Dortmund Data Bank
DDB Software Package

Chemical Thermodynamics and Physical Properties with DDB

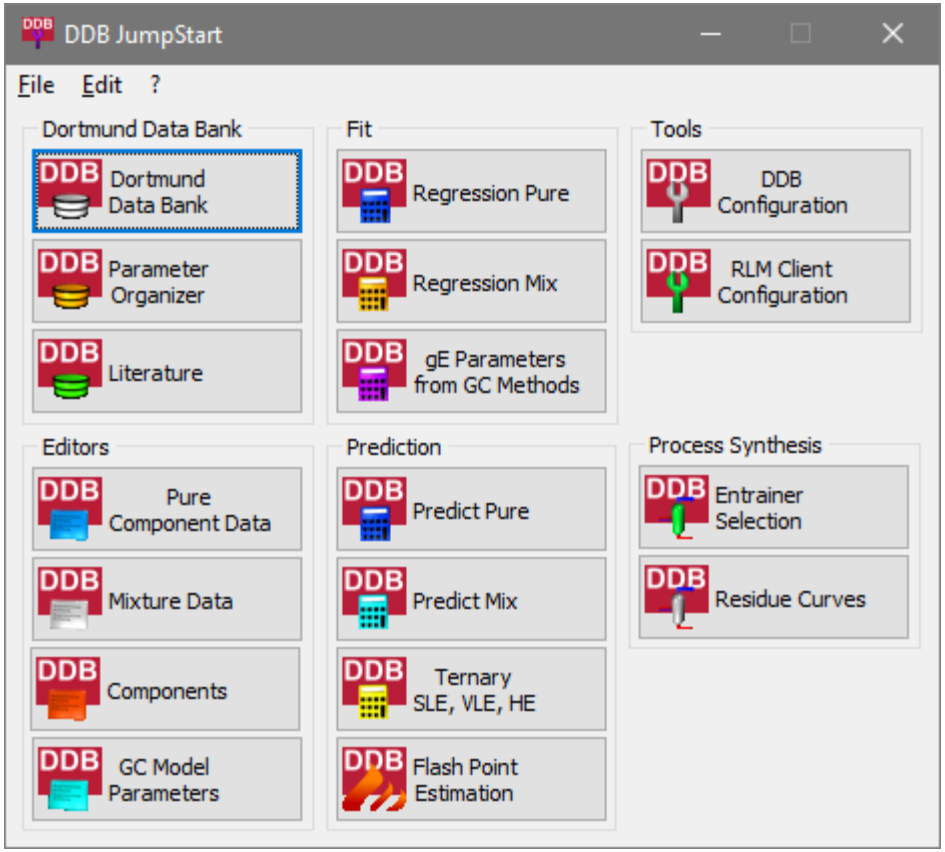
Contents

Parts of DDB

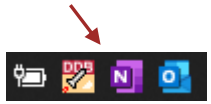
Lesson Objectives

- 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

DDB on your Computer - DDB Jumpstart



if not available here:



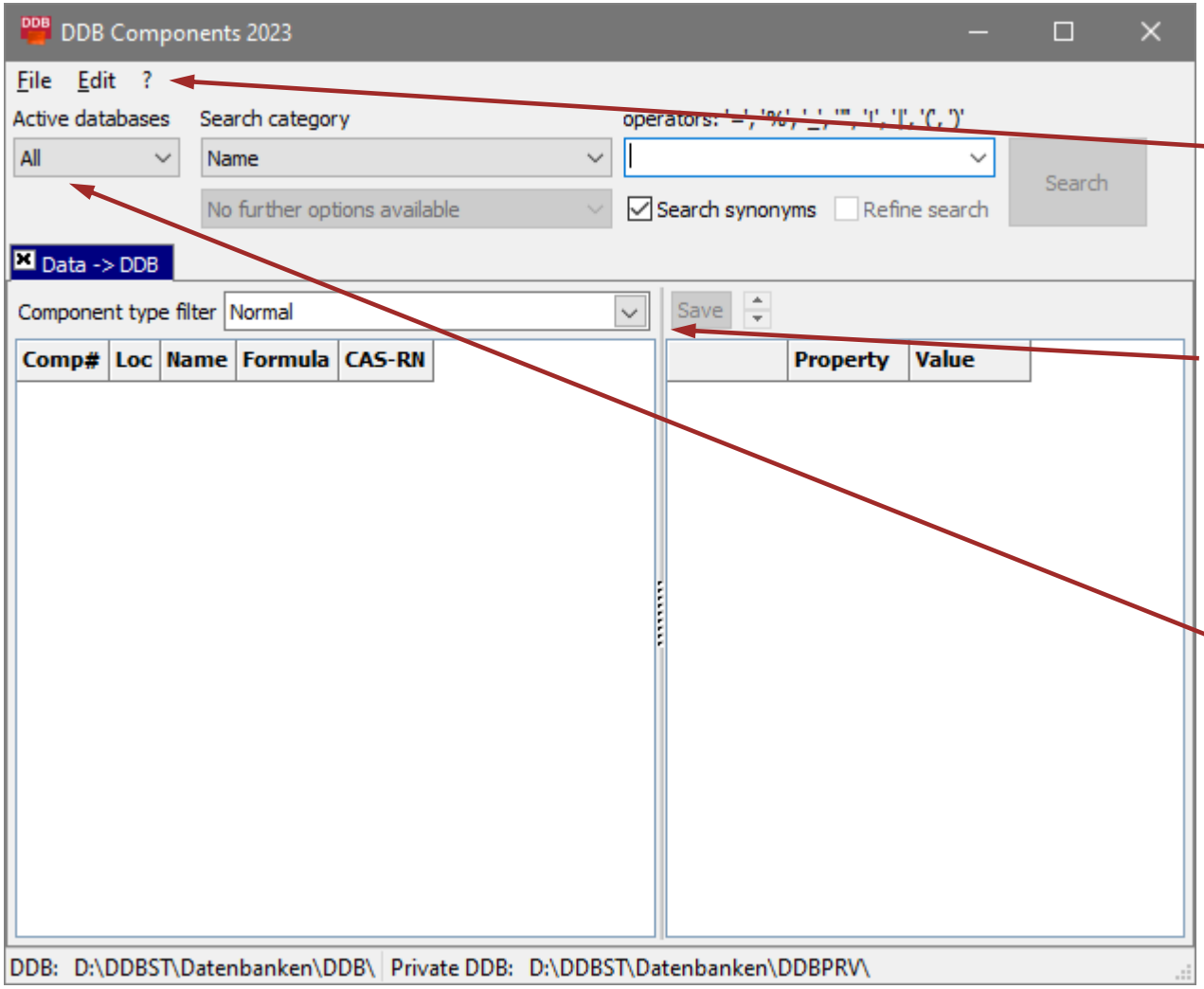
start via
Start – Programs – DDB 202x Client

Component Types and their Basic Data

- 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
- ….

Component Search Dialog

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

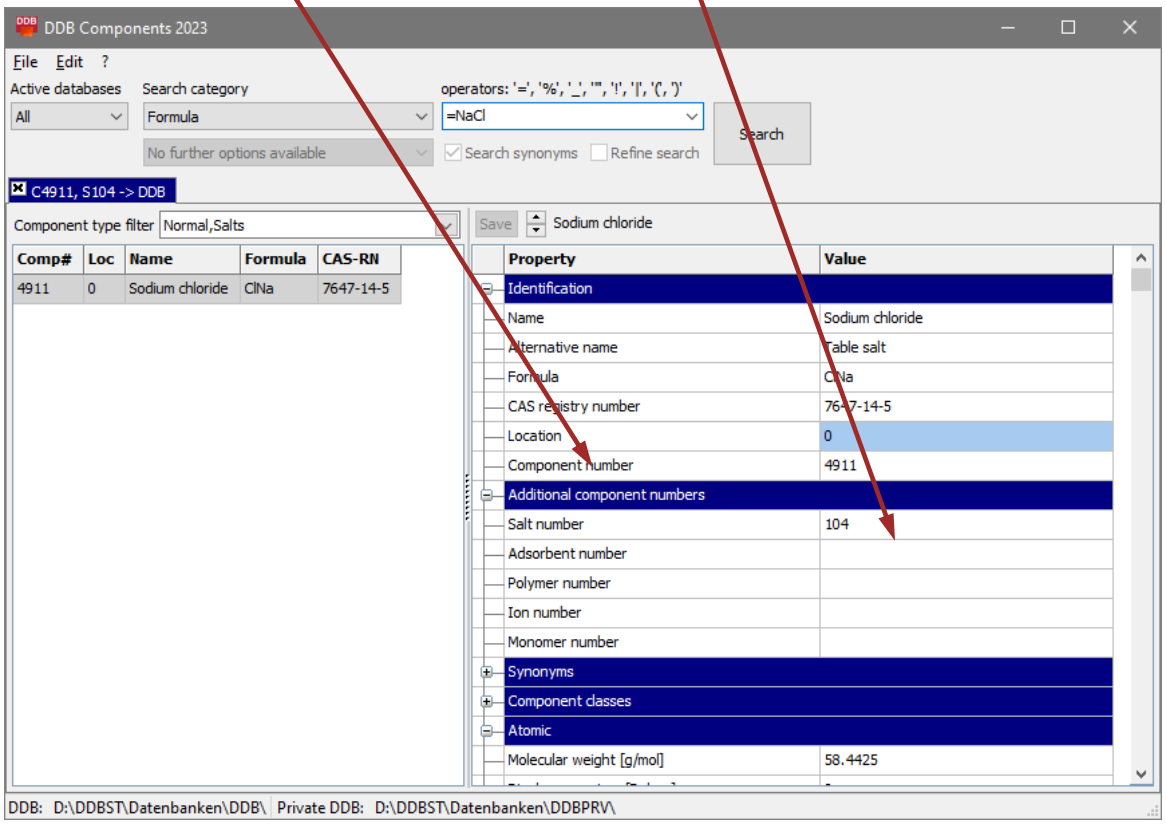
Connected Components/Salts

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
  ...



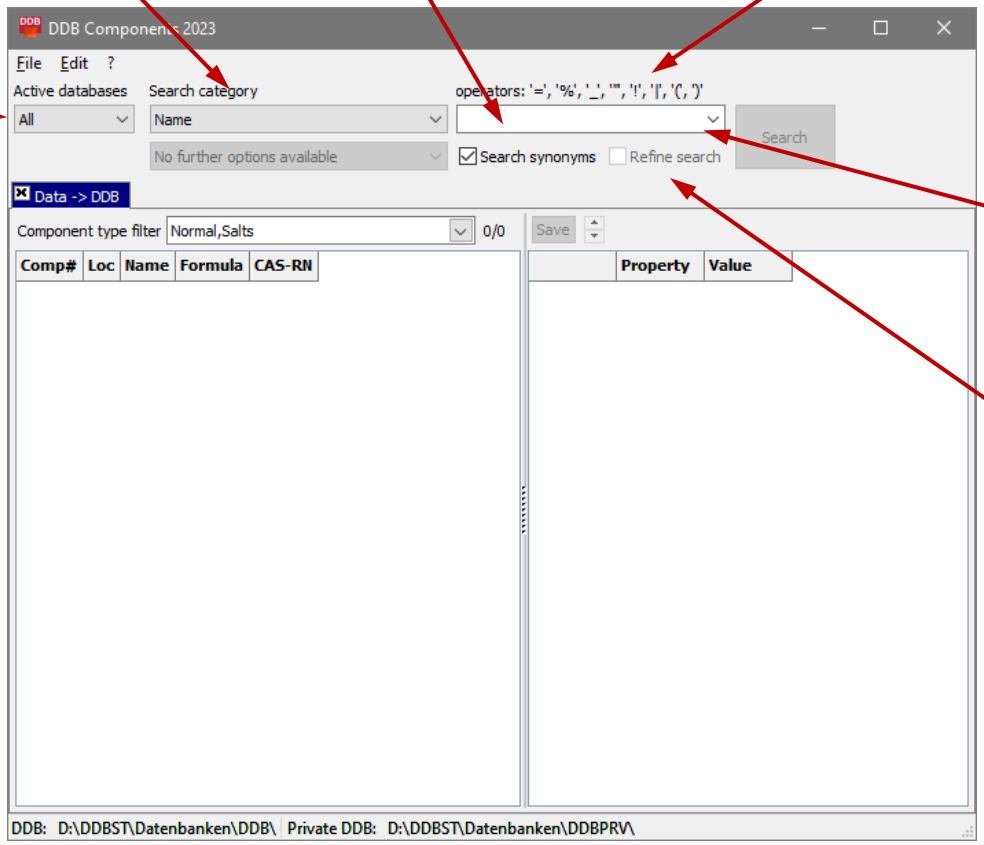
Search for Pure Components

what to search for

query expression

query syntax

active data bank

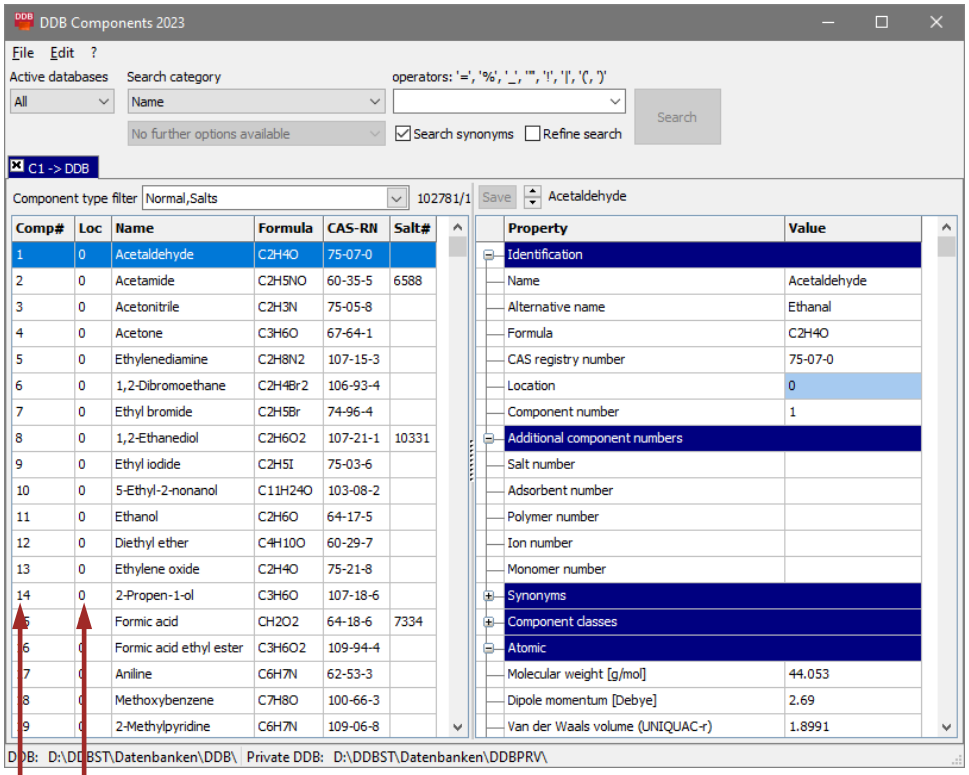


Select previous query from history

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, …).
…..

Select Components, Component Identification



location (DDB 0, private 1)

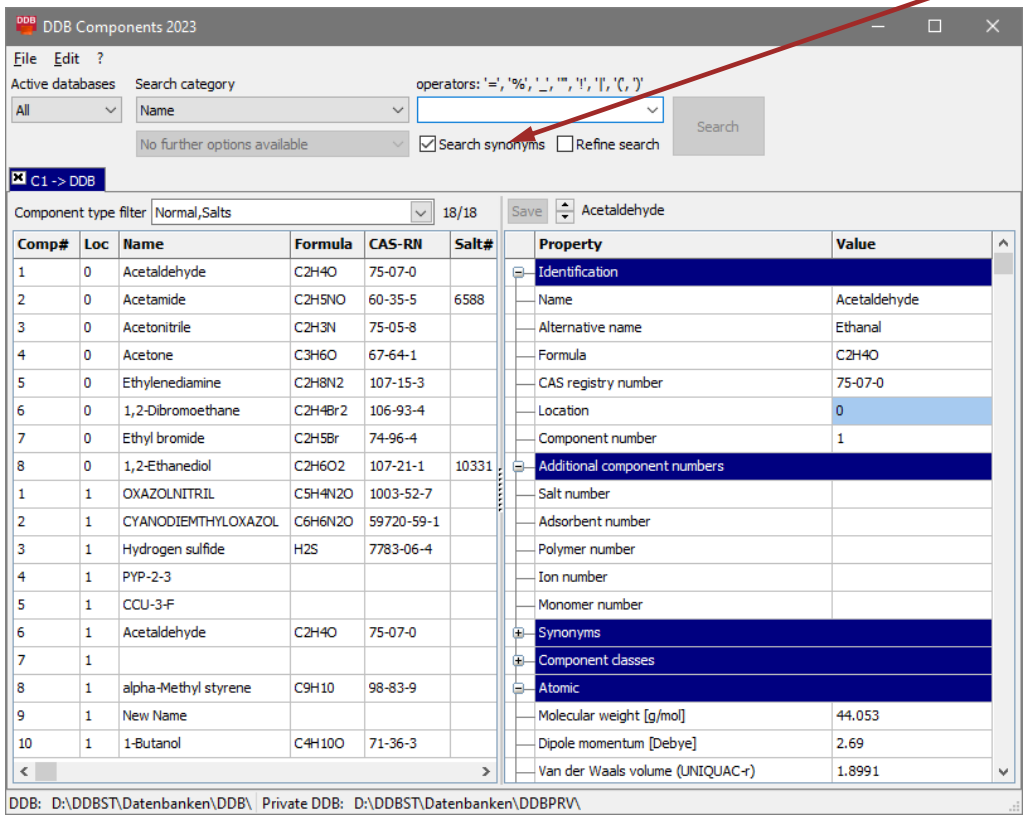
component code number

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.

Search for Pure Components - Synonyms



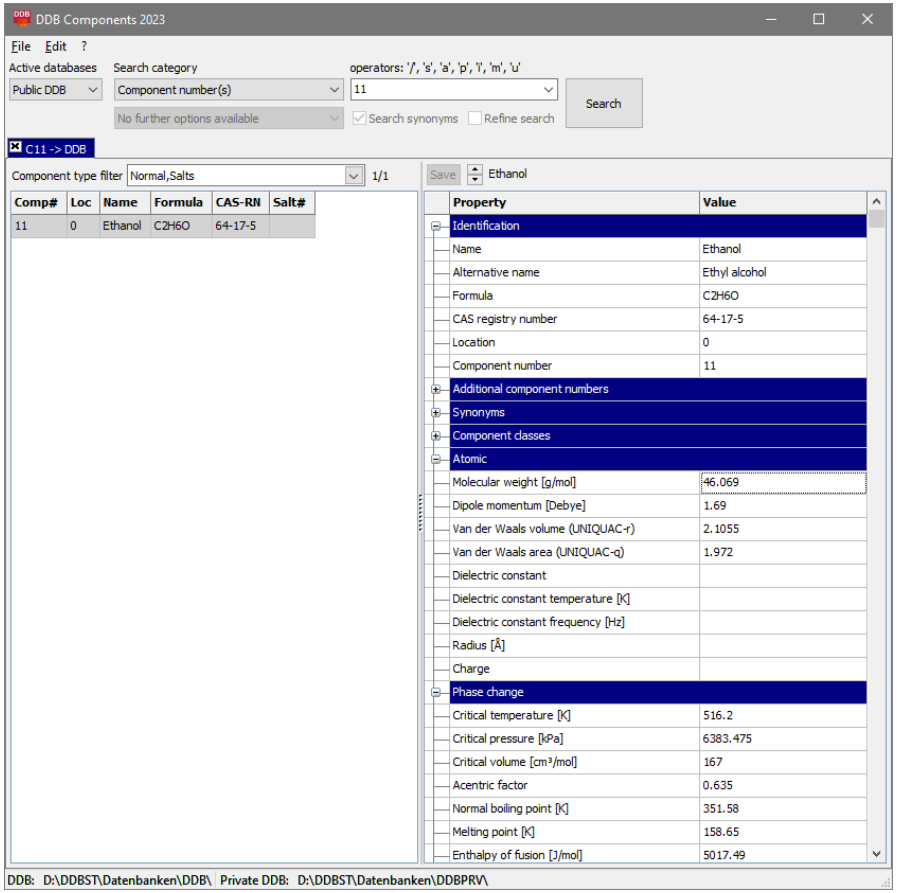
Search for synonyms

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

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

Searching synonyms is much slower …….

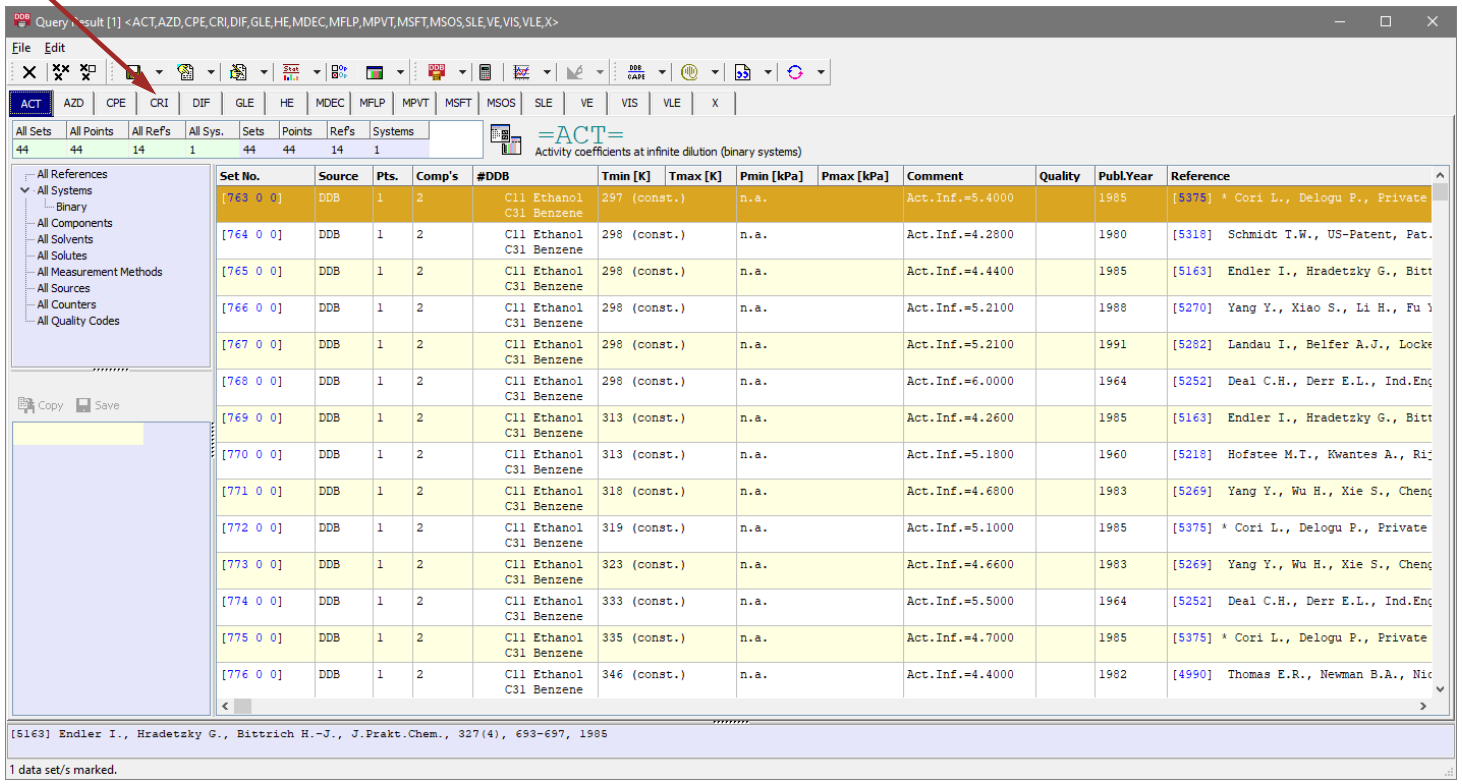
Basic Data (Usually Without Source Reference)



Molecular Structures (ChemDB)
Model Parameters (ParamDB)
Literature Sources,
Documents (LITERATURE)
COSMO σ-Profiles
…

Experimental Data (Nearly Strictly Only from Primary Reference)

Different Sheets for Each Data Bank



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 T.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

Component Selection Workshop

- 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)

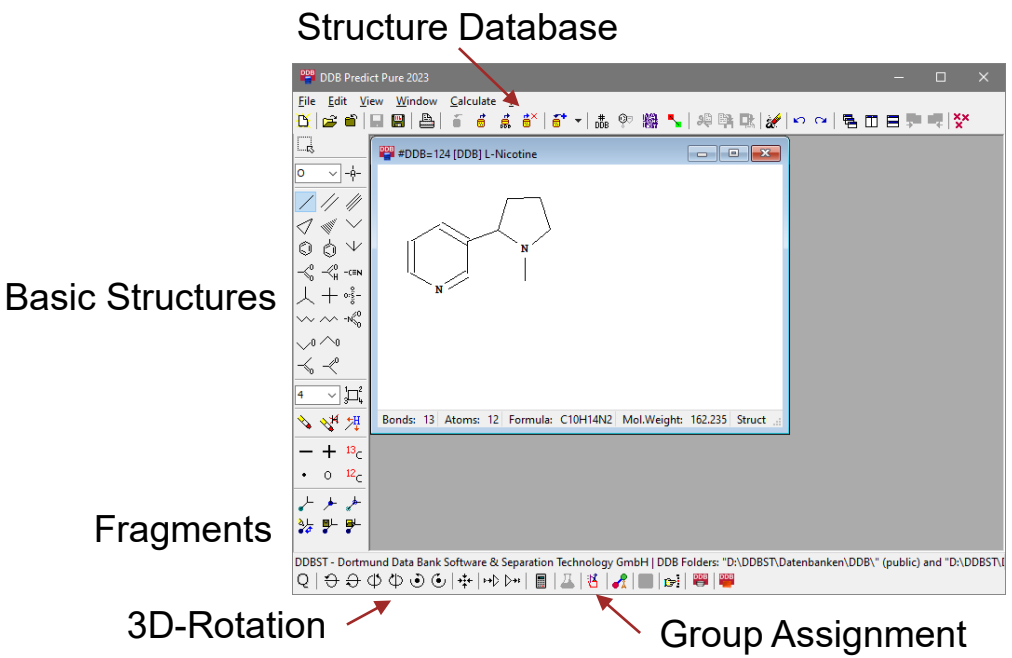
Molecular Structure Database and PredictPure

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

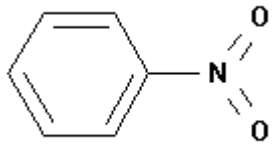


Demonstration

- Entering a structure in PredictPure.

