE data for the binary acetone - ethanol

The query result dialog should look like this:

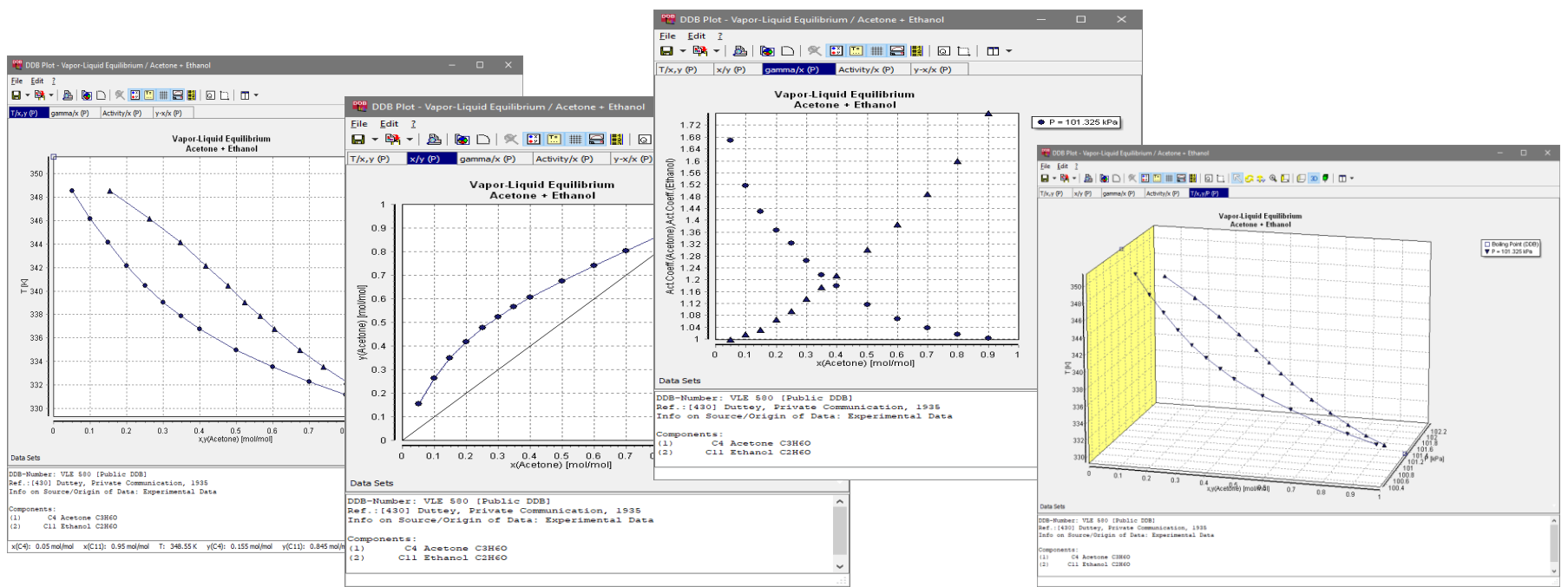
The screenshot displays the 'Query Result [2]' window in DDBST. The 'VLE' tab is selected, and the query is for 'Vapor-liquid equilibria (normal boiling points of all components above 0 °C)'. The table below shows the results for the C4 Acetone-C11 Ethanol system.

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	PubLYear	Reference
[579 0 0]	DDB	11	2	C4 Acetone C11 Ethanol	329	351	101 (const.)		Txy(P)		1956	[308] Amer H.H., Paxton R.R., van Winkle M.,
[580 0 0]	DDB	13	2	C4 Acetone C11 Ethanol	330	349	101 (const.)		Txy(P)		1935	[430] * Duttey, Private Communication, 1935
[581 0 0]	DDB	16	2	C4 Acetone C11 Ethanol	305 (const.)		12	41	Px(T)		1946	[309] Gordon A.R., Hines W.G., Can.J.Res.Sec
[582 0 0]	DDB	15	2	C4 Acetone C11 Ethanol	313 (const.)		18	57	Px(T)		1946	[309] Gordon A.R., Hines W.G., Can.J.Res.Sec
[583 0 0]	DDB	10	2	C4 Acetone C11 Ethanol	321 (const.)		27	76	Px(T)		1946	[309] Gordon A.R., Hines W.G., Can.J.Res.Sec
[584 0 0]	DDB	9	2	C4 Acetone C11 Ethanol	330	348	101 (const.)		Txy(P)		1953	[318] Hellwig L.R., van Winkle M., Ind.Eng.C
[1185 0 0]	DDB	5	2	C4 Acetone C11 Ethanol	303 (const.)		17	36	Px(T)		1973	[798] D'Avila S.G., Cotrim M.L., Rev.Bras.Te
[1186 0 0]	DDB	5	2	C4 Acetone C11 Ethanol	308 (const.)		22	44	Px(T)		1973	[798] D'Avila S.G., Cotrim M.L., Rev.Bras.Te
[1575 0 0]	DDB	14	2	C4 Acetone C11 Ethanol	305 (const.)		n.a.		xy(T)		1946	[309] Gordon A.R., Hines W.G., Can.J.Res.Sec
[1580 0 0]	DDB	14	2	C4 Acetone C11 Ethanol	313 (const.)		n.a.		xy(T)		1946	[309] Gordon A.R., Hines W.G., Can.J.Res.Sec
[1581 0 0]	DDB	12	2	C4 Acetone C11 Ethanol	321 (const.)		n.a.		xy(T)		1946	[309] Gordon A.R., Hines W.G., Can.J.Res.Sec
[3579 0 0]	DDB	10	2	C4 Acetone C11 Ethanol	328 (const.)		37	97	Pxy(T)		1966	[1417] Vinichenko I.G., Susarev M.P., J.Appl
[3861 0 0]	DDB	10	2	C4 Acetone C11 Ethanol	329	351	101 (const.)		Txy(P)		1966	[1417] Vinichenko I.G., Susarev M.P., J.Appl
[6681 0 0]	DDB	4	2	C4 Acetone C11 Ethanol	331	342	101 (const.)		Txy(P)		1968	[2101] Ravindran S., Srinivasan D., Laddha G

At the bottom of the window, the status bar indicates: 'Data Set: 1575 Source: 0 (Public DDB) Counter: 0' and '1 data set/s marked.'

# Workshop

Double-click data set 580 to display a data table. Close the data table. Mark all VLE data sets for the system acetone – ethanol, generate a plot of the data. The plot windows should contain these and more plots:



Zoom into an area in one of the 2D plots. Zoom full again. Change the P-axis in the Px-diagram to logarithmic scaling. Close all plot-windows.

## Workshop

In the query dialog, look at the comment column. Mark all data sets. Now run Consistency-automatic tests (marked sets). The comment column will show the result of the test (area test, point-to-point test):

- ? test not available
- + consistent
- inconsistent

Consistency – Single Set with options will show detailed results of the tests.

# Pure Component Data Regression

## Lesson Objectives

- Select and regress pure component property data
- Reduce the experimental data by removing unreliable data
- store the resulting parameters in the parameter data bank



“RegressionPure” allows to regress nearly all types of pure component data to a multitude of equations.

**DDB Regression Pure 2023**

Component: 222 Hydrogen peroxide

Equation: Antoine Equation

Key	Value
A	7.56571
B	1771.88
C	220.175
C1	222
EQID	4
Tmax	90.35
Tmin	4.65
User	jk
COUNT	1
DateD	23
DateM	9
DateY	2005

Buttons: Fit, Fit Simultaneously, Calculate, Plot, Details, Delete archive entry

**Vapor Pressure - Antoine**

Data Source: Pure Component Properties Database

Points: 34, Refs: 4, Component: 222 Hydrogen peroxide

Temperature Range: 277.8 363.5, Dependent Value Range: 0.0733273 9.63921

Fit Equation:  $F = \text{Sum}((y_{\text{exp}} - y_{\text{cal}}) / y_{\text{exp}})^2 / n$

Fit Options: Fit A,B only, Fit A,B,[C=Tb/-8], Fit Linear Reg.

Parameters: Tb=425.16 K

Source: PCP, Date: 2023-05-02

## Workshop

- In “Dortmund Databank”, select the component methanol, then select the vapor pressure data and run “RegressionPure”, select the Antoine equation and click the fit-button.
- In the fit-dialog, select the uppermost objective function from the pull-down menu, where the error is divided by the probable error.
- Click Fit, after the regression is finished, click plot.
- Exclude data points with a larger deviation.
- Refit the selected data and examine the deviations in the plot.
- Store the parameters in the private DDB.
- In “RegressionPure” plot the experimental data together with the curve from the newly fitted and saved parameters.

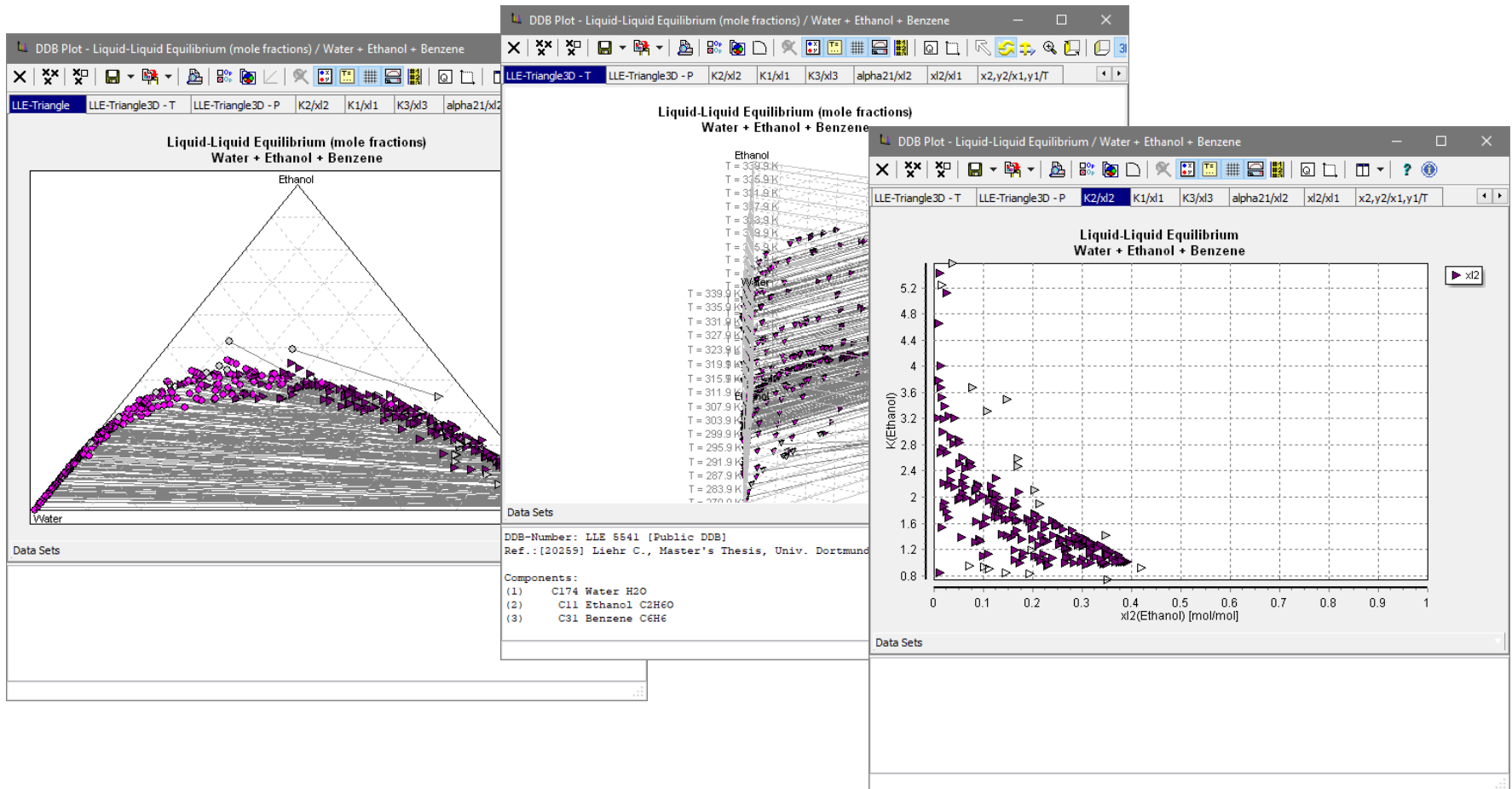
# Mixture Data Regression

## Lesson Objectives

- examine different possibilities for the regression of individual types of data or individual data types
- examine the regression results
- store regressed parameters in the parameter data bank

## Workshop

Search for data for the system ethanol – water - benzene.  
Fit/Plot the LLE-data at 298 K using the NRTL-model.  
Plot the partition coefficients of component 2.



## Workshop (continued)

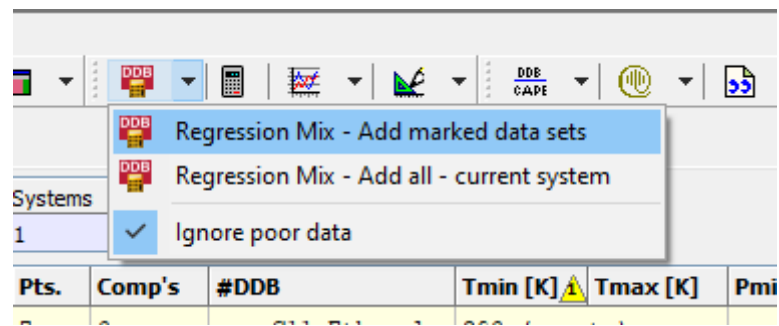
Store the regressed parameters in the parameter data bank and use them to calculate the VLE ethanol-water at 1 atm. Compare the results to experimental data.

# Simultaneous Mixture Data Regression

## Lesson Objectives

- inspect the different options required for simultaneous mixture property regression
- understand the interrelation between different kinds of mixture data
- regress reliable temperature dependent model parameters for a binary system

# Starting RegressionMix from the Data query Result dialog:



RegressionMix allows to correlate simultaneously VLE, HPV, ACT, AZD, LLE, HE and CPE-data using different  $g^E$ -models, compare the data to the results of UNIFAC or mod. UNIFAC, equations of state and simulator thermodynamics.

The different features of RegressionMix are demonstrated before the workshop.

### Workshop

Search for data for the system ethanol-ETBE (ethyl-tert.-butyl-ether) in Mixture Properties and start RegressionMix using all available data.

Save the project as ethanol-ETBE

Examine the different options in the Edit-menu and regress temperature dependent NRTL-parameters to the data. Remove data sets that are obviously wrong or of low quality.

In the first step, use ideal vapor phase. Switch to real vapor phase for the final regression.



DDB Regression Mix 2023

File Edit View ?

System

#	DDB Code	Component	Formula	r (UNIQUAC)	q (UNIQUAC)	v (Wilson) [cm³/mol]	Tm [K]	h (Fusion) [J/mol]	Tc [K]	Pc [kPa]	vc [cm³/mol]
1	1409	[Ethyl tert-butyl ether (ETBE)]	C6H14O	4.7422	4.1720	135.89	179.15	n.a.	509.40	2933.93	394.00
2	11	[Ethanol]	C2H6O	2.1055	1.9720	58.69	158.65	5017.5	516.20	6383.48	167.00

Experimental Data Recalculated Data Derived Azeotropic Point/s Fitted Parameters Fit Progress

VLE HE AZD CPE

VLE Weight: 1

Property

Temperature:  $((T_{exp} - T_{cal})/T_{exp})^2$

Pressure:  $((P_{exp} - P_{cal})/P_{exp})^2$

(368 Points)

#	x [mol/mol]	y [mol/mol]	T [K]	P [kPa]	Weight	+/-	Cons	Obj	Reference
15390 [0]	0 - 1		297.95	7.807 - 18.132	1.00	+/-	{??}	O	Rarey J., Horstmann S., Gmehling
15391 [0]	0 - 1		323.15	29.254 - 53.646	1.00	+/-	{??}	O	Rarey J., Horstmann S., Gmehling
15392 [0]	0 - 1		338.15	58.013 - 94.620	1.00	+/-	{??}	O	Rarey J., Horstmann S., Gmehling
15779 [0]	0.095 - 0.884	0.29 - 0.79	343.15		1.00	+/-	{??}	O	Peng C.-L., Chao K.-C., DIPPR Da
15780 [0]	0.057 - 0.884	0.161 - 0.795	363.15		1.00	+/-	{??}	O	Peng C.-L., Chao K.-C., DIPPR Da
18797 [0]	0.0151 - 0.9859	0.0647 - 0.9627	333.15		1.00	+/-	{??}	O	Oh J.-H., Park S.-J., J.Chem.Eng
18870 [0]	0 - 1	0 - 1	339.82 - 351.44	101.325	1.00	+/-	{++}	O	Arce A., Martinez-Ageitos J., Roc
18941 [0]	0 - 1		363.15	159.051 - 220.599	1.00	+/-	{??}	O	Rarey J., Horstmann S., Gmehling
23533 [0]	0 - 1	0 - 1	339.88 - 351.90	101.300	1.00	+/-	{-+}	O	Yang B., Wang H., J.Chem.Eng.D
26987 [0]	0.023 - 0.9796	0.1057 - 0.9653	313.15	19.580 - 34.350	1.00	+/-	{++}	O	Oh J.H., Park S.J., J.Ind.Eng.Che
37029 [0]	0.063 - 0.925	0.196 - 0.825	339.20 - 347.20	101.300	1.00	+/-	{++}	O	Watanabe T., Yonezawa S., Kobu

Model: NRTL/CT/Antoine/n.a.

