DDB and DDBSP

Delivery 2017

Changes and New Features

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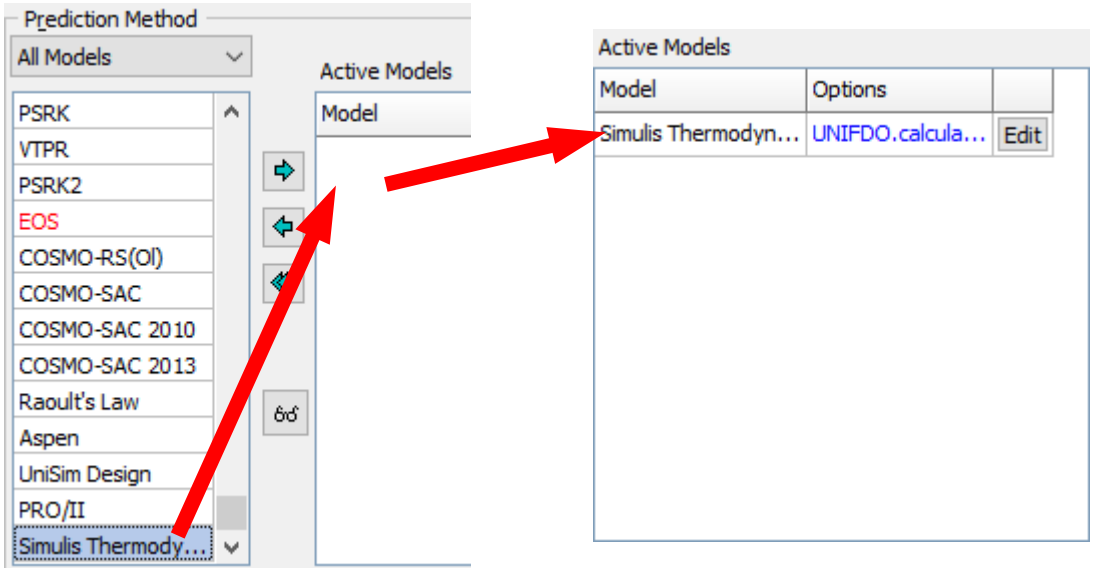
Contents

1 Connecting to Simulator Software

ProSim Simulis Thermodynamics

DDBST has added an interface to ProSim Simulis Thermodynamics. This allows calculating VLE, VLLE, and LLE within the Dortmund Data Bank by the Simulis Thermodynamics routines. Components from Simulis Thermodynamics calculator files can read and assigned to DDB numbers by a predefined mapping of Simulis and DDB components but a manual addition or override is also possible.

When predicting VLE/LLE data, Simulis Thermodynamics is added to the list possible models.



The settings are made within Simulis Thermodynamics (models, parameters, etc.).

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

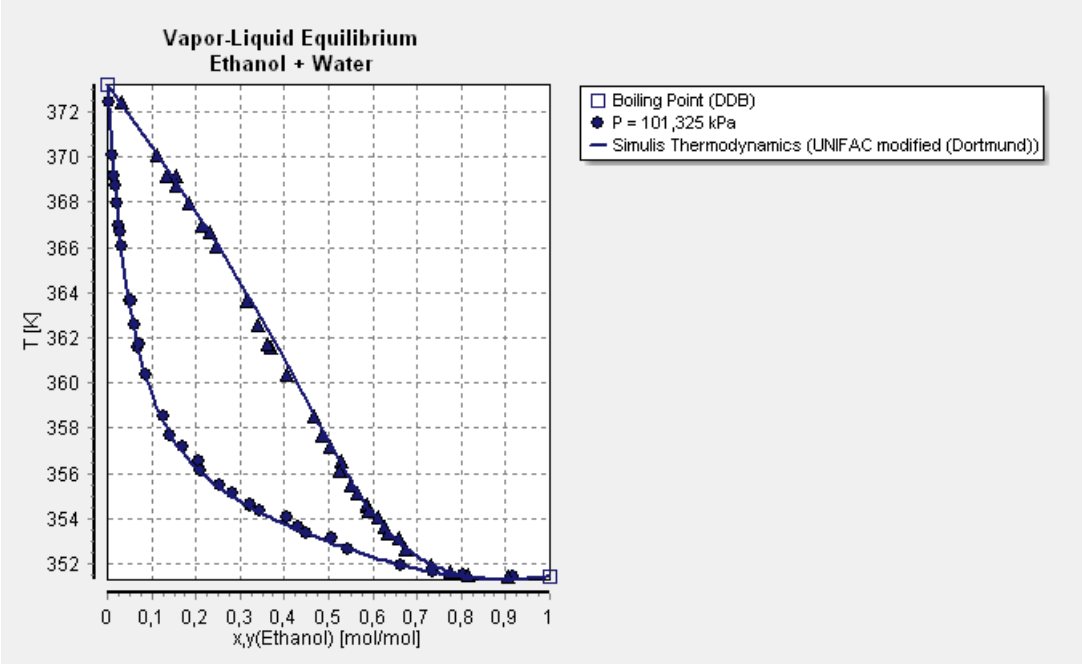


Figure 1: VLE T/x,y diagram

A more detailed description of the DDB-Simulis Thermodynamics connectivity can be found in the “Dortmund Data Bank” manual.