Workshop

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



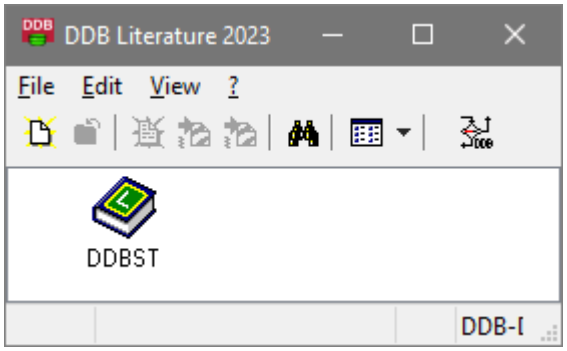
  - Search as sub-structure. Stop the search after the first 2,000 components.
  - Save the components matching the search structure as a list under the name "nitrobenzenes”

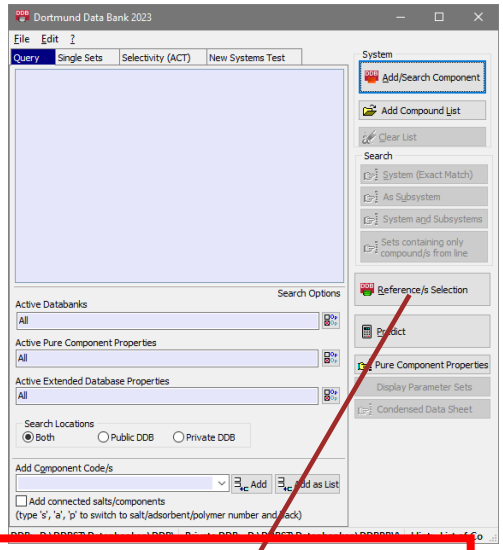
DDB Literature Management

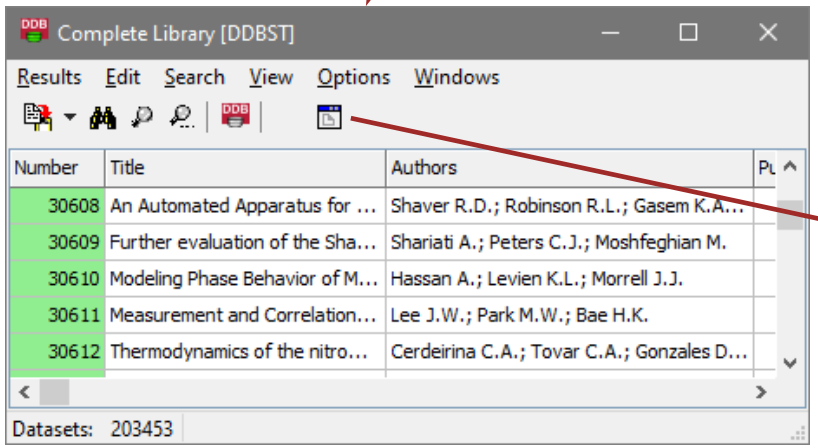
Lesson Objectives

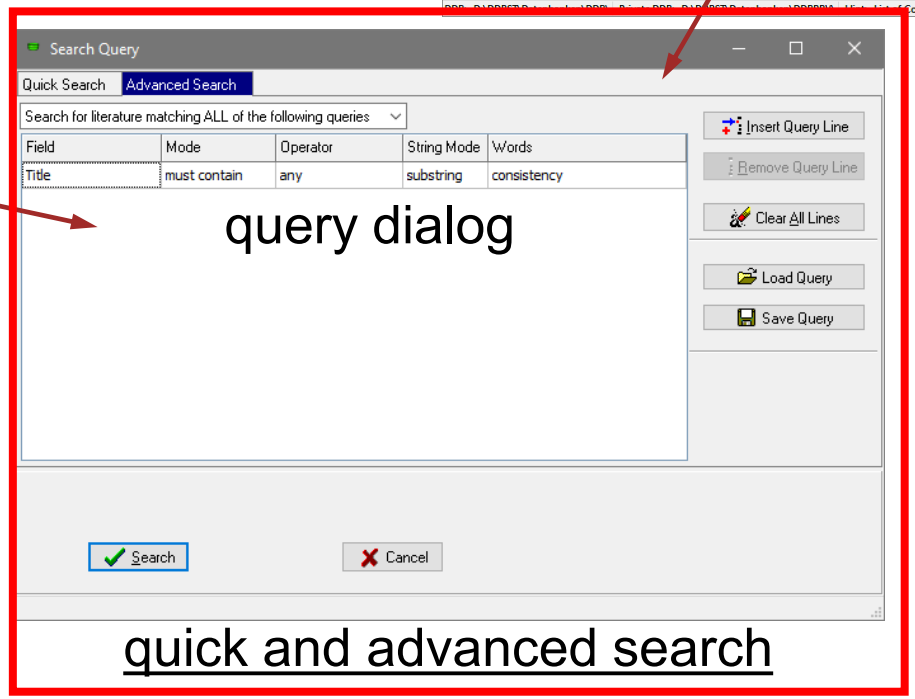
- Open and search Literature data banks
- Linked documents
- Links to data banks
- Find data from a reference

Search in Literature

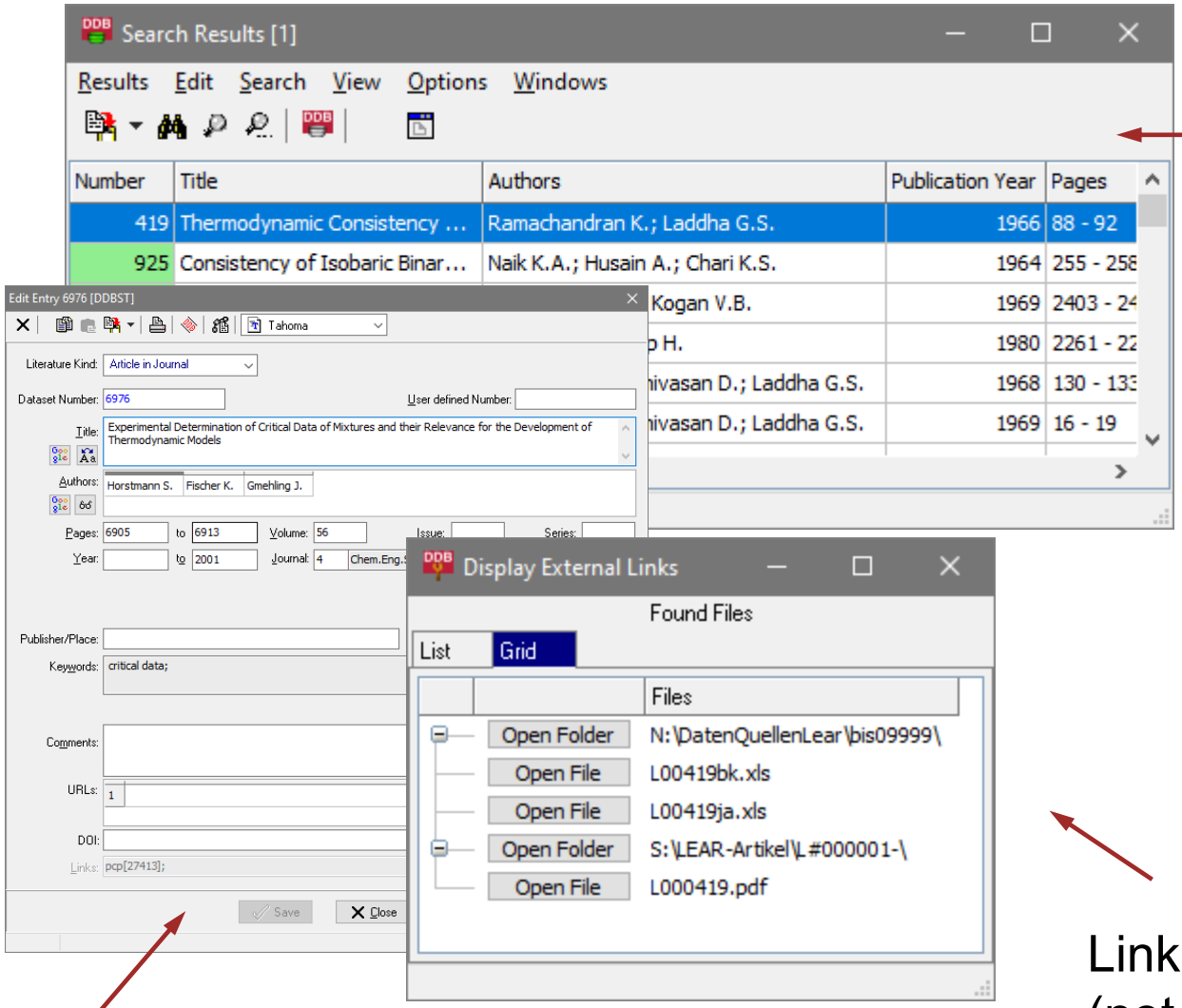








Linked Documents



query result list

query result data set

Linked document list (not in delivered Version)

Linked Documents Details

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.

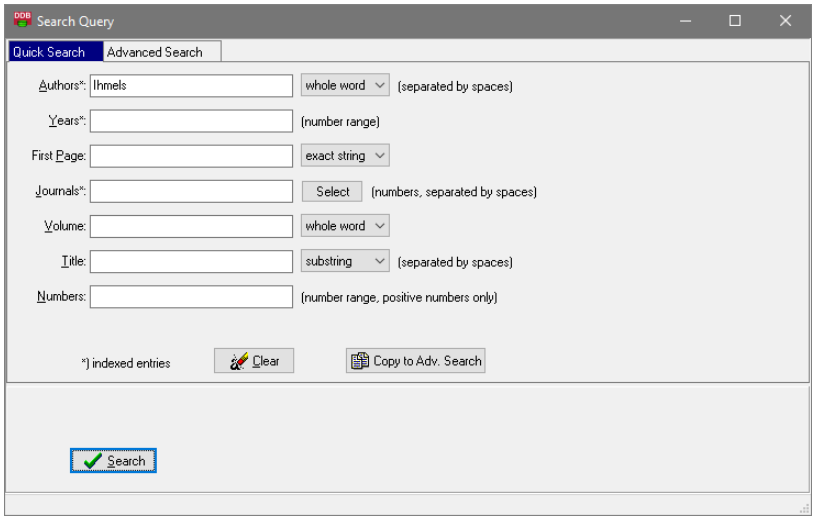
Document Linking can

- 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.

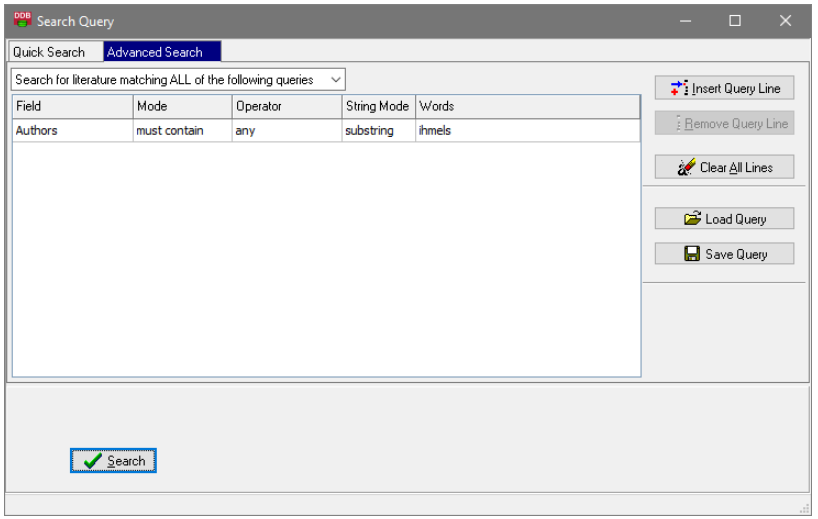
Mixture Properties Query via Reference

Workshop

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



or



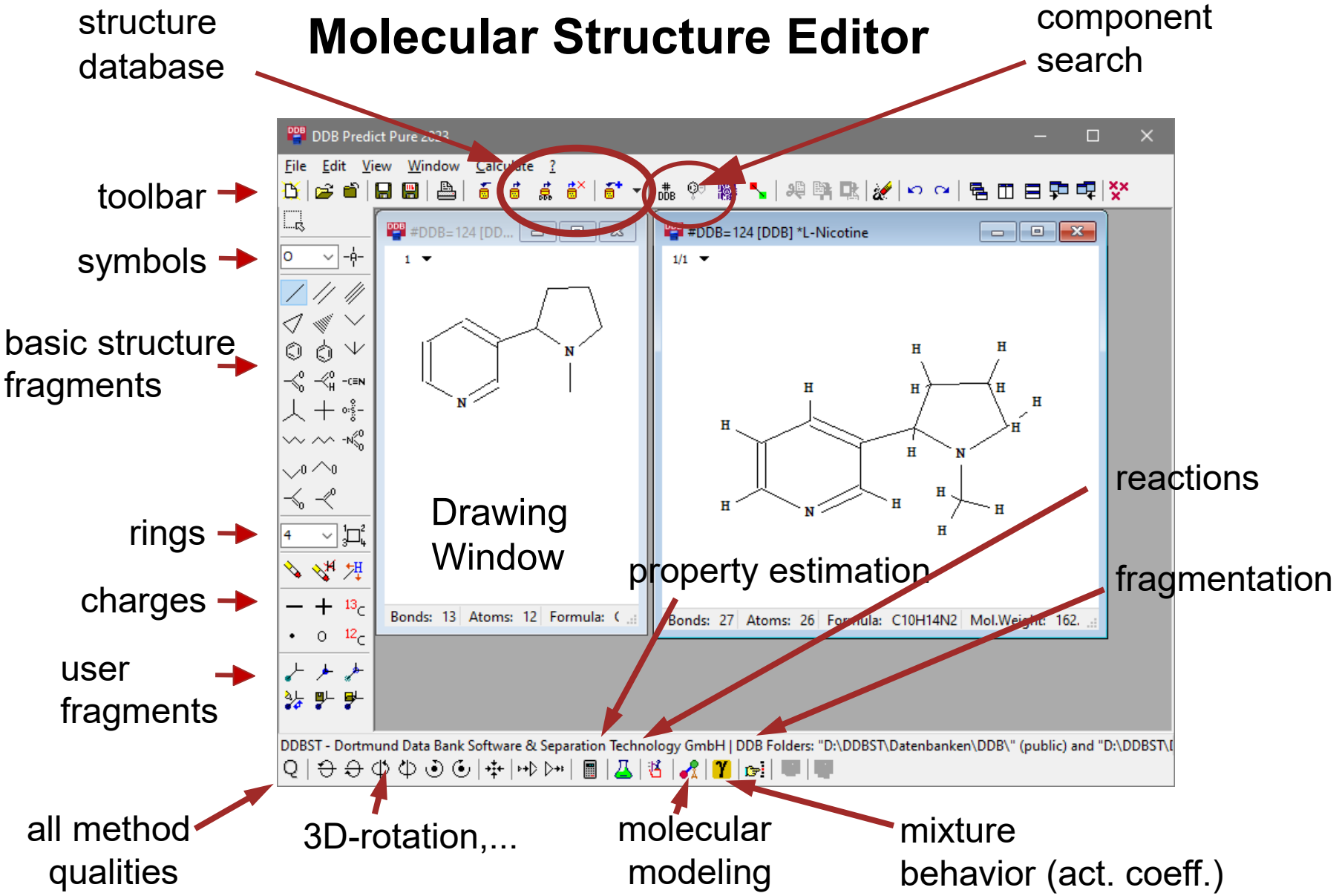
(in Literature, complex queries can be entered, saved and loaded)

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.

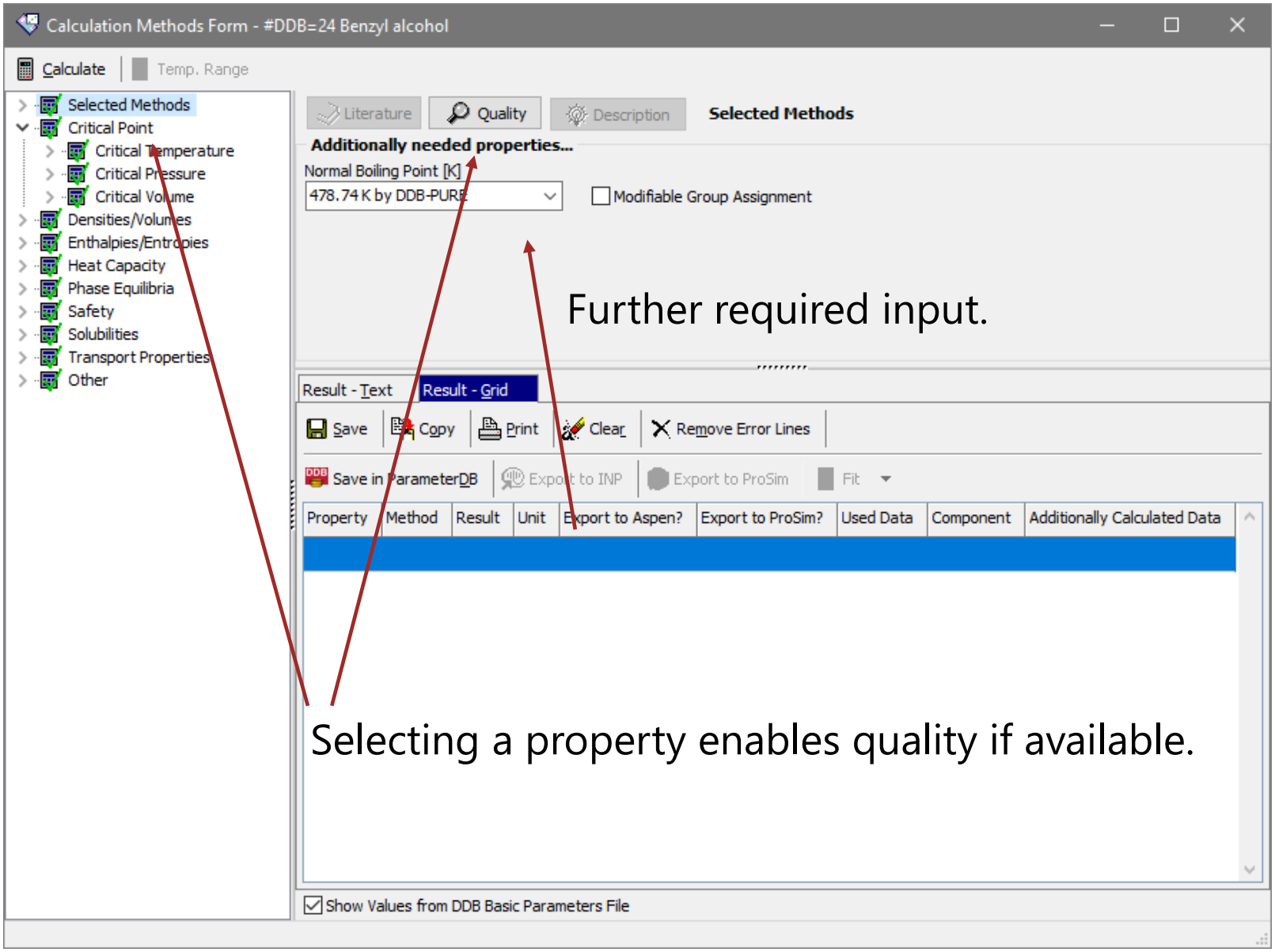
Lesson Objectives

- 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 (σ-Profile calculation)

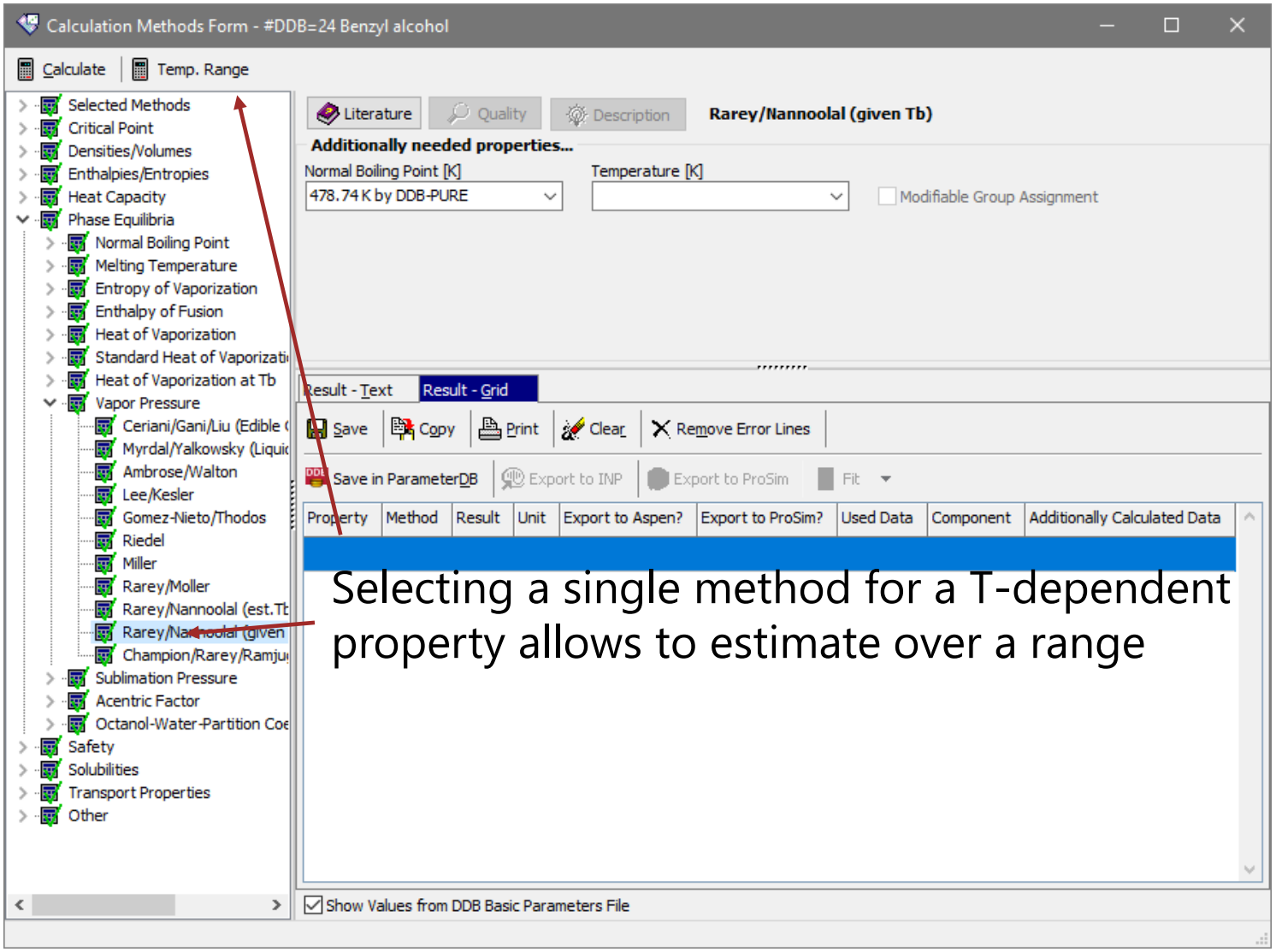
Molecular Structure Editor



PredictPure Calculation Dialog



PredictPure Calculation Dialog



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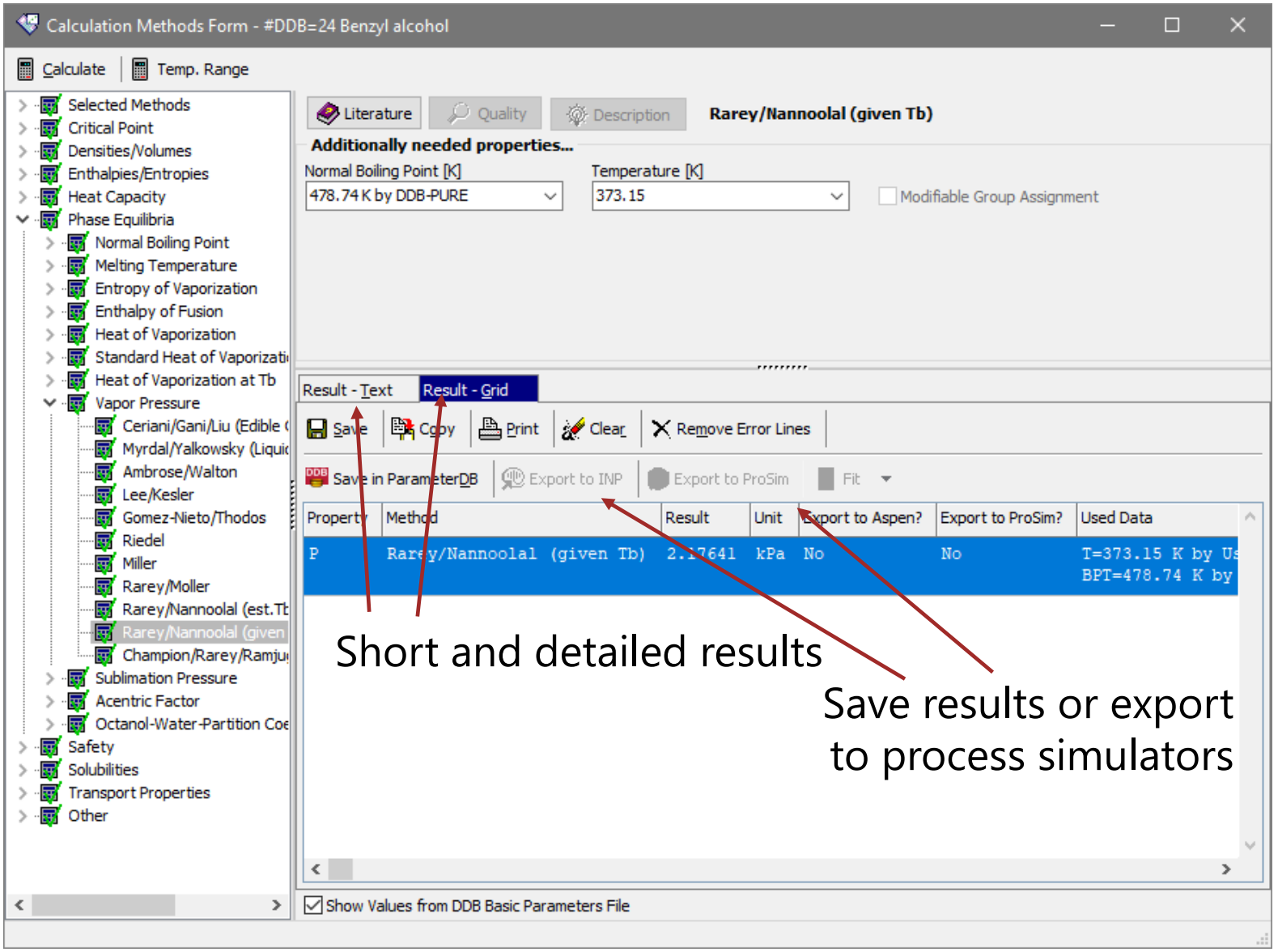
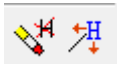
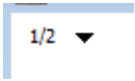
PredictPure Calculation Dialog



Workshop

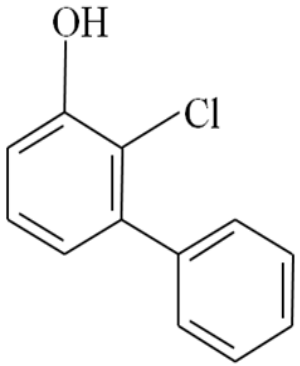
- Start PredictPure, open a new document window and draw the structure of 1,4-butanediol (HO-CH_2-CH_2-CH_2-CH_2-OH) using  .
- Use  to add and delete hydrogen atoms.
- Search the structure in the DDB (exact search).
- Accept the found component 614 

. 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.

Workshop 2

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

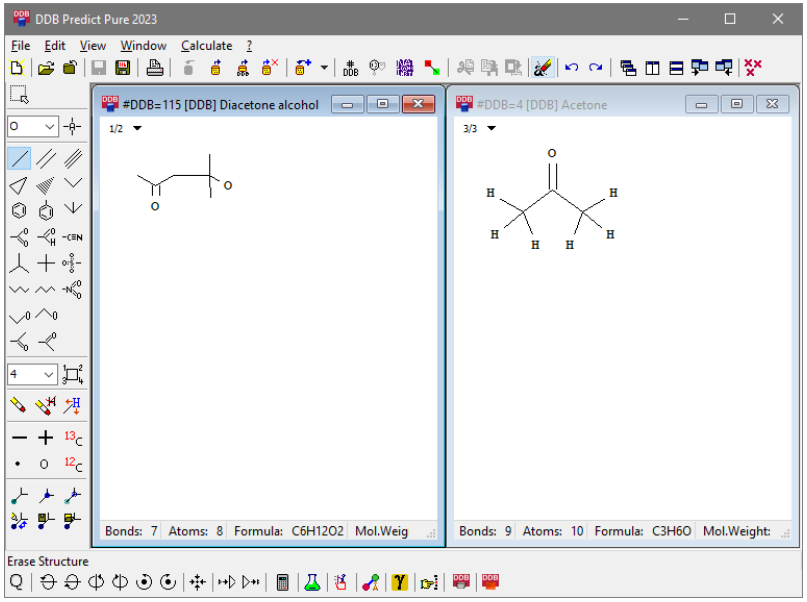


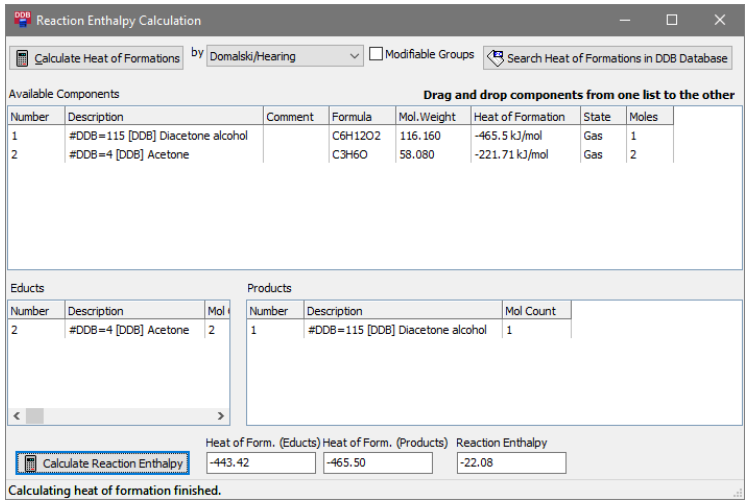
- Search this structure in the DDB as substructure
- Estimate important properties like critical data, normal boiling temperature and vapor pressure curve using different methods. Compare the results. (the experimental normal boiling point is 590.15 K)

- 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.





PredictPure - Structure Optimization - 1

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.

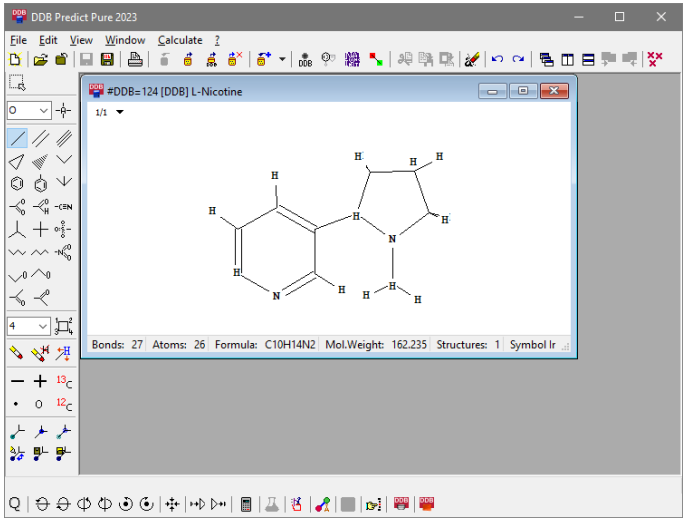
More rigorous structure optimization can be performed using the free packages MOPAC and Tinker.

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).

