
DDB and DDBSP Delivery

2016

Changes and New Features



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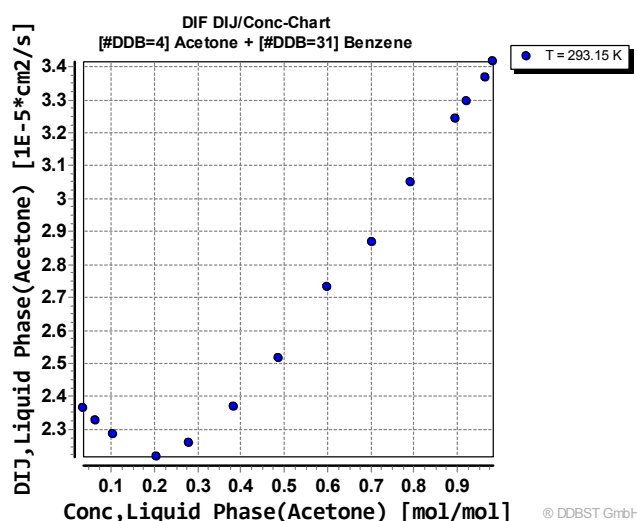
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1 New data bank for diffusion coefficients

A new data bank for diffusion coefficients is available. The chosen short term is “DIF” and it contains mostly mixture coefficients and only few pure component coefficients. Many pure component diffusion coefficients are stored in the separate data bank for pure component properties.

The data bank contains more than 1800 data sets with more than 13200 data points from more than 280 sources (articles, books, etc.) and more than a thousand mixtures are covered.



2 Pure component equation parameter fitting

1. The DIPPR 119 equation is now available for fitting parameters to liquid densities

$$\rho = A + B \cdot \tau^{\frac{1}{3}} + C \cdot \tau^{\frac{2}{3}} + D \cdot \tau^{\frac{5}{3}} + E \cdot \tau^{\frac{16}{3}} + F \cdot \tau^{\frac{43}{3}} + G \cdot \tau^{\frac{110}{3}} \quad \text{with} \quad \tau = 1 - \frac{T}{T_c}$$

2. The DIPPR 100 equation (just a polynomial) is now available for fitting parameters to vapor pressures
3. Antoine equation parameters can now be fitted by linear regression
4. Hoffmann-Florin equation added for saturated vapour pressures

$$P = \exp \left(A + B \left(\frac{1}{T} - 7.9151 \cdot 10^{-3} + 2.6726 \cdot 10^{-3} \cdot \log_{10}(T) - 0.8625 \cdot 10^{-6} \cdot T \right) \right)$$

3 Simultaneous regression tool (RecPar)

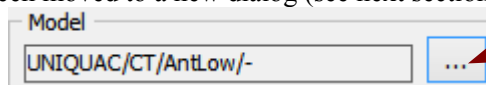
3.1 Some enhancements and changes

1. The Poynting corrections can be assigned per component now.
2. The result table does now contain a column for the contribution to the objective function.
3. The experimental data table does now display a summary line per data set only. The data points can be displayed by expanding the nodes. The summary does now contain – if applicable – the concentration range, the temperature range and the pressure range. Furthermore the data set weight and objective

#	x [mol/mol]	y [mol/mol]	T [K]	P [kPa]	Weight	+/-	Cons	Obj	Objective Functions
175 [0]	0.007 - 0.863	0.129 - 0.96	342.15 - 377.65	287.483	1.00	+/-	{-}	<input type="radio"/>	(T_exp - T_cal)/T_exp
176 [0]	0.065 - 0.933	0.251 - 0.967	378.15 - 400.15	721.847	1.00	+/-	{-?}	<input type="radio"/>	(T_exp - T_cal)/T_exp
177 [0]	0.039 - 0.943	0.217 - 0.984	363.15 - 382.55	515.011	1.00	+/-	{-}	<input type="radio"/>	(T_exp - T_cal)/T_exp

function is now visible, too. Finally a button to enable or disable a data set (or data point) and a button to modify the objective function properties for a data set (or data point) have been added.