Pro/II 10.0

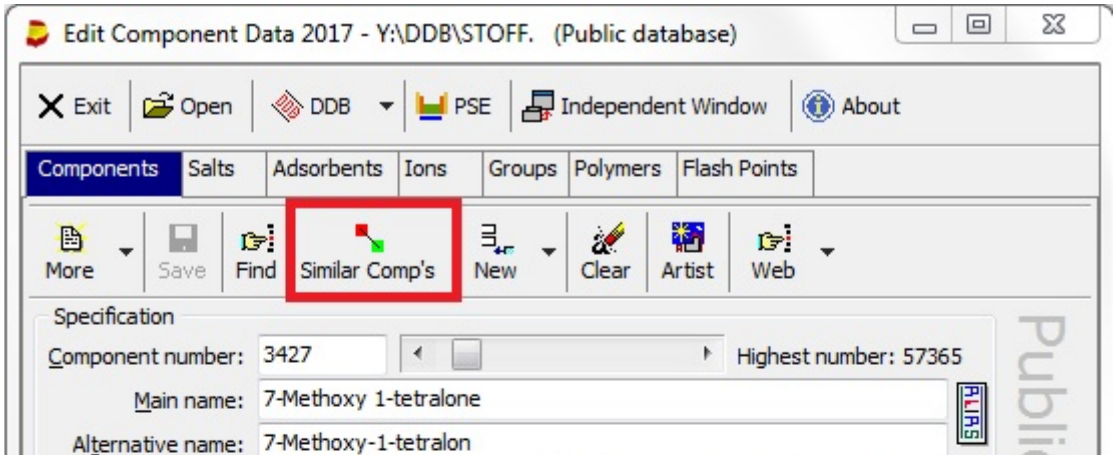
Support for the new Pro/II 10.0 version has been added.

UniSim Design R450

Support for the new UniSim Design version R450 has been added.

2 Component Data Base

Search for Similar Components



The similarity search is available in the Component Editor. There are three supported methods:

1. Finding related components for a given component.
2. Finding components within the same family of a given component. A family is defined by the presence of some functional groups.
3. A custom search with own criteria.

A detailed description of this new feature is given in the “Component Management” manual.

3 Component Selection

Two small improvements have been added:

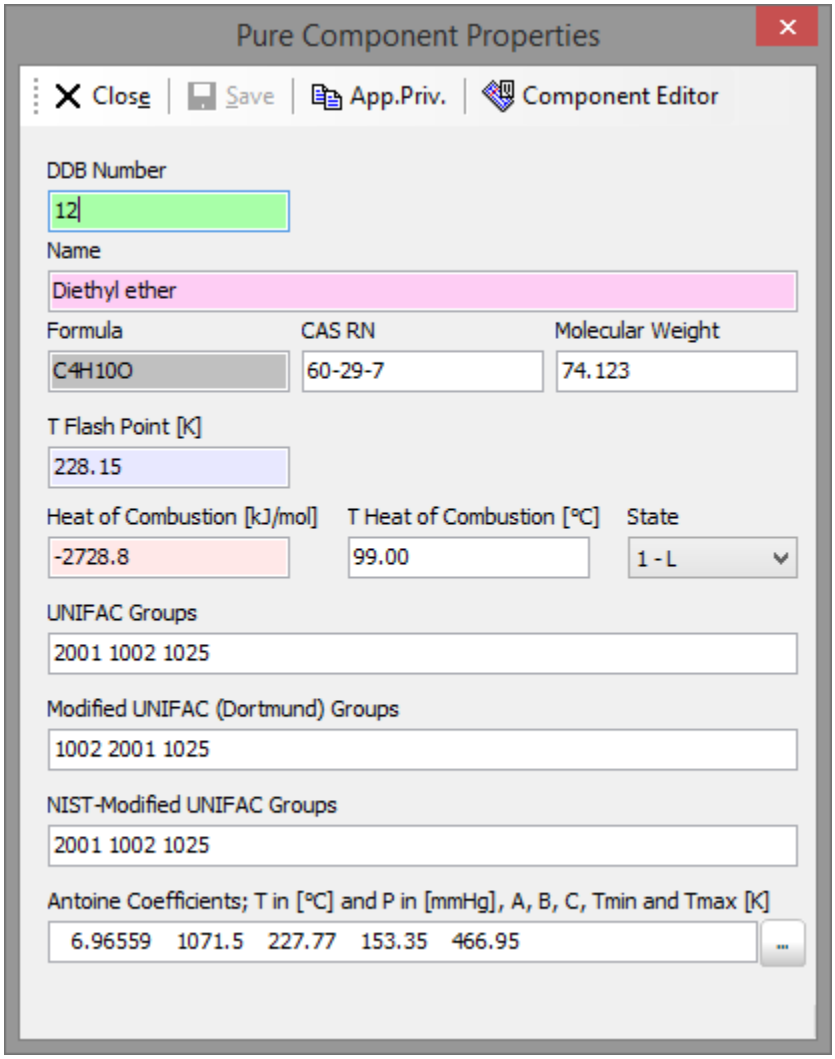
- **Support for polymer synonyms.**
  The polymer data bank contains some synonyms now available for search.
- **Improved search ignoring missing or redundant blanks**
  This feature makes it more probable to find components with different spellings regarding blanks.

4 Flash Point Prediction

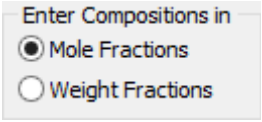
Four updates and additions are available:

- **Updated Data Base**
  A large number of pure component flash points and heats of combustion have been added.

- **Ideal Calculation Following Raoult's Law**
  Ideal calculation has been added as an option.
- **Editor for Component Database**
  A dialog for editing component specific data has been added.