Data Types Used For Fitting

VLE  HE  ACT  LLE

AZD  CPE  SLE

Show Result Diagrams

for all properties

for selected properties only

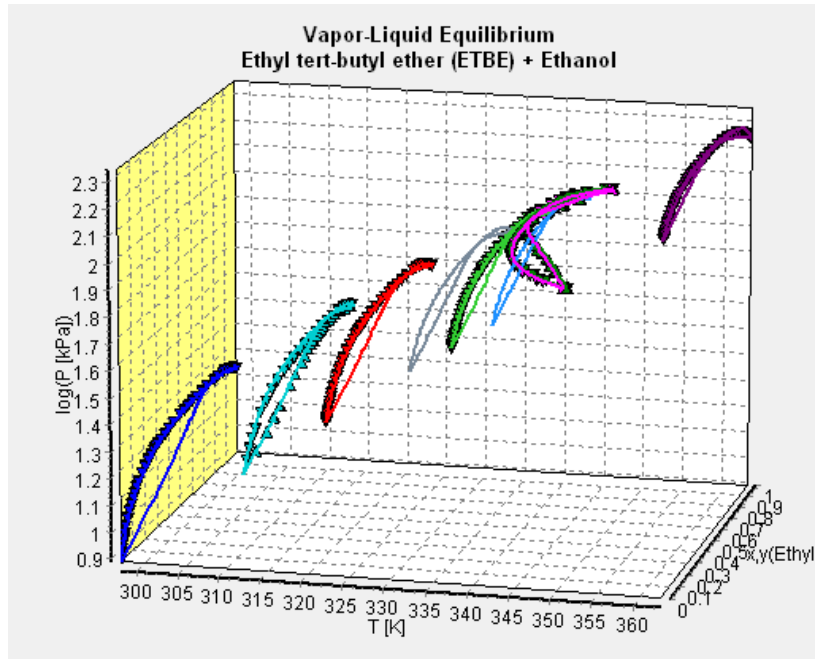
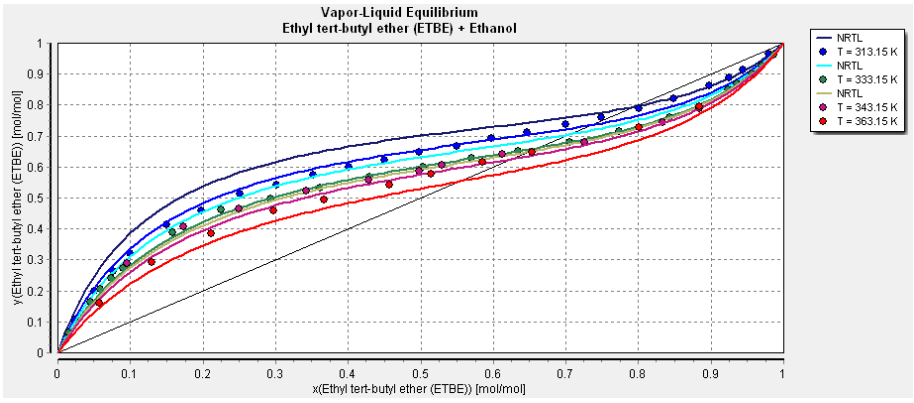
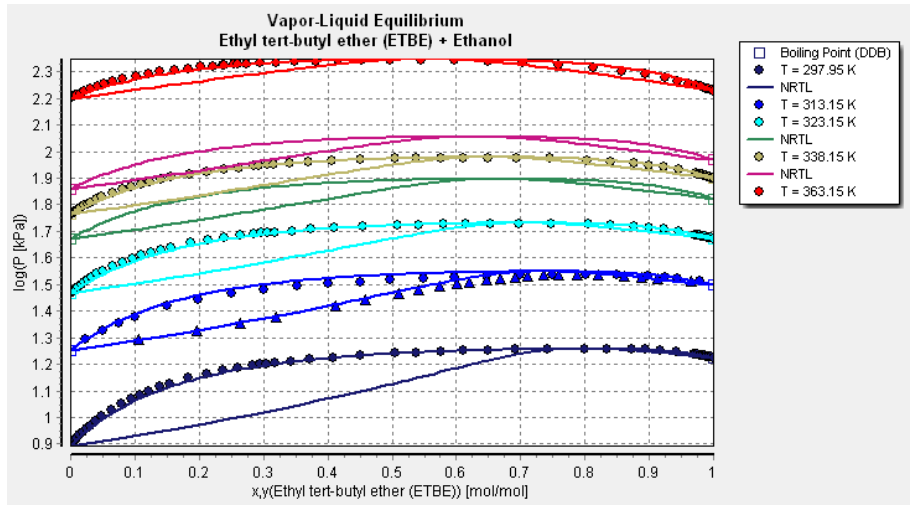
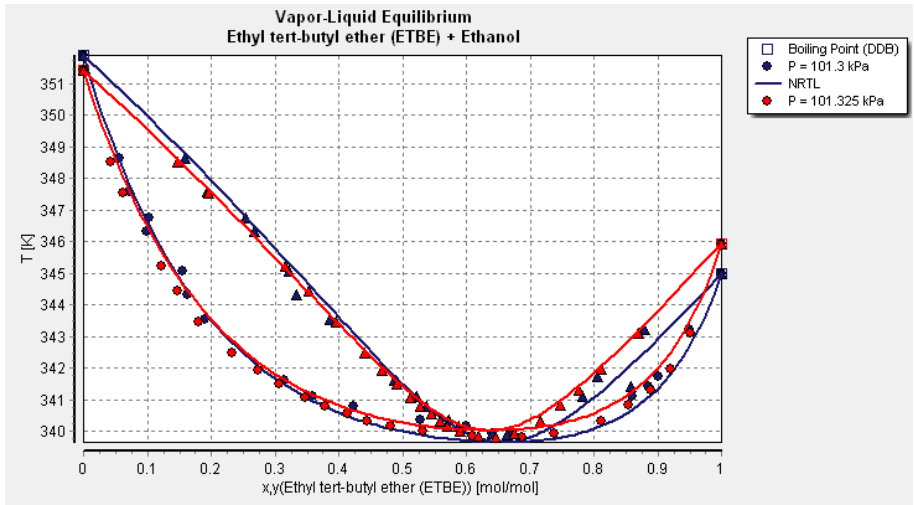
Hide disabled points in diagrams

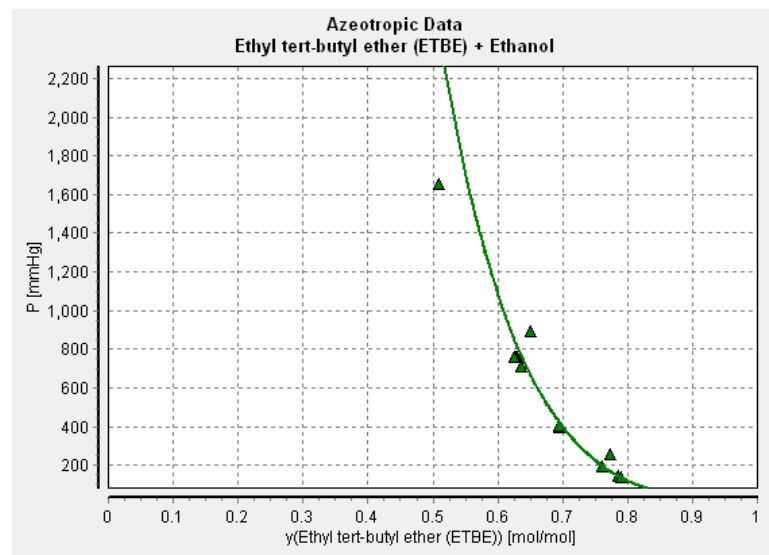
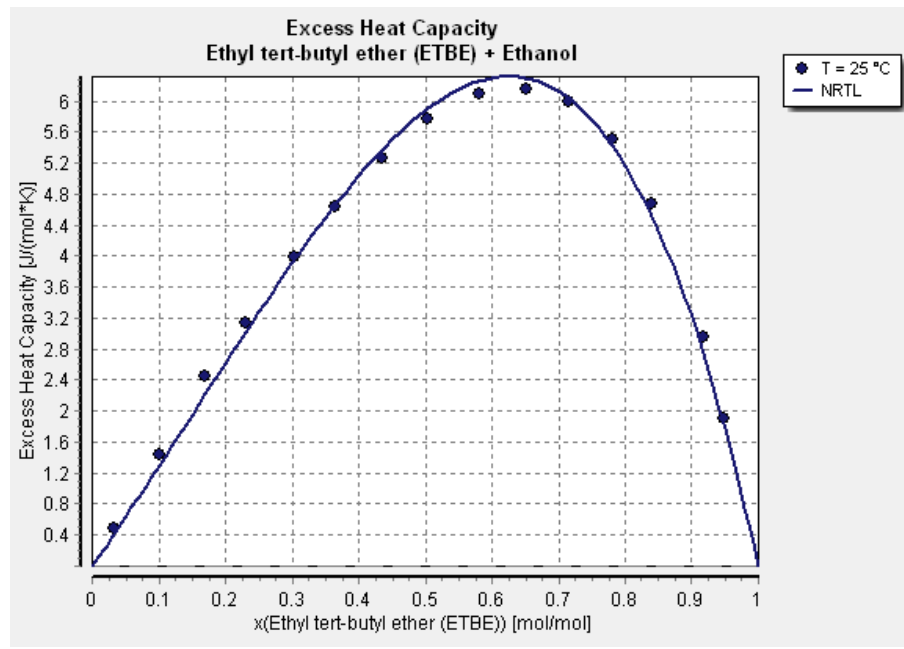
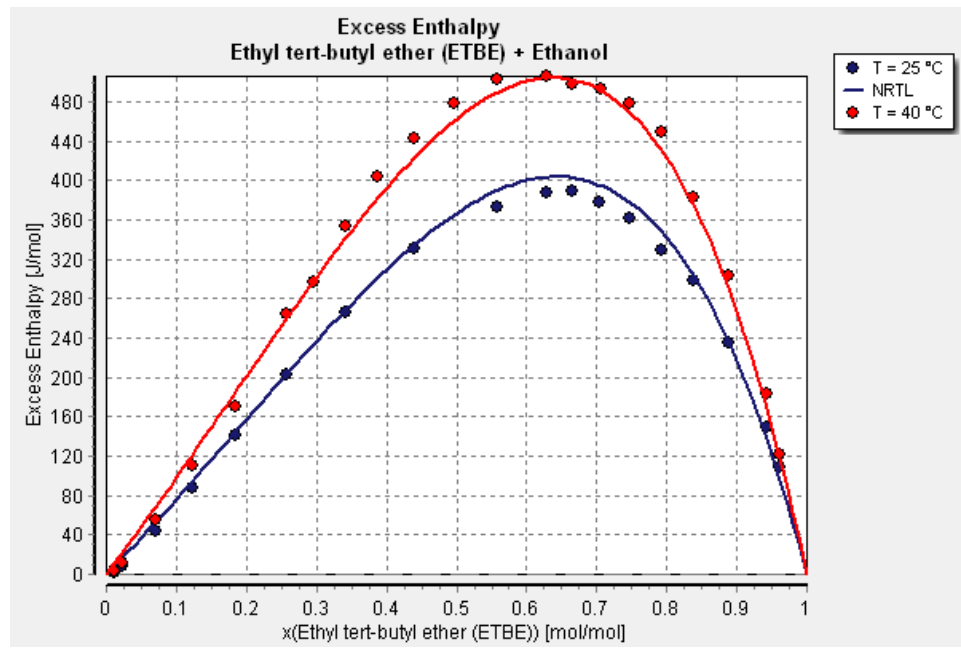
Fit Parameters

Systems (1)

11/1409 (441 points) Use

Ethanol Ethyl tert-butyl ether (ETBE) Process Batch





DDB Regression Mix 2023

#	DDB Code	Component	Formula	r [UNIQUEAC]	g [UNIQUEAC]	v [Wilson] [cm <sup>3</sup> /mol]	Tm [K]	h [Fusion] [J/mol]	Tc [K]	Pc [kPa]
1	1409	[Ethyl tert-butyl ether (ETBE)]	C8H14O	4.7422	4.1720	135.69	179.15	n.a.	509.40	2933.93
2	11	[Ethanol]	C2H6O	2.1055	1.9720	58.69	158.65	5017.5	516.20	6383.48

Experimental Data | Recalculated Data | Derived Azeotropic Points | **Fitted Parameters** | Fit Progress

Save as XLS | Copy | Clear

Model: NRTL/CT/Antoine,h.a.

**1 Set**

Set no.: 1

Model: NRTL/CT/Antoine,h.a.

Comp. 1: 1409 Ethyl tert-butyl ether (ETBE)

Comp. 2: 11 Ethanol

Parameters [cal/mol]

	a1	a2	b1	b2	c1	c2	d1	d2	e1	e2	f1	f2
1-2	-787.22011	148.21267	10.549514	-0.98714413	-0.018006211	0.0036468741	0	0	0	0	0	0

Obj. Function: Total=-3.53841 VLE=0.1837 HE=2.2198 CPE=0.1586 A2D=0.9763

Aspen [K]

	a1	a2	b1	b2	c1	c2	d1	d2	e1	e2	f1	f2
1-2	5.3087067	-0.49674882	-396.14343	74.583303	0.3	0.3	0	0	0	0	0	0

Fit Parameters

Systems (1)  
11/1409 (#11 points) Use  
Ethanol  
Ethyl tert-butyl ether (ETBE) Process Batch

# Mixture Data Estimation

## Lesson Objectives

- predict mixture data using group contribution methods
- examine the parameter matrices of the different methods
- learn, how to modify existing parameters or add new parameters

If no experimental data are available for a system, pseudo-experimental data can be estimated or predicted from a variety of methods and then be processed in the same way as experimental data.

### **Workshop**

Search for data for the system acetone – ethanol.

Now select predict from the Mixture Properties Query dialog and predict a VLE-data set at 1 atm using the mod. UNIFAC (Dortmund) group contribution method (use "Predict (Dataset/s returned to MixView)").

In the Query Result dialog, choose Predict and select the mod. UNIFAC (Lyngby) and COSMO-SAC model. Mark all sets and plot.

### **Note concerning Prediction in the Query Result window:**

Selected data sets and predicted data sets will be shown in a new Query Result dialog but can be moved to the previous result table by drag and drop.

The program GC-Models Parameter gives full access to the group interaction parameters of the different methods for the prediction of the real mixture behavior.

In case a local copy of the parameters is used and mapped to via file replacement, the user could enter or modify group interaction parameters. Use this feature with great care!

Interaction parameters for 756 group pairs (3066 parameters)

No. i	Subgroup name	Ri	Qi
1	CH3	0.6325	1.0608
2	CH2	0.6325	0.7081
3	CH	0.6325	0.3554
4	C	0.6325	0.0000
5	CH2=CH	1.2832	1.6016
6	CH=CH	1.2832	1.2489
7	CH2=C	1.2832	1.2489
8	CH=C	1.2832	0.8962
9	ACH	0.3763	0.4321
10	AC	0.3763	0.2113
11	ACCH3	0.9100	0.9490
12	ACCH2	0.9100	0.7962
13	ACCH	0.9100	0.3769
14	OH (P)	1.2302	0.8927
15	CH3OH	0.8585	0.9938
16	H2O	1.7334	2.4561
17	ACOH	1.0800	0.9750
18	CH3CO	1.7048	1.6700
19	CH2CO	1.7048	1.5542
20	CHO	0.7173	0.7710
21	CH3COO	1.2700	1.6286
22	CH2COO	1.2700	1.4228
23	HCOO	1.9000	1.8000
24	CH3O	1.1434	1.6022
25	CH2O	1.1434	1.2495
26	CHO	1.1434	0.8968
27	THF	1.7023	1.8784
28	CH3NH2	1.6607	1.6904
29	CH2NH2	1.6607	1.3377
30	CHNH2	1.6607	0.9850

# Test Process Simulator Parameters Prior to Process Simulation

## Lesson Objectives

- Check Aspen Plus calculation results against data from the DDB

Calculation using Simulator Thermodynamic to verify physical property issues prior to process simulation.

Example:

Aspen Plus:

VLE, HPV, LLE,  $h^E$ ,  $c_p^E$ ,  $v^E$ ,  $P^S$ ,  $c_p^L$ ,  $c_p^S$ ,  $c_p^V$

Next step:

- Additional properties
- Parameter regression

The screenshot shows the 'VLE/HPV Prediction' dialog box. The 'Components' list includes Acetone and Water. The 'Prediction Method' is set to 'All Models'. The 'Active Model' table shows 'Aspen' selected, with a red circle around it. The 'Type' section has 'Isobaric' selected at 101.325 kPa. The 'Mole Fraction Range' is set to 0.0 to 1.0 with a stepwidth of 0.01. The bottom of the window contains buttons for 'Predict (Table Output)', 'Predict and Plot', 'Predict (Result => Query Result)', 'Predict/Plot with Options', 'SCF Calculation (Separate Form)', '3D Predict and Plot', and 'Cancel'.