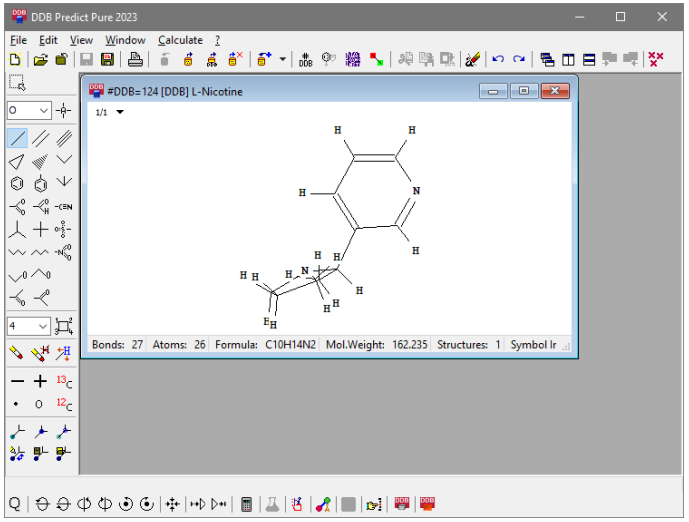
3D display is available via the free tool RasWin.

PredictPure - Structure Optimization - 2

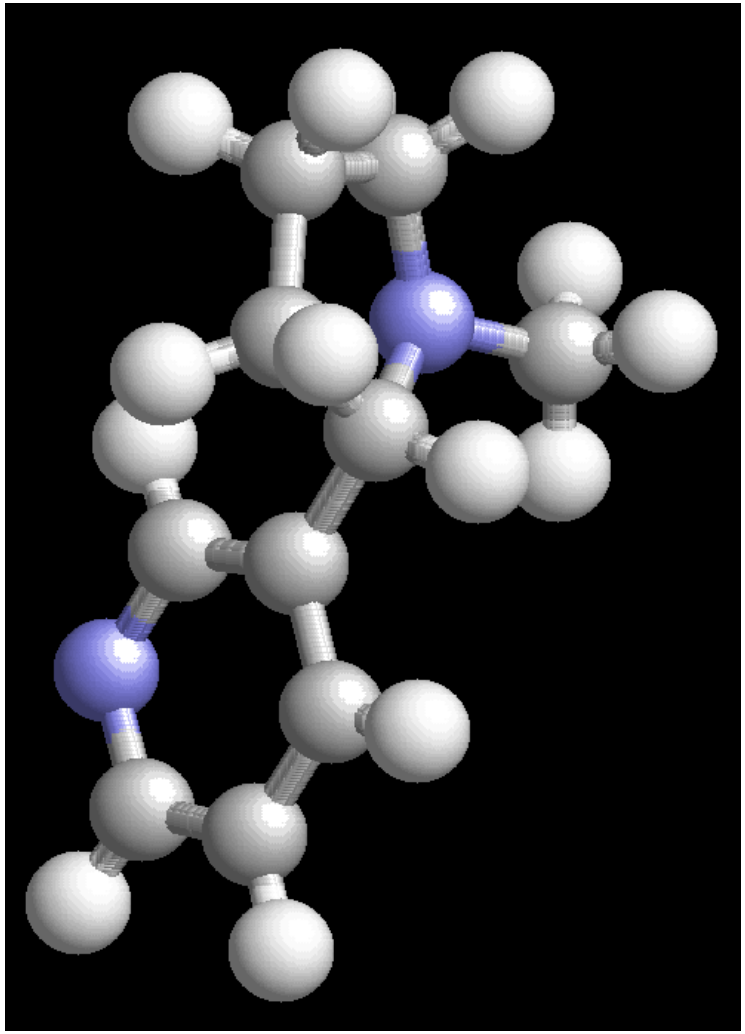
Load nicotine and add hydrogen atoms.



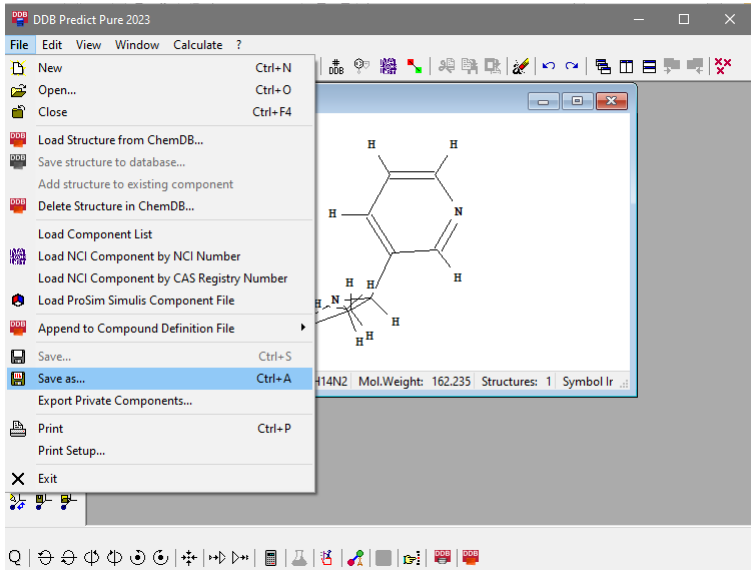
Calculate – MOPAC - run to optimize the molecular geometry, use coordinates.
Rotate the structure.



Display the structure using RasWin:



PredictPure - Gaussian Inputfile




```
%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

DDB - Pure Component Data Bank

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 2nd virial coefficient together with predictions using the RK, SRK and PR equations of state using  .

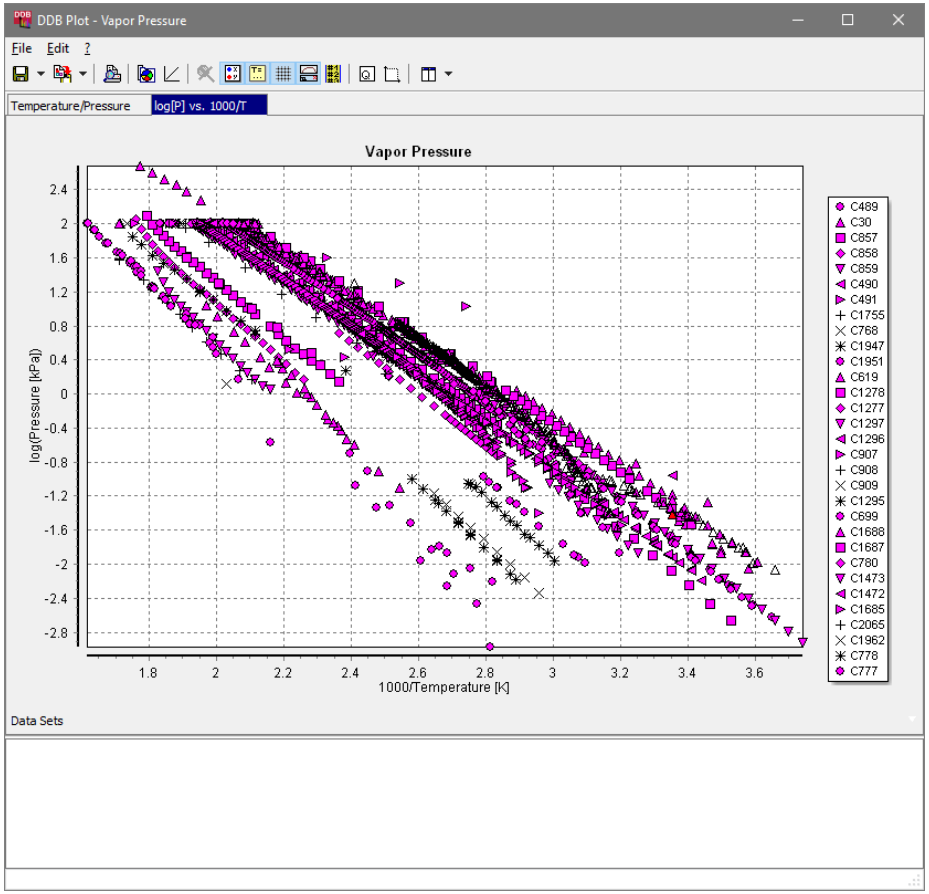
DDB - Pure Component Data Bank – Graphical Output

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

Workshop

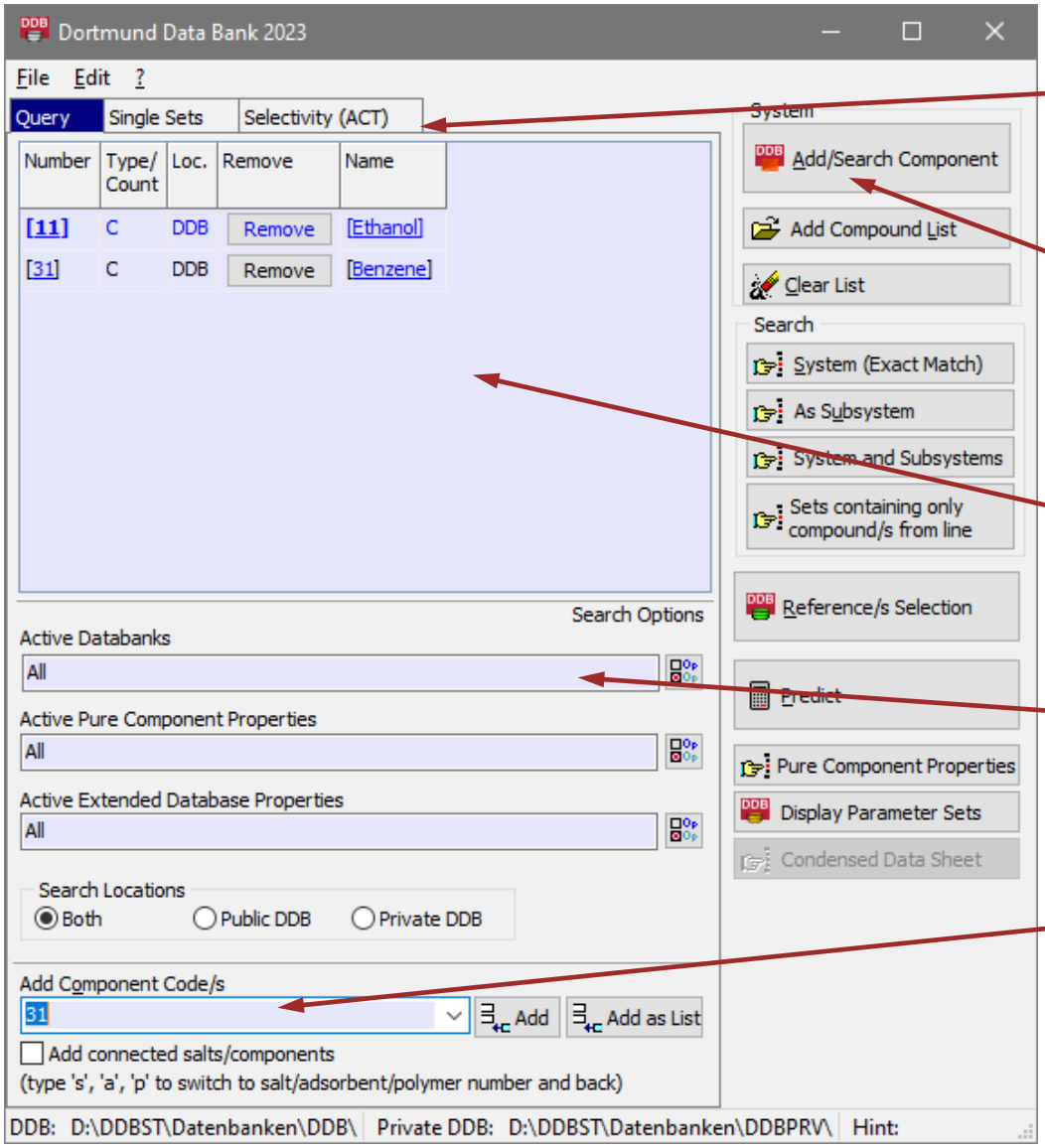
- Plot the vapor pressure of nitrobenzenes as log(P) vs. 1000/T.

Use the component list file previously stored from PredictPure.



DDB - Mixture Properties - Query

Search for a system via components



Special Selectivity Query

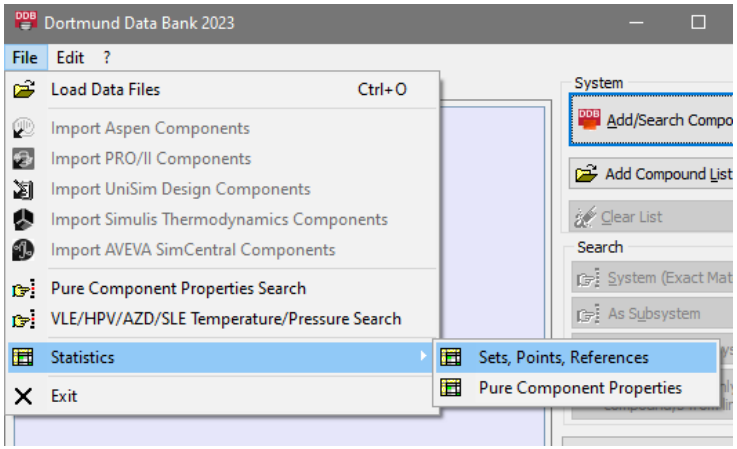
Add components via selection dialog, component lists via file open dialog

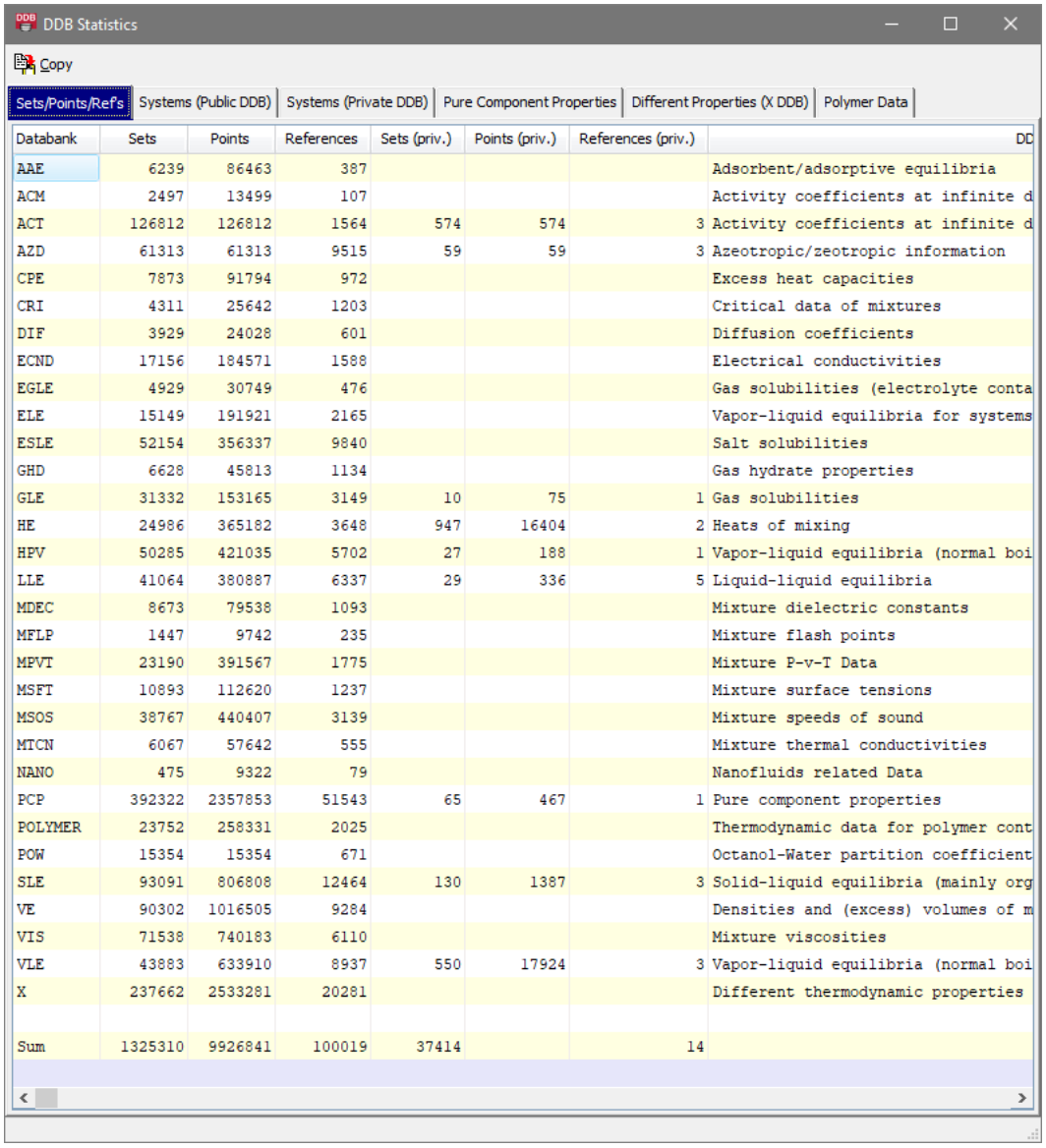
List of components or component lists

Select data banks to search (usually all)

Add components or component lists via code numbers

DDB - DDB Statistics

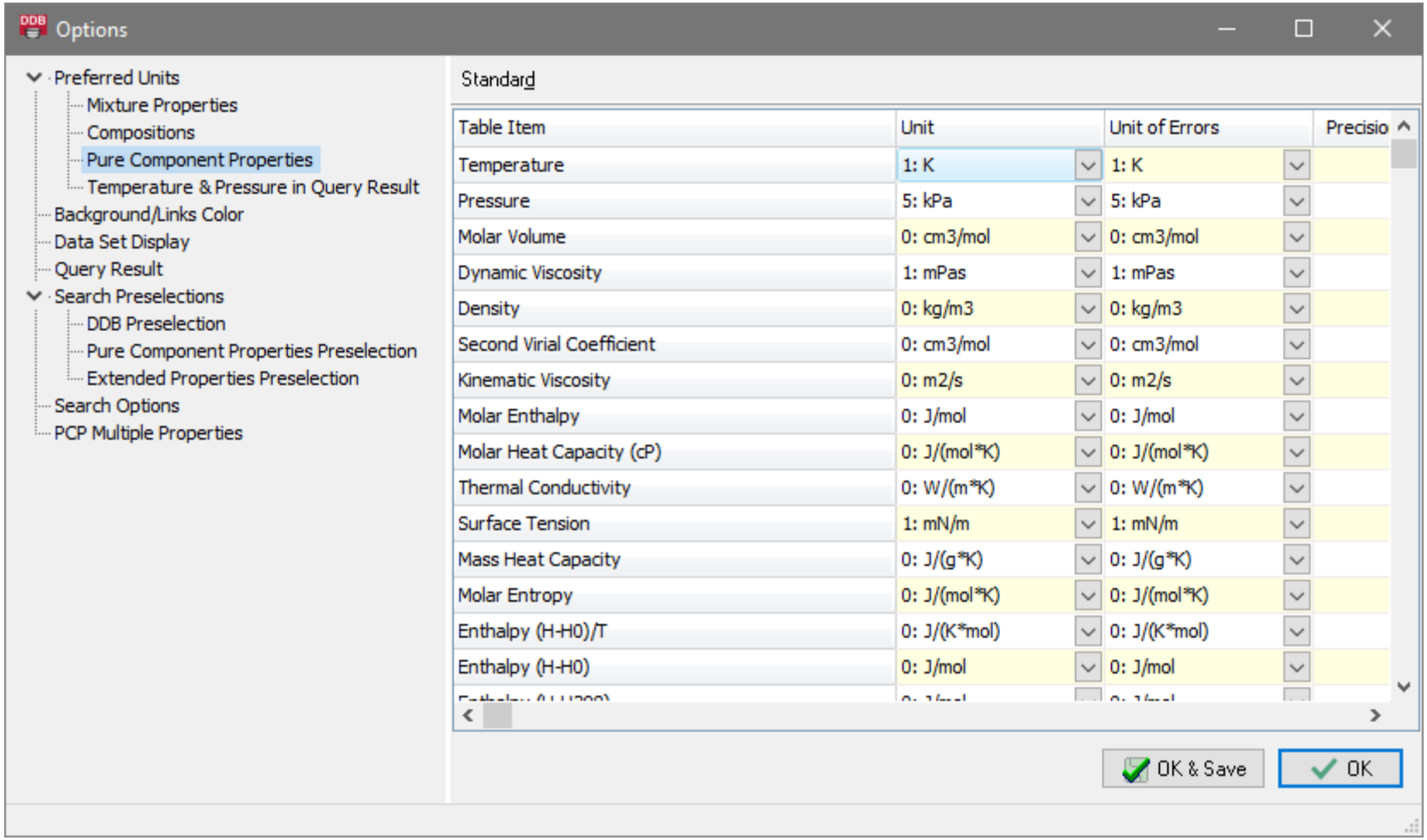




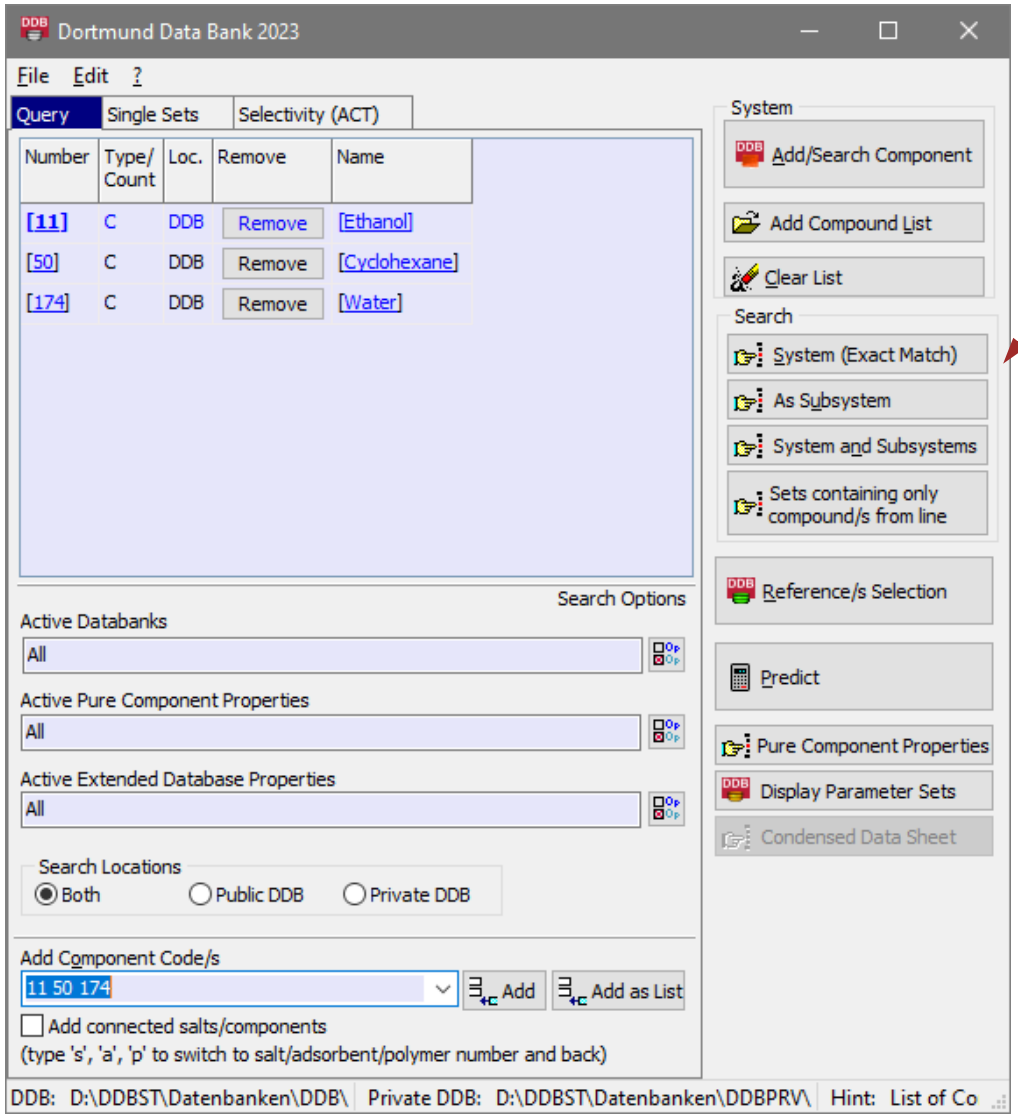
Databank	Sets	Points	References	Sets (priv.)	Points (priv.)	References (priv.)	DD
AAE	6239	86463	387				Adsorbent/adsorptive equilibria
ACM	2497	13499	107				Activity coefficients at infinite d
ACT	126812	126812	1564	574	574	3	Activity coefficients at infinite d
AZD	61313	61313	9515	59	59	3	Azeotropic/zeotropic 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



DDB - Mixture Properties - Query



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.

DDB - Mixture Properties – Query - Search for a System

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.

DDB - Mixture Properties – Query - Search for a System

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

DDB - Mixture Properties - Query - Result

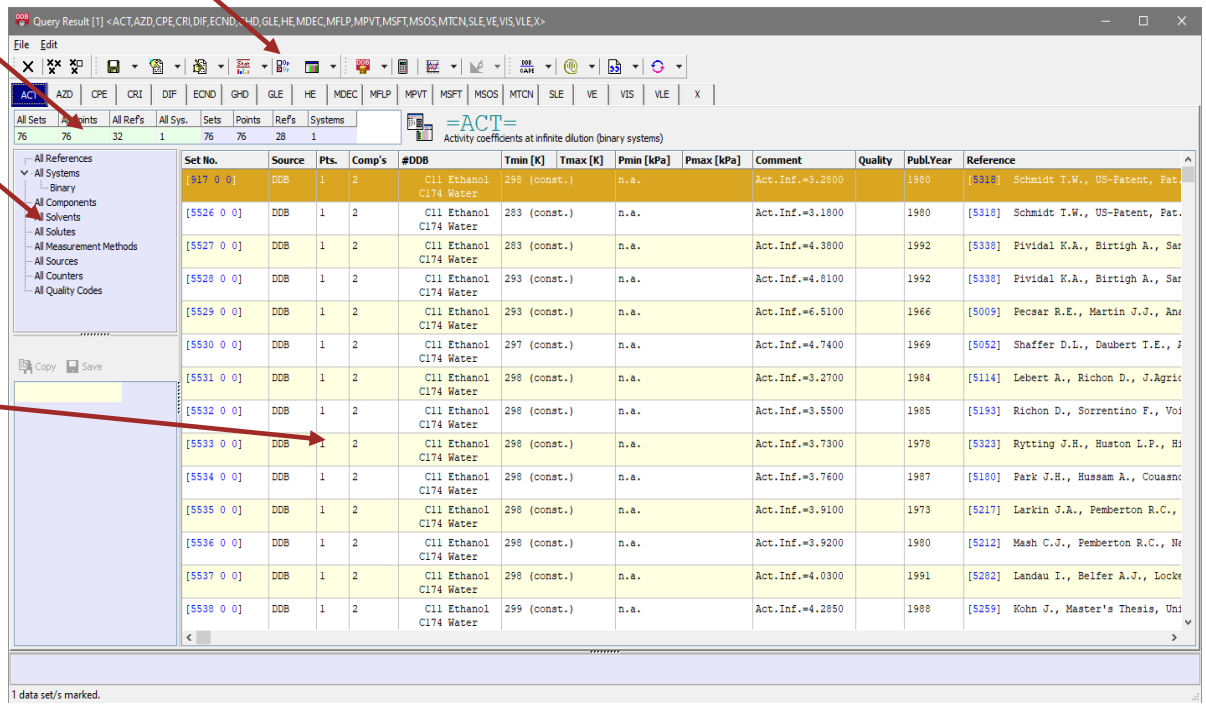
- **Data Bank Pages:**
show data sets of only one data bank. Switch between the data banks by a single-click on the data bank pages.

- **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



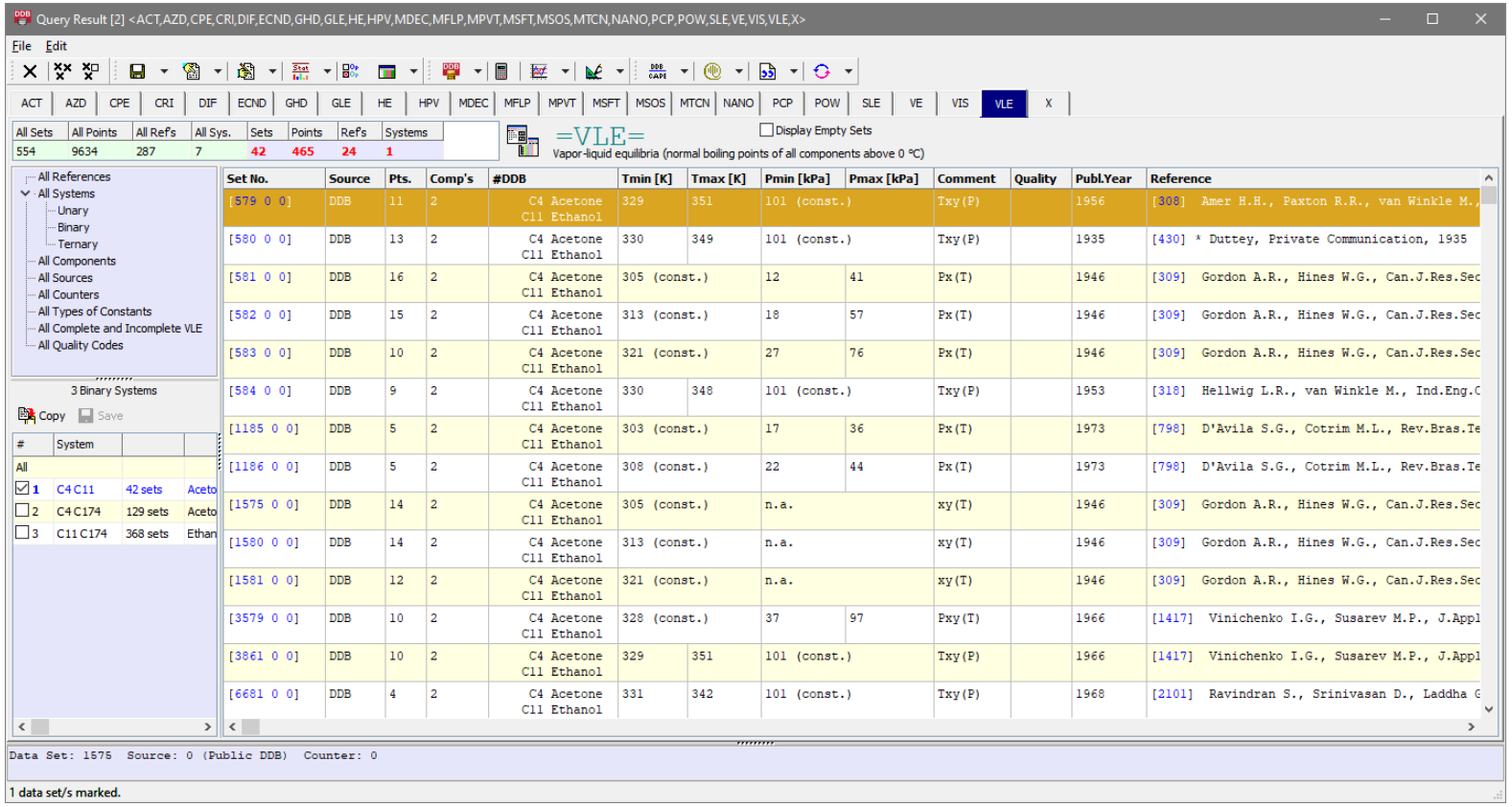
DDB - Mixture Properties Query - Result – Table - Workshop

Workshop

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

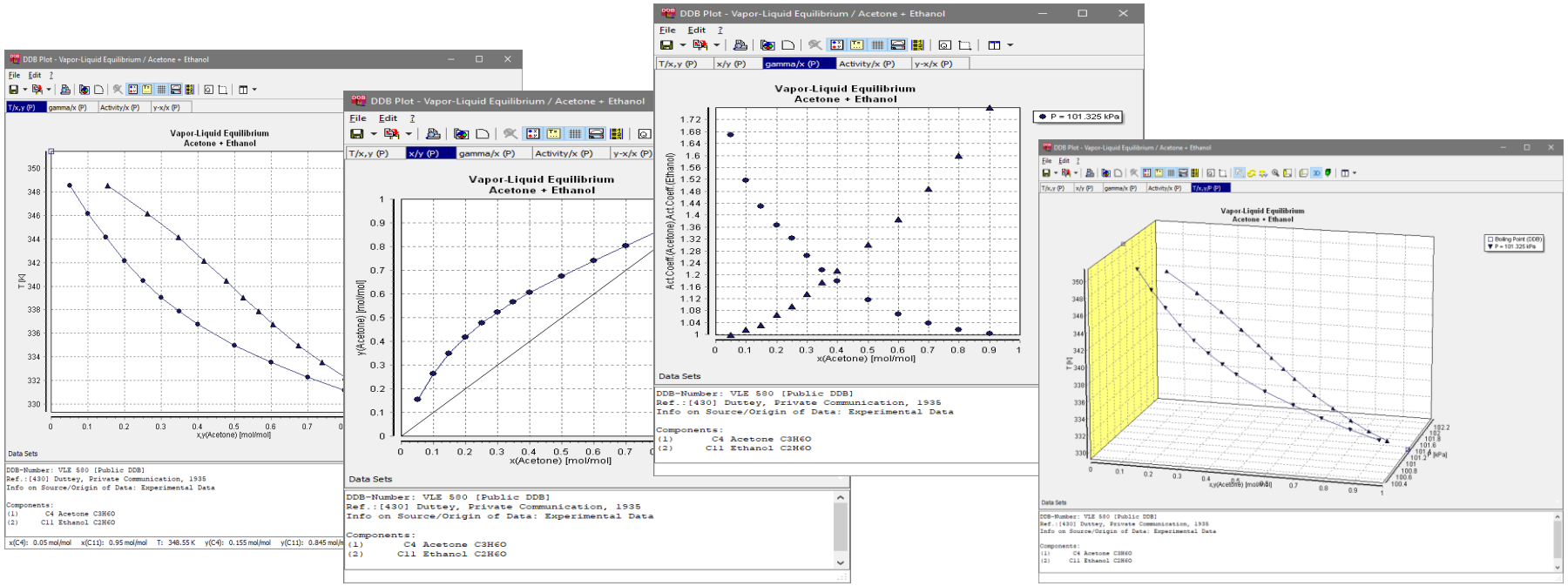
In the query result dialog, select VLE data for the binary acetone - ethanol

The query result dialog should look like this:



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.

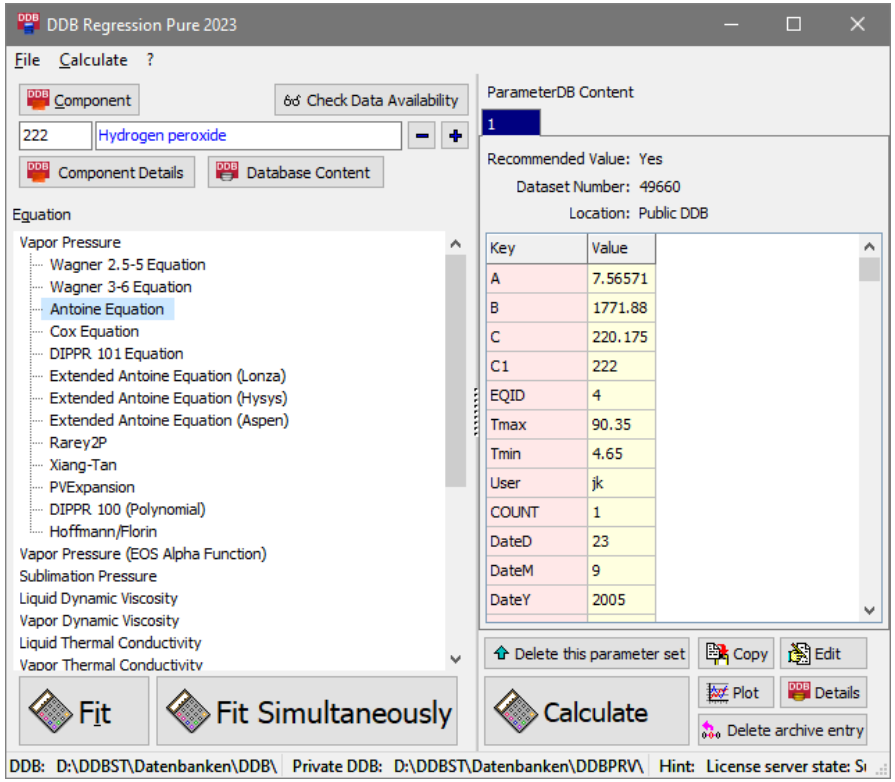
Pure Component Data Regression

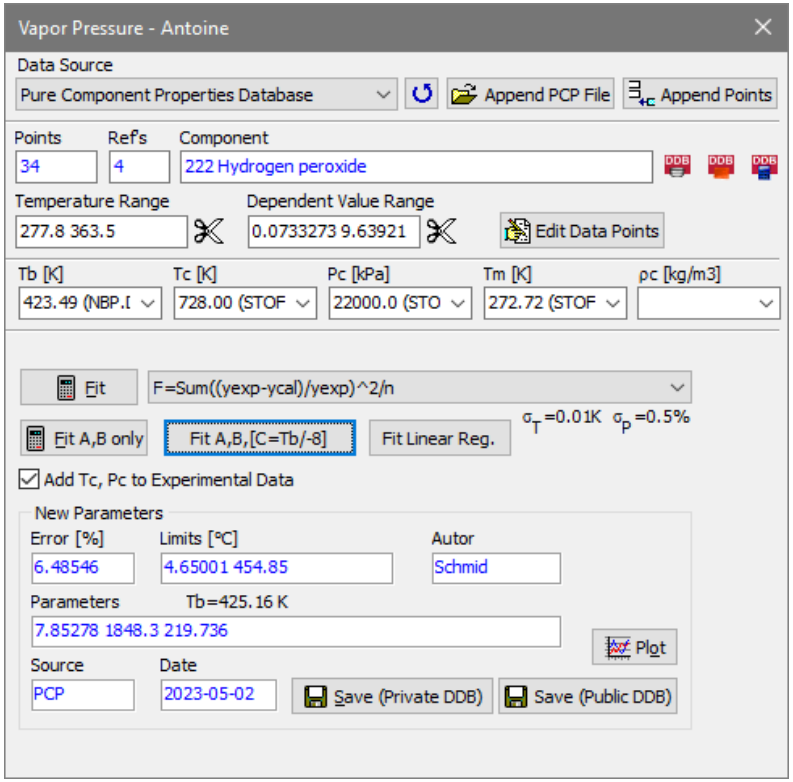
Lesson Objectives

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

DDB - Pure Component Data Regression

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





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

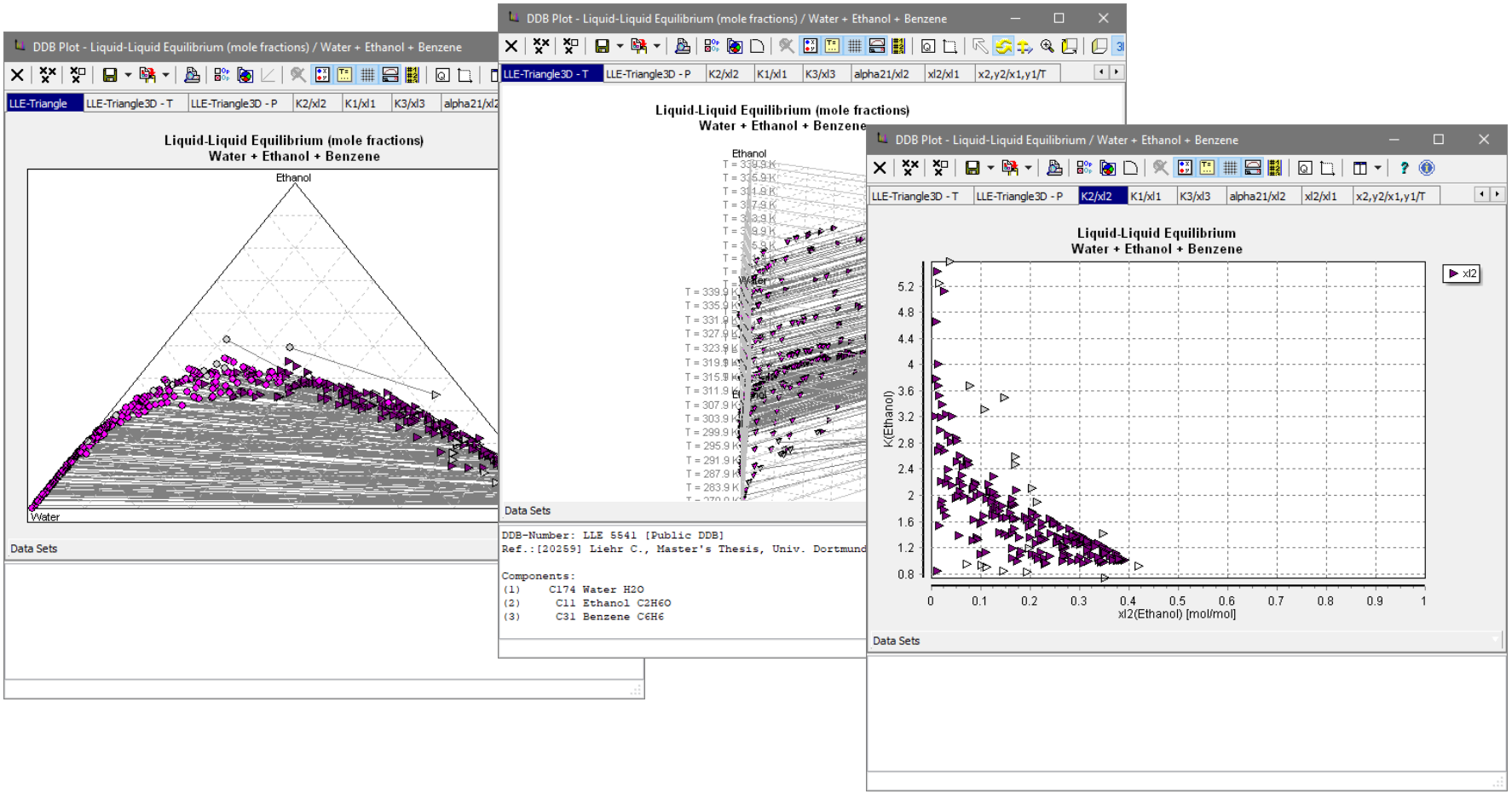
Lesson Objectives

- 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

DDB - Mixture Properties - Data Regression LLE - Workshop

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.

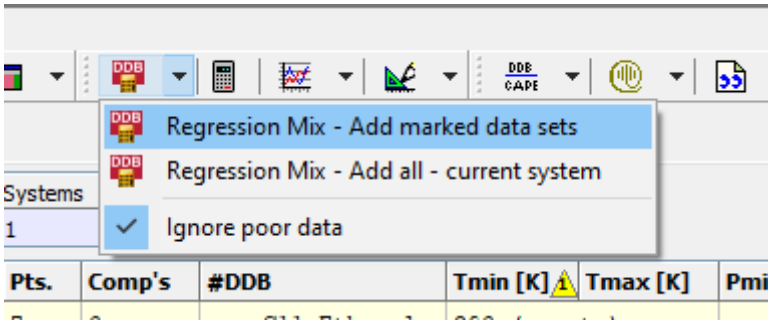
Simultaneous Mixture Data Regression

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

DDB - Mixture Properties – RegressionMix

Starting RegressionMix from the Data query Result dialog:



DDB - Mixture Properties – RegressionMix

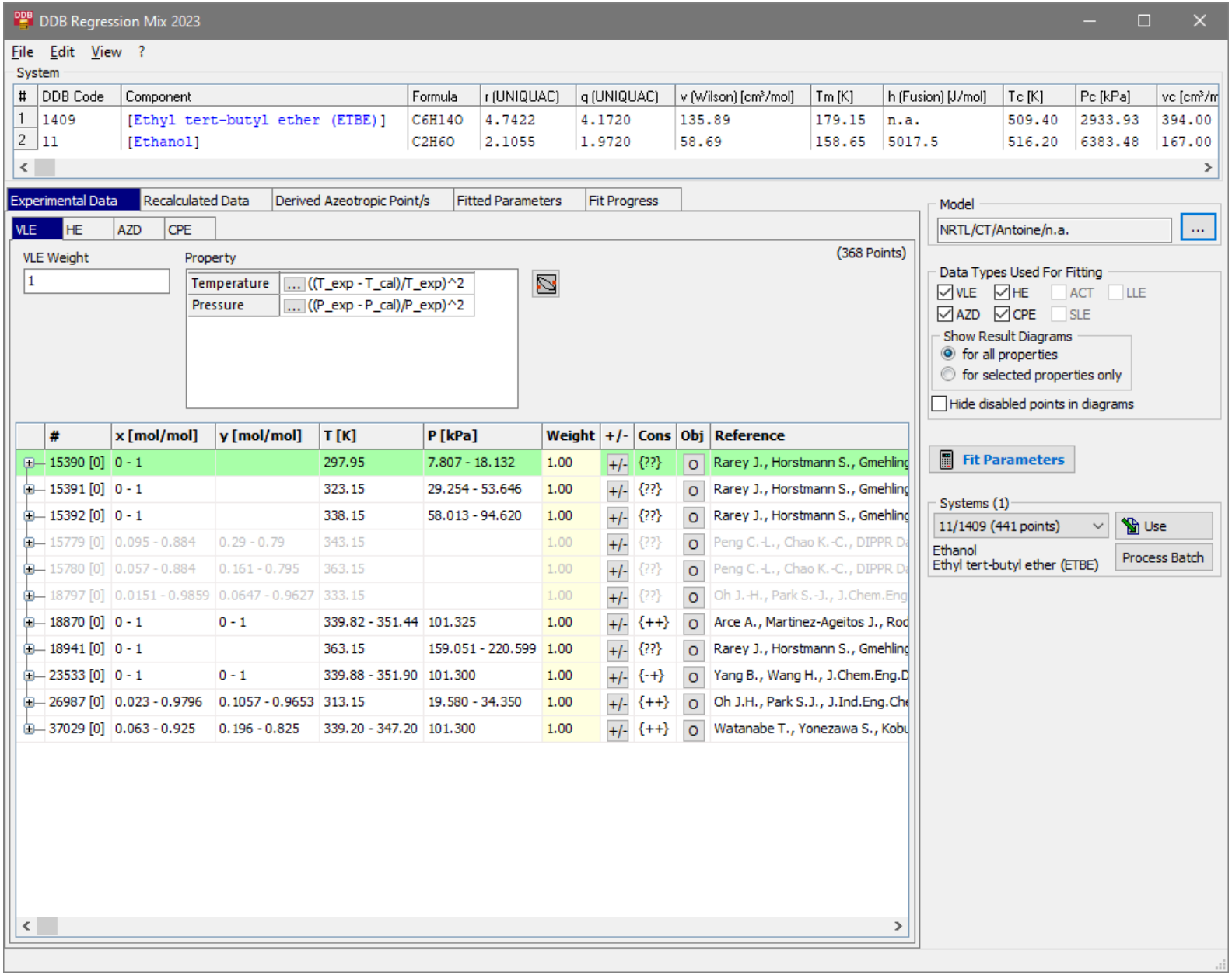
RegressionMix allows to correlate simultaneously VLE, HPV, ACT, AZD, LLE, HE and CPE-data using different g^E-models, compare the data to the results of UNIFAC or mod. UNIFAC, equations of state and simulator thermodynamics.

The different features of RegressionMix are demonstrated before the workshop.

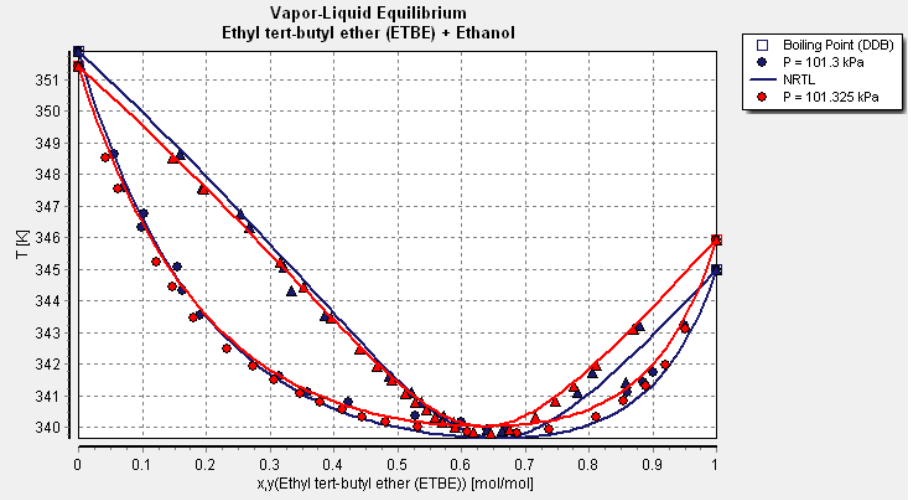