- **Support for Entering Compositions in Weight Fractions**
  Composition can now be entered in weight fractions.



5 Pure Component Equation Fit

Support for two new equations

- Polynomial in $^1/_T$ for Dynamic Viscosities

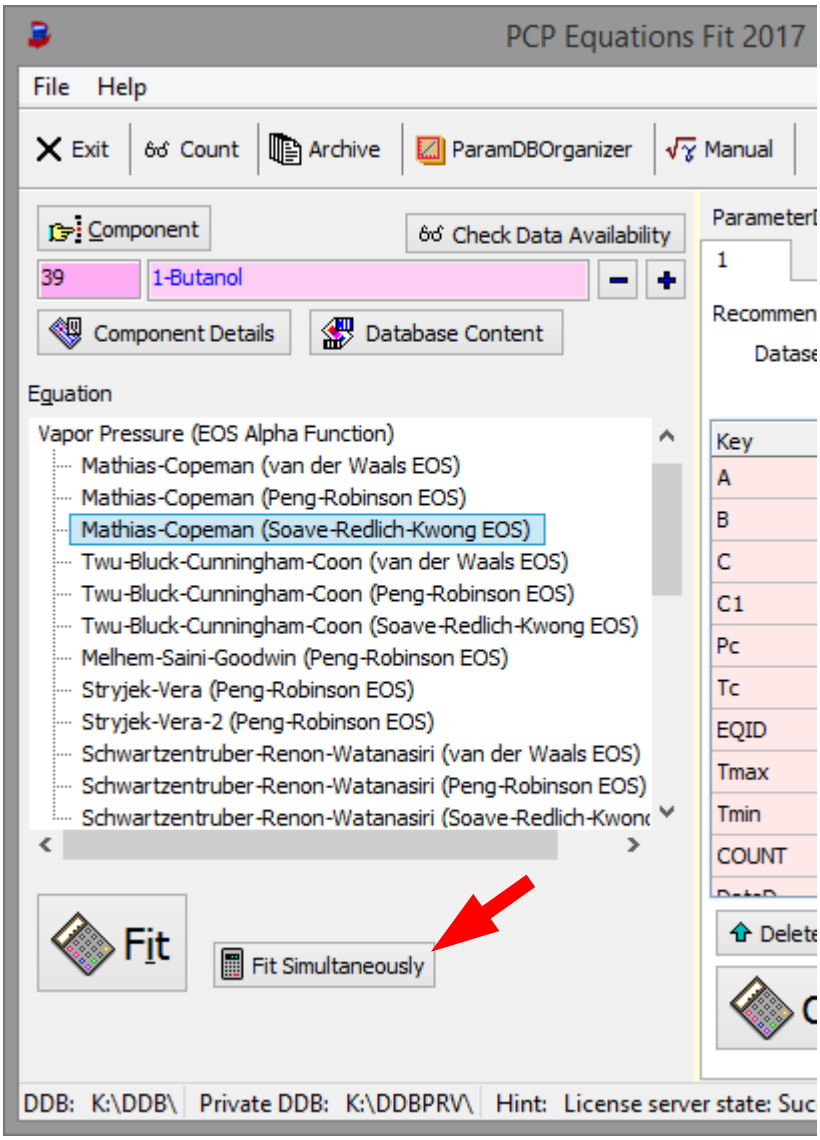
$$\eta = A + \frac{B}{T} + \frac{C}{T^2} + \frac{D}{T^3} + \frac{E}{T^4}$$

- Pitzer/Carruth/Kobayashi Equation for Heat of Vaporization

$$H_{vap} = A \cdot \tau^{\frac{1}{3}} + B \cdot \tau^{\frac{2}{3}} + C \cdot \tau \quad \text{with} \quad \tau = 1 - \frac{T}{T_c}$$

Simultaneous Regression for α Function Parameters

A new simultaneous fitting tools for α parameters is available for Mathias-Copeman constants for Soave-Redlich-Kwong (used in PSRK) and for Twu-Bluck-Cunningham-Coon constants for Peng-Robinson (used in VTPR).



The fitting routine supports the simultaneous fit of parameters to vapor pressures, heats of vaporization, second virial coefficients, and liquid heat capacities. A detailed description of this new feature is available in the "PCPEquationFit" manual.

6 Mixture Calculations

- **Prediction of Ternary Azeotropes**
  It is now possible to predict ternary azeotropes with all the models used already for binary azeotropes.

- **CPE, LLE, SLE Calculation with COSMO-SAC2010 and 2013**
  These rather new COSMO-based models can now be used to predict excess heat capacities, liquid-liquid equilibria, and solid-liquid equilibria.