# Import Project Components into Query

The screenshot shows the Dortmund Data Bank 2023 interface. The 'File' menu is open, highlighting 'Import Aspen Components'. Below it, the 'Import Aspen Components' dialog box is displayed, showing a table of components with columns for Use, Name, Alias, DDB No., DDB Name, DDB Formula, Change, and New. A red arrow points from the 'Import Aspen Components' menu item to the dialog box. Another red arrow points from the 'Add as New Component' button in the dialog box to the text 'Open Aspen Project File'.

#	Use	Name	Alias	DDB No.	DDB Name	DDB Formula	Change	New
1	<input checked="" type="checkbox"/>	WATER	H2O	174	Water	H2O	Change DDB Number	Add as New Component
2	<input checked="" type="checkbox"/>	METHA-01	CH4O	110	Methanol	CH4O	Change DDB Number	Add as New Component
3	<input checked="" type="checkbox"/>	ETHAN-01	C2H6O-2	11	Ethanol	C2H6O	Change DDB Number	Add as New Component
4	<input checked="" type="checkbox"/>	CHLOR-01	CHCL3	47	Chloroform	CHCL3	Change DDB Number	Add as New Component
5	<input checked="" type="checkbox"/>	BENZE-01	C6H6	31	Benzene	C6H6	Change DDB Number	Add as New Component
6	<input checked="" type="checkbox"/>	ACETO-01	C3H6O-1	4	Acetone	C3H6O	Change DDB Number	Add as New Component

Open Aspen Project File

The screenshot shows the Dortmund Data Bank 2023 software interface. The main window displays a table of search results under the 'Query' tab. The table has columns for Number, Type/Count, Loc., Remove, and Name. The results are as follows:

Number	Type/Count	Loc.	Remove	Name
[174]	C	DDB	Remove	[Water]
[110]	C	DDB	Remove	[Methanol]
[11]	C	DDB	Remove	[Ethanol]
[47]	C	DDB	Remove	[Chloroform]
[31]	C	DDB	Remove	[Benzene]
[4]	C	DDB	Remove	[Acetone]

Below the table, there are search options and active databanks. The 'Active Databanks' field contains 'ACT AZD GLE HE HPV LLE SLE VLE'. The 'Active Pure Component Properties' and 'Active Extended Database Properties' fields both contain 'All'. The 'Search Locations' section has radio buttons for 'Both' (selected), 'Public DDB', and 'Private DDB'. The 'Add Component Code/s' section has a dropdown menu and buttons for 'Add' and 'Add as List'. The status bar at the bottom shows the path 'DDB: D:\DDBST\Datenbanken\DDB\ Private DDB: D:\DDBST\Datenbanken\DDBPRV\ Hint'.

On the right side of the interface, there is a 'System' panel with several buttons: 'Add/Search Component', 'Add Compound List', 'Clear List', 'System (Exact Match)', 'As Subsystem', 'System and Subsystems', 'Sets containing only compound/s from line', 'Reference/s Selection', 'Predict', 'Pure Component Properties', 'Display Parameter Sets', and 'Condensed Data Sheet'. A red arrow points from the text 'Search for System and Subsystems' to the 'System and Subsystems' button.

Search for  
System and  
Subsystems

# Mark all VLE Data Sets Acetone-Water at 101 kPa - Select Prediction

Query Result [2] <ACT,AZD,GLE,HE,HPV,LLE,SLE,VLE>

File Edit

ACT AZD GLE HE HPV LLE SLE **VLE**

All Sets: 1627 | All Points: 25905 | All Refs: 679 | All Sys.: 40 | Sets: 129 | Points: 1929 | Refs: 62 | Systems: 1

**=VLE=**  Display Empty Sets  
Vapor-liquid equilibria (normal boiling points of all components above 0 °C)

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Quality	Pu ^
[11 0 0]	DDB	13	2	C4 Acetone C174 Water	331	368	101 (const.)		Txy (P)		19
[12 0 0]	DDB	12	2	C4 Acetone C174 Water	371	396	345 (const.)		Txy (P)		19
[13 0 0]	DDB	11	2	C4 Acetone C174 Water	399	424	689 (const.)		Txy (P)		19
[14 0 0]	DDB	13	2	C4 Acetone C174 Water	430	450	1379 (const.)		Txy (P)		19
[15 0 0]	DDB	12	2	C4 Acetone C174 Water	442	467	1724 (const.)		Txy (P)		19
[16 0 0]	DDB	10	2	C4 Acetone C174 Water	479	503	3447 (const.)		Txy (P)		19
[593 0 0]	DDB	13	2	C4 Acetone C174 Water	330	361	101 (const.)		Txy (P)		19
[766 0 0]	DDB	48	2	C4 Acetone C174 Water	329	373	101 (const.)		Txy (P)		19
[1043 0 0]	DDB	11	2	C4 Acetone C174 Water	298 (const.)		3	31	Pxy (T)		19
[1044 0 0]	DDB	11	2	C4 Acetone C174 Water	303 (const.)		4	37	Pxy (T)		19
[1045 0 0]	DDB	11	2	C4 Acetone C174 Water	318 (const.)		9	67	Pxy (T)		19
[1046 0 0]	DDB	11	2	C4 Acetone C174 Water	333 (const.)		20	115	Pxy (T)		19
[1047 0 0]	DDB	10	2	C4 Acetone C174 Water	328	371	97 (const.)		Txy (P)		19
[1048 0 0]	DDB	8	2	C4 Acetone C174 Water	293 (const.)		2	24	Pxy (T)		19

15 Binary Systems

Copy Save

#	System	sets
<input type="checkbox"/>	1 C4 C11	42 sets
<input type="checkbox"/>	2 C4 C31	66 sets
<input type="checkbox"/>	3 C4 C47	70 sets
<input type="checkbox"/>	4 C4 C110	98 sets
<input checked="" type="checkbox"/>	5 C4 C174	129 sets
<input type="checkbox"/>	6 C11 C31	151 sets
<input type="checkbox"/>	7 C11 C47	45 sets
<input type="checkbox"/>	8 C11 C110	61 sets
<input type="checkbox"/>	9 C11 C174	368 sets
<input type="checkbox"/>	10 C31 C47	51 sets
<input type="checkbox"/>	11 C31 C110	129 sets

[447] Othmer D.F., Chudgar M.M., Levy S.L., Ind.Eng.Chem., 44(8), 1872-1881, 1952

1 data set/s marked.

In the prediction dialog, the last selected Aspen project file is already given as default.

Base method:  
UNIQUAC

Select one of the options, in this example:  
Predict and Plot

**VLE/HPV Prediction**

Components  
[4] Acetone+[174] Water

4	Acetone	Tc=508.10 K	Pc=4701.5 kPa
174	Water	Tc=647.30 K	Pc=22048.3 kPa

Prediction Method  
All Models: NRTL, UNIQUAC, Wilson, Margules, van Laar, UNIFAC, Mod. UNIFAC (Do), NIST-mod. UNIFAC, Mod. UNIFAC (Ly), ASOG, PSRK, VTPR, PSRK2

Active Models

Model	Options	
Aspen	FlashCalculatio...	Edit

Type  
 Isobaric 101.325 kPa P.P  
 Isothermal K T.T  
 Calculate all pressures (2 Sets)  
 Calculate all points (2 Sets)

Recalculate  
 Recalculate Data Points

Activity Coefficient Model Options  
 Vapor Pressure Equation: Antoine-Low  
 Vapor Phase Fugacity Model: Ideal  
 Poynting Correction: No Correction

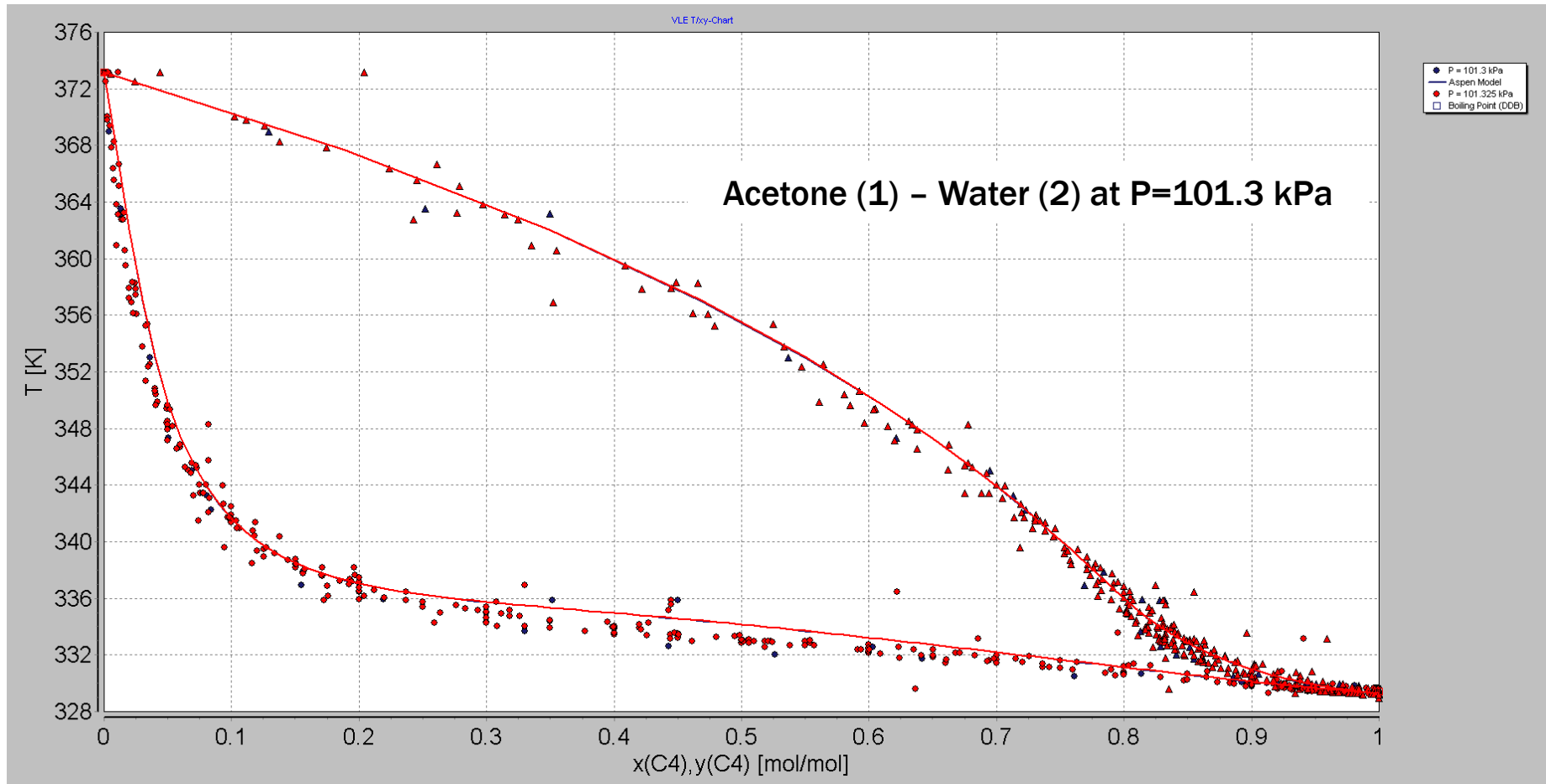
Antoine/Mathias-Copeman/Twu-B.C.C. Equations  
 Use Experimental Vapor Pressure

Mole Fraction Range  
 Min. x: 0.0, Max. x: 1.0, Stepwidth: 0.01  
 Create Data Points  
 Special Data Point Creation  
 0 Points

x [4] x [174]

Predict (Table Output) Predict and Plot  
 Predict (Result => Query Result) Predict/Plot with Options  
 SCF Calculation (Separate Form) 3D Predict and Plot Cancel

## Temperature as function of liquid and vapor phase composition



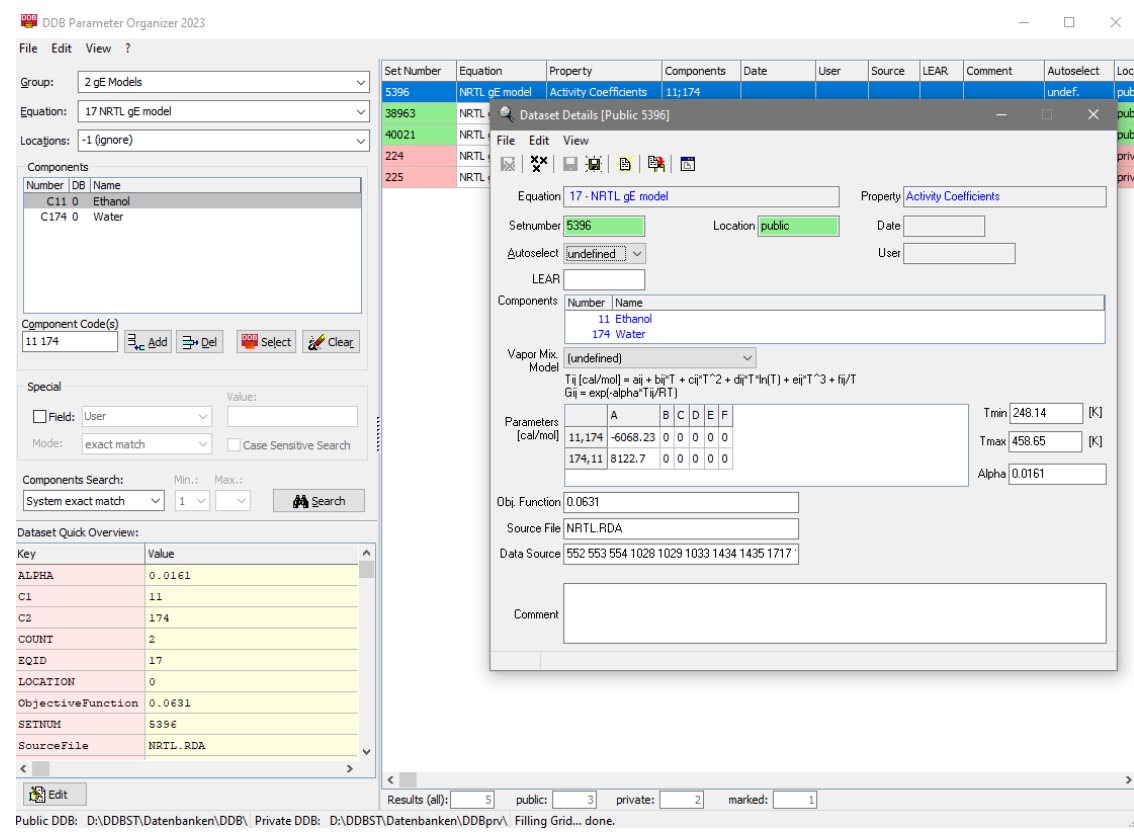
Workshop: Carefully examine the different diagrams, repeat the procedure for a system of your choice.

# DDB Parameter Data Bank

## Lesson Objectives

- examine the DDB parameter data bank
- learn, how to search for parameters
- learn about the possibility to use the Parameter DB for your own in-house parameters

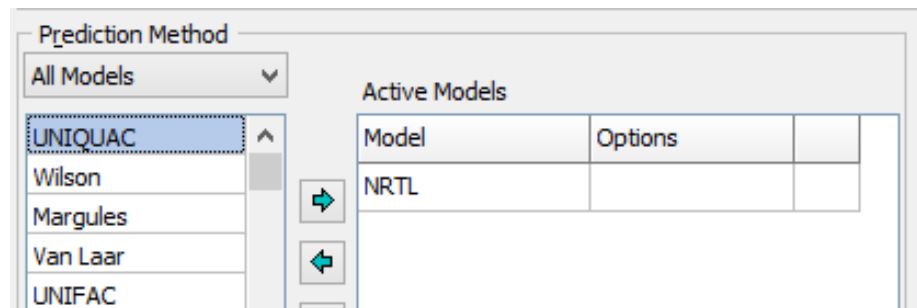
The DDB parameter data bank can hold all types of pure component or mixture properties and parameters and can be accessed via *Editors* – *Parameter DDB Organizer*:



It is integrated into the software and is automatically accessed when values or parameters are required.

## Workshop

Use the previous example but instead of Aspen Plus, use NRTL to predict the VLE data of acetone-water at 1 atm.



In the  $g^E$ -Model Interaction Parameters Manager, select a parameter set from the data bank.

Examine the option to copy/paste Aspen Plus parameters.