Workshop

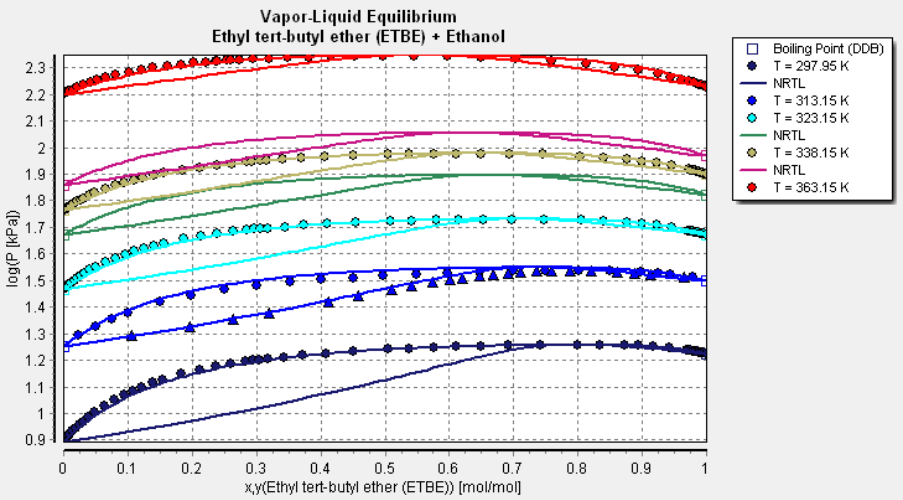
Search for data for the system ethanol-ETBE (ethyl-tert.-butyl-ether) in Mixture Properties and start RegressionMix using all available data.
Save the project as ethanol-ETBE
Examine the different options in the Edit-menu and regress temperature dependent NRTL-parameters to the data. Remove data sets 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.

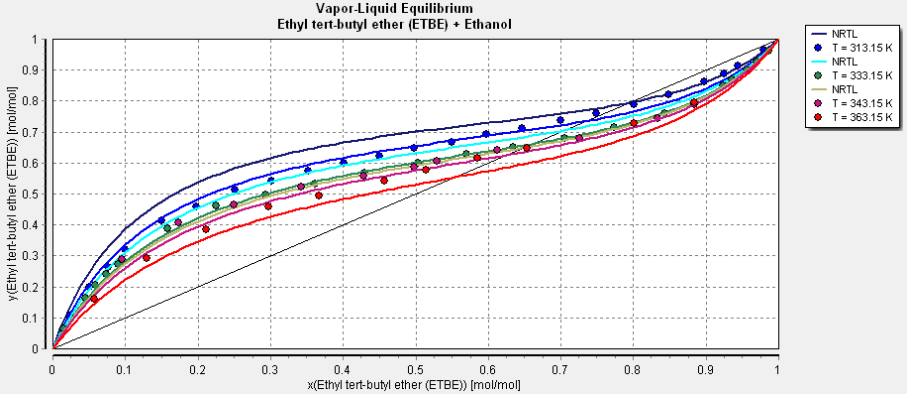
RegressionMix - Regression Dialog

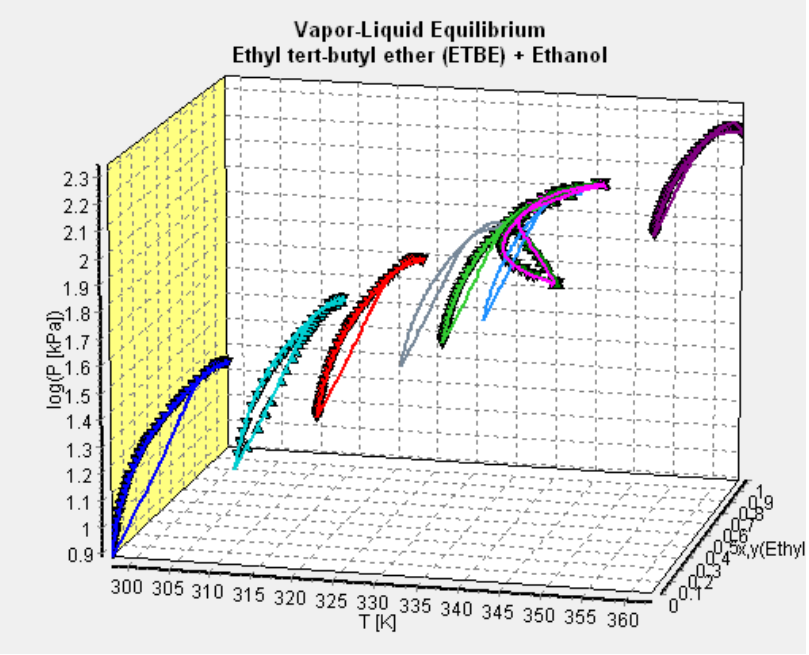


RegressionMix - Results

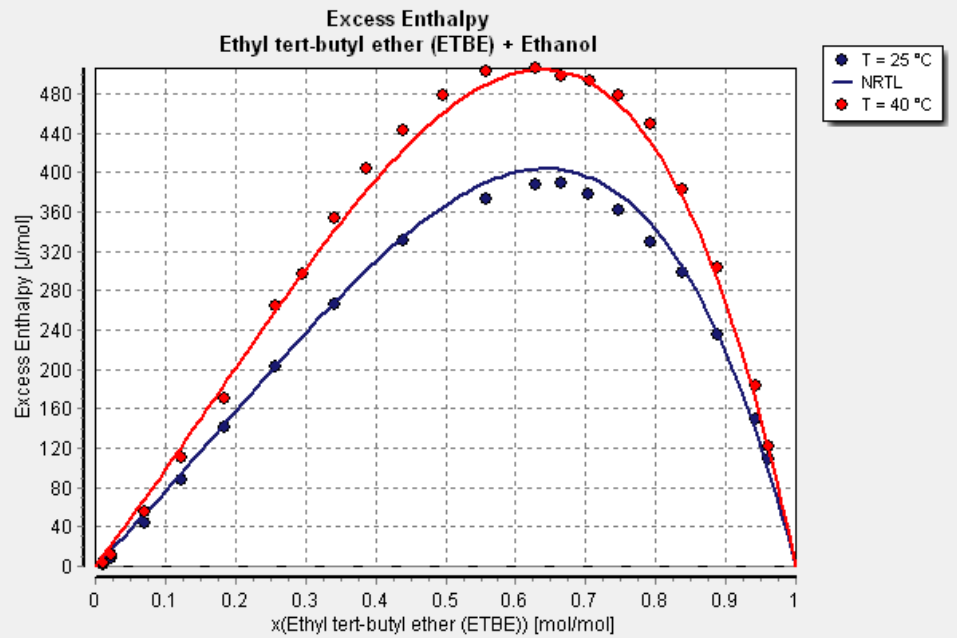


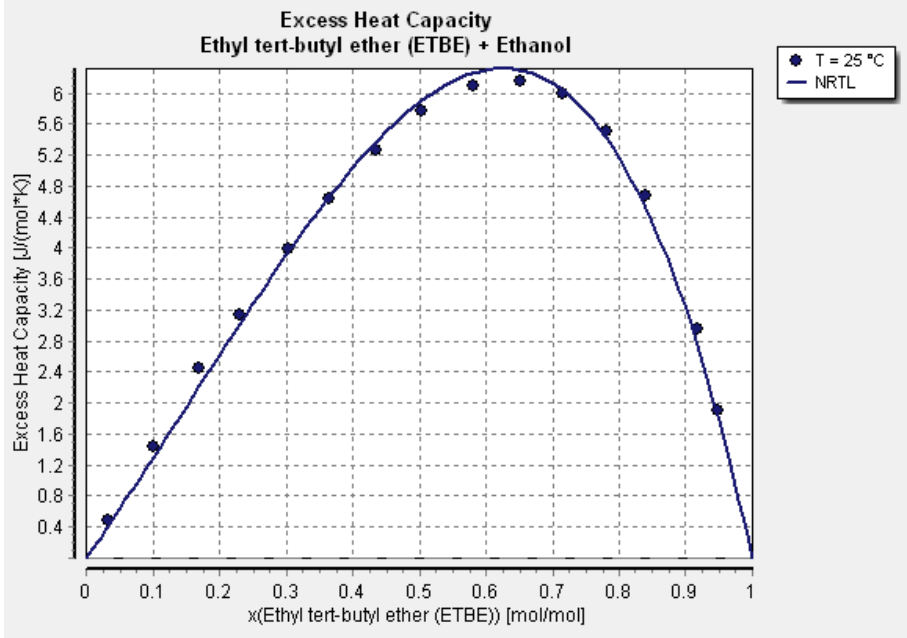


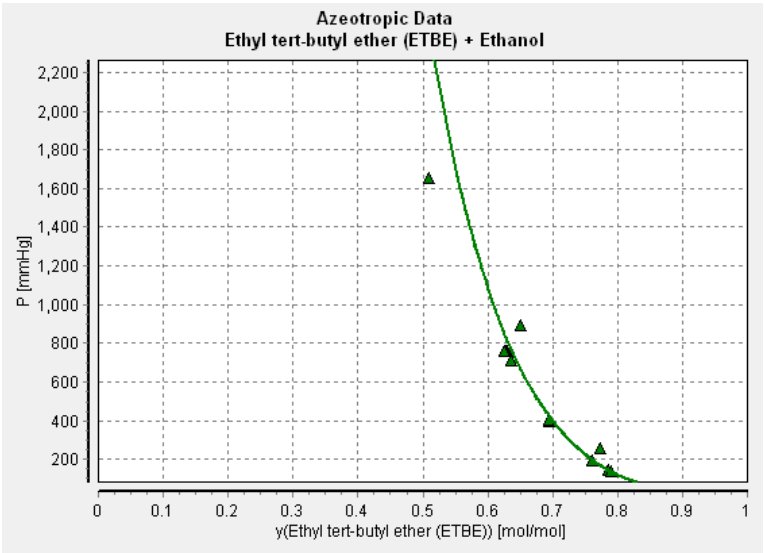


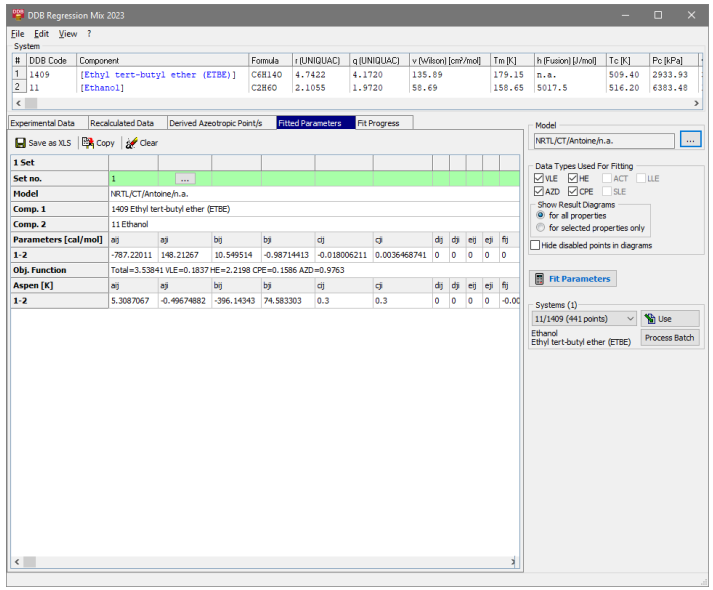


RegressionMix - Results









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

DDB - Mixture Data Estimation – Predict Data

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.

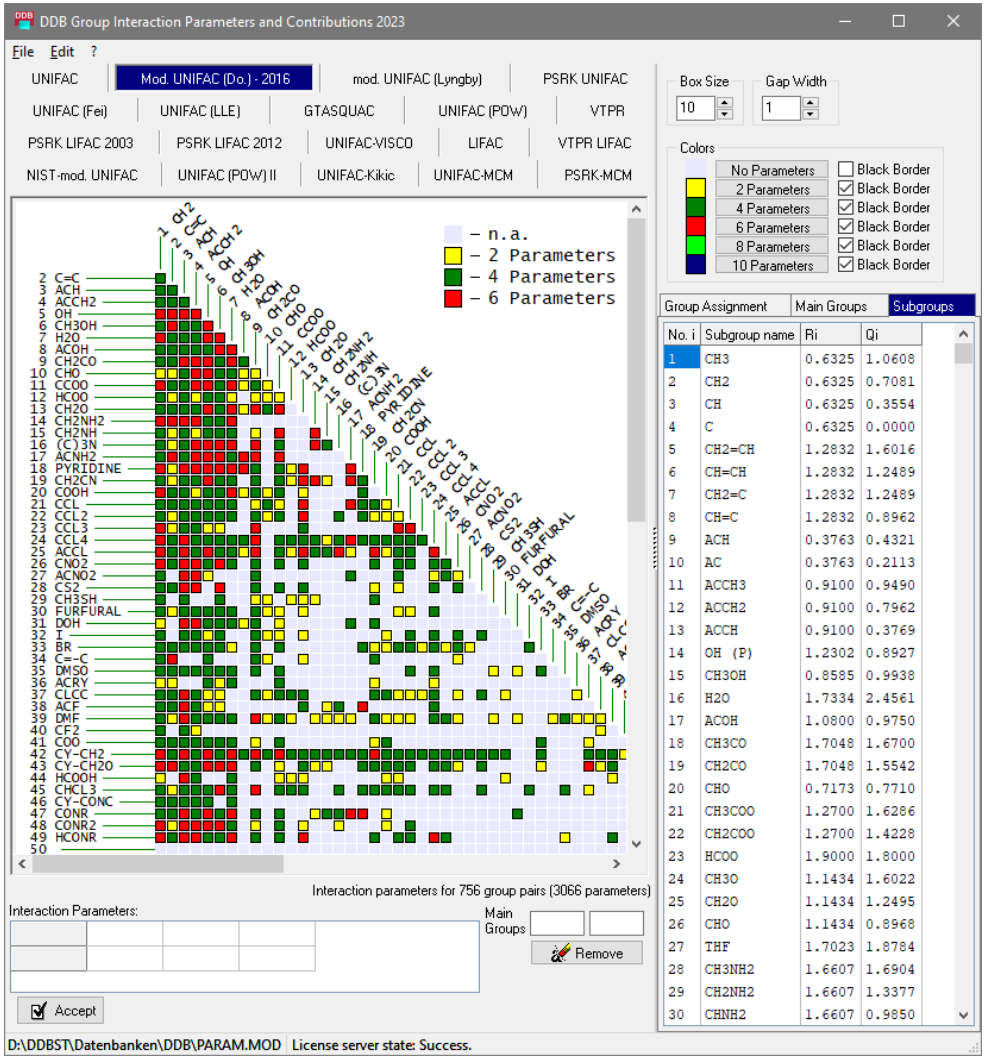
Note concerning Prediction in the Query Result window:

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.

DDB - Group Contribution Models Parameter

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!



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

Simulator Thermo Engine Support

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

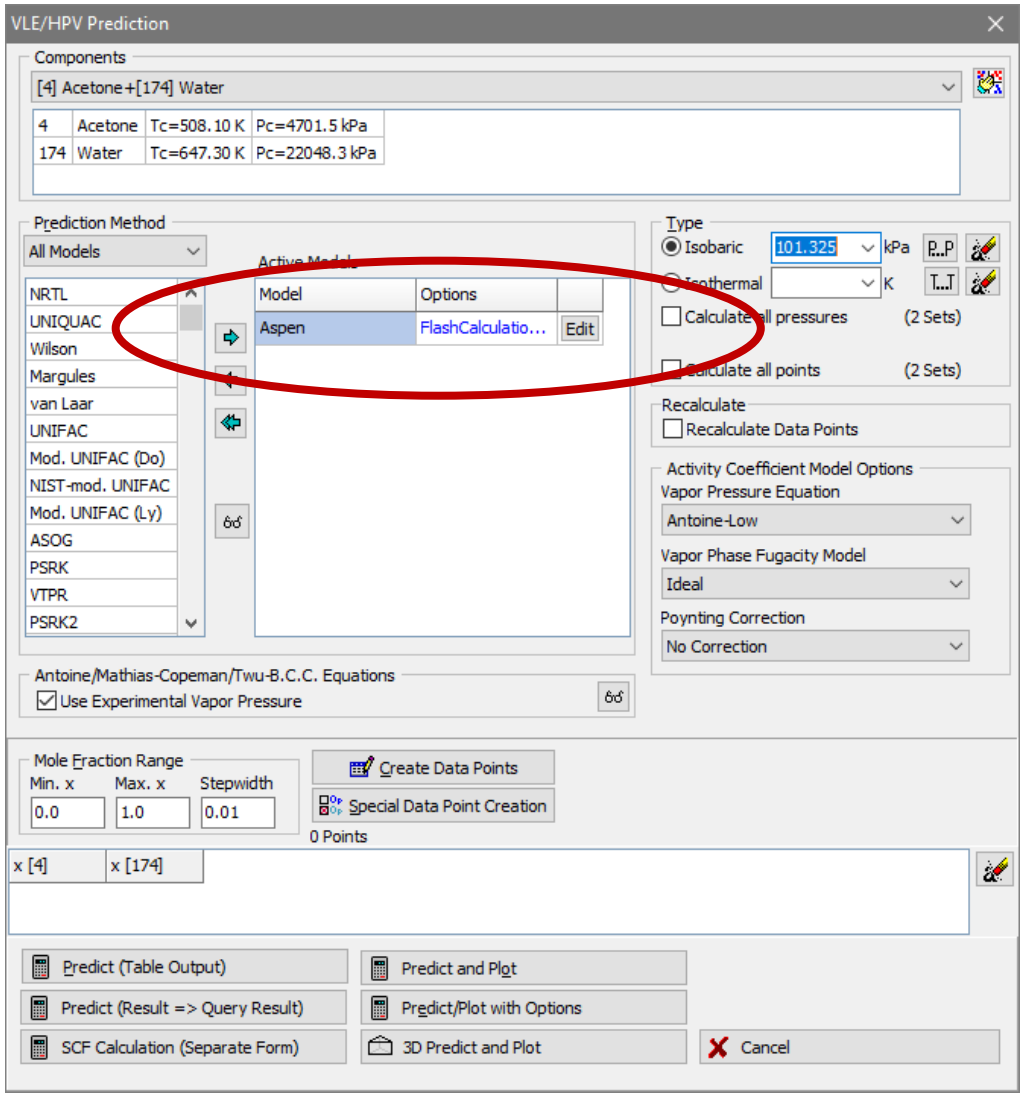
Example:

<u>Aspen Plus:</u>

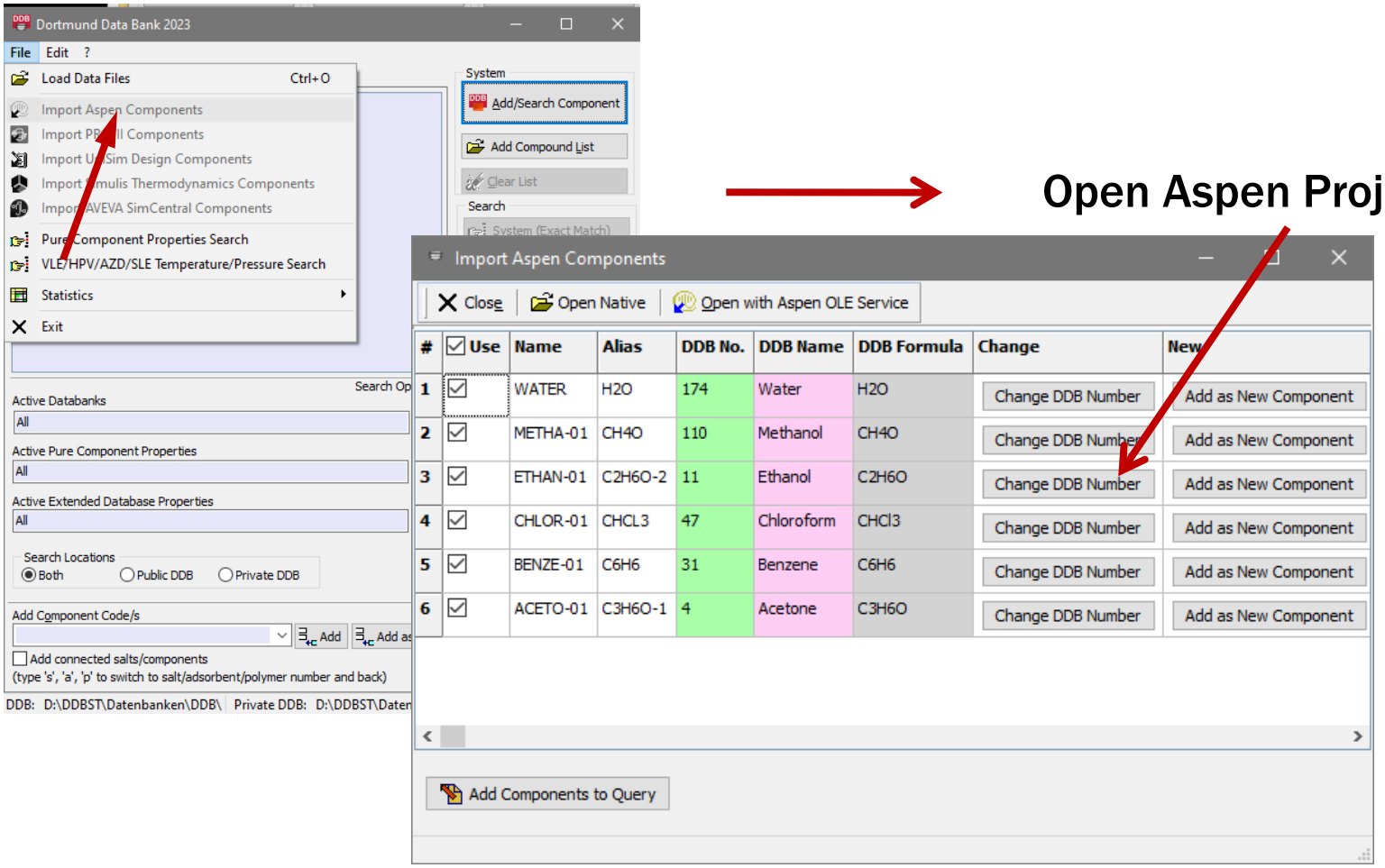
VLE, HPV, LLE, h^E, c_P^E, v^E, P^S, c_P^L, c_P^s, c_P^V

Next step:

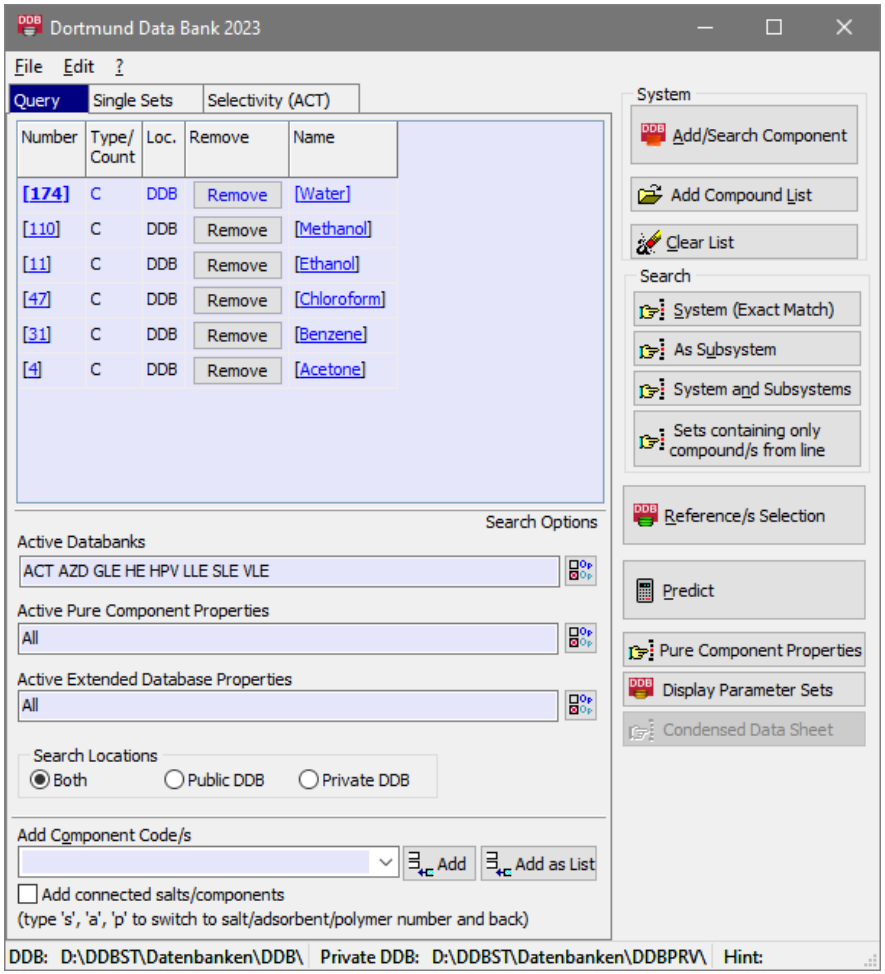
- Additional properties
- Parameter regression



Import Project Components into Query

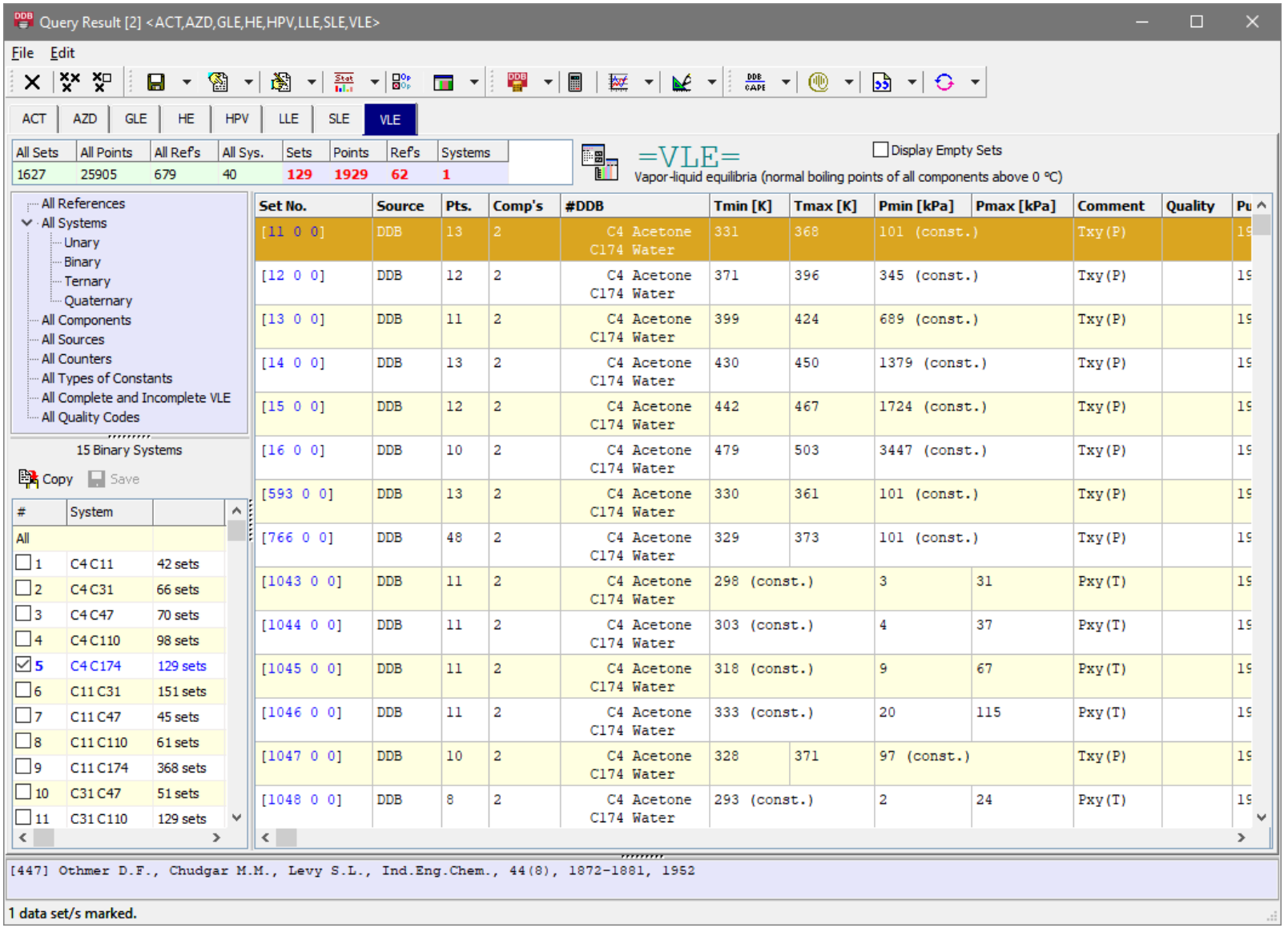


Search for Data



Search for System and Subsystems

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

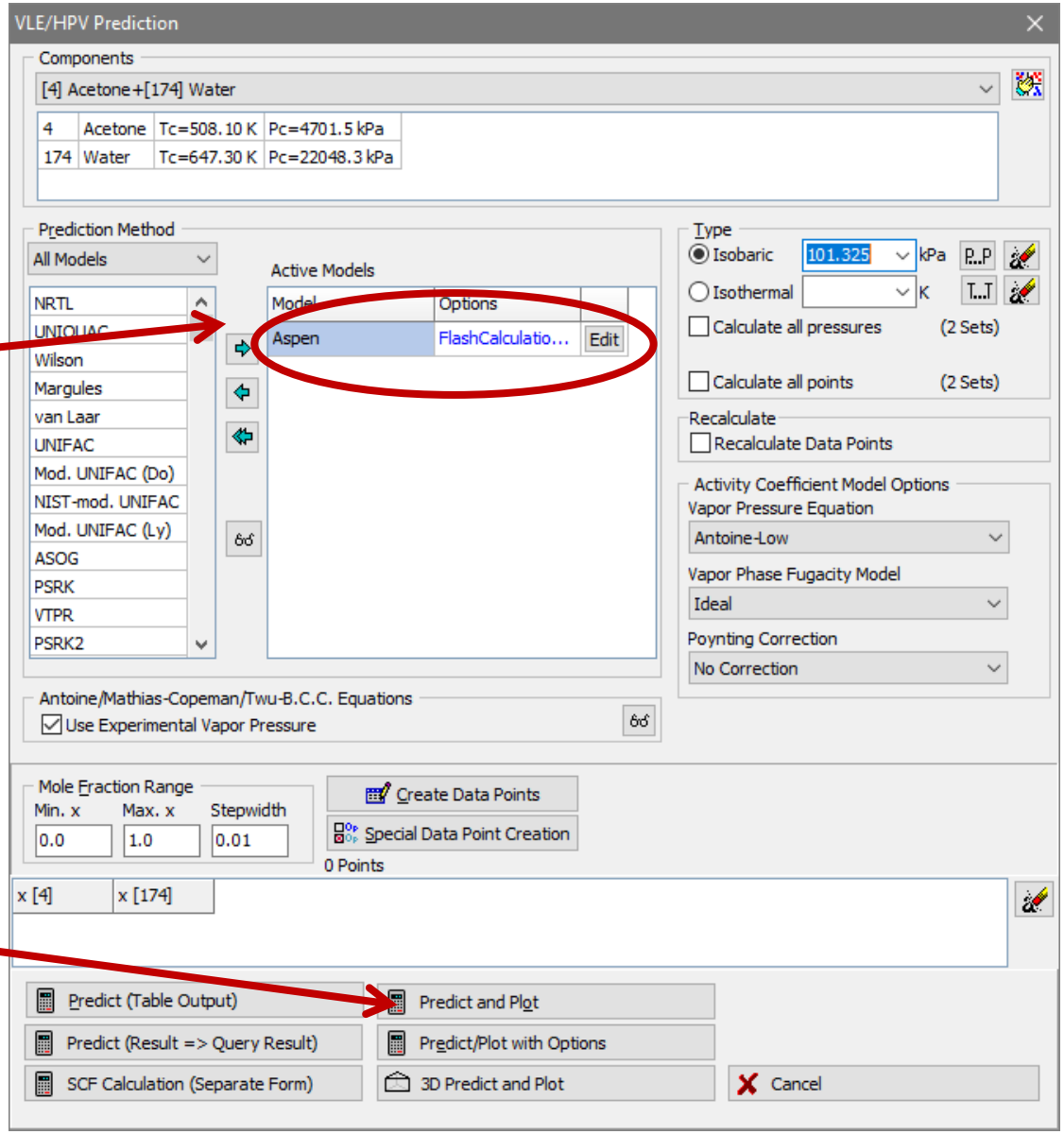


Prediction Dialog

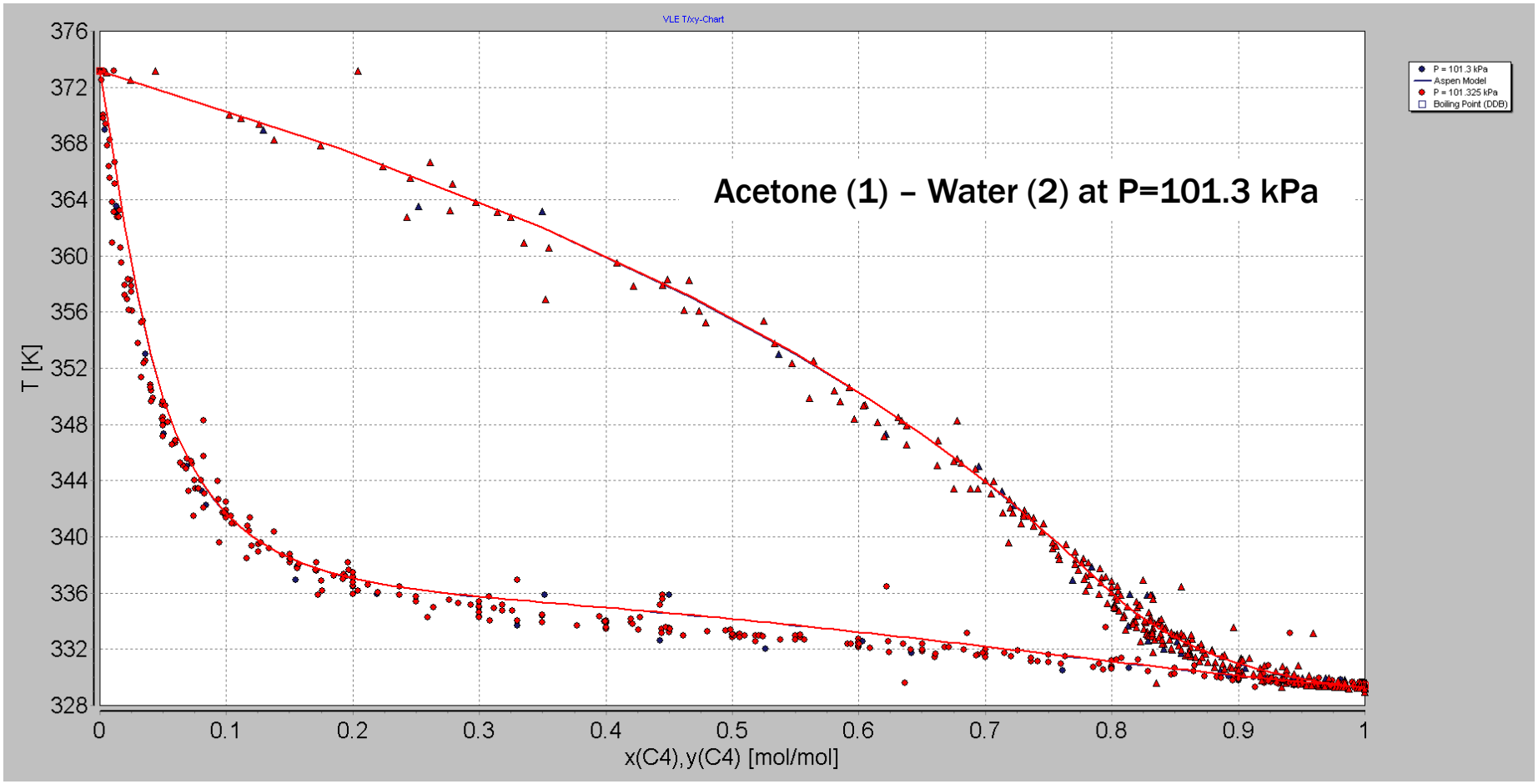
In the prediction dialog, the last selected Aspen project file is already given as default.

Base method: UNIQUAC

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



Temperature as function of liquid and vapor phase composition



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

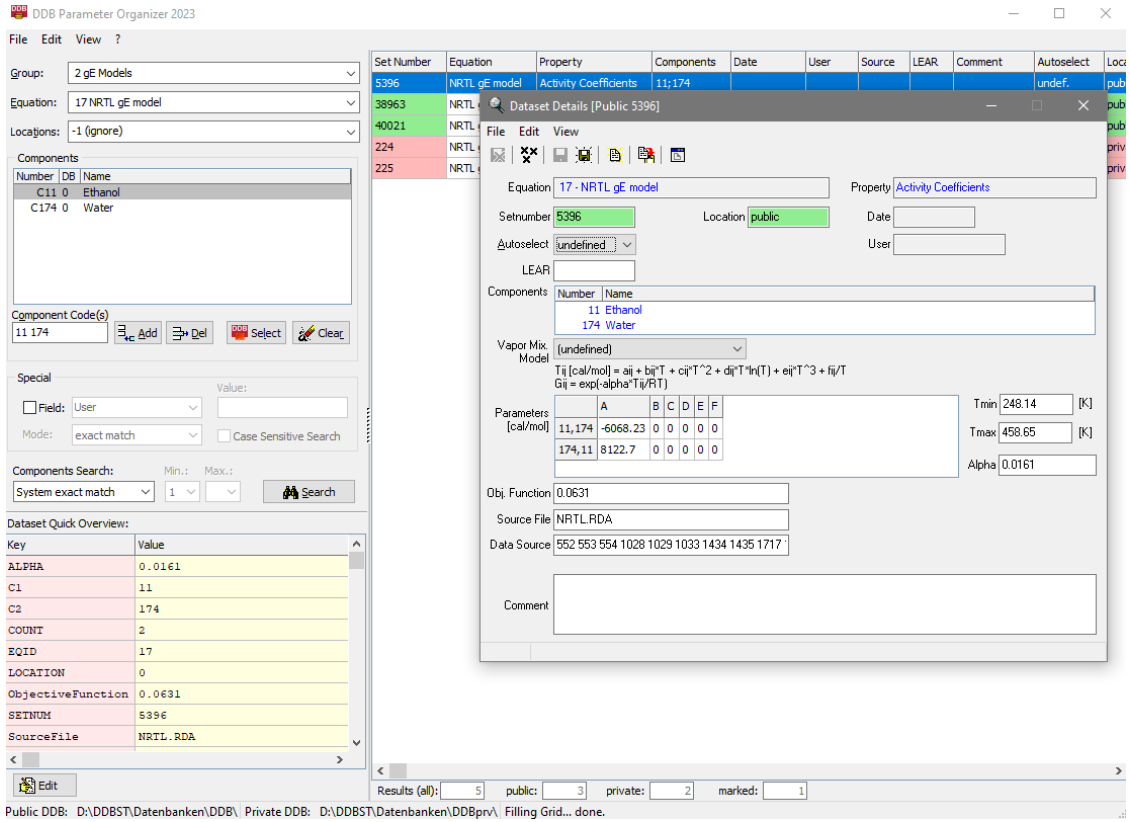
DDB Parameter Data Bank

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

DDB - Parameter Data Bank

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:*

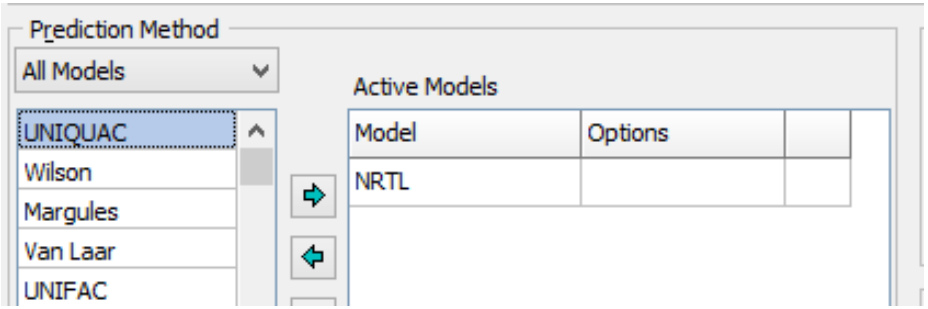


It is integrated into the software and is automatically accessed when values or parameters are required.

Parameters Retrieval From the DDB

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

Process Synthesis – Residual Curves

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.

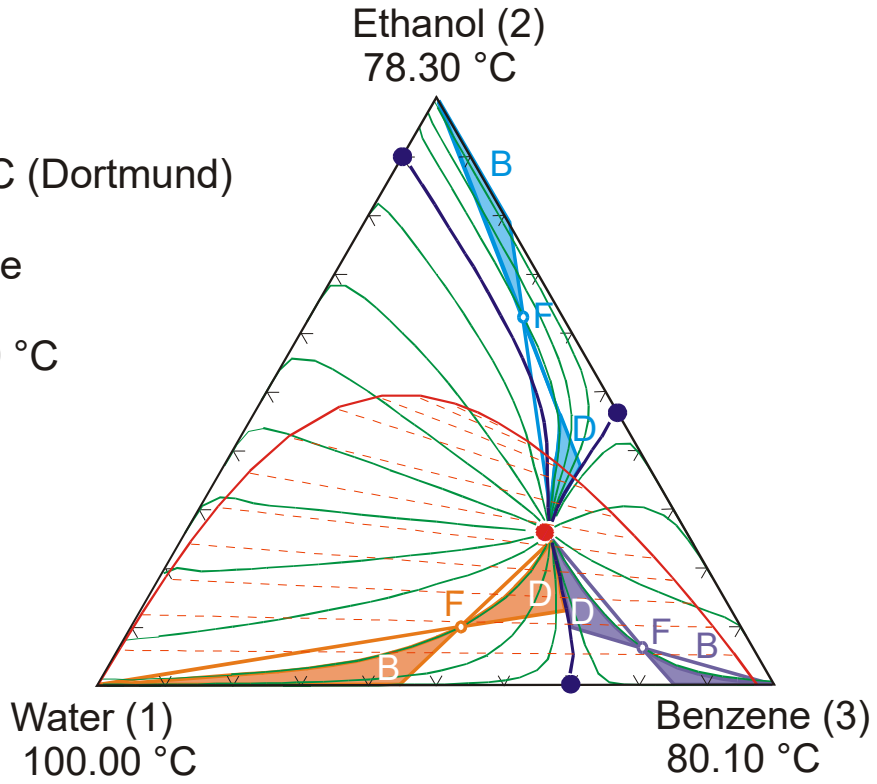
In DDB, these plots can be generated using Process Synthesis – Residual Curves. The plot on the right shows feasible product regions for two different feed compositions in a complex 3 component system with miscibility gap.

P = 1 atm

Modified UNIFAC (Dortmund)

ideal vapor phase

(1)-(2)-(3) 64.89 °C
(1)-(2) 78.14 °C
(1)-(3) 69.23 °C
(2)-(3) 67.66 °C



Workshop

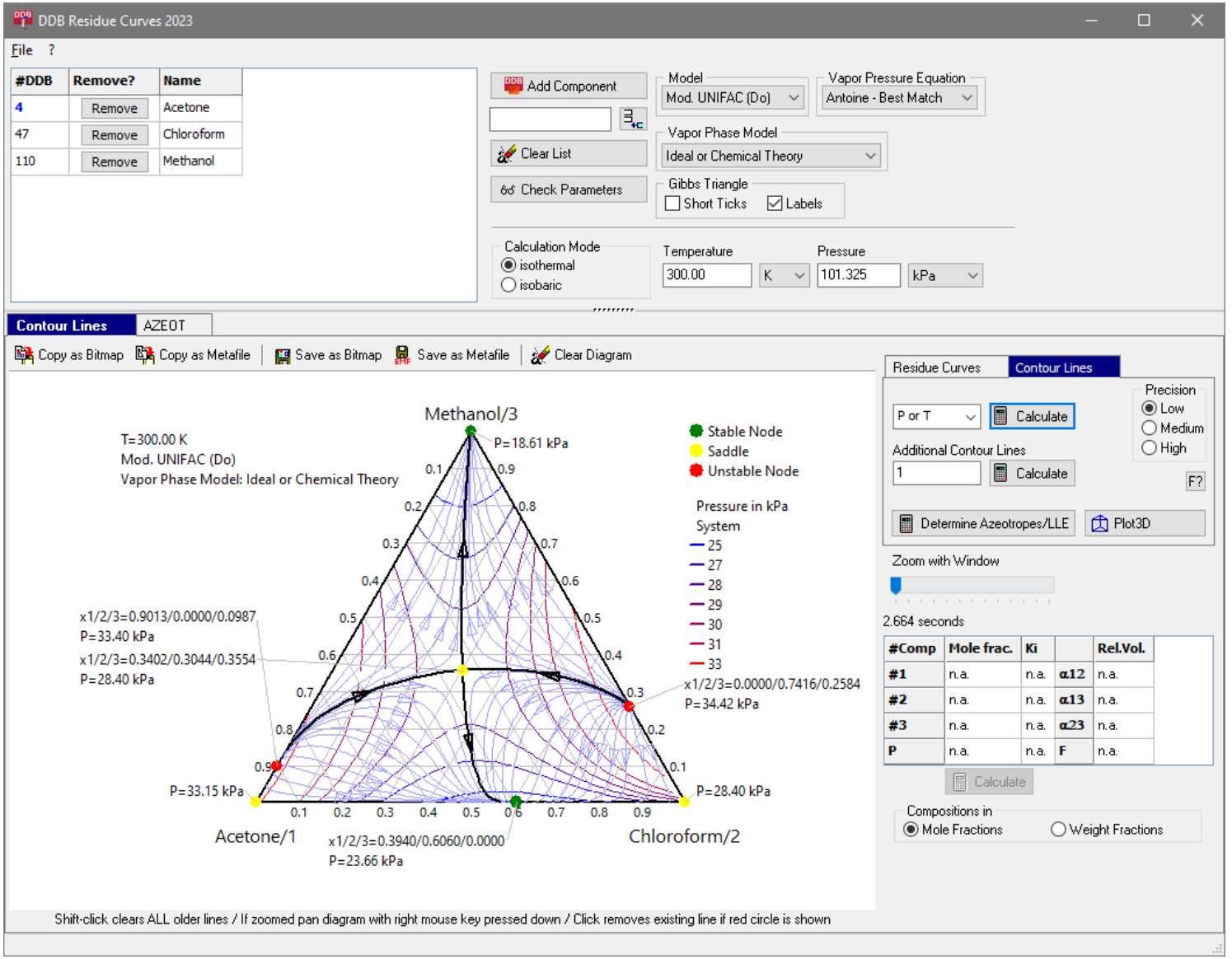
Plot the azeotropes, boundary curves and residual curves for the mixture acetone – chloroform – methanol using mod. UNIFAC (Do) at 300 K.

Examine and explain the result.

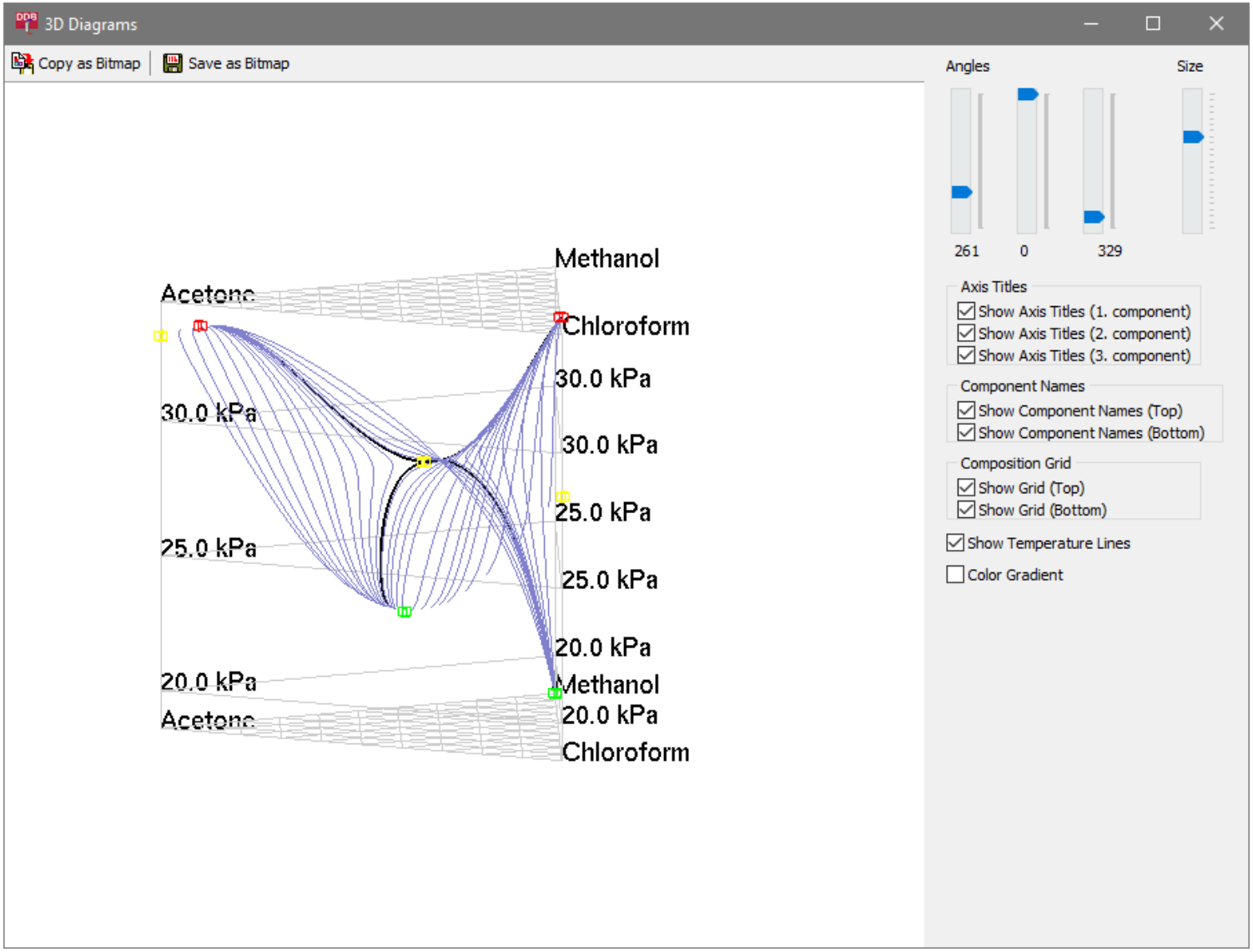
Add the temperature contour lines to the plot.

Generate the 3D plot.

Process Synthesis – Residual Curves Workshop



Process Synthesis – Residual Curves Workshop



Process Synthesis – Entrainer Selection

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

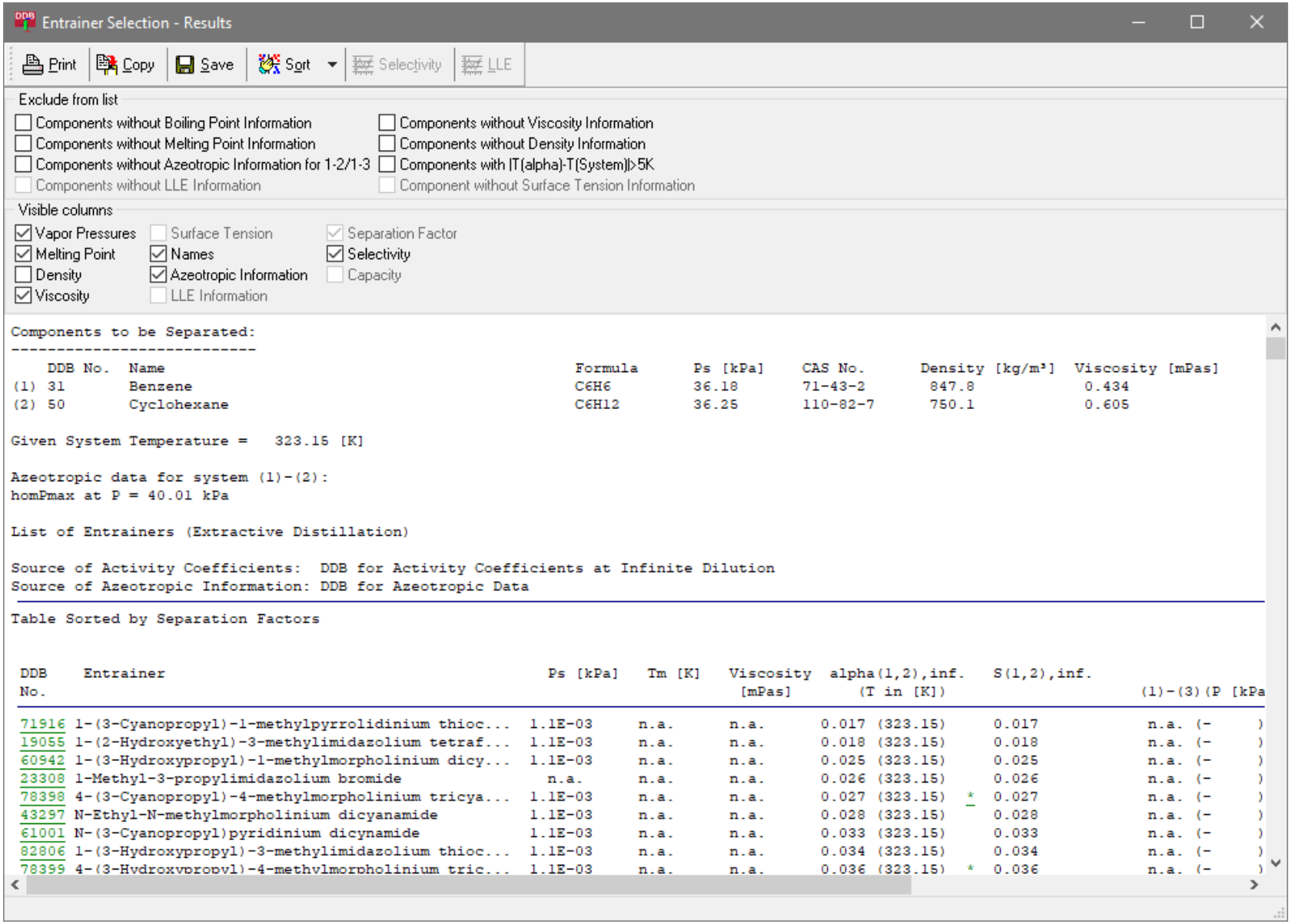
Select the components benzene - cyclohexane