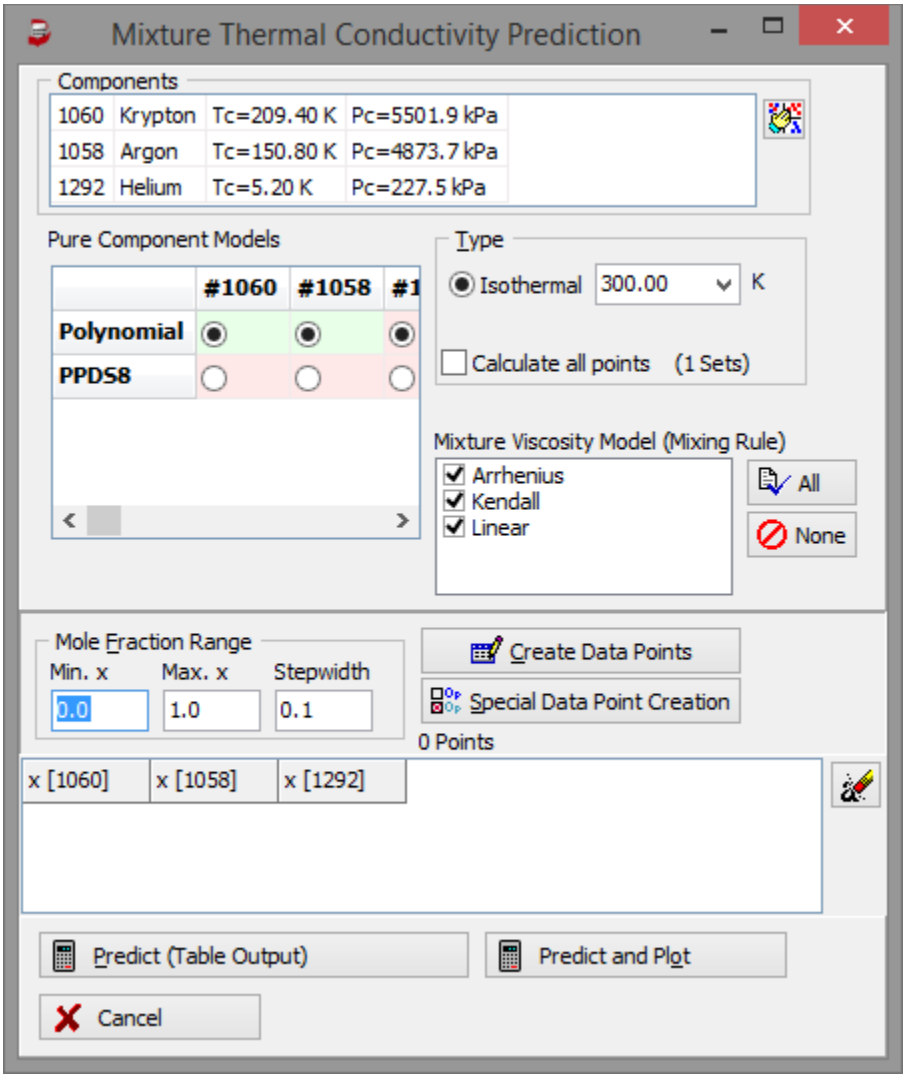
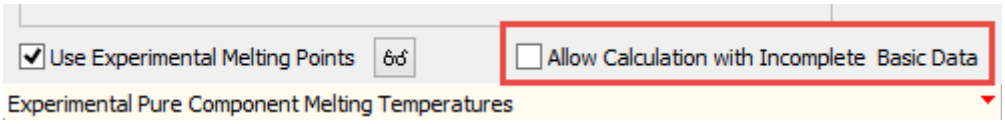


Figure 2: Prediction of Mixture Thermal Conductivities

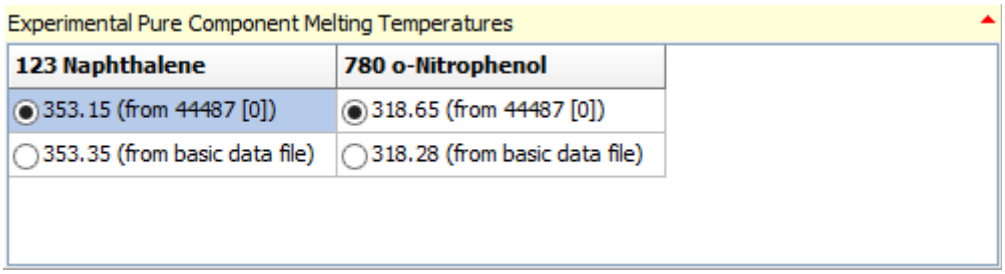
- **Prediction of Mixture Thermal Conductivities**
  This prediction uses some simple miscibility rules together with pure component data calculated by the equations PPDS8 and polynomial. The parameter have to be fitted with PCPEquationFit.

- **Calculation of single SLE branch**
  This option allows the calculation of a solid-liquid equilibrium even if the needed pure component properties are available only for single components and not for the entire mixture.



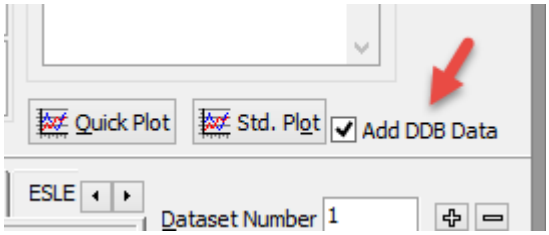
- **SLE Prediction: Selection of Experimental Melting Points**
  For the recalculation of experimental data it is sometimes necessary to modify the standard melting

temperature stored in the DDB by a melting point that matches the experimental values; otherwise an offset would be created. If the experimental data contain a pure component melting temperature it is normally best to select that T_m. This option allow switching between these values and the value from the DDB basic component data file.