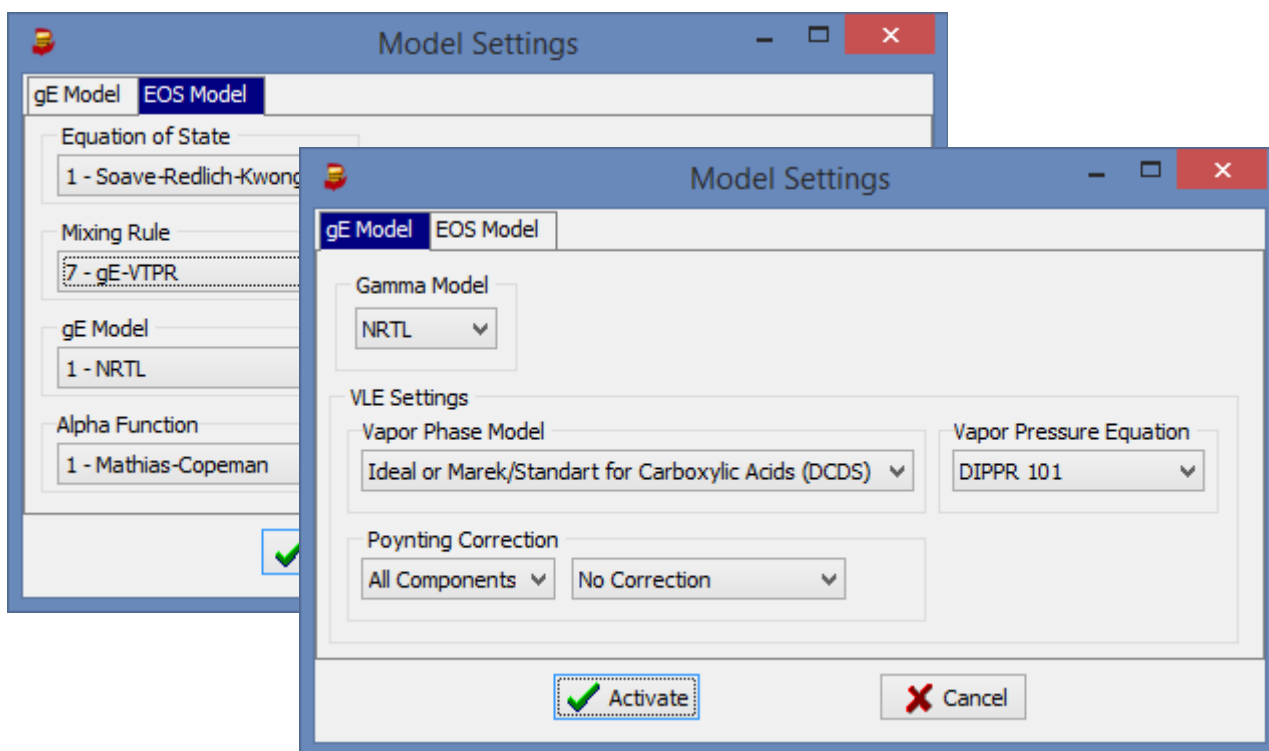
- The model selection has been moved to a new dialog (see next section).



- The start parameters dialog is now displayed when the fit button is pressed.

3.2 Integration of fitting parameters for equation of state mixing rules

The new RecPar combines the fitting of g^E model parameters already known from the old RecVal tool with the fitting of parameters for equation of state mixing rule previously implemented in a different tool (GenPar).



This integration allows fitting these parameters to other than only VLE data, as before. Supported properties are mixing enthalpies, activity coefficients, solid-liquid and liquid-liquid equilibrium data, and excess heat capacities.



In addition to GenPar the model Peng-Robinson 1978 is now supported.

Furthermore the temperature dependency term for g^E mixing rules has been extended:

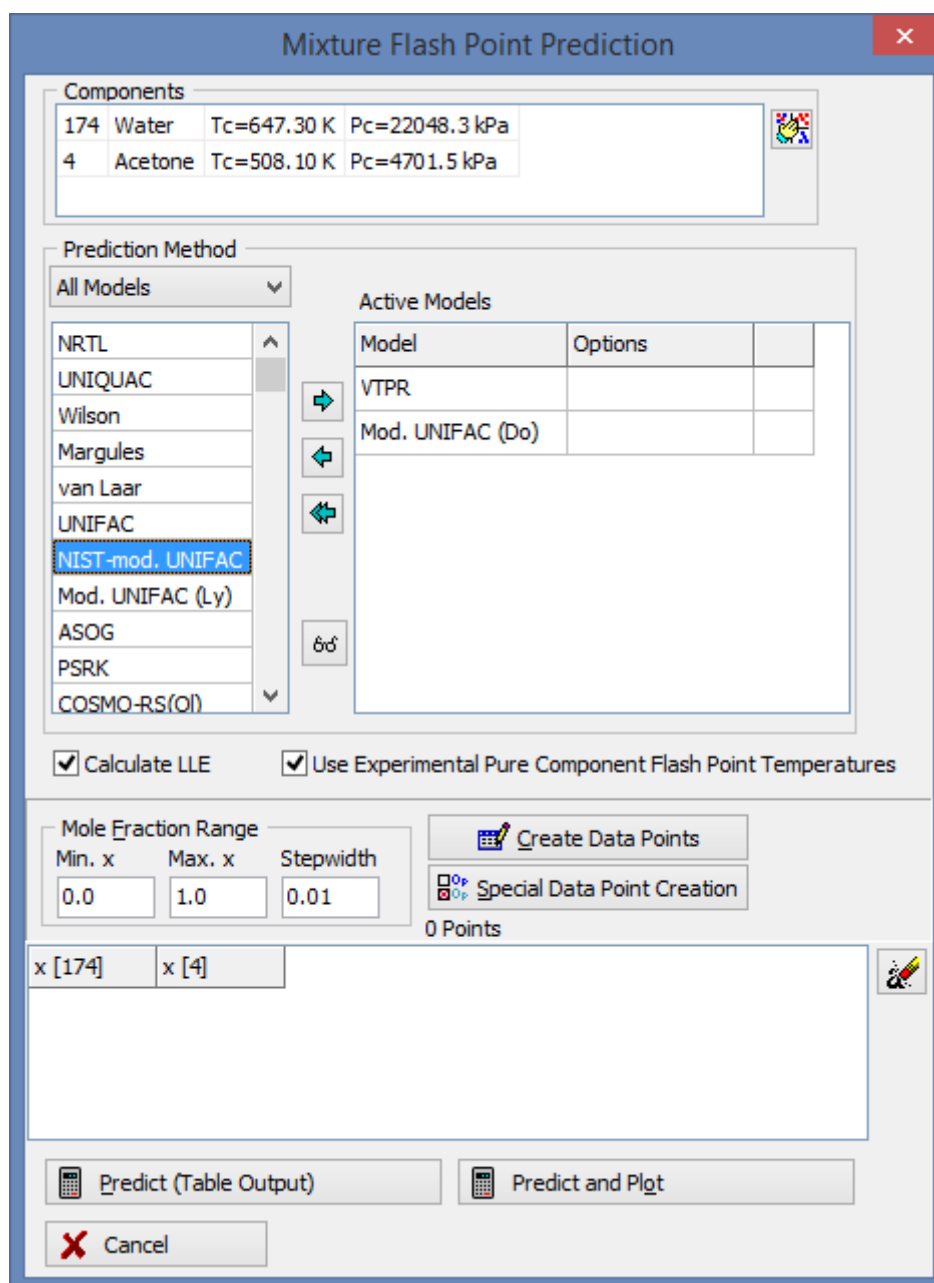
$$k_{ij} = a_{ij} + b_{ij}T + c_{ij} + \frac{d_{ij}}{T} + e_{ij}T \ln T + f_{ij}T^3 .$$

The terms for e_{ij} and f_{ij} have been added.