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



Entrainer Selection - Results

Print | Copy | Save | Sort | Selectivity | LLE

Exclude from list

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

Visible columns

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

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)

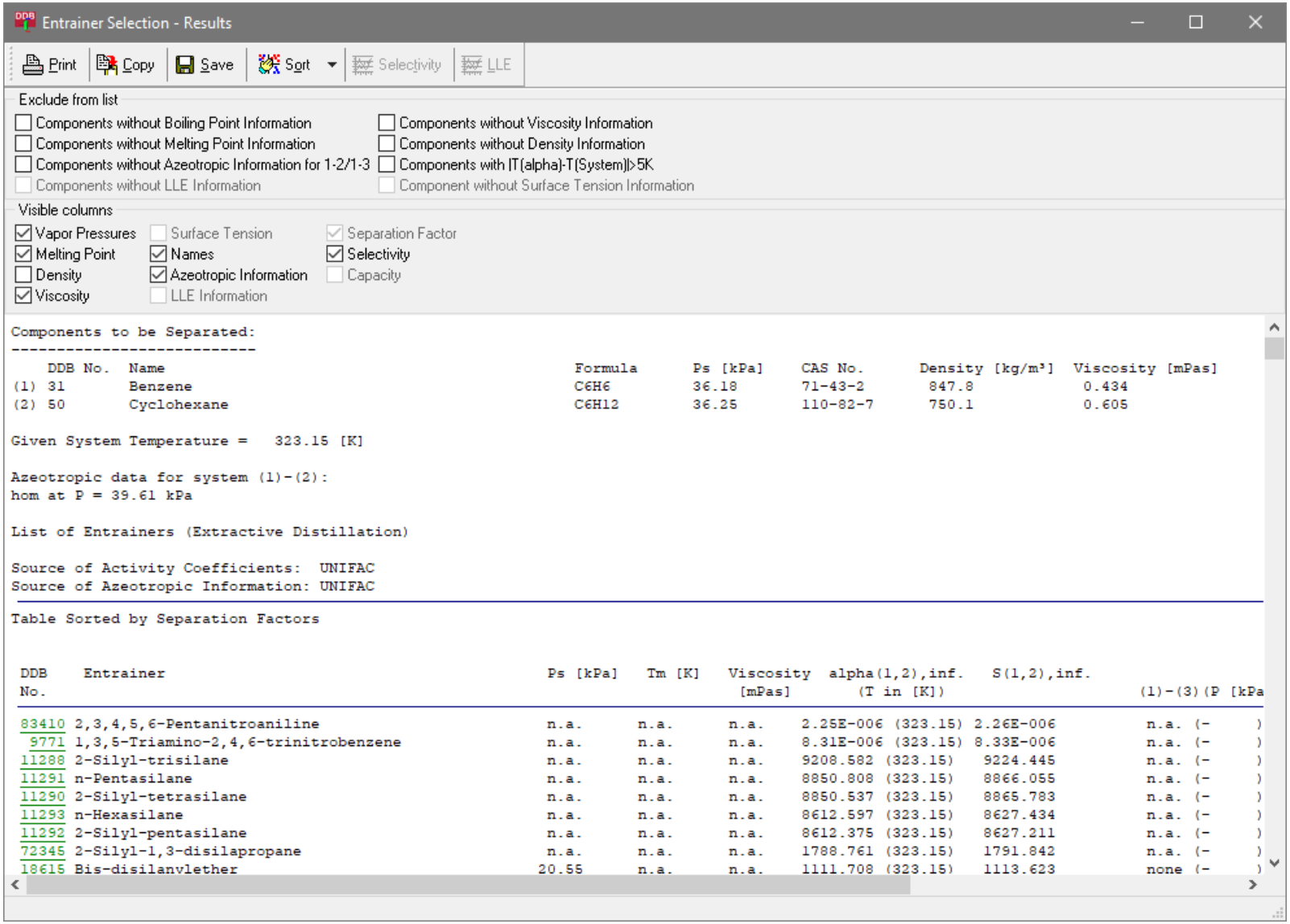
Source of Activity Coefficients: DDB for Activity Coefficients at Infinite Dilution
Source of Azeotropic Information: DDB for Azeotropic Data

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 dicynamide	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. (-)

Entrainer Selection (UNIFAC)

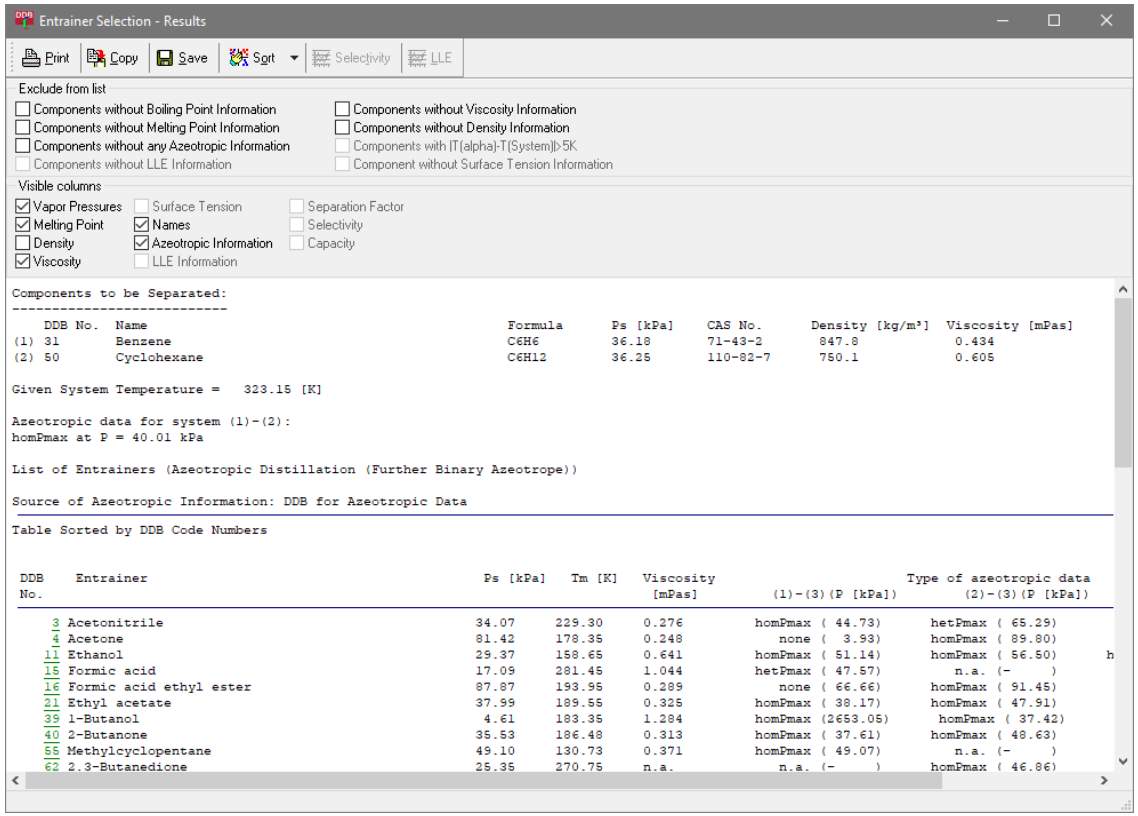
Search for selective solvents using the predictive method UNIFAC.



Entrainer Selection

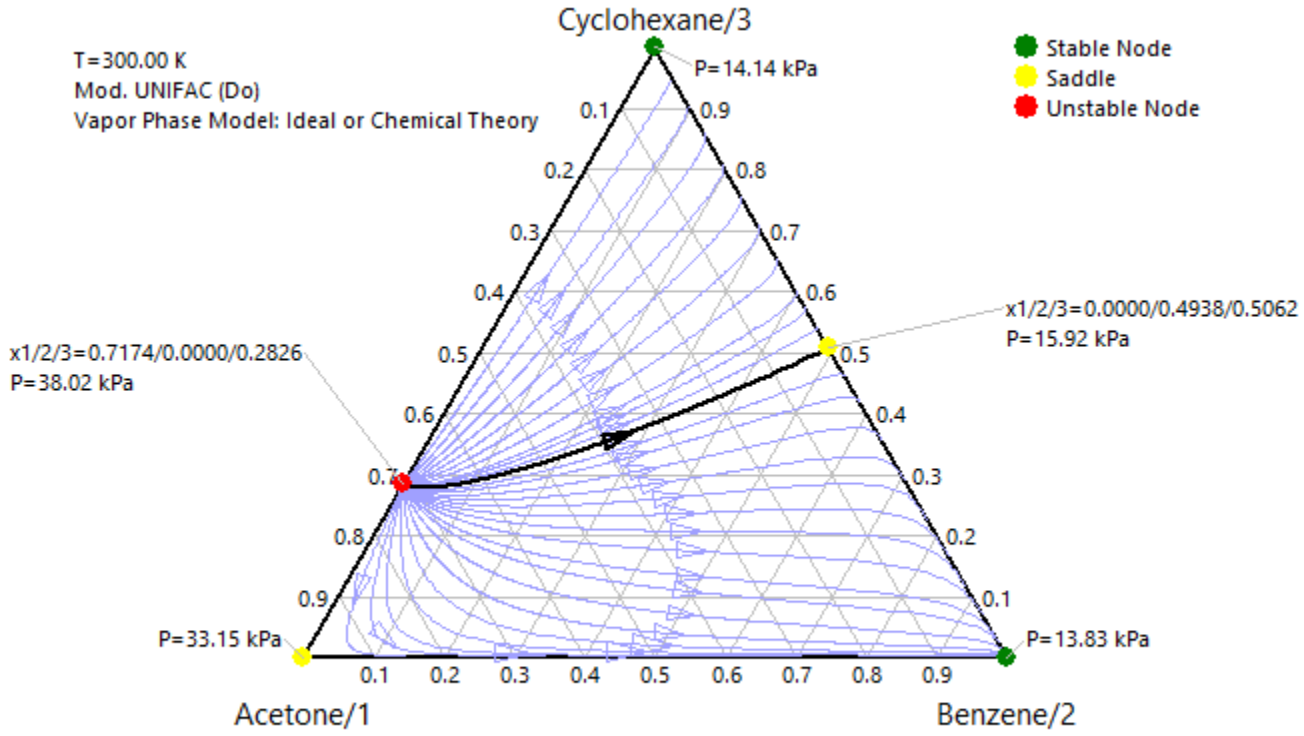
Instead of using a selective solvent for extractive distillation, it is also possible to add an entrainer that forms a binary azeotrope with one of the components or a ternary heterogeneous azeotrope. Components of industrial use for the aliphatics – aromatics separation in case of aromatic-rich mixtures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



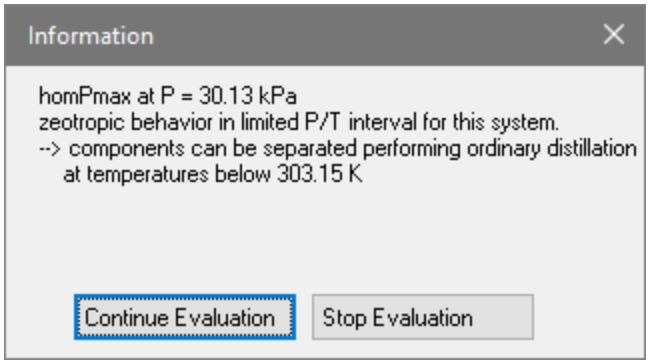
Entrainer Selection

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



Entrainer Selection

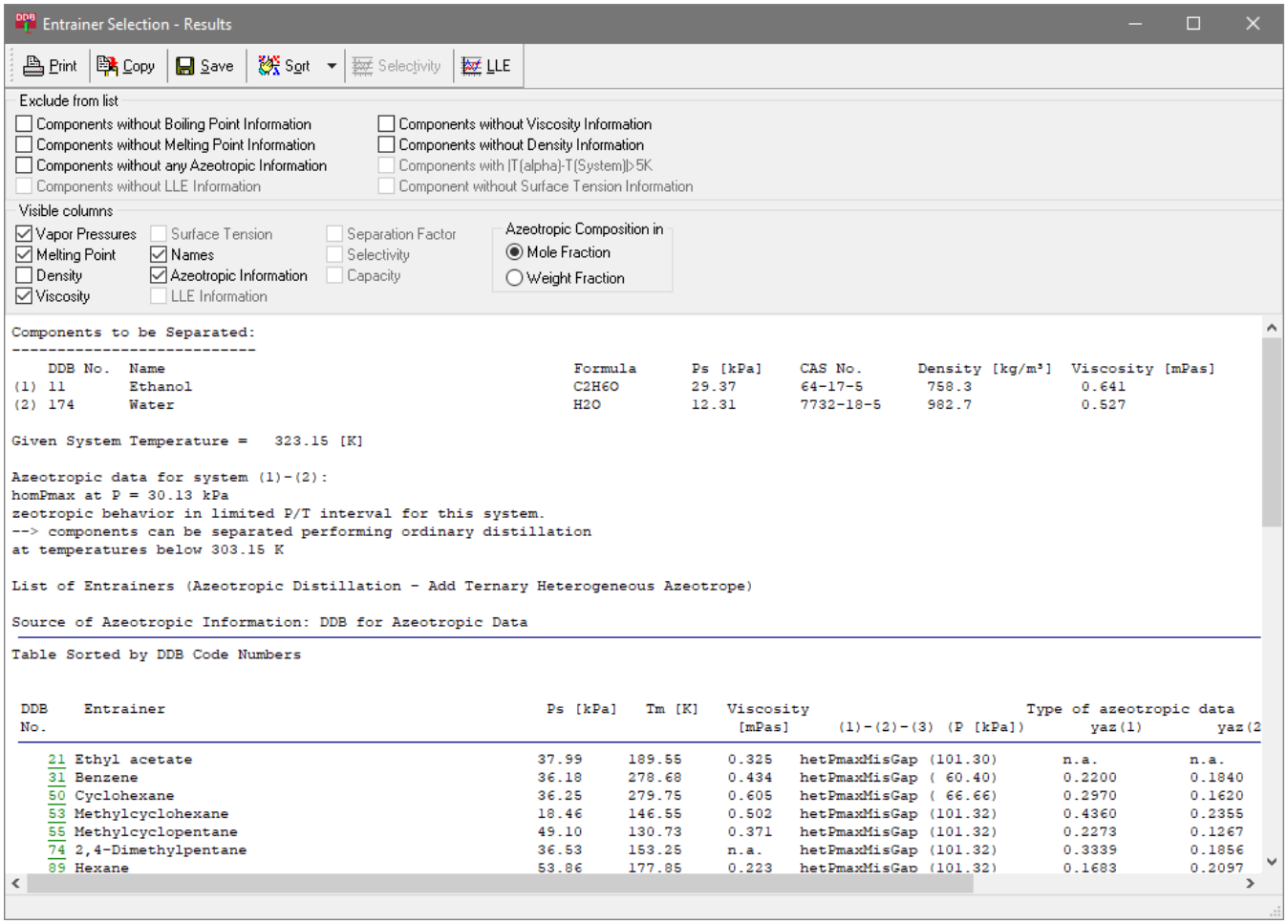
Another possibility is the introduction of a heterogeneous ternary azeotrope. Look for an entrainer for the separation of the system ethanol – water. The program will first display the following message:



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

Entrainer Selection

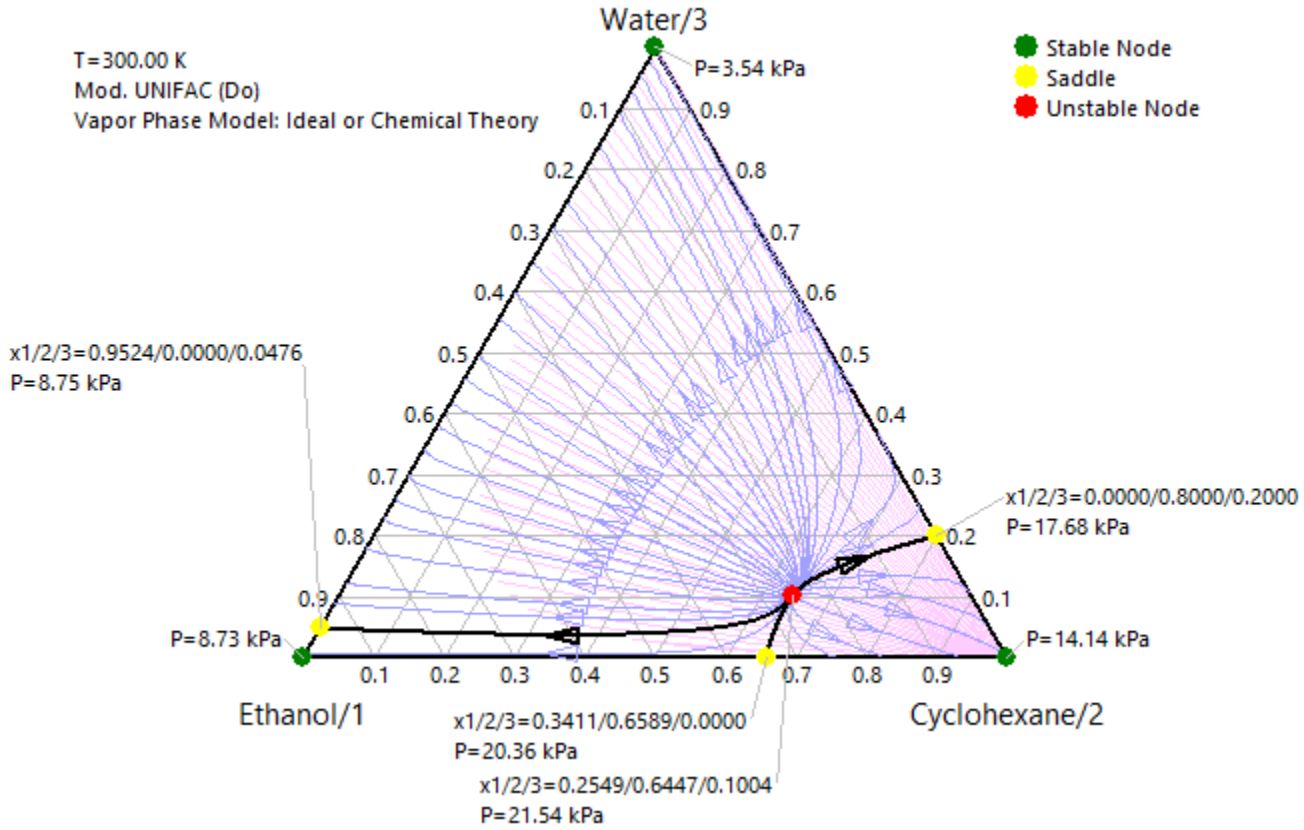
The following list of entrainers is shown:



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

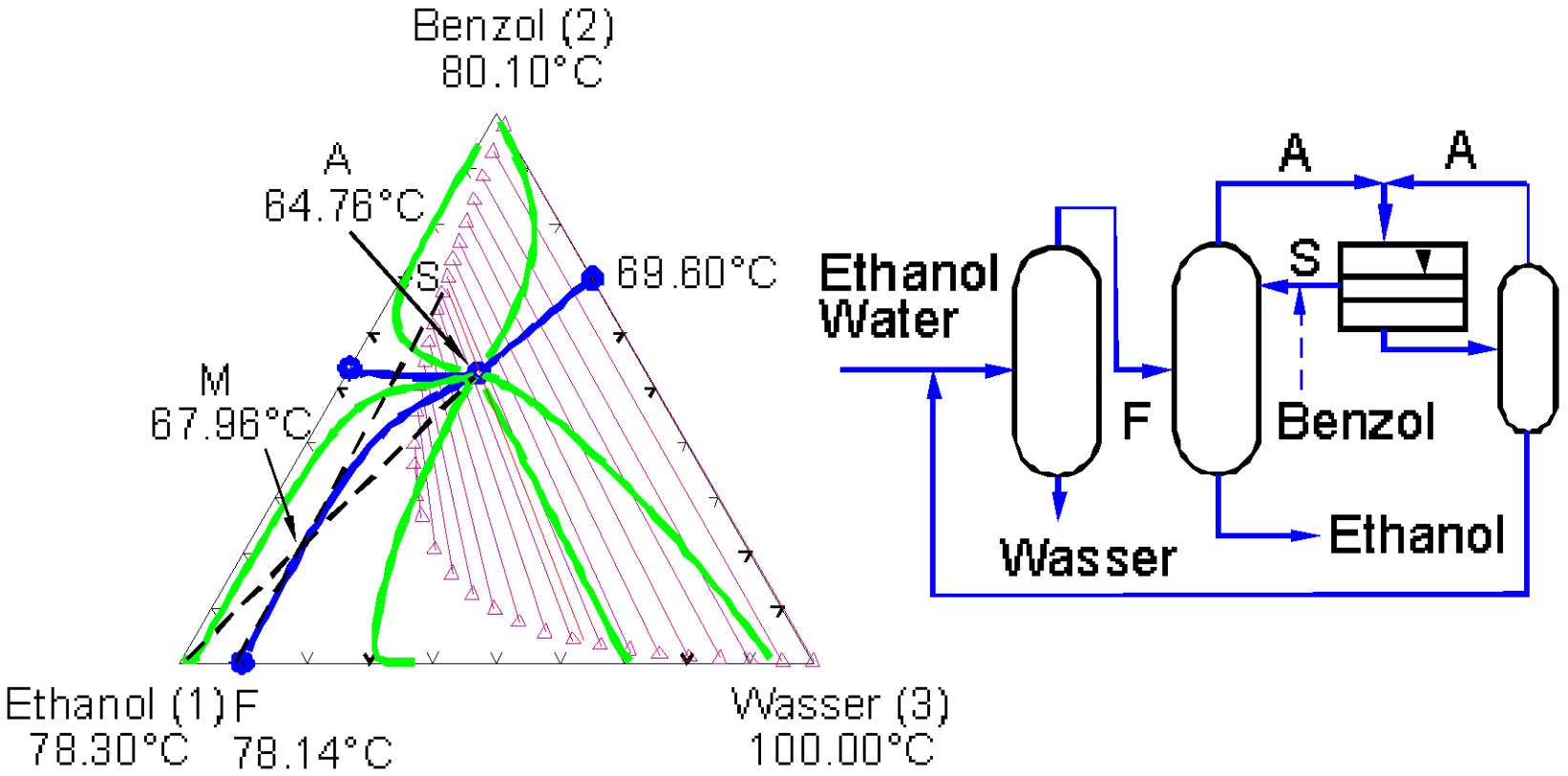
Entrainer Selection

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



Entrainer Selection

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

DDB - 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.

Not in Explorer Version

DDB - Private DDB

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

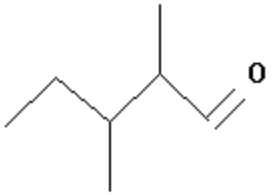
For the following workshops, start with an empty private folder.

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.

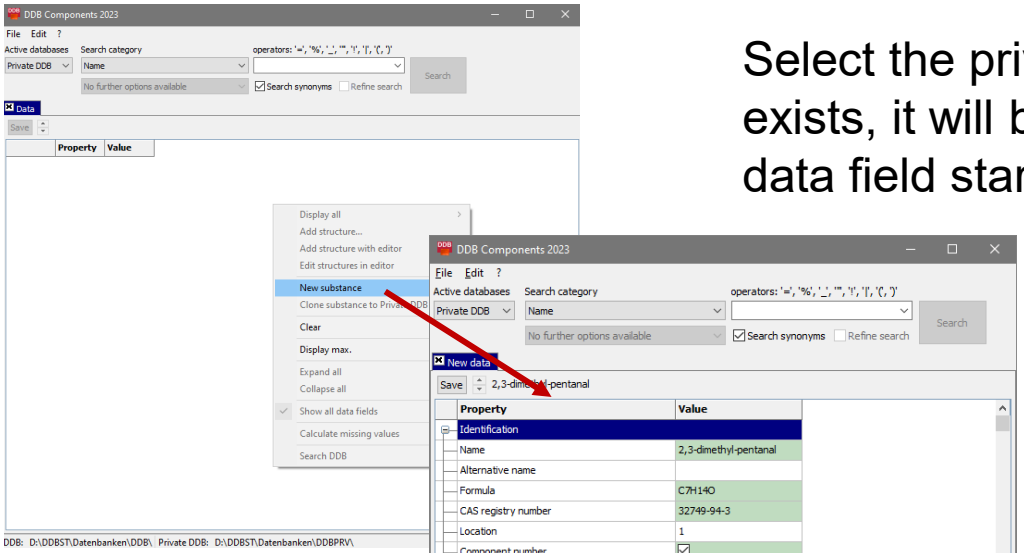
Workshop

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



2,3-dimethyl-pentanal
Beilstein Registry Number 1901854

Start the program *Components*



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

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"

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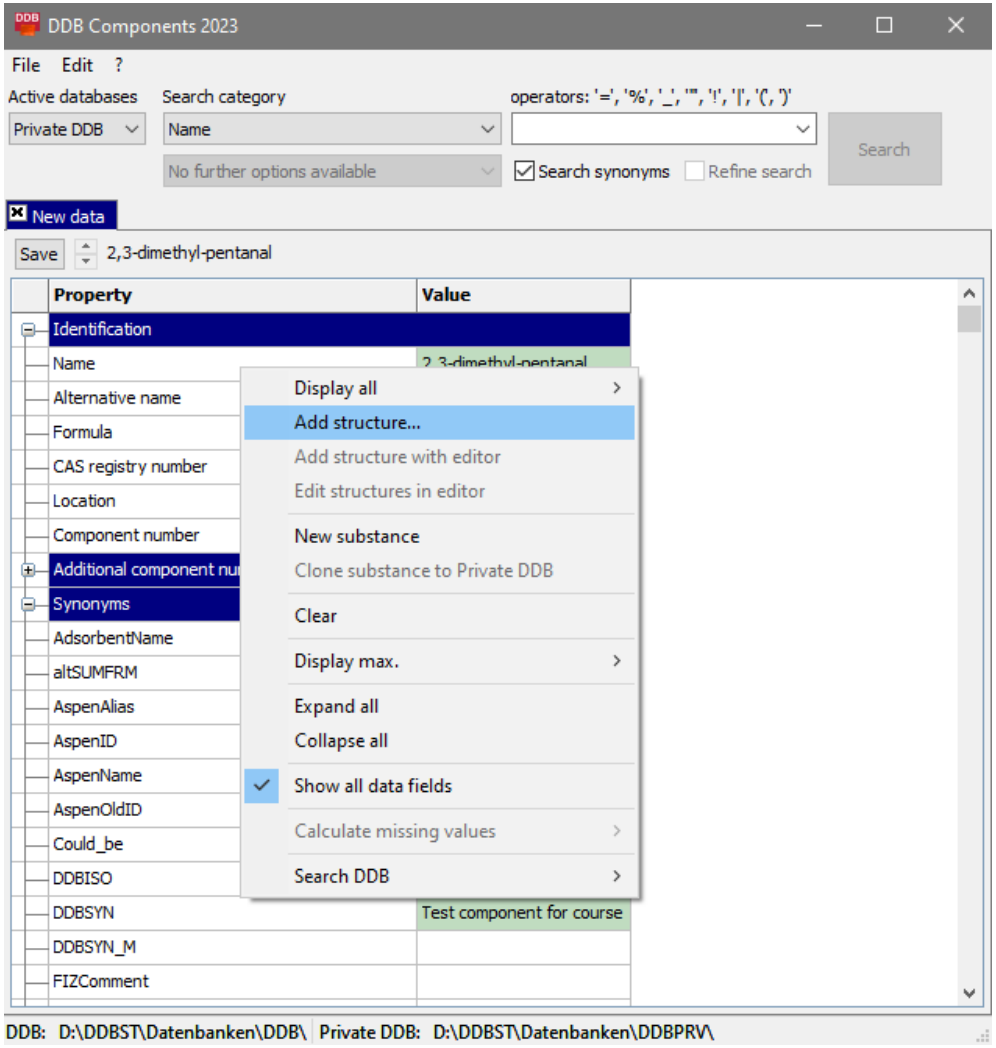
DDB - Private Component

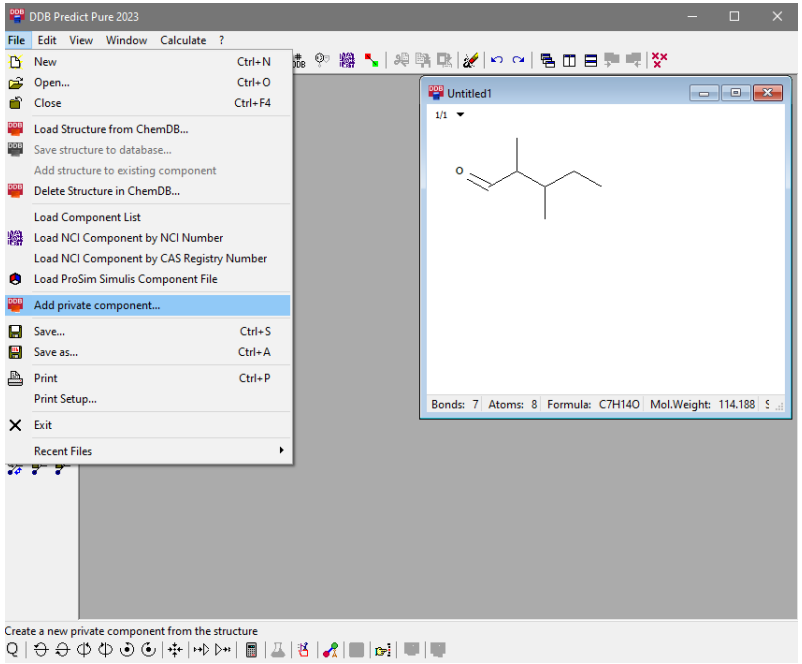
Selecting *add structure* from the right-click menu allows the import of *.mol files.



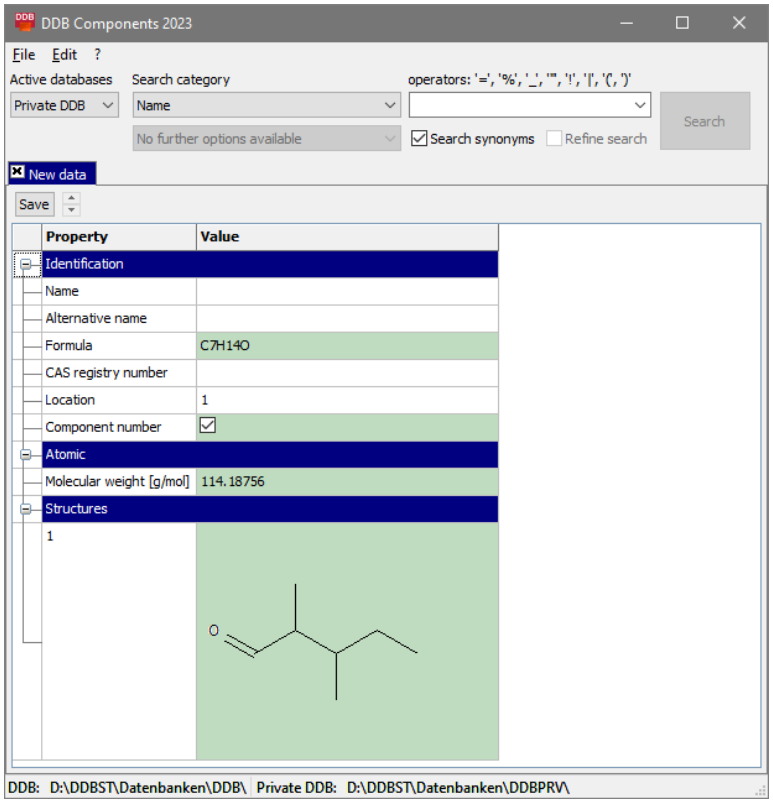
not in Explorer Version

DDB - Private Component 2

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



Selecting *Add private component* from the *file* menu brungs up Componens and transfers the structure as well as formular and molecular weight.

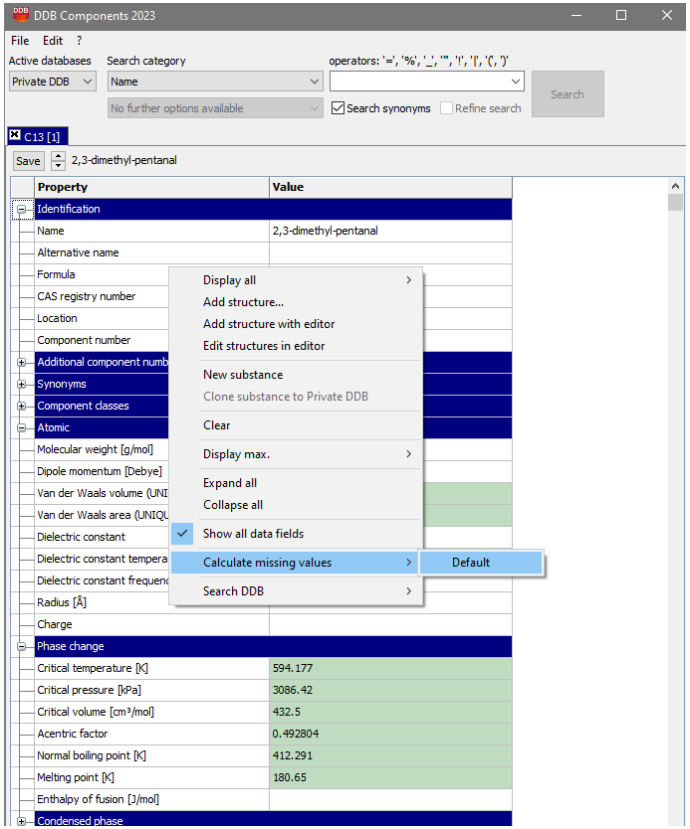


The further procedure is as shown before. Once completed, press the *save* button to store the new component. A component number will be assigned automatically.

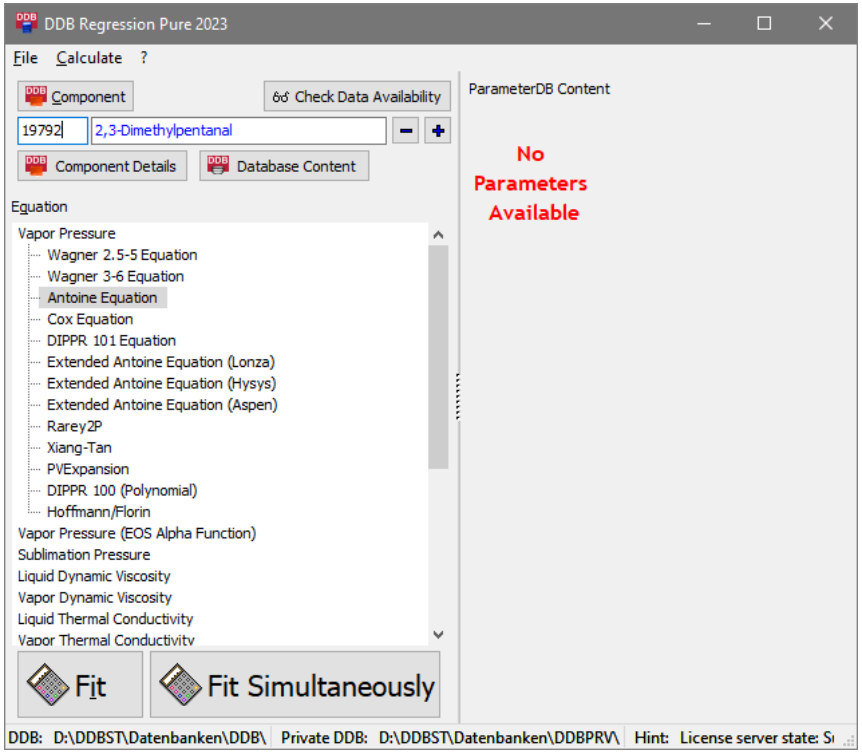
not in Explorer Version

DDB - Private Component 3

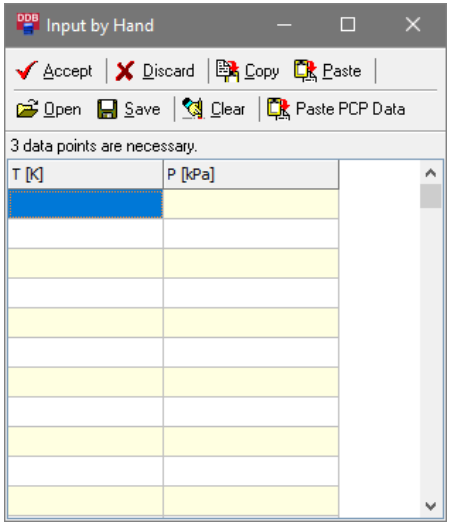