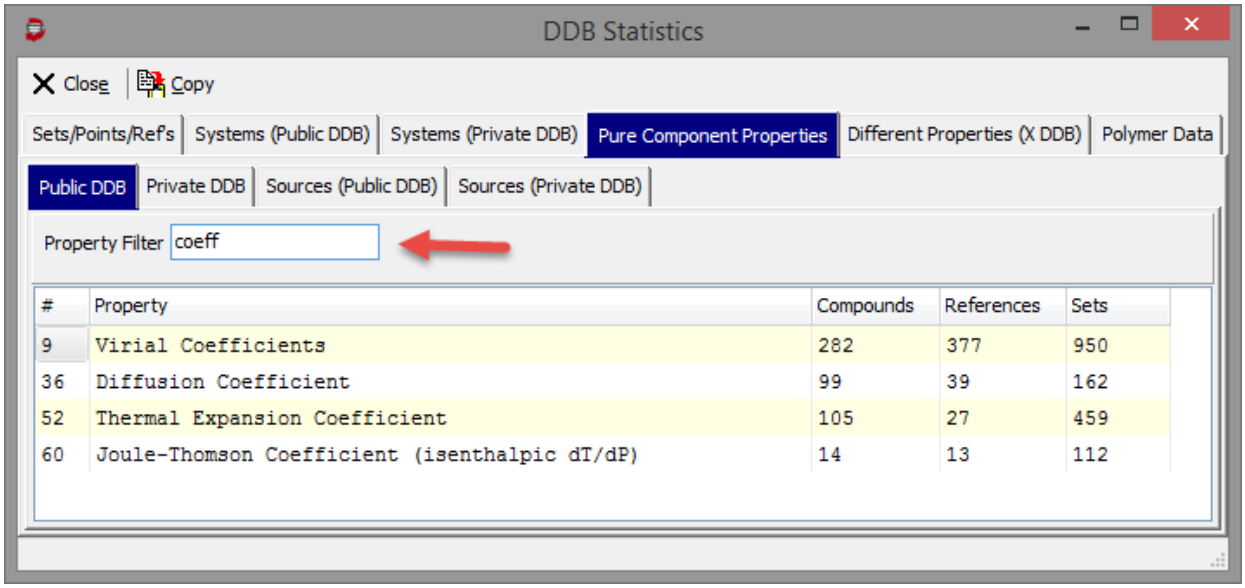
7 Edit Mixture Data

The editor supports to plot stored experimental data together with the newly added data.



8 Dortmund Data Bank

1. The statistics displaying the content of the pure component properties data bank (PCPDDB) allows filtering for properties.



2. It is now possible to plot VLE data containing pure component data. These sets are converted to pure component data and then displayed.

9 RecPar

Support for single point VLE data sets has been added.

10 Compound List Editor

Import components from PIN and QR files

PIN (prediction input) and QR (query result) files are created within the DDB software package and contain mixture and component information. The Compound List Editor is now capable of extracting this information and display the components. PIN and QR files can either be ‘dragged and dropped’ or opened.

Transfer single components or component lists to query of

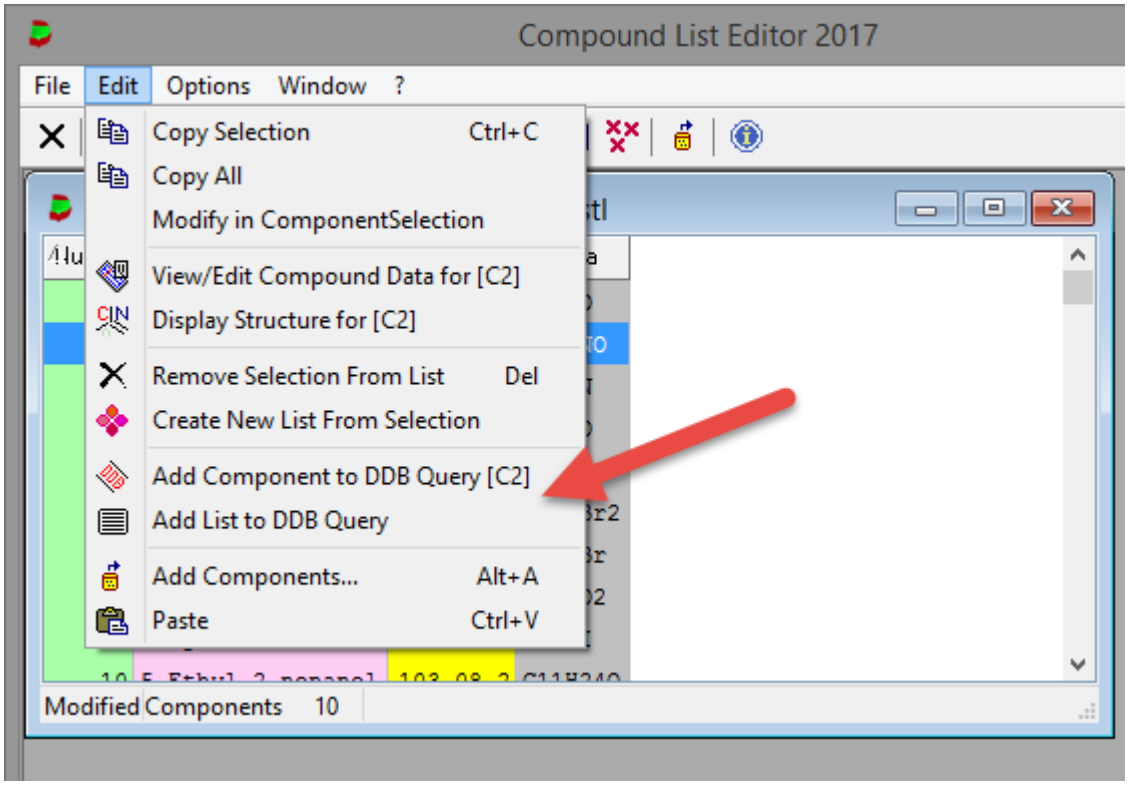
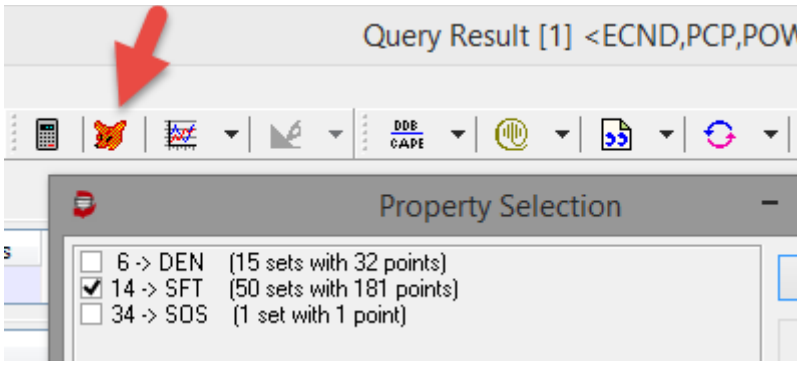