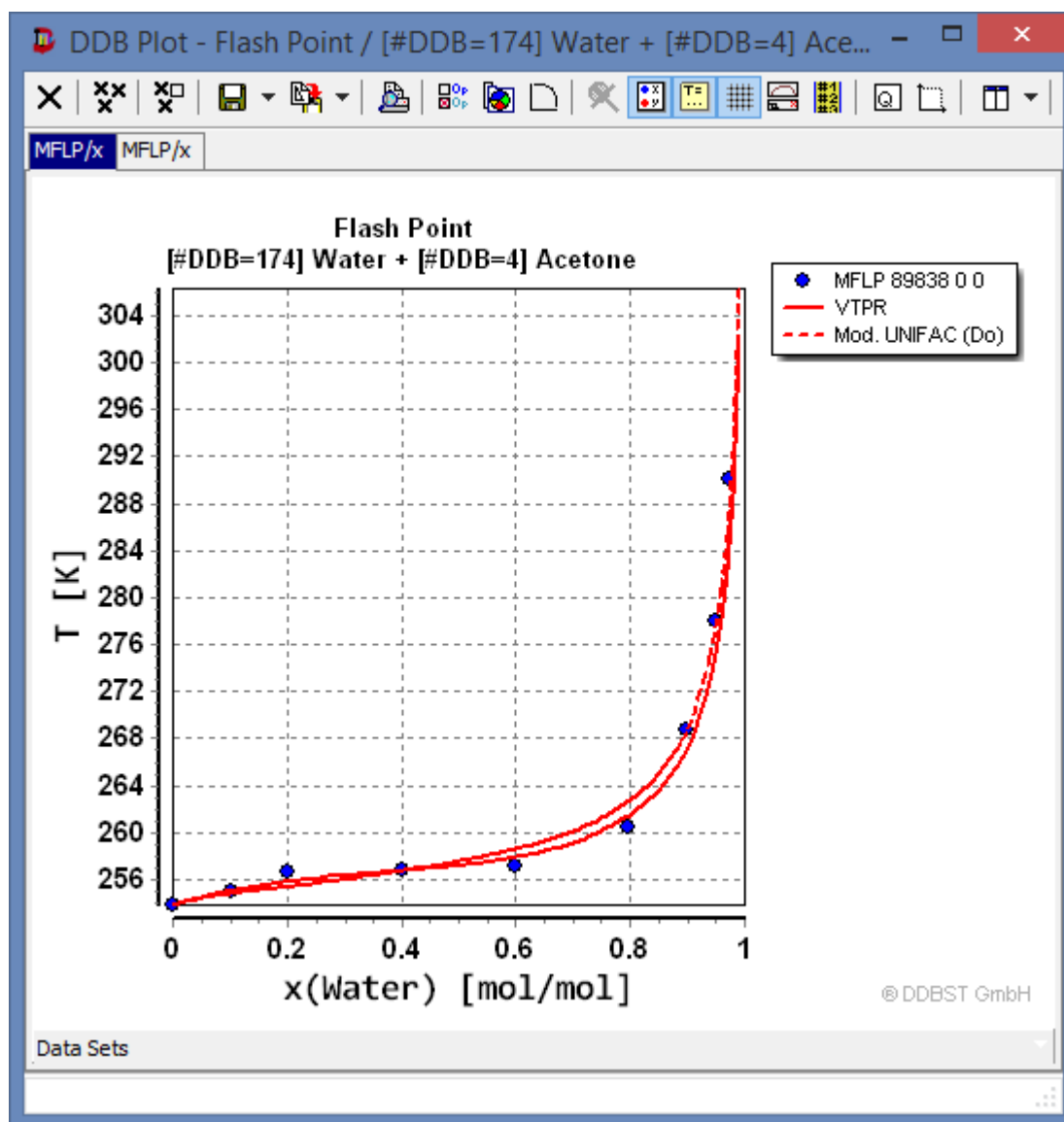
3.3 Parallel installation of old and new EOS mixing rule parameter fit tool

Currently the old GenPar tool is still distributed to allow customers to use the old and new software together for a transition time.