Various missing properties can automatically be estimated using some pre-defined methods via right-click menu, *Calculate missing values – Default*. The calculation itself is performed by PredictPure in the background which also allows to choose different methods for e.g. different substance classes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



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

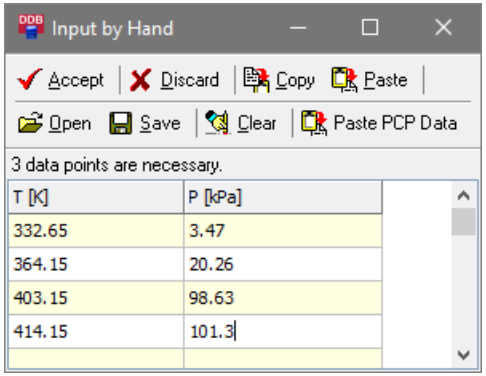


Select *Fit* and data source *Hand* to bring up the following dialog :

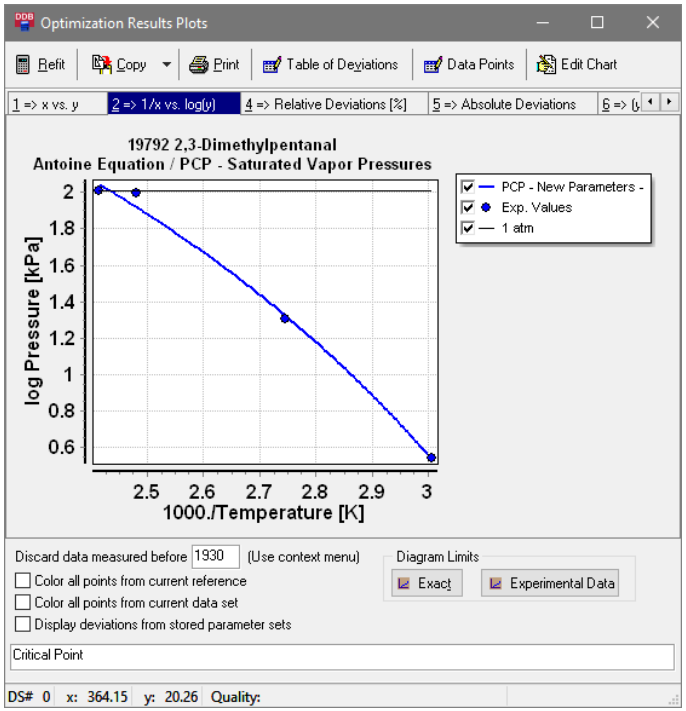


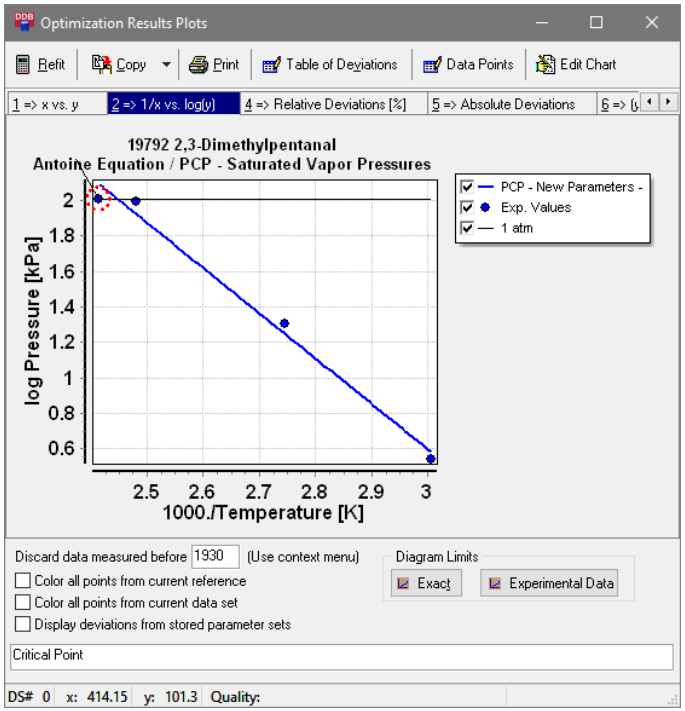
Enter the following data and accept your input:

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:





DDB - Private Component - Pure Component Data Input

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 it's primary source.

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

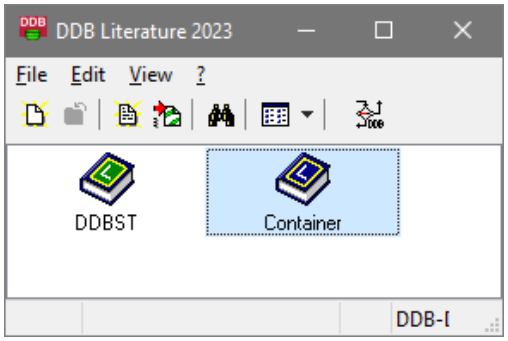
Experimental pure component or mixture data sets in DDB are linked to the component(s) in the component definition and the source reference in the literature data bank LEAR.

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

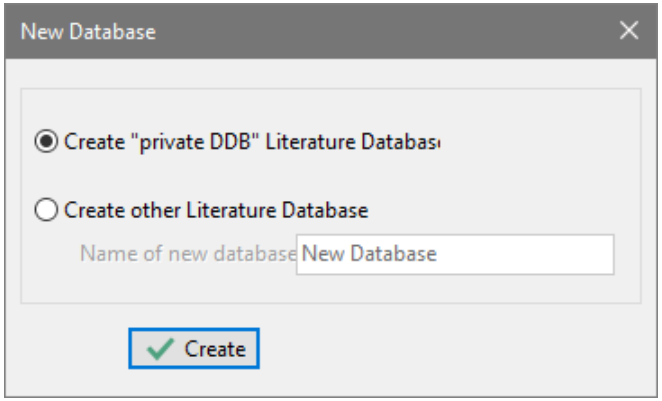
As we entered 2,3-Dimethyl-Pentanal as a new component in the private data pure component definition file, we now must enter the reference for the first data set (the patent found via CAS).

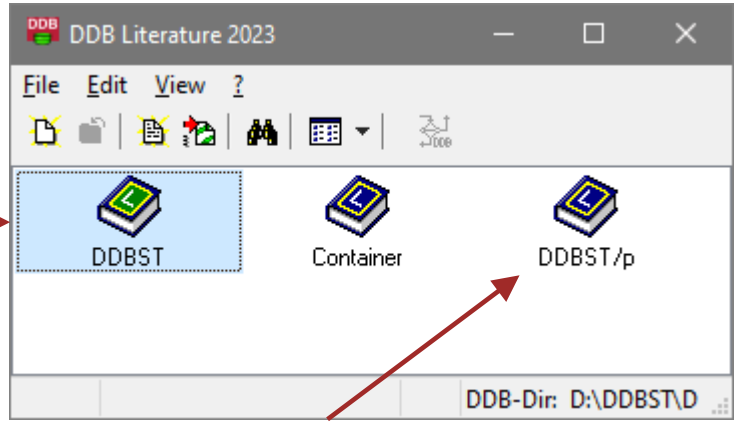
DDB - Private Data - Reference Input

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.

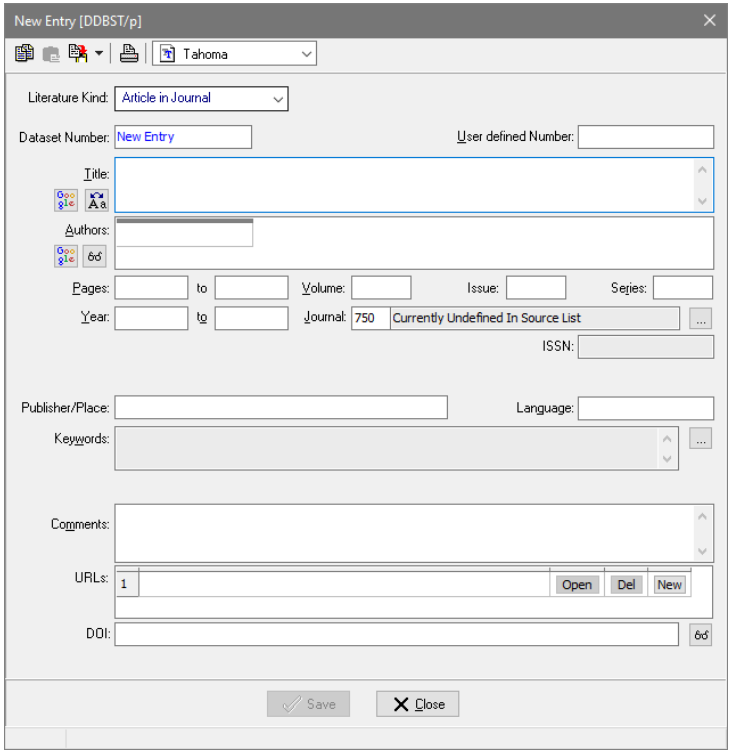




Private reference database

DDB - Private Data - Reference Input

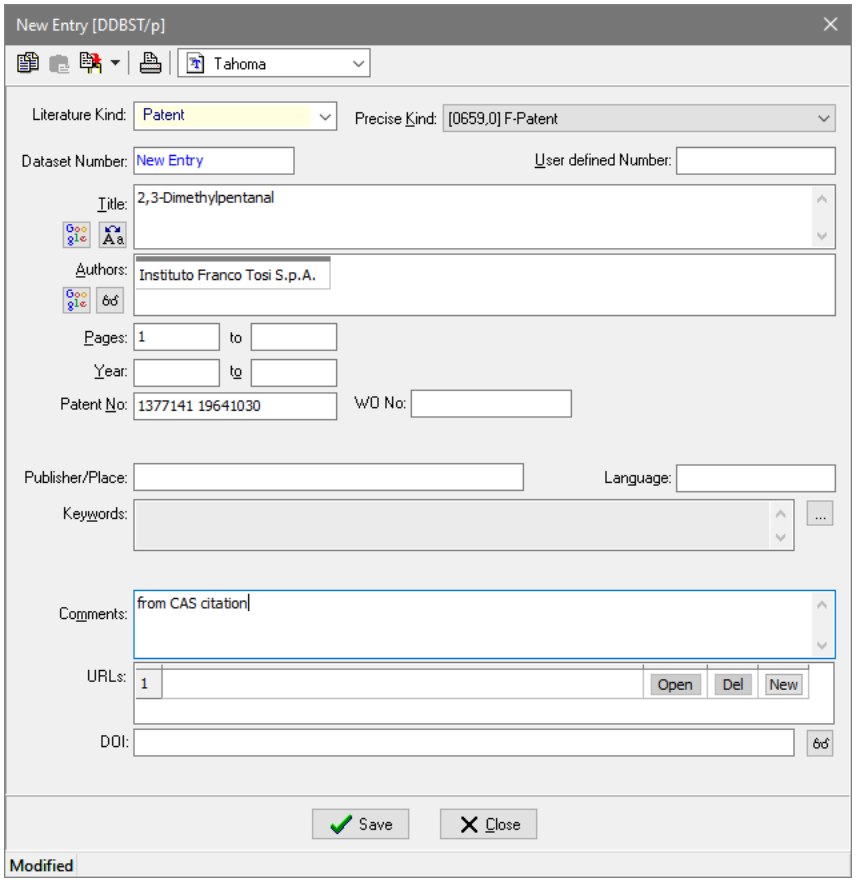
Double-click DDBST/p to open the data view dialog and select Edit – New Data Set:



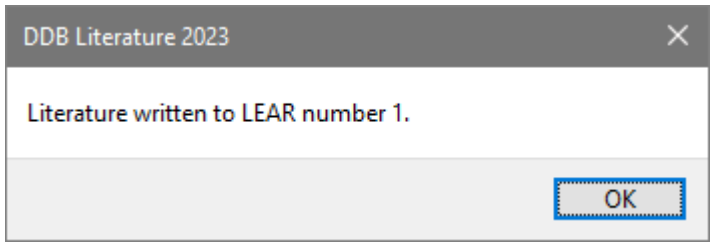
Now enter the reference information as shown on the next slide.

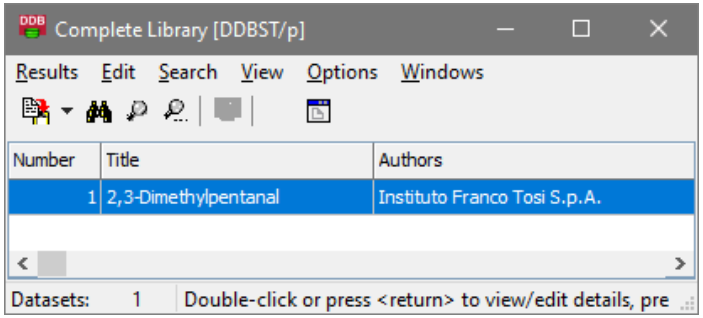
not in Explorer Version

DDB - Private Data - Reference Input



Save the Reference:



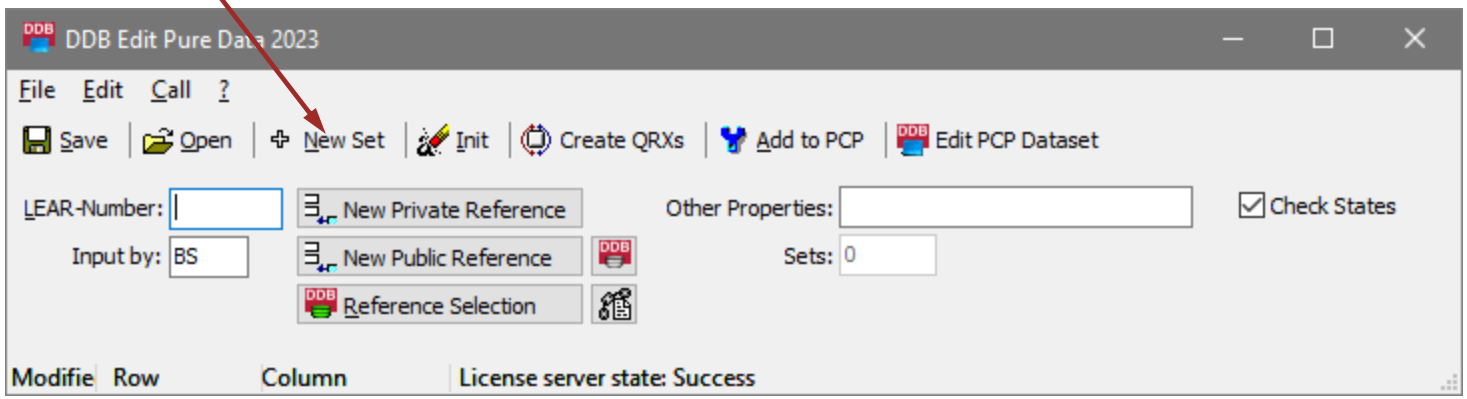


not in Explorer Version

DDB - Private Data - Reference Input

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

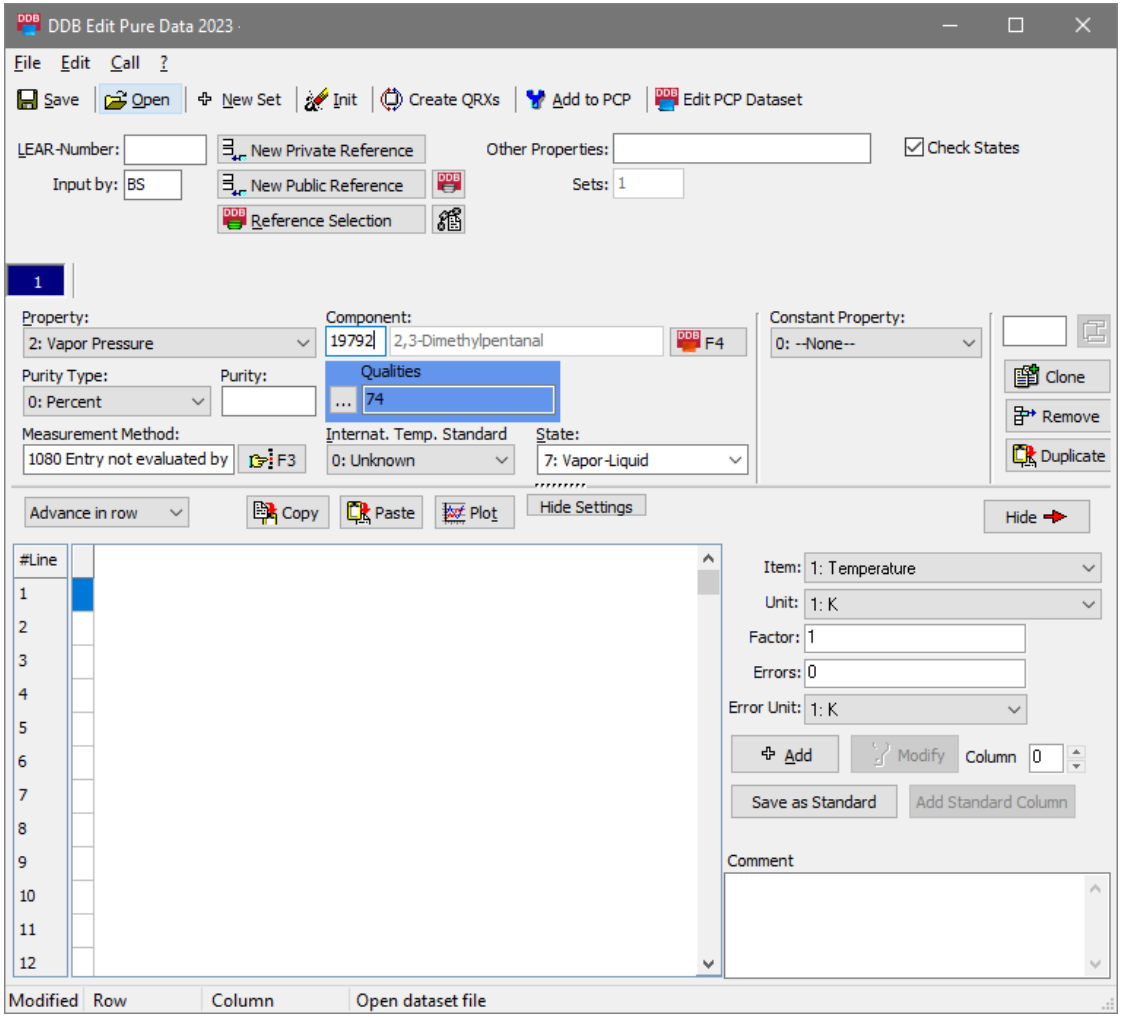
Select *New Set*



not in Explorer Version

DDB - Pure Component Data Input

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



not in Explorer Version

DDB - Pure Component Data Input

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

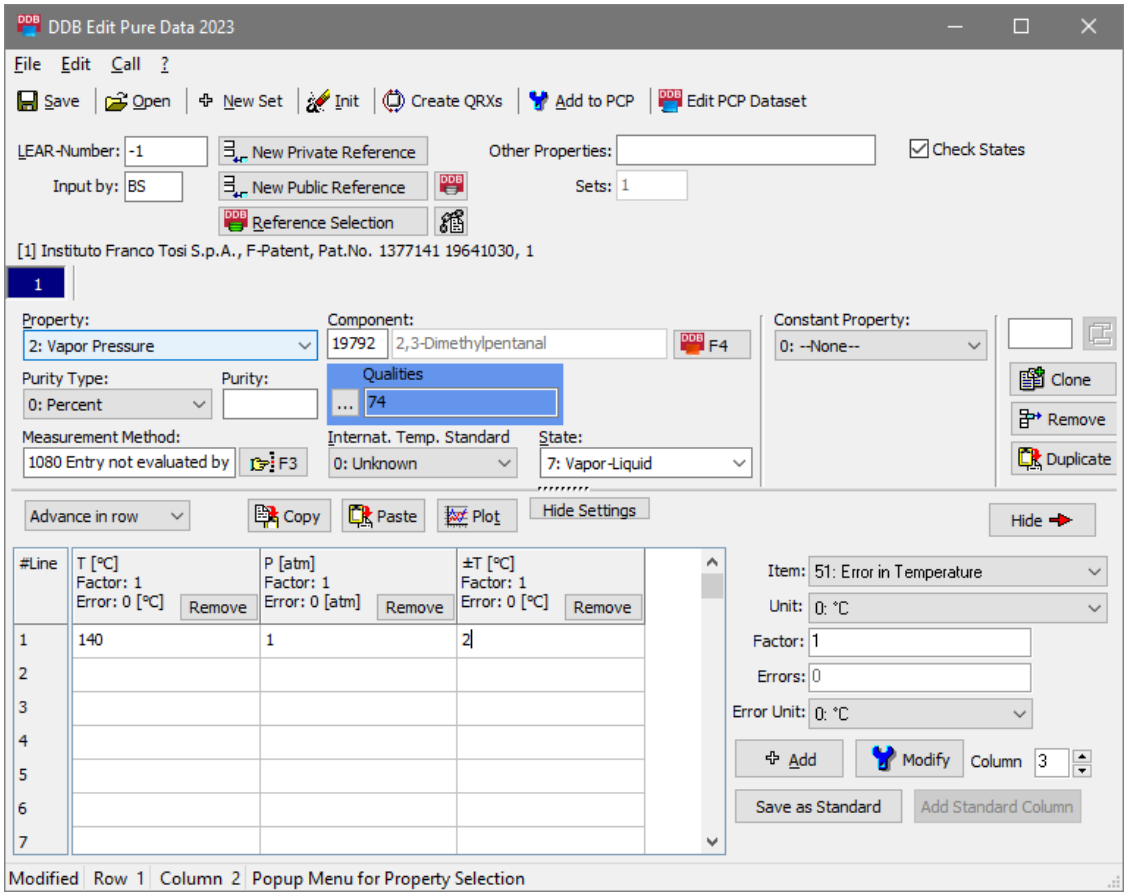
B an explicit error column can be introduced for absolute or relative errors of each property in each table line

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.

not in Explorer Version

DDB - Pure Component Data Input

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 "Lear Number is equal 1"):

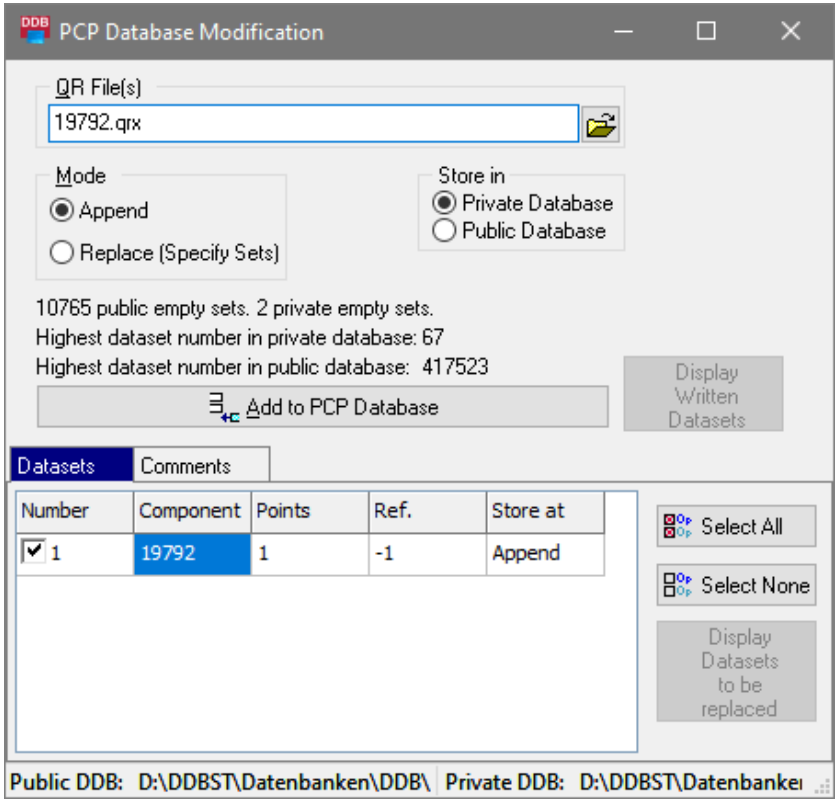


Now save the file and select Add to PCP.

not in Explorer Version

DDB - Pure Component Data Input

The following dialog will be shown:



And select "Add to PCP Database"

not in Explorer Version

DDB - Pure Component Data Input

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.

not in Explorer Version

DDB - Mixture Data Input

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

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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-C_6H_{10}) + oxolane (tetrahydrofuran, C_4H_8O), + oxane (tetrahydropyran, $C_5H_{10}O$), + 1,3-dioxolane (1,3-$C_3H_6O_2$), + 1,4-dioxane (1,4-$C_4H_8O_2$), and + cyclohexane (c-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-$C_3H_6O_2$ + c-C_6H_{10}, $H^E(x = 0.5) = 1155.5$ J mol^{-1}; and for 1,4-$C_4H_8O_2$ + c-C_6H_{10}, $H^E(x = 0.5) = 909.7$ J mol^{-1}. The excess enthalpy for C_4H_8O + c-C_6H_{10} is considerably smaller, i.e., $H^E(x = 0.5) = 285.5$ J mol^{-1}, and $C_5H_{10}O$ + c-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-C_6H_{12} + c-C_6H_{10} the excess enthalpy is rather symmetric, with $H^E(x = 0.5) = 97.3$ J mol^{-1}.