Figure 3: Transfer of Components or Component Lists to DDB Query

Dortmund Data Bank program.

11 Pure Component Prediction

Prediction of Surface Tensions by DIPPR106 and PPDS14 Equations



This allows to calculate surface tensions by the two mentioned equations within the Dortmund Data Bank main retrieval program. The parameters are taken from the ParameterDDB and must have been fitted with the PCP equation fit software tool.

12 Artist

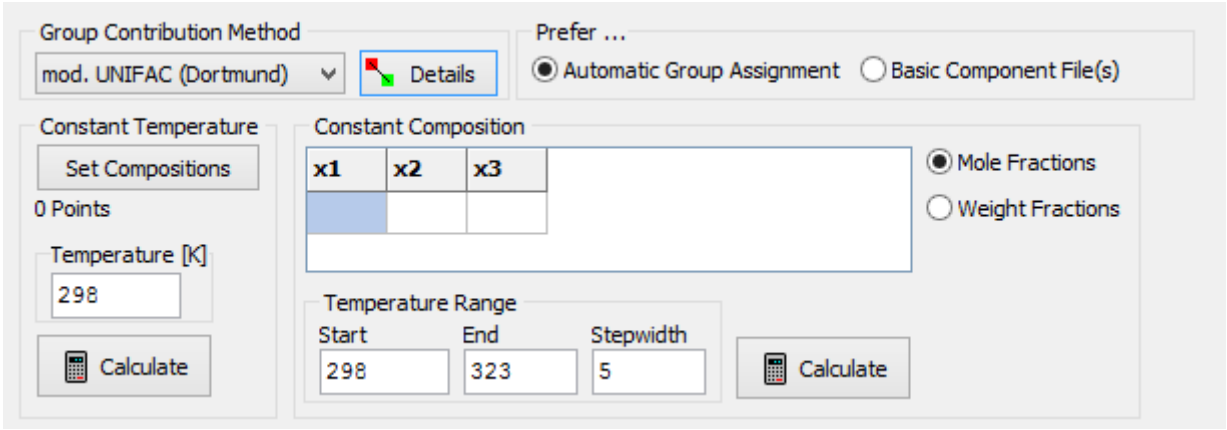
Added Fedors Method for Critical Temperatures

Implemented from “Fedors R.F., "A Relationship Between Chemical Structure and the Critical Temperature", Chem.Eng.Commun., 16, 149-151, 1982”.

Support for SDF files

SDF files can now be opened. SDF files contain a single molecular structure or lists of molecular structures in ‘mol’ format.

Improved Dialog for Activity Coefficient Calculations



- The dialog now contains a button (“Details”) which allows to invoke the detailed display of available group assignments and interaction parameters for the specified model.
- An option (“Prefer...”) has been added that allows to use stored group assignments for DDB components instead of using group lists from the Artist internal automatic group assignment function. This allows altering group assignments manually in the component editor.

SMILES

Artist has limited support for loading molecular structures in the SMILES format. Artist does not load or save SMILES itself, it uses OpenBabel for that purpose. OpenBabel is not delivered with Artist but must be downloaded and installed separately.

OpenBabel, if available, is also used for creating 2D and 3D structures.

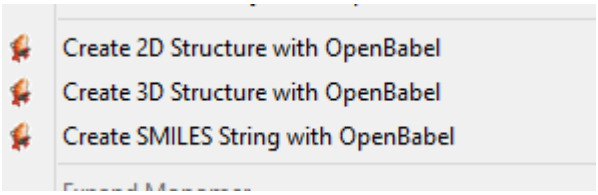


Figure 4: Part of drawing window's context menu

13 Mixture Plots

Two small improvements have been added:

- Users can modify and save/restore plot options.
- The normal pressure (1 atm) and P_c are shown in diagrams, where appropriate.

14 AZEOT (Prediction of Azeotropes)

Two small improvements have been added:

1. Predicted azeotropic points can now be shown in a diagram
2. The LLE test can be deactivated which may make sense if the LLE prediction is not reliable (model and system specific).