# Process Synthesis

## Lesson Objectives

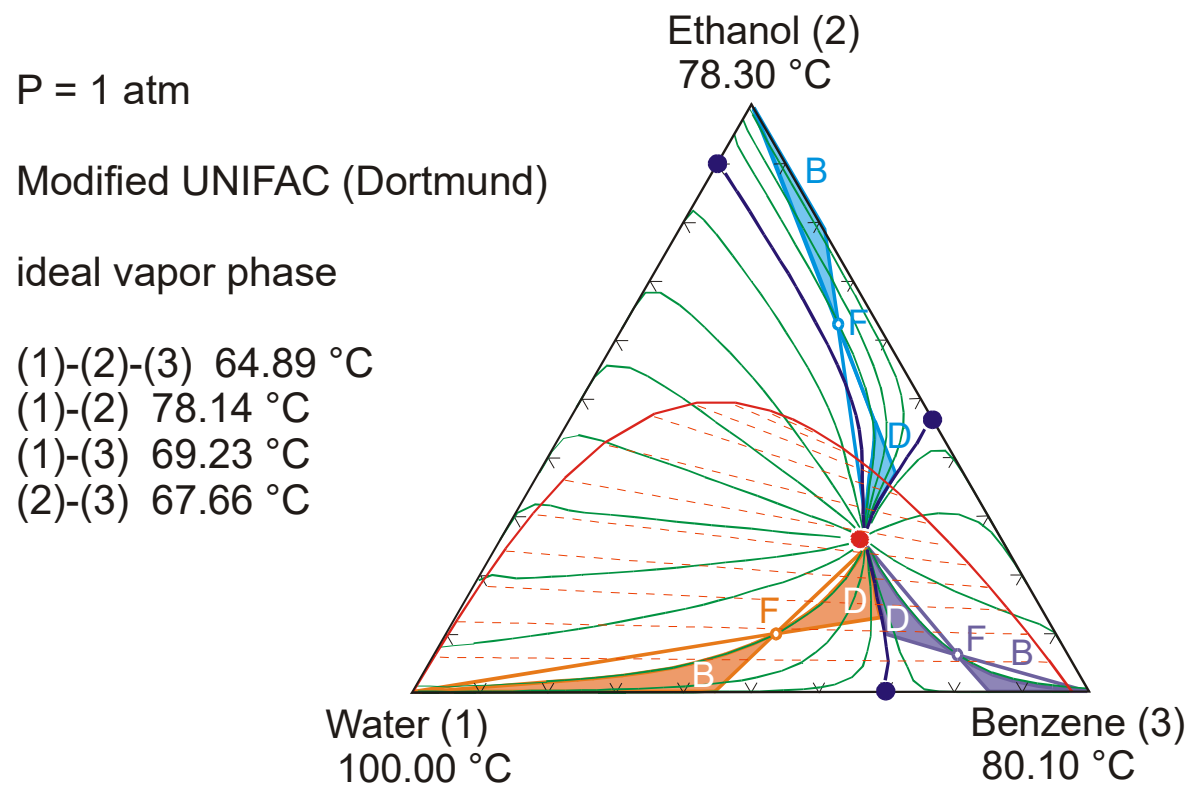
- examine the different programs in the process synthesis package.
- select a selective solvent for extractive distillation and verify its performance
- select an entrainer for azeotropic distillation

When designing a simple 3 component distillation with feed, top and bottom product, feasible products are not always obvious.

In a ternary diagram, feed, bottom and top product must be on a straight line. Top and bottom product must be on the same distillation curve.

Instead of distillation curves, often the qualitatively identical but easier to calculate residual curves are plotted.

In DDB, these plots can be generated using Process Synthesis – Residual Curves. The plot on the right shows feasible product regions for two different feed compositions in a complex 3 component system with miscibility gap.



## Workshop

Plot the azeotropes, boundary curves and residual curves for the mixture acetone – chloroform – methanol using mod. UNIFAC (Do) at 300 K.

Examine and explain the result.

Add the temperature contour lines to the plot.

Generate the 3D plot.

DDB Residue Curves 2023
— □ ×

File ?

#DDB	Remove?	Name
4	<input type="button" value="Remove"/>	Acetone
47	<input type="button" value="Remove"/>	Chloroform
110	<input type="button" value="Remove"/>	Methanol

Model: Mod. UNIFAC (Do)

Vapor Pressure Equation: Antoine - Best Match

Vapor Phase Model: Ideal or Chemical Theory

Gibbs Triangle:  Short Ticks  Labels

Calculation Mode:  isothermal  isobaric

Temperature: 300.00 K

Pressure: 101.325 kPa

**Contour Lines**    AZEOT

Residue Curves    **Contour Lines**

P or T

Additional Contour Lines: 1

Zoom with Window

2.664 seconds

#Comp	Mole frac.	Ki		Rel.Vol.
#1	n.a.	n.a.	$\alpha_{12}$	n.a.
#2	n.a.	n.a.	$\alpha_{13}$	n.a.
#3	n.a.	n.a.	$\alpha_{23}$	n.a.
P	n.a.	n.a.	F	n.a.

Compositions in:  Mole Fractions  Weight Fractions

**Methanol/3**

T=300.00 K  
Mod. UNIFAC (Do)  
Vapor Phase Model: Ideal or Chemical Theory

x1/2/3=0.9013/0.0000/0.0987  
P=33.40 kPa

x1/2/3=0.3402/0.3044/0.3554  
P=28.40 kPa

x1/2/3=0.0000/0.7416/0.2584  
P=34.42 kPa

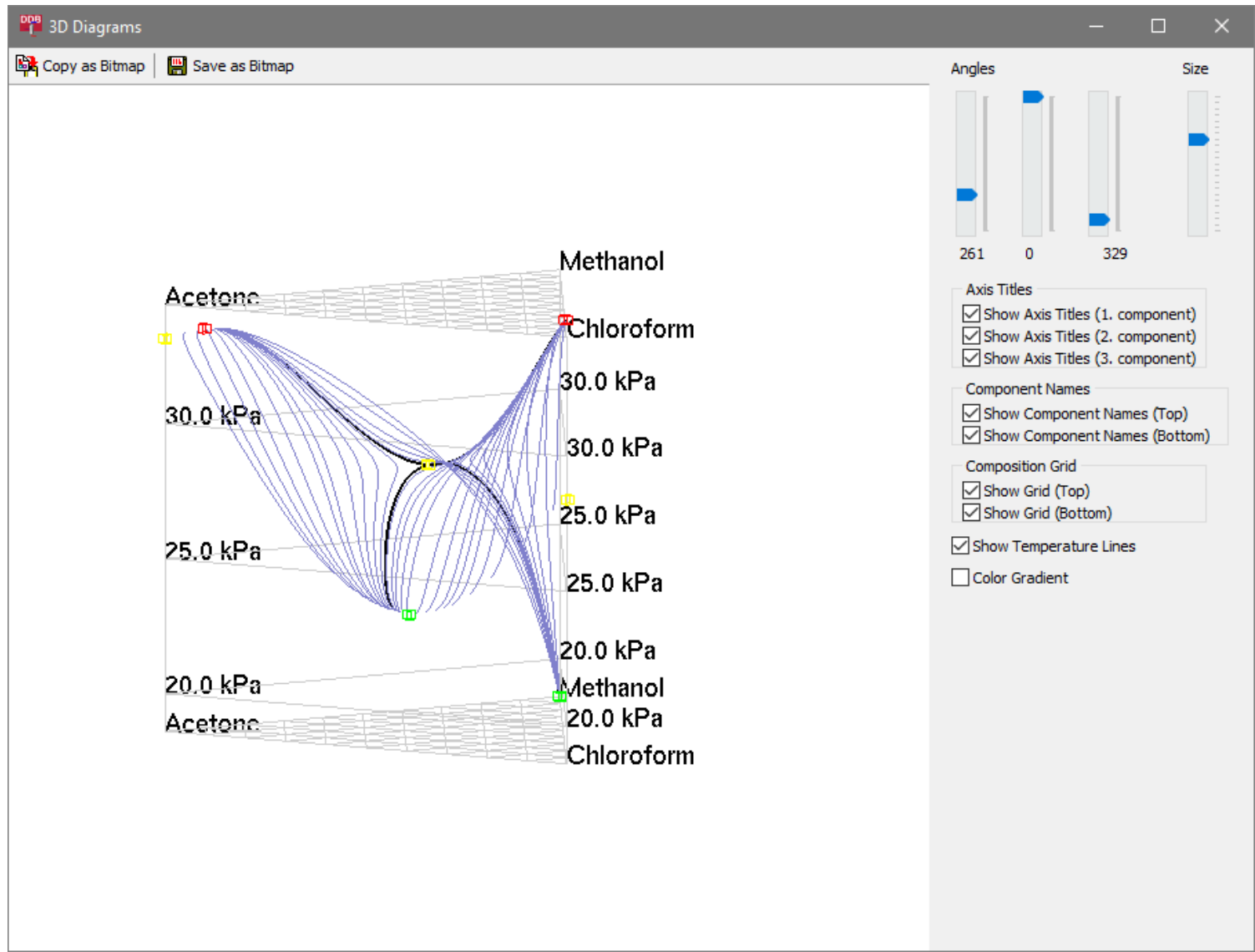
Acetone/1      Chloroform/2

x1/2/3=0.3940/0.6060/0.0000  
P=23.66 kPa

- Stable Node
- Saddle
- Unstable Node

- 25
- 27
- 28
- 29
- 30
- 31
- 33

Shift-click clears ALL older lines / If zoomed pan diagram with right mouse key pressed down / Click removes existing line if red circle is shown



A typical task for process engineers is the selection of a suitable solvent for azeotropic or extractive distillation, extraction, ...

DDB can assist via Process Synthesis – Entrainer Selection.

The action of an entrainer for extractive distillation results from the different activity coefficients of the components to be separated using an entrainer. The greatest effect is usually observed when the components are infinitely diluted in the entrainer.

The effect of the entrainer on the activity coefficients can result in an azeotropic point of one of the components with the entrainer, which should be avoided.

Solvent Selection either uses the DDB or the results of predictive models (e.g. UNIFAC) as a source for activity coefficients (ACT) or azeotropic data (AZD). The program is very powerful and has many important options, only a very simple example is shown here.

If the components are chemically very similar (as in case of isomeric compounds), usually no suitable entrainer can be found!

## Workshop

Start Process Synthesis – Entrainer Selection

Go to the Distillation Process sheet, select the Extractive Distillation

Select the components benzene - cyclohexane

Run entrainer selection by DDB access. After a short time the result dialog on the next slide will be shown.

The green hyperlink in front of the solvent names leads to the thermophysical properties and mixture data the selection is based on.

Examine further options in the dialog.

Entrainer Selection - Results

Print Copy Save Sort Selectivity LLE

Exclude from list

Components without Boiling Point Information     Components without Viscosity Information  
 Components without Melting Point Information     Components without Density Information  
 Components without Azeotropic Information for 1-2/1-3     Components with |T(alpha)-T(System)|>5K  
 Components without LLE Information     Component without Surface Tension Information

Visible columns

Vapor Pressures     Surface Tension     Separation Factor  
 Melting Point     Names     Selectivity  
 Density     Azeotropic Information     Capacity  
 Viscosity     LLE Information

Components to be Separated:

DDB No.	Name	Formula	Ps [kPa]	CAS No.	Density [kg/m³]	Viscosity [mPas]
(1) 31	Benzene	C6H6	36.18	71-43-2	847.8	0.434
(2) 50	Cyclohexane	C6H12	36.25	110-82-7	750.1	0.605

Given System Temperature = 323.15 [K]

Azeotropic data for system (1)-(2):  
homPmax at P = 40.01 kPa

List of Entrainers (Extractive Distillation)

Source of Activity Coefficients: DDB for Activity Coefficients at Infinite Dilution  
Source of Azeotropic Information: DDB for Azeotropic Data

Table Sorted by Separation Factors

DDB No.	Entrainer	Ps [kPa]	Tm [K]	Viscosity [mPas]	alpha(1,2), inf. (T in [K])	S(1,2), inf.	(1)-(3) (P [kPa])
71916	1-(3-Cyanopropyl)-1-methylpyrrolidinium thioc...	1.1E-03	n.a.	n.a.	0.017 (323.15)	0.017	n.a. (- )
19055	1-(2-Hydroxyethyl)-3-methylimidazolium tetraf...	1.1E-03	n.a.	n.a.	0.018 (323.15)	0.018	n.a. (- )
60942	1-(3-Hydroxypropyl)-1-methylmorpholinium dicy...	1.1E-03	n.a.	n.a.	0.025 (323.15)	0.025	n.a. (- )
23308	1-Methyl-3-propylimidazolium bromide	n.a.	n.a.	n.a.	0.026 (323.15)	0.026	n.a. (- )
78398	4-(3-Cyanopropyl)-4-methylmorpholinium tricya...	1.1E-03	n.a.	n.a.	0.027 (323.15)	* 0.027	n.a. (- )
43297	N-Ethyl-N-methylmorpholinium dicyanamide	1.1E-03	n.a.	n.a.	0.028 (323.15)	0.028	n.a. (- )
61001	N-(3-Cyanopropyl)pyridinium dicyanamide	1.1E-03	n.a.	n.a.	0.033 (323.15)	0.033	n.a. (- )
82806	1-(3-Hydroxypropyl)-3-methylimidazolium thioc...	1.1E-03	n.a.	n.a.	0.034 (323.15)	0.034	n.a. (- )
78399	4-(3-Hydroxypropyl)-4-methylmorpholinium tric...	1.1E-03	n.a.	n.a.	0.036 (323.15)	* 0.036	n.a. (- )



## Search for selective solvents using the predictive method UNIFAC.

DDB Entrainer Selection - Results
\_ □ ×

Print Copy Save Sort Selectivity LLE

Exclude from list

<input type="checkbox"/> Components without Boiling Point Information	<input type="checkbox"/> Components without Viscosity Information
<input type="checkbox"/> Components without Melting Point Information	<input type="checkbox"/> Components without Density Information
<input type="checkbox"/> Components without Azeotropic Information for 1-2/1-3	<input type="checkbox"/> Components with $ T(\alpha) - T(\text{System})  > 5\text{K}$
<input type="checkbox"/> Components without LLE Information	<input type="checkbox"/> Component without Surface Tension Information

Visible columns

<input checked="" type="checkbox"/> Vapor Pressures	<input type="checkbox"/> Surface Tension	<input checked="" type="checkbox"/> Separation Factor
<input checked="" type="checkbox"/> Melting Point	<input checked="" type="checkbox"/> Names	<input checked="" type="checkbox"/> Selectivity
<input type="checkbox"/> Density	<input checked="" type="checkbox"/> Azeotropic Information	<input type="checkbox"/> Capacity
<input checked="" type="checkbox"/> Viscosity	<input type="checkbox"/> LLE Information	

Components to be Separated:

DDB No.	Name	Formula	Ps [kPa]	CAS No.	Density [kg/m³]	Viscosity [mPas]
(1) 31	Benzene	C6H6	36.18	71-43-2	847.8	0.434
(2) 50	Cyclohexane	C6H12	36.25	110-82-7	750.1	0.605

Given System Temperature = 323.15 [K]

Azeotropic data for system (1)-(2):  
hom at P = 39.61 kPa

List of Entrainers (Extractive Distillation)

Source of Activity Coefficients: UNIFAC  
Source of Azeotropic Information: UNIFAC

---

Table Sorted by Separation Factors

DDB No.	Entrainer	Ps [kPa]	Tm [K]	Viscosity [mPas]	alpha(1,2), inf. (T in [K])	S(1,2), inf.	(1)-(3) (P [kPa])
83410	2,3,4,5,6-Pentanitroaniline	n.a.	n.a.	n.a.	2.25E-006 (323.15)	2.26E-006	n.a. (- )
9771	1,3,5-Triamino-2,4,6-trinitrobenzene	n.a.	n.a.	n.a.	8.31E-006 (323.15)	8.33E-006	n.a. (- )
11288	2-Silyl-trisilane	n.a.	n.a.	n.a.	9208.582 (323.15)	9224.445	n.a. (- )
11291	n-Pentasilane	n.a.	n.a.	n.a.	8850.808 (323.15)	8866.055	n.a. (- )
11290	2-Silyl-tetrasilane	n.a.	n.a.	n.a.	8850.537 (323.15)	8865.783	n.a. (- )
11293	n-Hexasilane	n.a.	n.a.	n.a.	8612.597 (323.15)	8627.434	n.a. (- )
11292	2-Silyl-pentasilane	n.a.	n.a.	n.a.	8612.375 (323.15)	8627.211	n.a. (- )
72345	2-Silyl-1,3-disilapropane	n.a.	n.a.	n.a.	1788.761 (323.15)	1791.842	n.a. (- )
18615	Bis-disilanvlether	20.55	n.a.	n.a.	1111.708 (323.15)	1113.623	none (- )