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 alkanoic 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-C_6H_{10}) + oxolane (tetrahydrofuran, C_4H_8O), + oxane (tetrahydropyran, $C_5H_{10}O$), + 1,3-dioxolane (1,3-$C_3H_6O_2$), + 1,4-dioxane (1,4-$C_4H_8O_2$), and + cyclohexane (c-C_6H_{12}). These measurements will be used later to assess, in terms of group-contribution theory (*6*), the influence of various structural parameters (ring size, proximity of oxygen in diethers, n–π interaction, etc.) on the thermodynamic behavior of such mixtures.

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Table I. Densities (ρ) of Pure Component Liquids at 298.15 K

compd	ρ/(kg m^{-3}) exptl	lit.
cyclohexene	806.0	806.09 (*9*), 806.3,[a] 805.66 (*11*), 805.9 (*12*), 805.70 (*13*)
cyclohexane	773.9	773.89 (*14*)
oxane	879.1	879.22[b]
oxolane	881.9	881.97 (*16*)
1,4-dioxane	1028.2	1028.21 (*17*), 1027.97 (*18*)
1,3-dioxolane	1059.1	1053.8[c]

[a] Interpolated value from ref *10*. [b] Interpolated value from ref *15*. [c] 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) + Cyclohexane ($1 - x$) with the Results of Marsh (*20*)

x	H^E/(J mol^{-1}) exptl	Marsh (*20*)	δ[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

[a] Percentage deviation $\delta = 100(H^E_{exptl} - H^E_{Marsh})/H^E_{Marsh}$.

Experimental Section

Materials. Source and treatment of the cycloethers have been given previously (*1*). Cyclohexene (from Fluka, puriss.,

0021-9568/82/1727-0333$01.25/0

Table III. Molar Excess Enthalpy H^E for Cyclic Ether + Cyclohexene and for Cyclohexane + Cyclohexene at 298.15 K[a]

x	H^E/(J mol^{-1})	x	H^E/(J mol^{-1})
	x c-C_6H_{12} + $(1-x)$ c-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-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-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-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-$C_3H_6O_2$ + $(1-x)$ c-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		

[a] Mole fraction of cyclic ether or cyclohexane is x.

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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

not in Explorer Version

DDB – Data Export

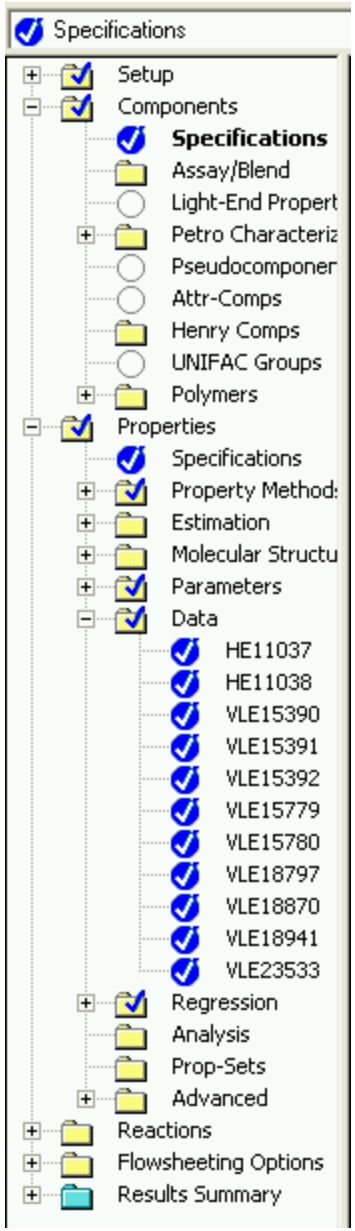
DDB-data and Parameters can be exported in a variety of ways:

- 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.



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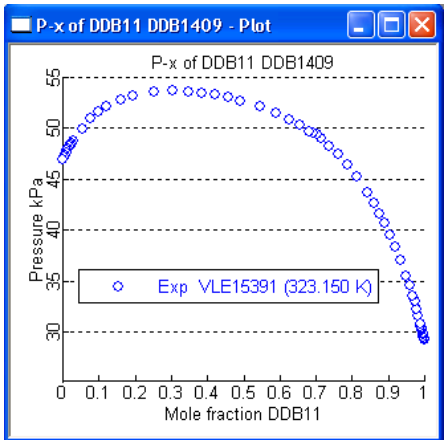
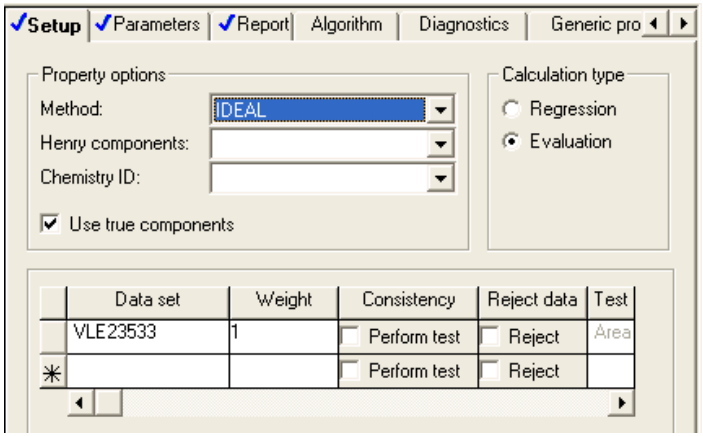
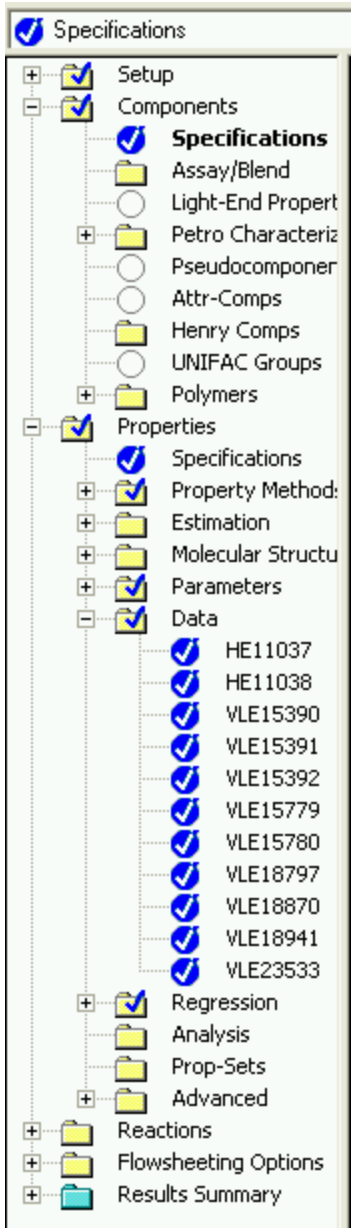
DDB - Data Export

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

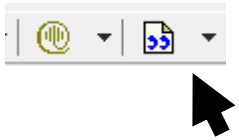


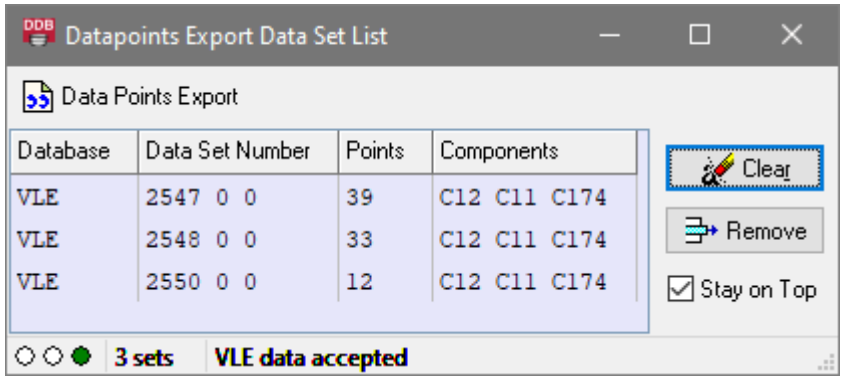
The regression case defined in the inp-file specifies ideal, evaluation and includes only the first data set. Change these settings as desired:





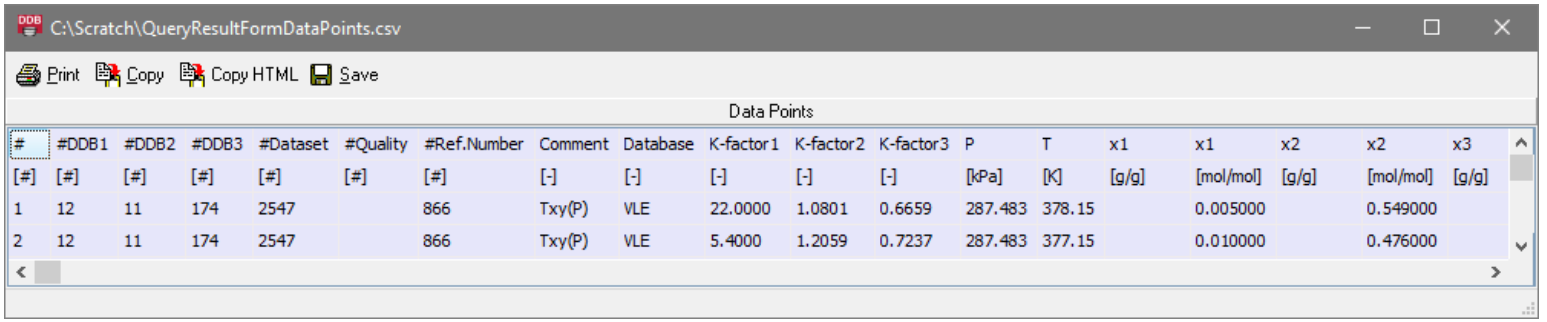
Complete Table Creation For Spreadsheets





Collecting data sets by drag and drop

Table creation and copying to Windows clipboard



#	#DDB1	#DDB2	#DDB3	#Dataset	#Quality	#Ref.Number	Comment	Database	K-factor1	K-factor2	K-factor3	P	T	x1	x1	x2	x2	x3
[#]	[#]	[#]	[#]	[#]	[#]	[#]	[-]	[-]	[-]	[-]	[-]	[kPa]	[K]	[g/g]	[mol/mol]	[g/g]	[mol/mol]	[g/g]
1	12	11	174	2547		866	Txy(P)	VLE	22.0000	1.0801	0.6659	287.483	378.15		0.005000		0.549000	
2	12	11	174	2547		866	Txy(P)	VLE	5.4000	1.2059	0.7237	287.483	377.15		0.010000		0.476000	

Conclusion

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 for updates and patches.

Thank you very much for your interest.