15 CalculateX3

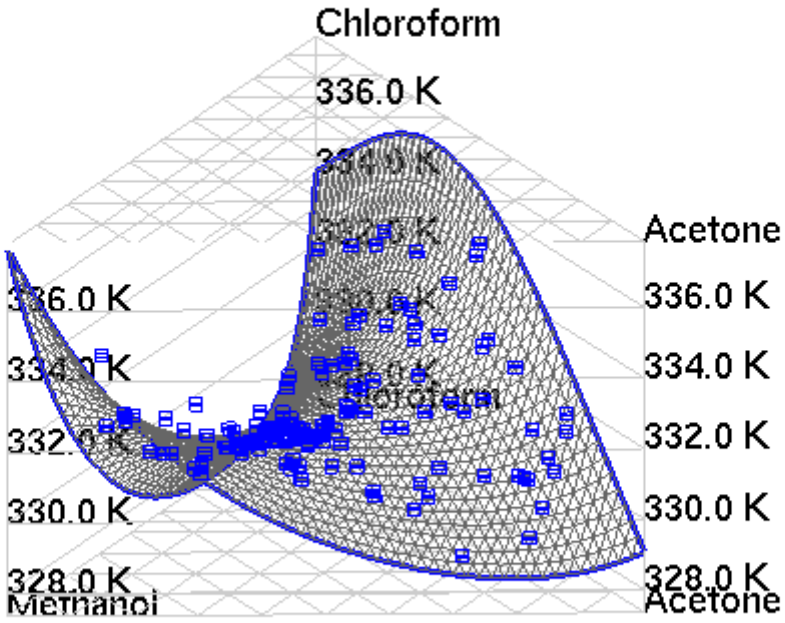


Figure 5: VLE of Chloroform/Methanol/Acetone Calculated with PSRK

The calculation of vapor-liquid equilibria and heats of mixing is now possible with PSRK and VTPR.

16 PredictiveEOS

The support for predicting **excess volumes** with PSRK and VTPR has been added. PSRK has its limitations, though, and the accuracy is rather limited, whereas VTPR mostly delivers usable results.

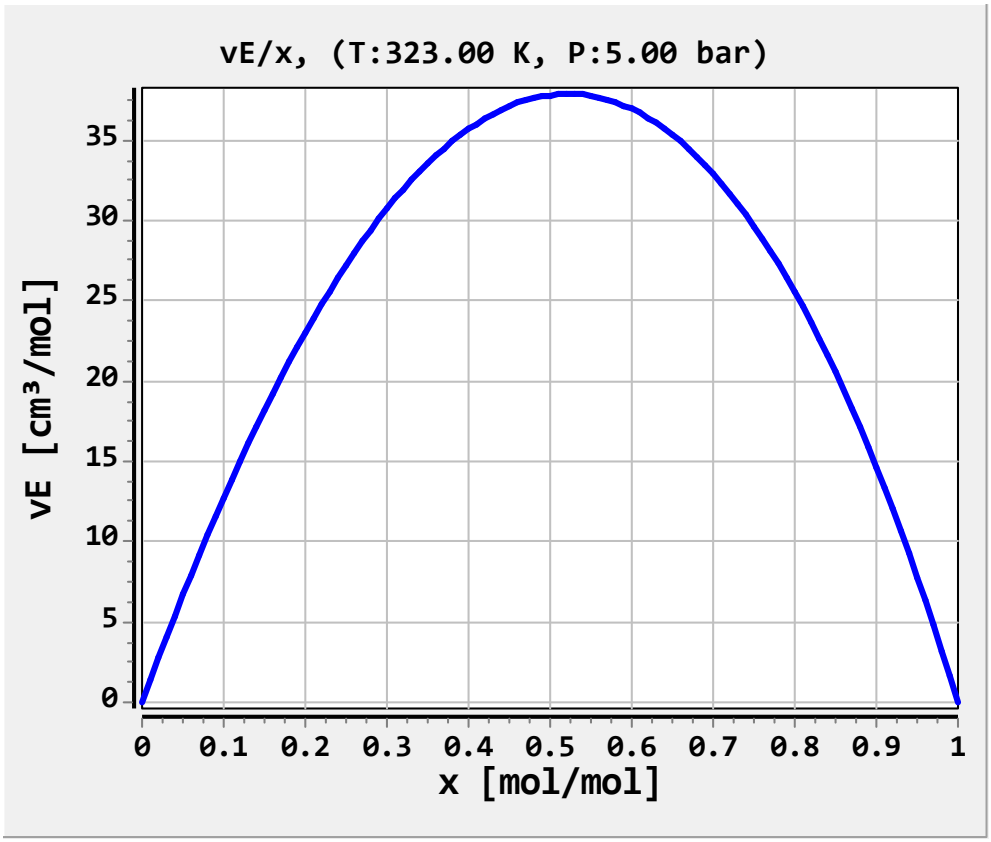


Figure 6: Excess Volume of Propane and Carbon Dioxide Calculated by VTPR

17 Parameters for Modified UNIFAC (Dortmund)

The parameters of “Hector T., Gmehling J., "Present status of the modified UNIFAC model for the prediction of phase equilibria and excess enthalpies for systems with ionic liquids", Fluid Phase Equilib., 371, 82-92, 2014” and “Constantinescu D., Gmehling J., "Further Development of Modified UNIFAC (Dortmund): Revision and Extension 6", J.Chem.Eng.Data, 61(8), 2738-2748, 2016” are now included.

18 Dortmund Data Bank Progress

The Dortmund Data Bank 2017 has more than 58000 new data sets and more than 455000 new data points. Data from more than 4100 sources have been added.