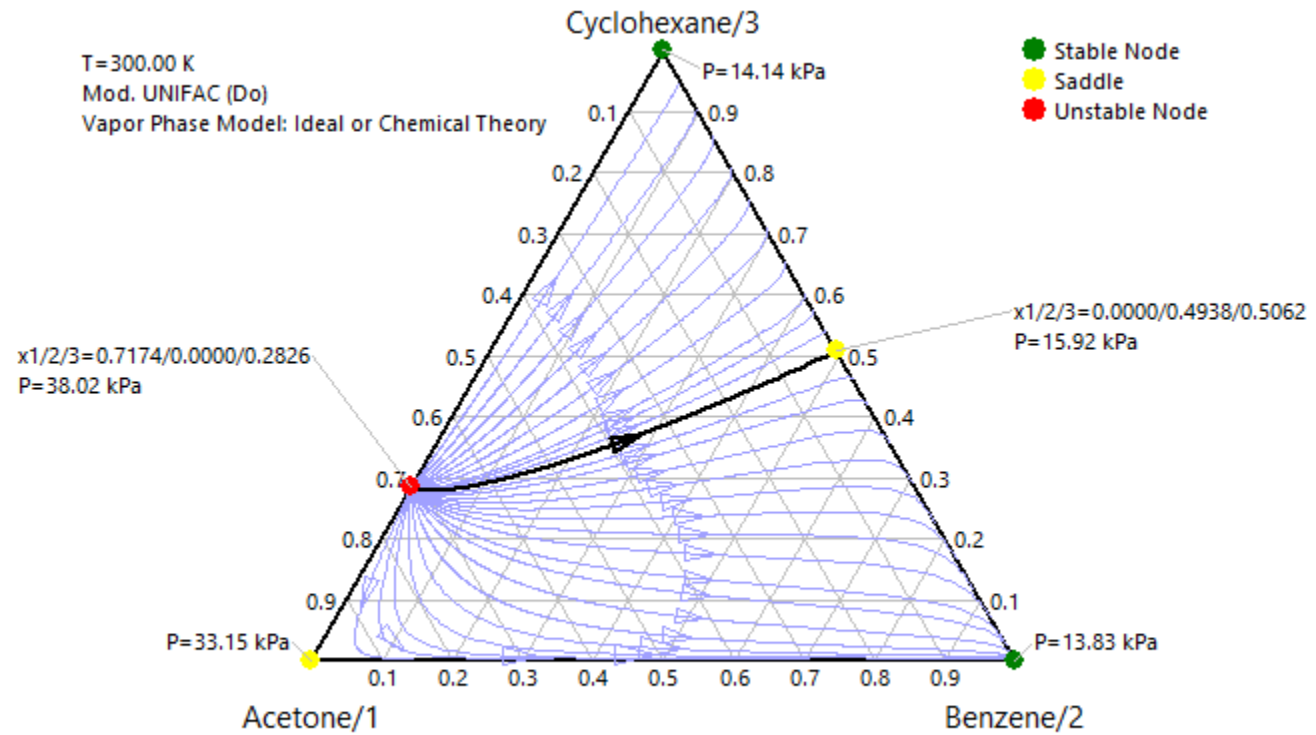
Instead of using a selective solvent for extractive distillation, it is also possible to add an entrainer that forms a binary azeotrope with one of the components or a ternary heterogeneous azeotrope. Components of industrial use for the aliphatics – aromatics separation in case of aromatic-rich mixtures like acetone or 2-butanone are found when searching for an entrainer for azeotropic distillation:

Search for an entrainer introducing at least one further binary azeotrope with DDB-access leads to the output on the right:

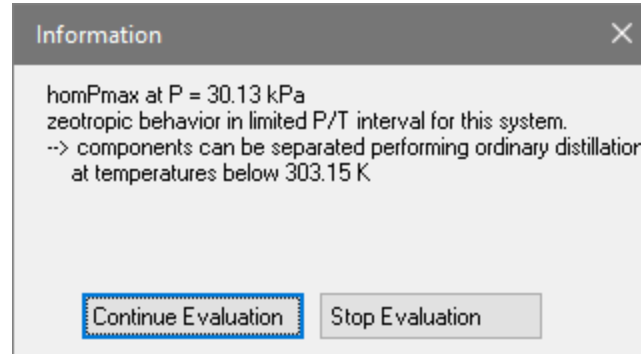
The screenshot shows the 'Entrainer Selection - Results' window. It includes a menu bar with 'Print', 'Copy', 'Save', 'Sort', 'Selectivity', and 'LLE'. Below the menu is a section for 'Exclude from list' with several checkboxes. A 'Visible columns' section has checkboxes for 'Vapor Pressures', 'Melting Point', 'Density', 'Viscosity', 'Surface Tension', 'Names', 'Azeotropic Information', 'LLE Information', 'Separation Factor', 'Selectivity', and 'Capacity'. The main area displays 'Components to be Separated:' with a table for Benzene and Cyclohexane. It also shows 'Given System Temperature = 323.15 [K]' and 'Azeotropic data for system (1)-(2): homPmax at P = 40.01 kPa'. The 'List of Entrainers (Azeotropic Distillation (Further Binary Azeotrope))' section is followed by a table of entrainers sorted by DDB code numbers.

DDB No.	Entrainer	Ps [kPa]	Tm [K]	Viscosity [mPas]	(1)-(3) (P [kPa])	Type of azeotropic data (2)-(3) (P [kPa])
3	Acetonitrile	34.07	229.30	0.276	homPmax ( 44.73)	hetPmax ( 65.29)
4	Acetone	81.42	178.35	0.248	none ( 3.93)	homPmax ( 89.80)
11	Ethanol	29.37	158.65	0.641	homPmax ( 51.14)	homPmax ( 56.50)
15	Formic acid	17.05	281.45	1.044	hetPmax ( 47.57)	n.a. ( - )
16	Formic acid ethyl ester	87.87	193.95	0.289	none ( 66.66)	homPmax ( 91.45)
21	Ethyl acetate	37.95	189.55	0.325	homPmax ( 38.17)	homPmax ( 47.91)
39	1-Butanol	4.61	183.35	1.284	homPmax (2653.05)	homPmax ( 37.42)
40	2-Butanone	35.53	186.48	0.313	homPmax ( 37.61)	homPmax ( 48.63)
55	Methylcyclopentane	49.10	130.73	0.371	homPmax ( 49.07)	n.a. ( - )
62	2,3-Butanedione	25.35	270.75	n.a.	n.a. ( - )	homPmax ( 46.86)

Addition of e.g. acetone will send the binary azeotrope with cyclohexane to the top of the column.



Another possibility is the introduction of a heterogeneous ternary azeotrope. Look for an entrainer for the separation of the system ethanol – water. The program will first display the following message:



"Continue Evaluation" as we do not consider a vacuum distillation with unfavorable separation factor.

The following list of entrainers is shown:

Entrainer Selection - Results

Exclude from list

- Components without Boiling Point Information
- Components without Melting Point Information
- Components without any Azeotropic Information
- Components without LLE Information
- Components without Viscosity Information
- Components without Density Information
- Components with  $|T[\alpha]-T[\text{System}]| > 5K$
- Component without Surface Tension Information

Visible columns

- Vapor Pressures
- Melting Point
- Density
- Viscosity
- Surface Tension
- Names
- Azeotropic Information
- LLE Information
- Separation Factor
- Selectivity
- Capacity
- Azeotropic Composition in
  - Mole Fraction
  - Weight Fraction

Components to be Separated:

DDB No.	Name	Formula	Ps [kPa]	CAS No.	Density [kg/m <sup>3</sup> ]	Viscosity [mPas]
(1) 11	Ethanol	C <sub>2</sub> H <sub>6</sub> O	29.37	64-17-5	759.3	0.641
(2) 174	Water	H <sub>2</sub> O	12.31	7732-18-5	982.7	0.527

Given System Temperature = 323.15 [K]

Azeotropic data for system (1)-(2):  
 homPmax at P = 30.13 kPa  
 azeotropic behavior in limited P/T interval for this system.  
 --> components can be separated performing ordinary distillation  
 at temperatures below 303.15 K

List of Entrainers (Azeotropic Distillation - Add Ternary Heterogeneous Azeotrope)

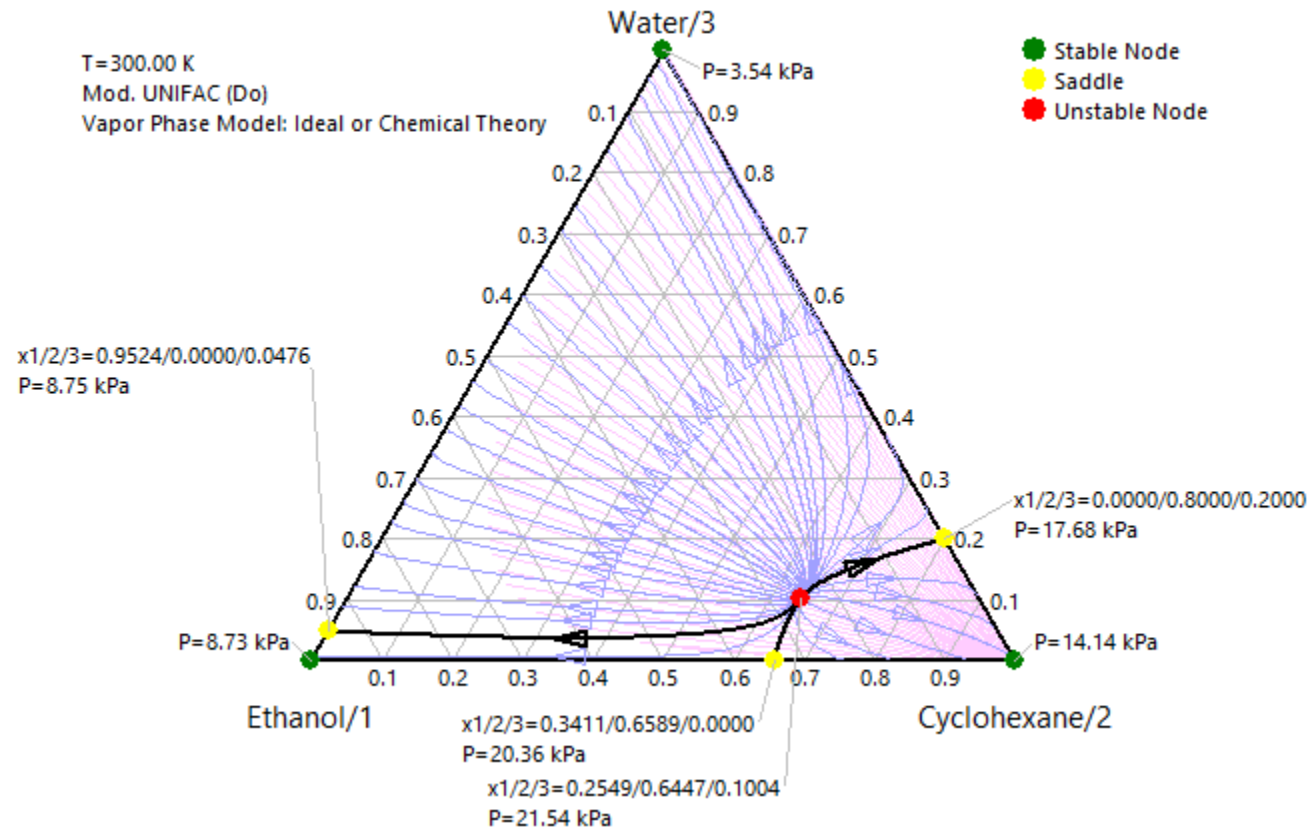
Source of Azeotropic Information: DDB for Azeotropic Data

Table Sorted by DDB Code Numbers

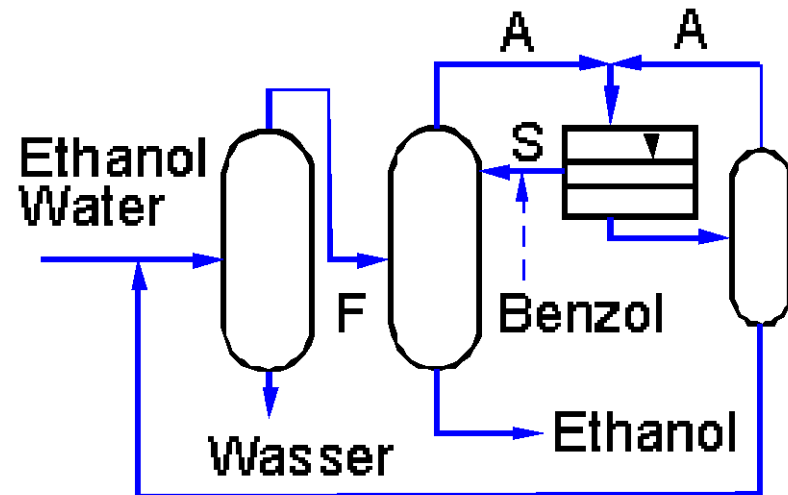
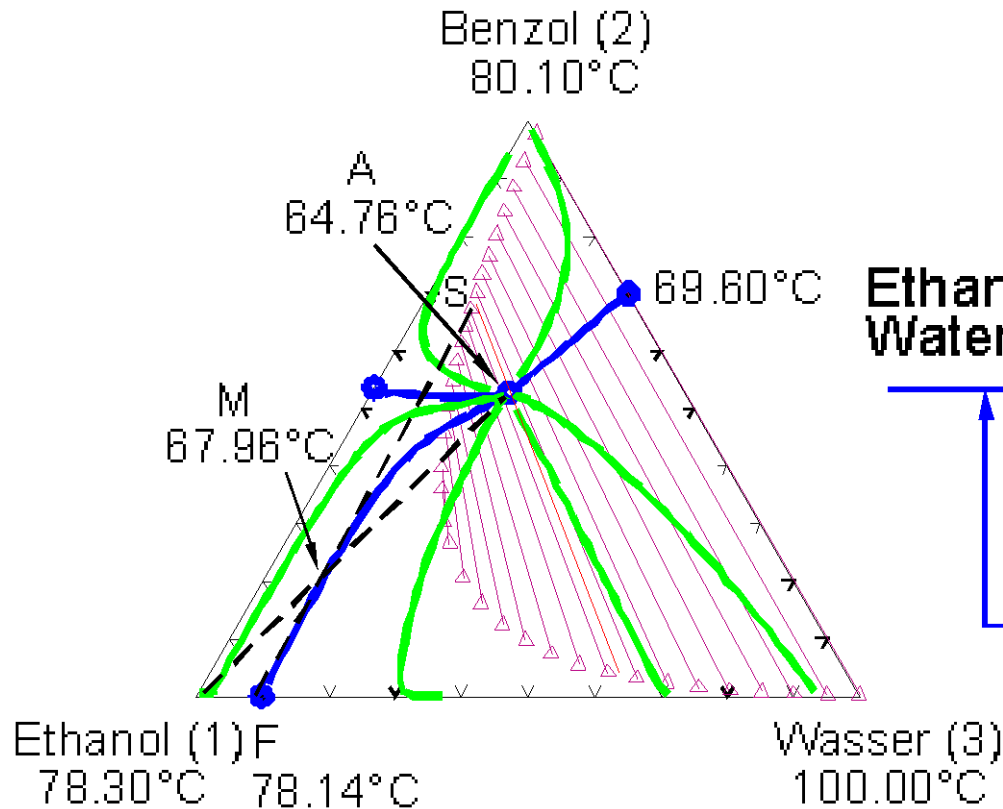
DDB No.	Entrainer	Ps [kPa]	Tm [K]	Viscosity [mPas]	Type of azeotropic data		
					(1)-(2)-(3) (P [kPa])	yaz(1)	yaz(2)
21	Ethyl acetate	37.99	189.55	0.325	hetPmaxMisGap (101.30)	n.a.	n.a.
31	Benzene	36.18	278.68	0.434	hetPmaxMisGap ( 60.40)	0.2200	0.1840
50	Cyclohexane	36.25	279.75	0.605	hetPmaxMisGap ( 66.66)	0.2970	0.1620
53	Methylcyclohexane	18.46	146.55	0.502	hetPmaxMisGap (101.32)	0.4360	0.2355
55	Methylcyclopentane	49.10	130.73	0.371	hetPmaxMisGap (101.32)	0.2273	0.1267
74	2,4-Dimethylpentane	36.53	153.25	n.a.	hetPmaxMisGap (101.32)	0.3339	0.1856
89	Hexane	53.86	177.85	0.223	hetPmaxMisGap (101.32)	0.1683	0.2097

The list contains components like benzene and cyclohexane used in large scale ethanol dehydration.

Using mod. UNIFAC (Do), the following residual curve plot can be calculated:



The actual implementation of the process is shown here using benzene as entrainer:



# Data Input

## Lesson Objectives

- enter a new pure component into the private basic data file
- Estimate and enter the most important properties required for calculations
- Enter a mixture property data set
- Test the data and append the data set to the private DDB



Users can store references, new components, pure component and mixture data, model parameters, molecular structures, ... in their own data bank.

Files and formats are identical to the DDB but files reside on a separate directory. Currently only one private data bank can be active at a time.

For data input, easy to use data editors are available.

Data input is described in detail in the manuals

*Edit Mixture Data Tutorial*

*Edit Pure Data Tutorial*

*Component Management Tutorial*

*Lear Tutorial*

in the documentation folder.

For data input, easy to use data editors are available.

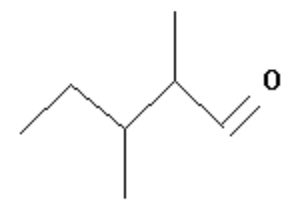
For the following workshops, start with an empty private folder.

First we introduce a new private component and enter the structure and basic properties to be used as defaults for further calculations in the structure database and the component definition file.

For these entries, no links to data sources etc. are stored and the user should document his input separately.

# Workshop

Task: Enter the component on the right as a new component into the private DDB.



Start the program *Components*

2,3-dimethyl-pentanal  
Beilstein Registry Number 1901854

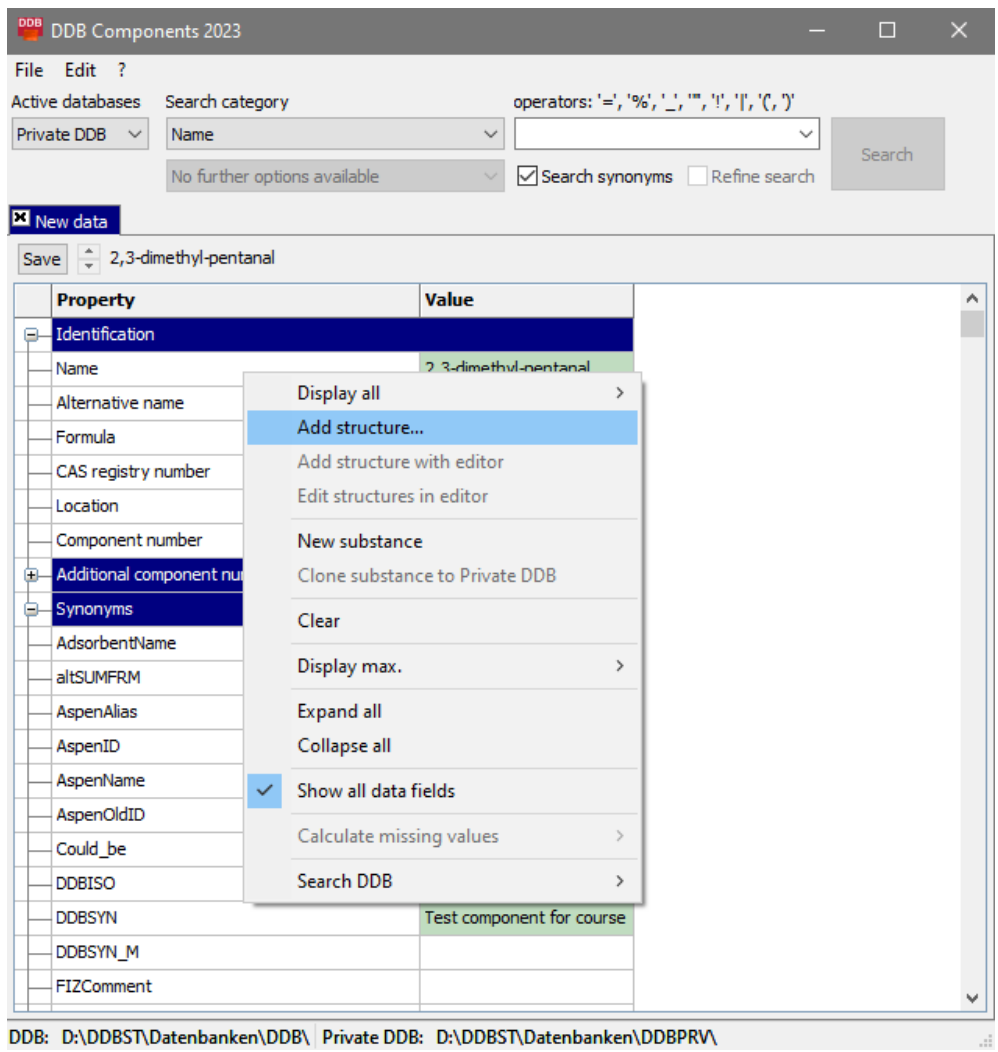
Select the private data bank. If the file does not exist, it will be generated. A right-click in the data field starts the procedure.

The screenshot shows the 'DDB Components 2023' interface. A context menu is open over the 'New data' section, with 'New substance' highlighted. The main window shows a table with the following data:

Property	Value
<b>Identification</b>	
Name	2,3-dimethyl-pentanal
Alternative name	
Formula	C7H14O
CAS registry number	32749-94-3
Location	1
Component number	<input checked="" type="checkbox"/>
<b>Additional component numbers</b>	
<b>Synonyms</b>	
AdsorbentName	
alSUMFRM	
AspenAlias	
AspenID	
AspenName	
AspenOldID	
Could_be	
DDBISO	
DDBSYN	Test component for course
DDBSYN_M	
FIZComment	

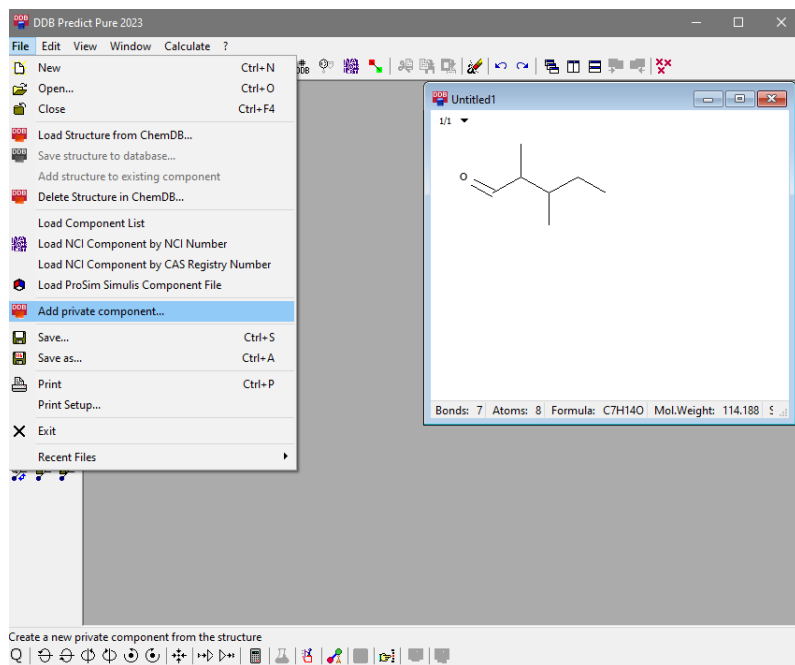
Enter the English name 2,3-dimethyl-pentanal. Enter the empirical formula.  
Enter the CAS-number 32749-94-3  
Enter the DDB-synonym "Test component for course"

Selecting *add structure* from the right-click menu allows the import of \*.mol files.



not in Explorer Version

Start *PredictPure* and draw the molecular structure of 2,3-dimethyl-pentanal



The further procedure is as shown before. Once completed, press the save button to store the new component. A component number will be assigned automatically.

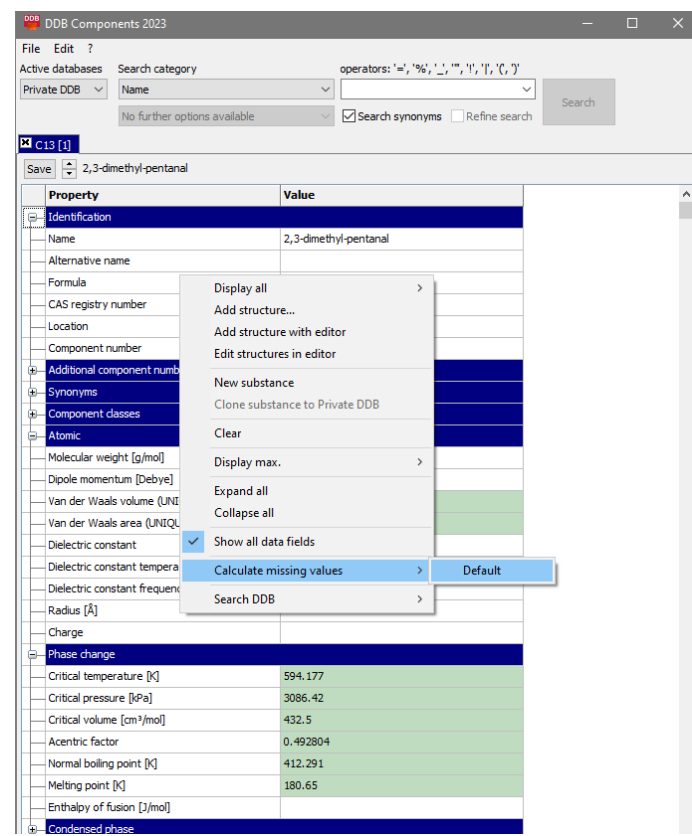
Selecting *Add private component* from the *file* menu brings up Components and transfers the structure as well as formula and molecular weight.

The screenshot shows the 'DDB Components 2023' application window. The 'New data' table is displayed with the following properties and values:

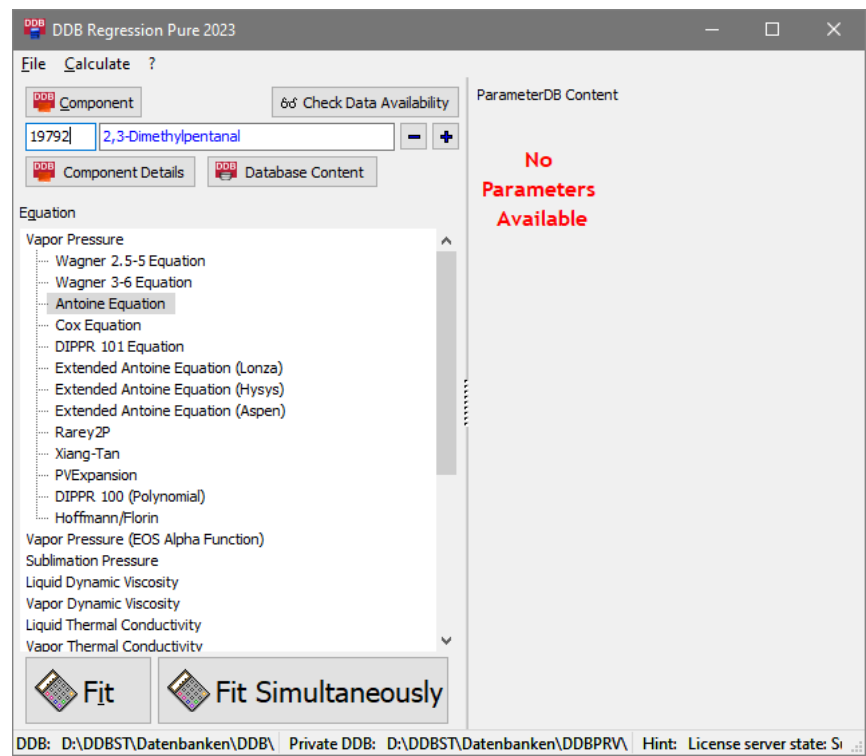
Property	Value
<b>Identification</b>	
Name	
Alternative name	
Formula	C7H14O
CAS registry number	
Location	1
Component number	<input checked="" type="checkbox"/>
<b>Atomic</b>	
Molecular weight [g/mol]	114.18756
<b>Structures</b>	
1	

The status bar at the bottom indicates: DDB: D:\DDBST\Datenbanken\DDB\ Private DDB: D:\DDBST\Datenbanken\DDBPRV\

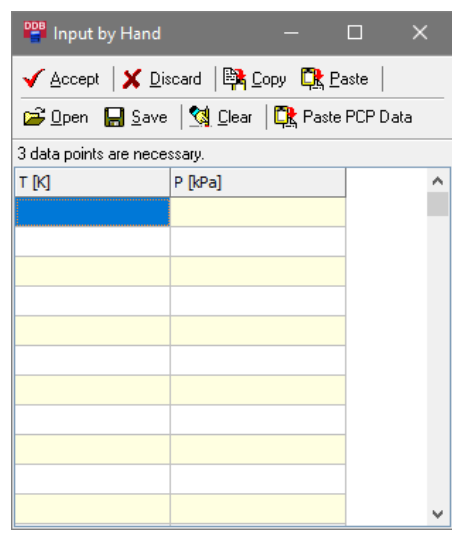
Various missing properties can automatically be estimated using some pre-defined methods via right-click menu, *Calculate missing values – Default*. The calculation itself is performed by PredictPure in the background which also allows to choose different methods for e.g. different substance classes (see manual).



Start Regression Pure and select 2,3-dimethyl-pentanal from the DDB:

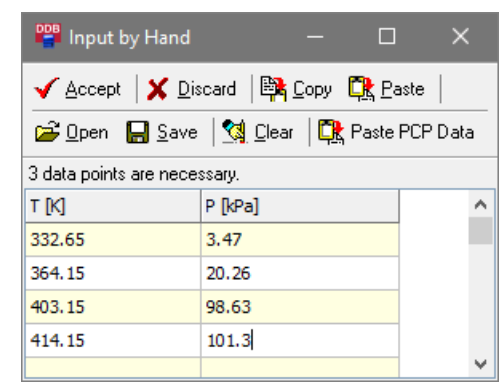


Select *Fit* and data source *Hand* to bring up the following dialog :

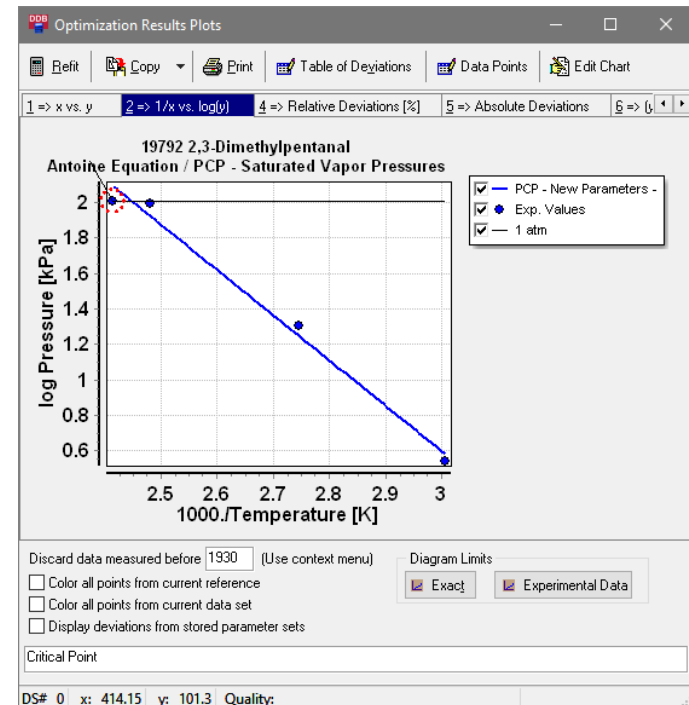
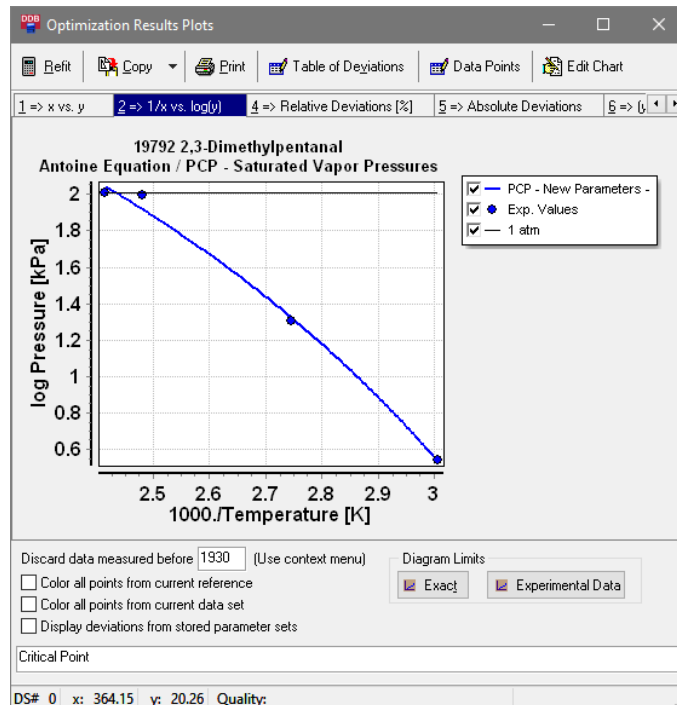


Enter the following data and accept your input:

T / °C	P / mmHg	T / K	P / kPa
59.5	26	332.65	3.47
91	152	364.15	20.26
130	740	403.15	98.63
141	760	414.15	101.30



After the fit the left plot can be shown. The vapor pressure curve shows a strong curvature, which is the combined result of the low quality of the data and the ability of the Antoine equation to describe this non-linear behavior. Nevertheless, it is very unlikely that the component of interest has such a vapor pressure curve. Select Refit and fit only A and B of the Antoine equation. This will result in the more realistic vapor pressure curve shown on the right:





Instead of entering the vapor pressure data into *RegressionPure* by hand, it would have been better to store them in the PCP data bank.

All data points could be stored in 2 data sets with the references CAS and Beilstein or each value could be stored separately with its primary source.