	2017			2016			Absolute Gain			Relative Gain		
Data Bank	Sets	Points	References	Sets	Points	References	Sets	Points	References	Sets	Points	References
AAE	4846	60645	295	4592	57044	283	+254	+3601	+12	5,53 %	6,31 %	4,24 %
ACM	1774	10599	83	1725	10312	75	+49	+287	+8	2,84 %	2,78 %	10,67 %
ACT	96392	96392	1418	90047	90047	1380	+6345	+6345	+38	7,05 %	7,05 %	2,75 %
AZD	57427	57427	8684	56632	56632	8548	+795	+795	+136	1,40 %	1,40 %	1,59 %
CPE	6819	78380	823	6472	74844	794	+347	+3536	+29	5,36 %	4,72 %	3,65 %
CRI	3361	22975	1051	3295	22520	1019	+66	+455	+32	2,00 %	2,02 %	3,14 %
DIF	2136	14757	370	1820	13297	303	+316	+1460	+67	17,36 %	10,98 %	22,11 %
ECND	9956	103690	927	8827	93230	822	+1129	+10460	+105	12,79 %	11,22 %	12,77 %
EGLE	3450	19968	275	2863	16805	222	+587	+3163	+53	20,50 %	18,82 %	23,87 %
ELE	13465	169308	1865	11898	148575	1680	+1567	+20733	+185	13,17 %	13,95 %	11,01 %
ESLE	41911	289024	7798	40469	280257	7592	+1442	+8767	+206	3,56 %	3,13 %	2,71 %
GHD	4281	31505	774	3850	28833	698	+431	+2672	+76	11,19 %	9,27 %	10,89 %
GLE	24140	115492	2356	22971	110002	2219	+1169	+5490	+137	5,09 %	4,99 %	6,17 %
HE	23174	342613	3370	22792	336850	3314	+382	+5763	+56	1,68 %	1,71 %	1,69 %
HPV	41090	353411	4695	39829	340551	4547	+1261	+12860	+148	3,17 %	3,78 %	3,25 %
LLE	32479	293285	5084	30824	272370	4831	+1655	+20915	+253	5,37 %	7,68 %	5,24 %
MDEC	7289	66887	885	6762	62846	813	+527	+4041	+72	7,79 %	6,43 %	8,86 %
MFLP	639	5381	121	567	5148	105	+72	+233	+16	12,70 %	4,53 %	15,24 %
MPVT	14457	253545	1177	12804	222746	1026	+1653	+30799	+151	12,91 %	13,83 %	14,72 %
MSFT	6217	69251	772	5691	64957	697	+526	+4294	+75	9,24 %	6,61 %	10,76 %
MSOS	20469	247558	1930	17654	218973	1681	+2815	+28585	+249	15,95 %	13,05 %	14,81 %

	2017			2016			Absolute Gain			Relative Gain		
Data Bank	Sets	Points	References	Sets	Points	References	Sets	Points	References	Sets	Points	References
MTCN	4828	42864	390	4764	41872	377	+64	+992	+13	1,34 %	2,37 %	3,45 %
PCP	302232	1928014	40086	286294	1832577	37919	+15938	+95437	+2167	5,57 %	5,21 %	5,71 %
POLYMER	21072	219139	1758	20539	210443	1704	+533	+8696	+54	2,60 %	4,13 %	3,17 %
POW	14686	14686	602	14359	14359	581	+327	+327	+21	2,28 %	2,28 %	3,61 %
SLE	60270	496984	8715	56175	462449	8176	+4095	+34535	+539	7,29 %	7,47 %	6,59 %
VE	75911	851635	8000	71391	801218	7545	+4520	+50417	+455	6,33 %	6,29 %	6,03 %
VIS	44796	473077	4228	40909	435572	3895	+3887	+37505	+333	9,50 %	8,61 %	8,55 %
VLE	38696	562155	8015	37457	547223	7832	+1239	+14932	+183	3,31 %	2,73 %	2,34 %
X	32226	310762	3549	27832	273621	3024	+4394	+37141	+525	15,79 %	13,57 %	17,36 %
Sum	**1010489**	**7601409**	**78210**	**952104**	**7146173**	**74108**	**+58385**	**+455236**	**+4102**	**6,13 %**	**6,37 %**	**5,54 %**

Disclaimer: The numbers presented here may be different for a specific delivery because of corrections or other necessary changes.

The data base short terms are:
AAE: Adsorbent/Adsorptive equilibria – ACM: Activity coefficients at infinite dilution of a solute in a binary solvent – ACT: Activity coefficients at infinite dilution of a solute in a pure solvent – AZD: Azeotropic data points – CPE: Heat capacities and excess heat capacities – CRI: Critical data of mixtures – DIF: Diffusion coefficients – ECND: Electrical conductivities – EGLE: Gas solubilities in electrolyte-containing mixtures – ELE: Vapor-liquid equilibria of electrolyte-containing mixture – ESLE: Salt solubilities – GHD: Gas hydrate data – GLE: Gas solubilities (gas-liquid equilibria) – HE: excess enthalpies – HPV: Vapor-liquid equilibria (at least one component has a normal boiling point below 0°C) – LLE: Liquid-liquid equilibria (miscibility gaps) – MDEC: Mixture dielectric constants – MFLP: Mixture Flash Points – MPVT: Mixture P-v-T data – MSFT: Mixture surface tensions – MSOS: Mixture speeds of sound – MTCN: Mixture thermal conductivities – PCP: Pure component properties (several dozen different properties) - POLYMER: Polymer related data (VLE, LLE, etc.) – POW: Octanol-Water partition coefficients – SLE: Solid-liquid equilibria (solubilities) – VE: volumes, densities and excess volumes of mixtures – VIS: Mixture viscosities – VLE: Vapor-liquid equilibria (all components with a normal boiling point above 0°C) – X: Different thermodynamic properties.