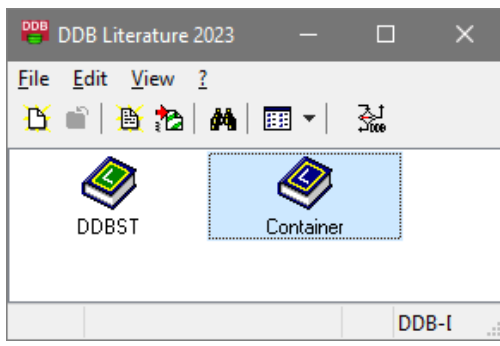
**Important Notice:** In the DDB, data are only extracted from the primary source, which is nearly always available at DDBST GmbH.

Experimental pure component or mixture data sets in DDB are linked to the component(s) in the component definition and the source reference in the literature data bank LEAR.

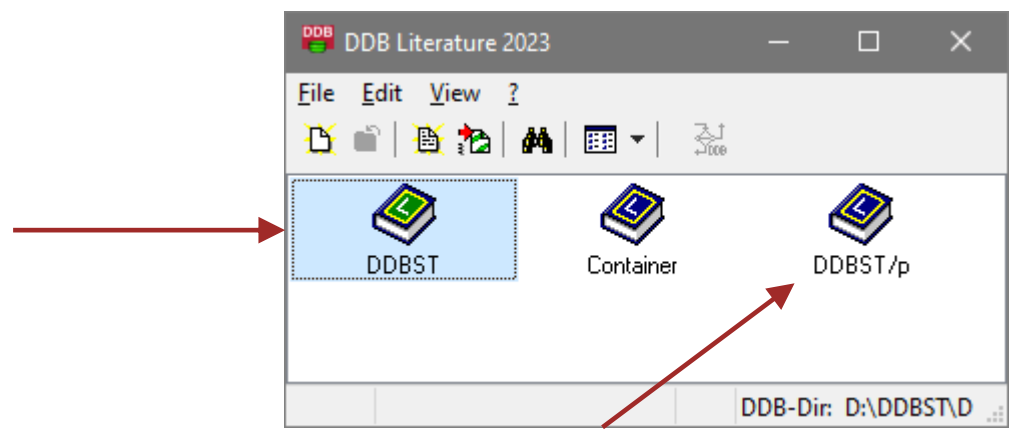
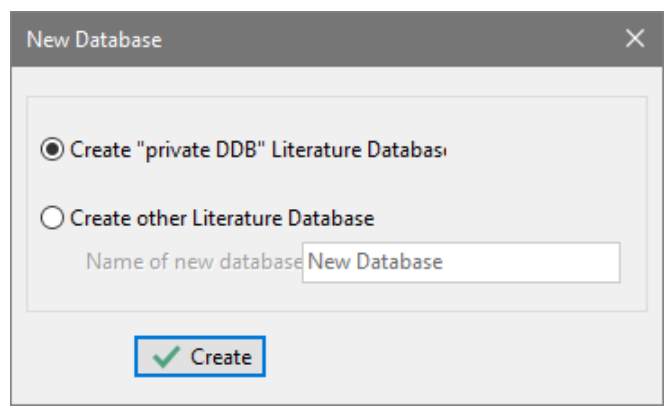
When data sets are added, the component and reference entries must be available.

As we entered 2,3-Dimethyl-Pentanal as a new component in the private data pure component definition file, we now must enter the reference for the first data set (the patent found via CAS).

Start the program LITERATURE. The following dialog will be shown:

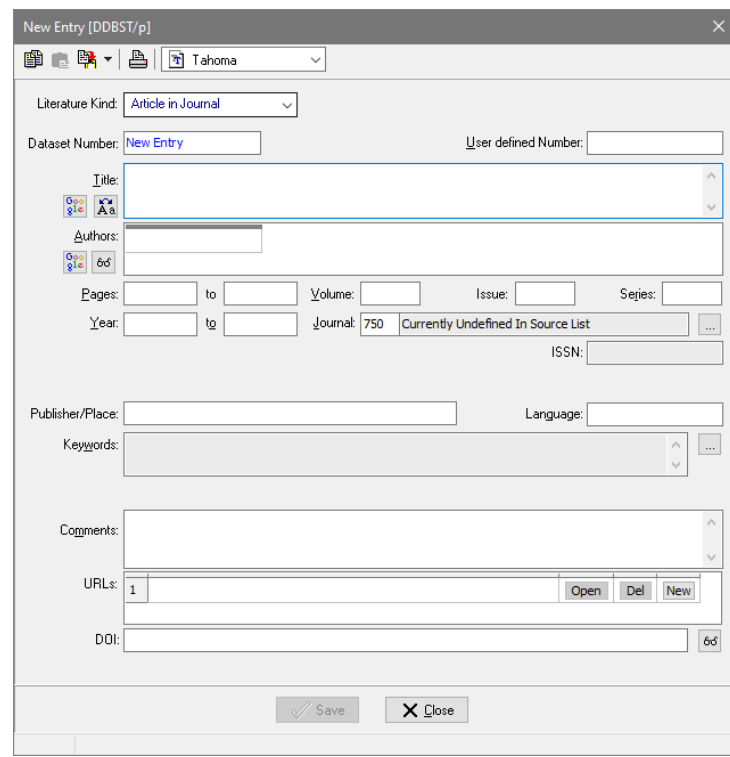


As there currently is no private reference database, we need to create it. Select New – New Library. In the next dialog, select Create.



Private reference database

Double-click DDBST/p to open the data view dialog and select Edit – New Data Set:



Now enter the reference information as shown on the next slide.

New Entry [DDBST/p]

Literature Kind: Patent Precise Kind: [0659.0] F-Patent

Dataset Number: New Entry User defined Number:

Title: 2,3-Dimethylpentanal

Authors: Istituto Franco Tosi S.p.A.

Pages: 1 to Year: Patent No: 1377141 19641030 WD No:

Publisher/Place: Language:

Keywords:

Comments: from CAS citation

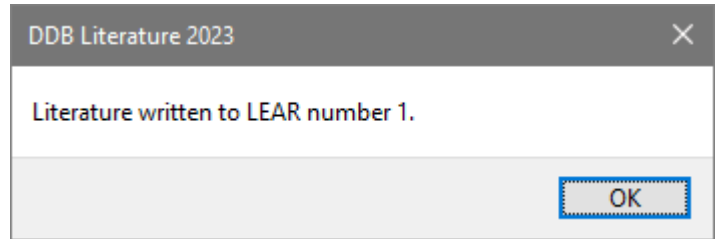
URLs: 1 Open Del New

DOI:

Save Close

Modified

## Save the Reference:



Complete Library [DDBST/p]

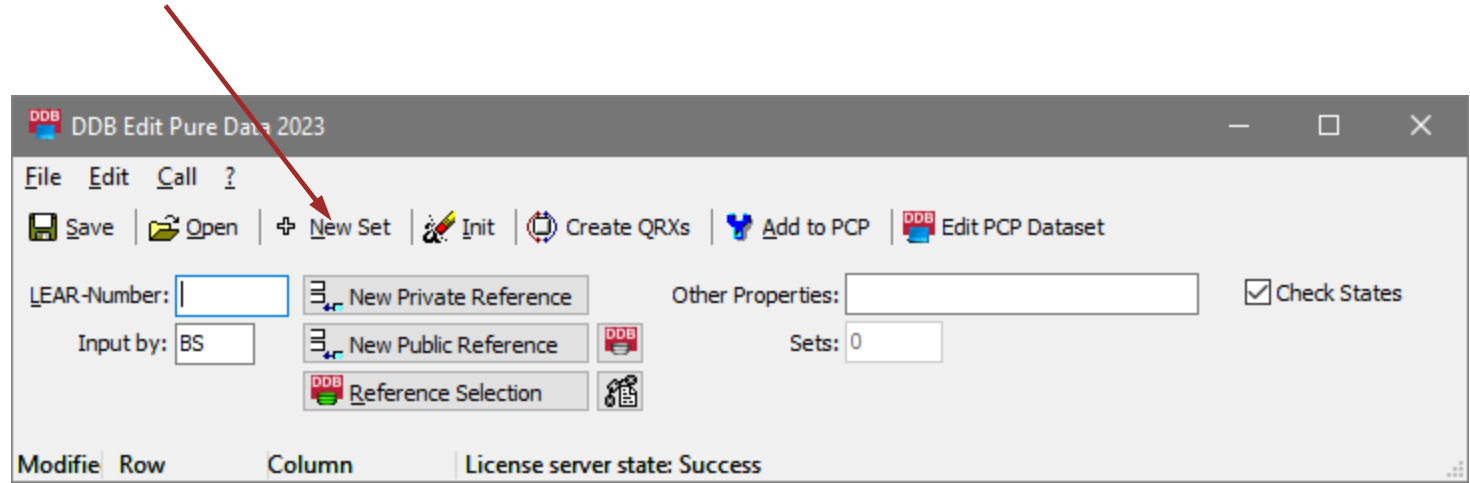
Results Edit Search View Options Windows

Number	Title	Authors
1	2,3-Dimethylpentanal	Instituto Franco Tosi S.p.A.

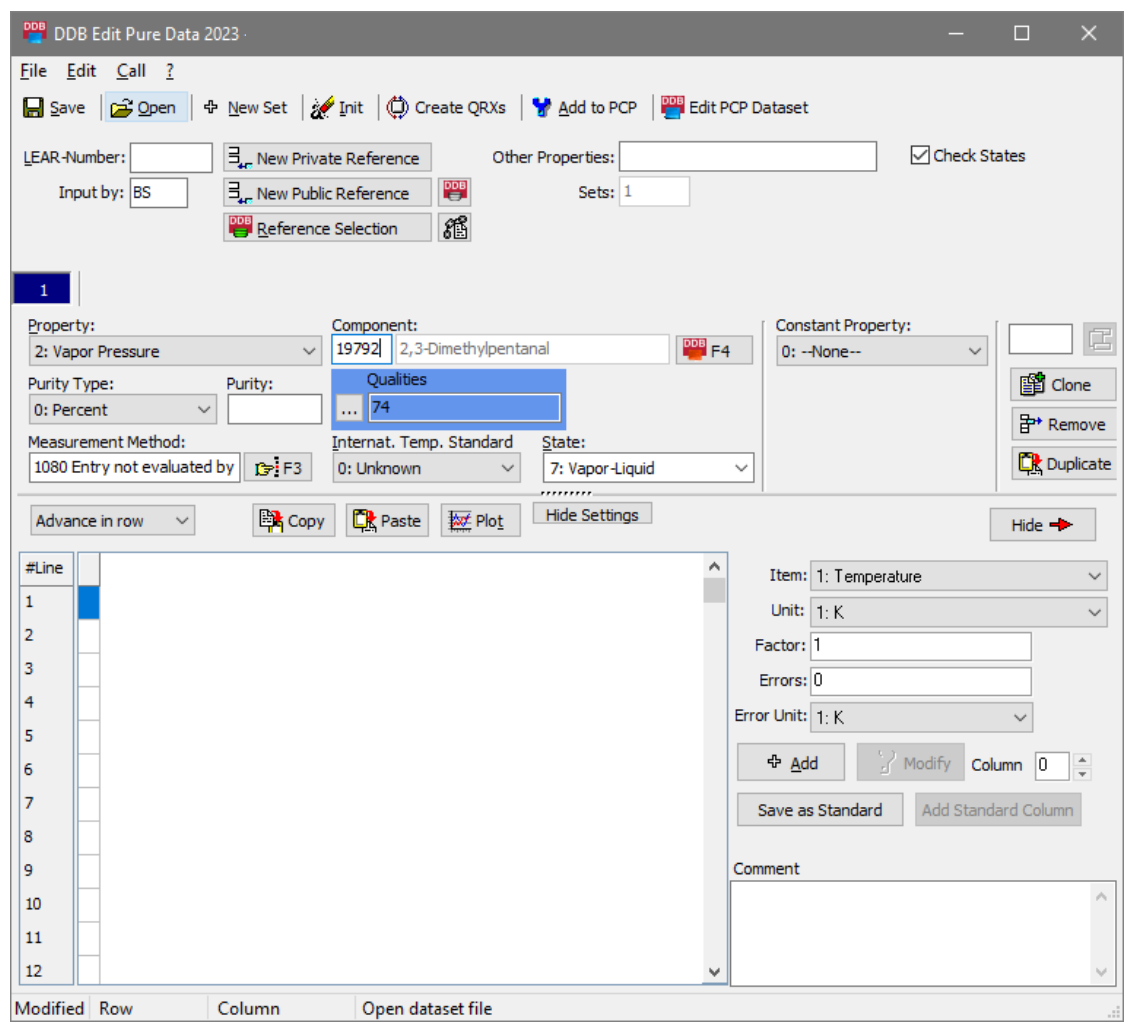
Datasets: 1 Double-click or press <return> to view/edit details, pre

Let us enter the data with their primary source using Edit Pure Data:

## Select *New Set*



In the dialog below, select vapor pressure as property, select the component 2,3-dimethyl-pentanal from the DDB, select vapor-liquid as state.



The next step is to define the table entries in the small floating dialog. Let us enter the normal boiling point found via CAS. The columns should be temperature in °C, pressure in atm and temperature error in °C.

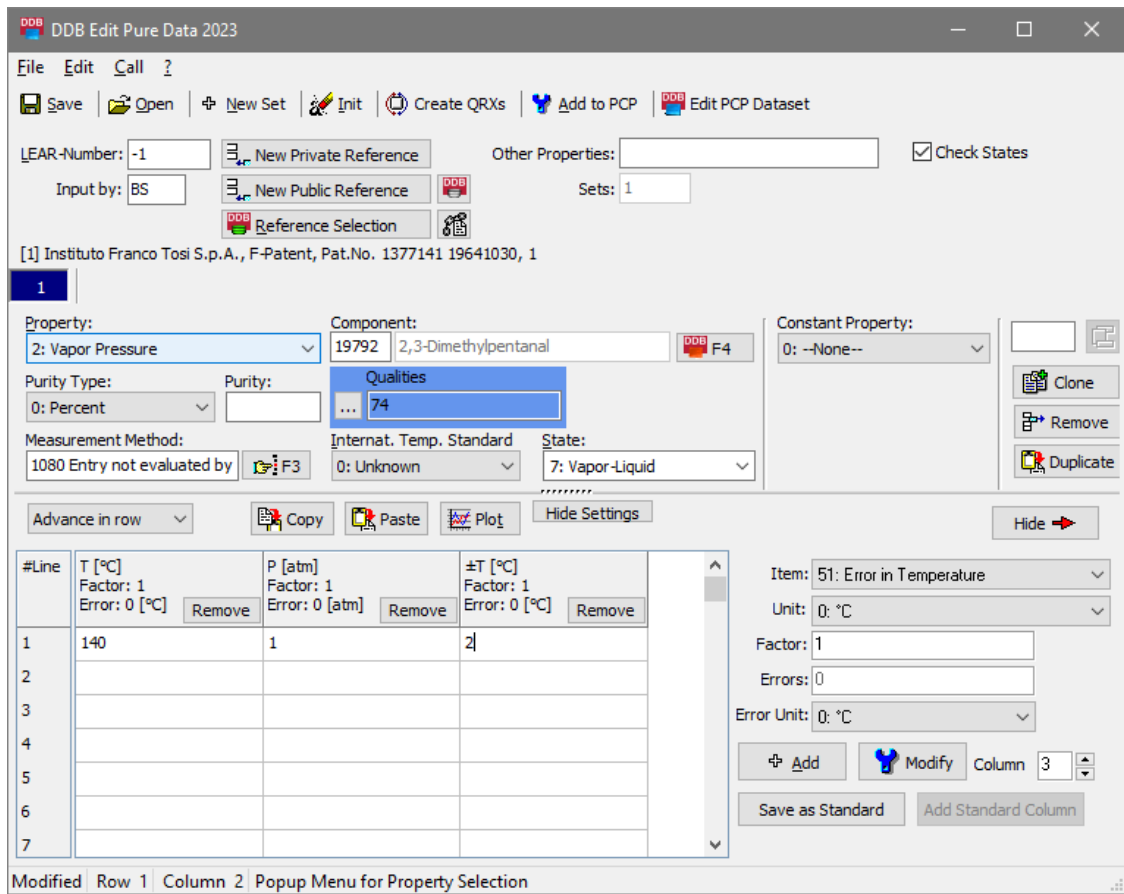
Factor is always 1 in our example. It is used in case the authors present a table in which all column values have to be multiplied with a common factor (e.g.  $10^3$ ).

There are 2 ways to specify errors:

- A in the column definition, an absolute or relative error can be specified for all data in the column
- B an explicit error column can be introduced for absolute or relative errors of each property in each table line

In case of data sets with one data point, both choices are equally valid. Normally one would use option A and save the additional column.

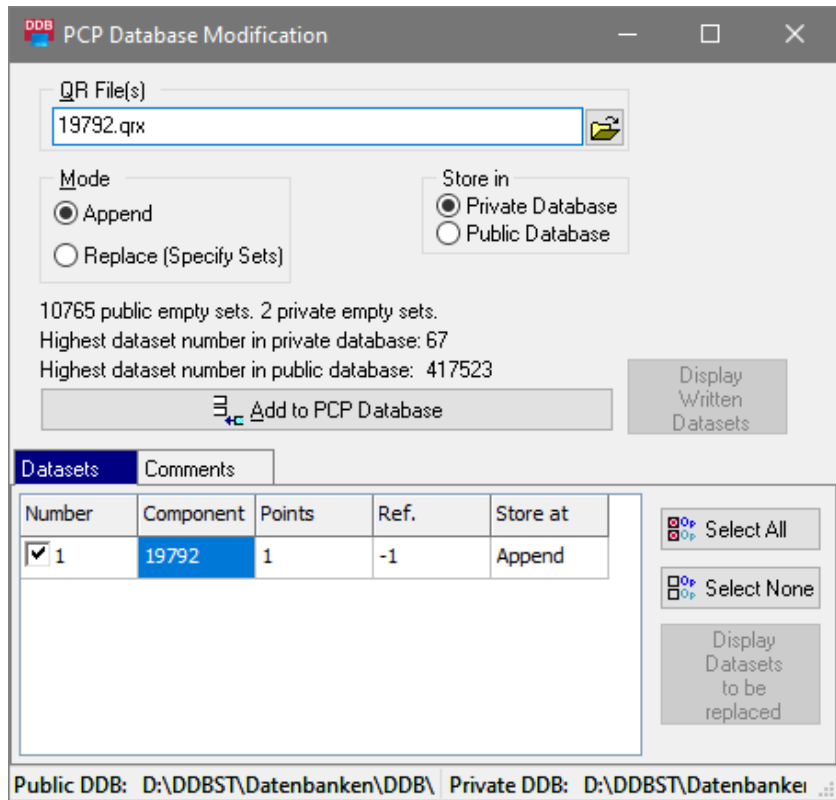
Now that the data columns are available, enter the data and select the reference from the private reference file via F1 (search private file with "Learn Number is equal 1"):



Now save the file and select Add to PCP.



The following dialog will be shown:



And select "Add to PCP Database"

## Remark on Private Databanks:

Out of historical reasons, private data set numbers, reference numbers and component numbers are stored as negative numbers. This allows for exactly two databanks, one public and one private.

Newer developed programs use 3 integer numbers to identify the number and the data bank plus additional information, which will allow to handle the public and a large number of private data banks (company, group, individual user, ...) simultaneously.

Editor programs show the actually used negative numbers in the dialogs.

The input of mixture data works in a similar way as the pure component data input shown before.

## Workshop

Enter the following  $h^E$ -data set into the private mixture data bank:

### Excess Enthalpies of Binary Systems of Cyclic Ether + Cyclohexene

Jean-Pierre E. Grollier,<sup>\*†</sup> Americo Ingleso,<sup>‡</sup> and Emmerich Wilhelm<sup>§</sup>

Centre de Thermodynamique et de Microcalorimétrie du C.N.R.S., F-13003 Marseille, France

The molar excess enthalpy  $H^E$  has been measured as a function of mole fraction  $x$  at atmospheric pressure and 298.15 K for the binary liquid systems cyclohexene ( $C_6H_{10}$ ) + oxolane (tetrahydrofuran,  $C_4H_8O$ ), + oxane (tetrahydropyran,  $C_5H_{10}O$ ), + 1,3-dioxolane (1,3- $C_3H_4O_2$ ), + 1,4-dioxane (1,4- $C_4H_8O_2$ ), and + cyclohexane ( $C_6H_{12}$ ), by using a flow calorimeter of the Picker design. The mixtures with cyclic diethers exhibit relatively large positive excess enthalpies: for 1,3- $C_3H_4O_2$  +  $C_6H_{10}$ ,  $H^E(x=0.5) = 115.5$  J mol<sup>-1</sup>; and for 1,4- $C_4H_8O_2$  +  $C_6H_{10}$ ,  $H^E(x=0.5) = 909.7$  J mol<sup>-1</sup>. The excess enthalpy for  $C_6H_8O$  +  $C_6H_{10}$  is considerably smaller, i.e.,  $H^E(x=0.5) = 285.5$  J mol<sup>-1</sup>, and  $C_5H_{10}O$  +  $C_6H_{10}$  shows S-shaped dependence of  $H^E$  on  $x$ , with the very small negative section being located at small mole fractions of the cyclic ether ( $x < 0.0899$ ). For  $C_6H_{12}$  +  $C_6H_{10}$  the excess enthalpy is rather symmetric, with  $H^E(x=0.5) = 97.3$  J mol<sup>-1</sup>.

#### Introduction

Excess enthalpies of binary liquid mixtures composed of either five- or six-membered cyclic ethers and various second components (ranging from  $n$ -alkanes to alkanic acids) were reported in ref 1-5. As a sequel, we present here measurements of the molar excess enthalpy  $H^E$  at 298.15 K of the binary systems cyclohexene ( $C_6H_{10}$ ) + oxolane (tetrahydrofuran,  $C_4H_8O$ ), + oxane (tetrahydropyran,  $C_5H_{10}O$ ), + 1,3-dioxolane (1,3- $C_3H_4O_2$ ), + 1,4-dioxane (1,4- $C_4H_8O_2$ ), and + cyclohexane ( $C_6H_{12}$ ). These measurements will be used later to assess, in terms of group-contribution theory (6), the influ-

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<sup>†</sup> Present address: Istituto di Chimica Fisica, Università di Bari, Bari, Italy.

<sup>‡</sup> On leave from Institut für Physikalische Chemie, Universität Wien, Währingerstrasse 42, A-1090 Wien, Austria.

Table I. Densities ( $\rho$ ) of Pure Component Liquids at 298.15 K

compd	$\rho$ (kg m <sup>-3</sup> )	
	exptl	lit.
cyclohexene	806.0	806.09 (9), 806.3, <sup>a</sup> 805.66 (11), 805.9 (12), 805.70 (13)
		773.89 (14)
cyclohexane	773.9	773.89 (14)
oxane	879.1	879.22 <sup>b</sup>
oxolane	881.9	881.97 (16)
1,4-dioxane	1028.2	1028.21 (17), 1027.97 (18)
1,3-dioxolane	1059.1	1053.8 <sup>c</sup>

<sup>a</sup> Interpolated value from ref 10. <sup>b</sup> Interpolated value from ref 15. <sup>c</sup> Extrapolated value from ref 19.

Table II. Comparison of Experimental Molar Excess Enthalpies  $H^E$  at 298.15 K of the Test System Benzene (x) + Cyclohexene (1-x) with the Results of Marsh (20)

x	$H^E$ (J mol <sup>-1</sup> )		
	exptl	Marsh (20)	$\delta^a$
0.2118	519.3	523.8	-0.9
0.3064	667.2	669.7	-0.4
0.4015	756.2	761.8	-0.7
0.4920	793.7	798.5	-0.6
0.5768	779.9	787.2	-0.9
0.6581	729.3	733.8	-0.6
0.7400	638.3	636.2	+0.3
0.9334	214.6	214.7	0.0

<sup>a</sup> Percentage deviation  $\delta = 100(H^E_{\text{exptl}} - H^E_{\text{Marsh}})/H^E_{\text{Marsh}}$ .

ence of various structural parameters (ring size, proximity of oxygen in diethers,  $n$ - $\pi$  interaction, etc.) on the thermodynamic behavior of such mixtures.

#### Experimental Section

**Materials.** Source and treatment of the cycloethers have been given previously (7). Cyclohexene (from Fluka, puriss.,

Table III. Molar Excess Enthalpy  $H^E$  for Cyclic Ether + Cyclohexene and for Cyclohexane + Cyclohexene at 298.15 K<sup>a</sup>

x	$H^E$ / (J mol <sup>-1</sup> )	x	$H^E$ / (J mol <sup>-1</sup> )
$x$ $C_6H_{12}$ + (1-x) $C_6H_{10}$			
0.0451	14.4	0.5431	97.3
0.1442	45.0	0.6297	91.7
0.1883	58.0	0.7265	80.0
0.2738	75.9	0.8238	60.0
0.3604	88.7	0.9178	31.5
0.4512	95.2		
$x$ $C_5H_{10}O$ + (1-x) $C_6H_{10}$			
0.0495	-11.5	0.5825	148.1
0.0794	-1.5	0.6697	136.6
0.2270	69.8	0.7540	114.3
0.3195	109.4	0.8704	66.9
0.4965	148.5	0.9597	18.4
$x$ $C_4H_8O$ + (1-x) $C_6H_{10}$			
0.0591	14.6	0.6126	279.2
0.1831	132.5	0.6935	251.2
0.2358	181.4	0.7794	207.0
0.3341	242.2	0.8615	144.6
0.4285	276.8	0.9369	69.4
0.5224	286.0		
$x$ 1,4- $C_4H_8O_2$ + (1-x) $C_6H_{10}$			
0.0899	362.7	0.6151	850.7
0.2518	755.1	0.6990	762.7
0.3498	860.4	0.7784	629.8
0.5304	900.3	0.8850	368.0
$x$ 1,3- $C_3H_4O_2$ + (1-x) $C_6H_{10}$			
0.1080	520.4	0.7400	898.3
0.2920	1008.3	0.8115	726.3
0.3973	1133.9	0.9042	414.3
0.5806	1112.7	0.9709	133.7
0.6620	1028.4		

<sup>a</sup> Mole fraction of cyclic ether or cyclohexane is  $x$ .

## Workshop

After storing the data in the private data bank, use the different possibilities to plot and regress the data and to compare them to results of predictive models.

Various editor programs are available for the input and test of new components, references as well as pure component and mixture data.

In case a larger number of data is to be included from in-house data banks, please inquire about our batch import tools.

# Data Import and Export

## Lesson Objectives

- get an overview on the different possibilities of data export from DDB to
  - the Aspen simulator
  - Spreadsheets like Microsoft Excel

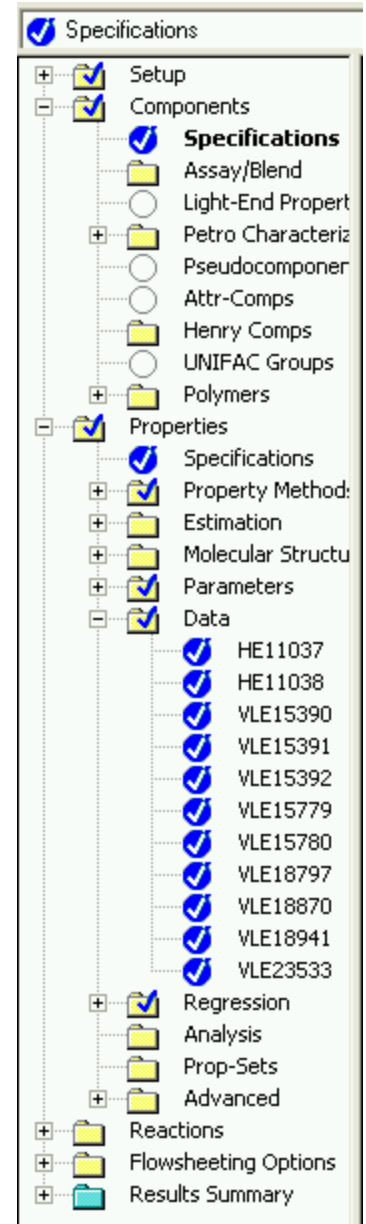
DDB-data and Parameters can be exported in a variety of ways:

- Cut/copy and paste
- DDB-format data files
- Aspen inp-files
- PPDX-files (Physical Property Data Exchange (IK-CAPE))

**Workshop**

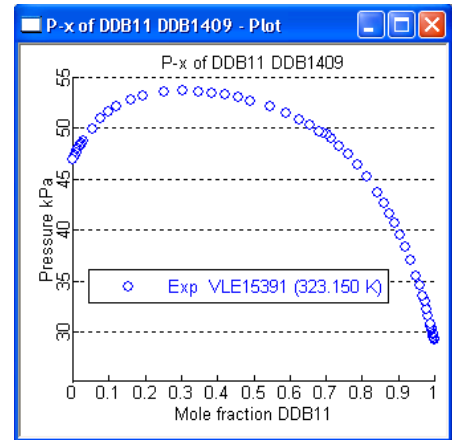
- In Mixture Properties, search for data for the system ethanol-ETBE.
- Export the data to an inp-file (Aspen inp export, show form, all possible data sets, Aspen inp export)
- Start the Aspen User interface and open the inp-file

As shown on the right all data sets and further specifications are set in the Aspen project.



not in Explorer Version

The data can directly be visualized using the Aspen plot wizard:



The regression case defined in the inp-file specifies ideal, evaluation and includes only the first data set. Change these settings as desired:

Setup Parameters Report Algorithm Diagnostics Generic pro

Property options

Method: IDEAL

Henry components:

Chemistry ID:

Use true components

Calculation type

Regression

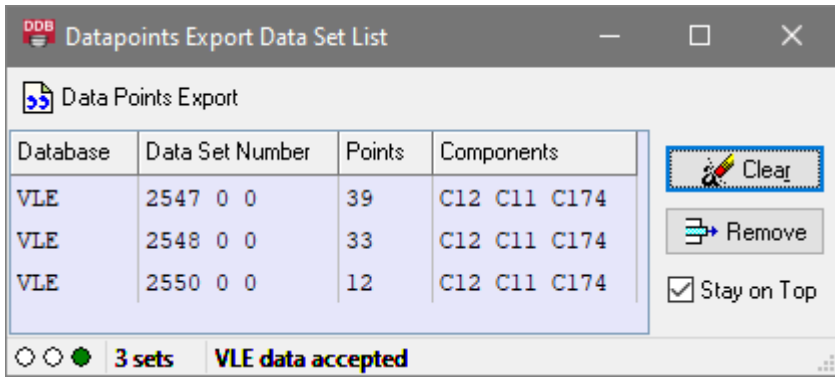
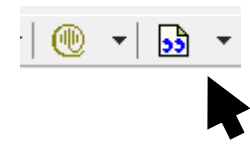
Evaluation

Data set	Weight	Consistency	Reject data	Test
VLE23533	1	<input type="checkbox"/> Perform test	<input type="checkbox"/> Reject	Area
*		<input type="checkbox"/> Perform test	<input type="checkbox"/> Reject	

Specifications

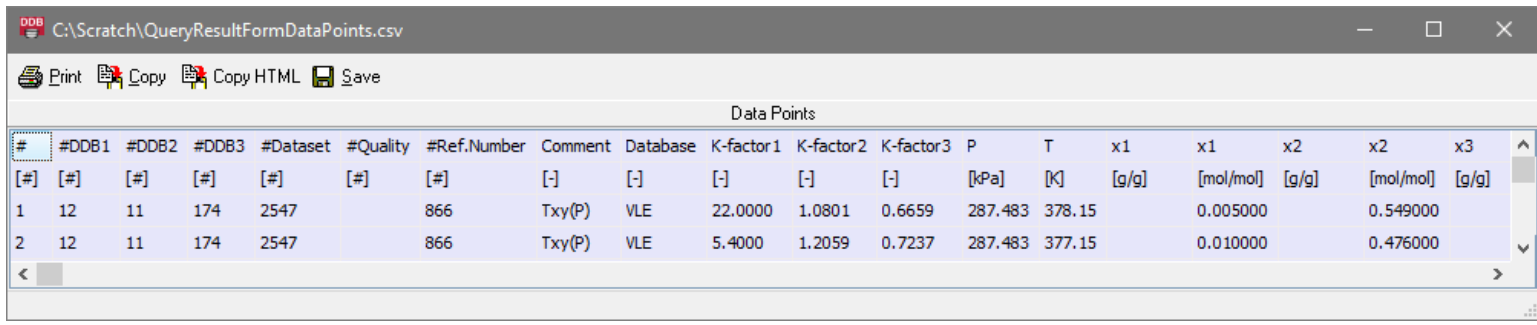
- Setup
- Components
  - Specifications
  - Assay/Blend
  - Light-End Propert
  - Petro Characteriz
  - Pseudocomponer
  - Attr-Comps
  - Henry Comps
  - UNIFAC Groups
  - Polymers
- Properties
  - Specifications
  - Property Method:
  - Estimation
  - Molecular Structu
  - Parameters
  - Data
    - HE11037
    - HE11038
    - VLE15390
    - VLE15391
    - VLE15392
    - VLE15779
    - VLE15780
    - VLE18797
    - VLE18870
    - VLE18941
    - VLE23533
  - Regression
  - Analysis
  - Prop-Sets
  - Advanced
- Reactions
- Flowsheeting Options
- Results Summary

## Complete Table Creation For Spreadsheets



Collecting data sets by  
drag and drop

## Table creation and copying to Windows clipboard





Only a rather rough walkthrough could have been presented in this part of the course.

This course did not cover any of the important aspects of mixture thermodynamic basics and applications. For this subject, special courses are available in German as well as English language .

When applying DDB to your own problems, please consult the manual or the hotline (support@ddbst.com).

In case of problems or special requirements, help including software patches can usually supplied quickly.

We are very busy improving and extending DDB. Please check [ww.ddbst.de](http://ww.ddbst.de) for updates and patches.

Thank you very much for your interest.