4 Mixture flash point predictions

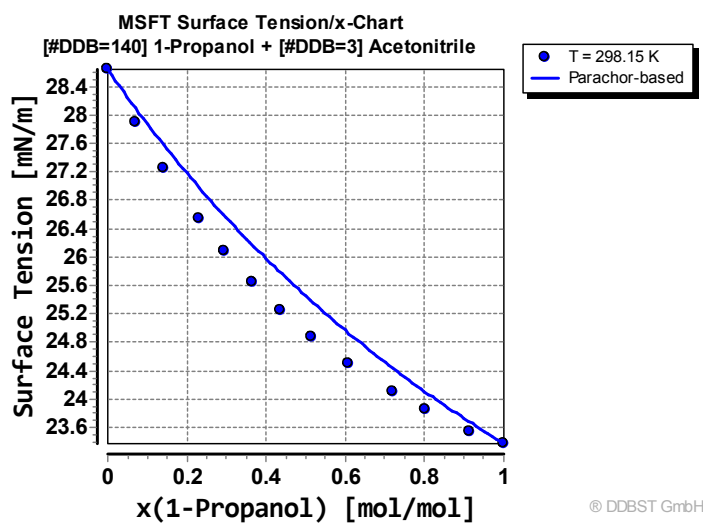
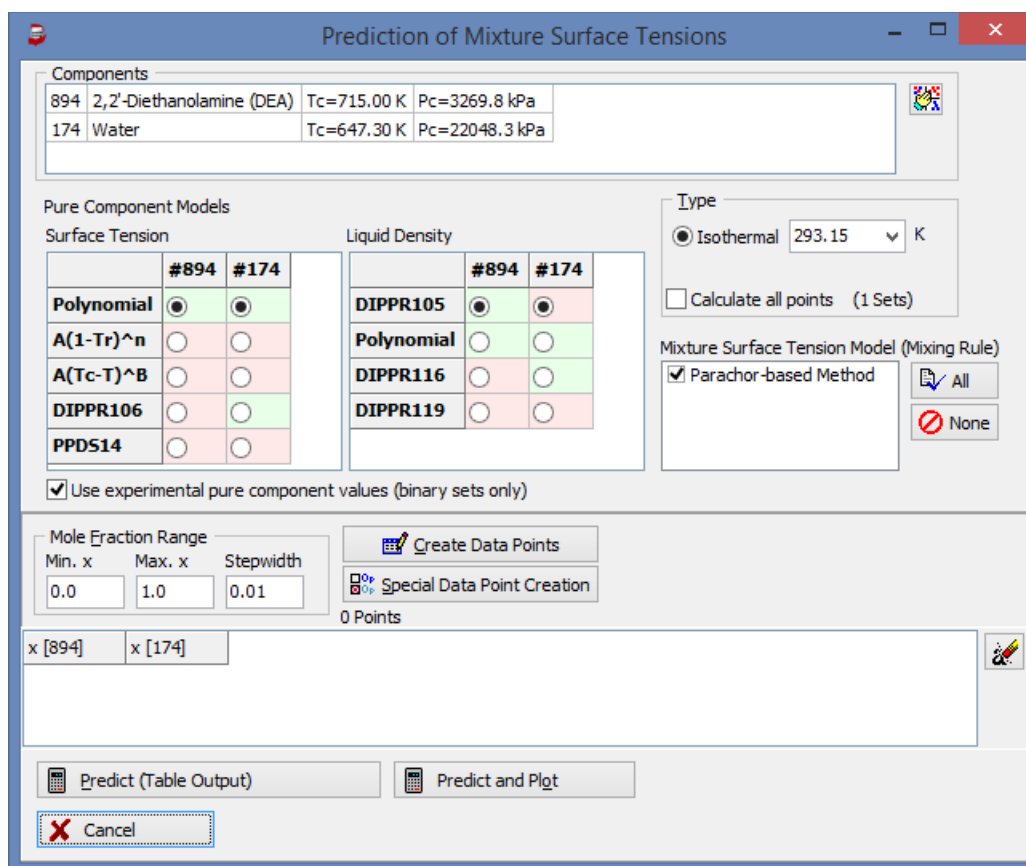


Mixture flash points can now be predicted with some common models like UNIFAC and PSRK. The prediction method is based on the same model as used in the stand-alone flash point estimation tool but has the limitation of not being able to add needed parameters if they are missing in the data banks.



5 Mixture surface tension predictions

Mixture surface tension can now be predicted with a mixing rule based on parachors. Needed pure component surface tensions and liquid densities are calculated with several correlations and parameters taken from the ParameterDDB.



6 Other prediction enhancements

6.1 Enabled flash point prediction without a heat of combustion.

A missing heat of combustion has not much influence and the quality of the predicted is only somewhat deteriorated. But, on the positive side, the calculation becomes possible for much more components and their mixtures.

6.2 Support for COSMO-SAC 2010 and COSMO-SAC 2013

The mixture properties prediction and the residue curves program do now support the models COSMO-SAC 2010 and COSMO-SAC 2013. The authors of COSMO-SAC 2013 have added a dispersion term to COSMO-SAC 2010 to improve the predictive quality.

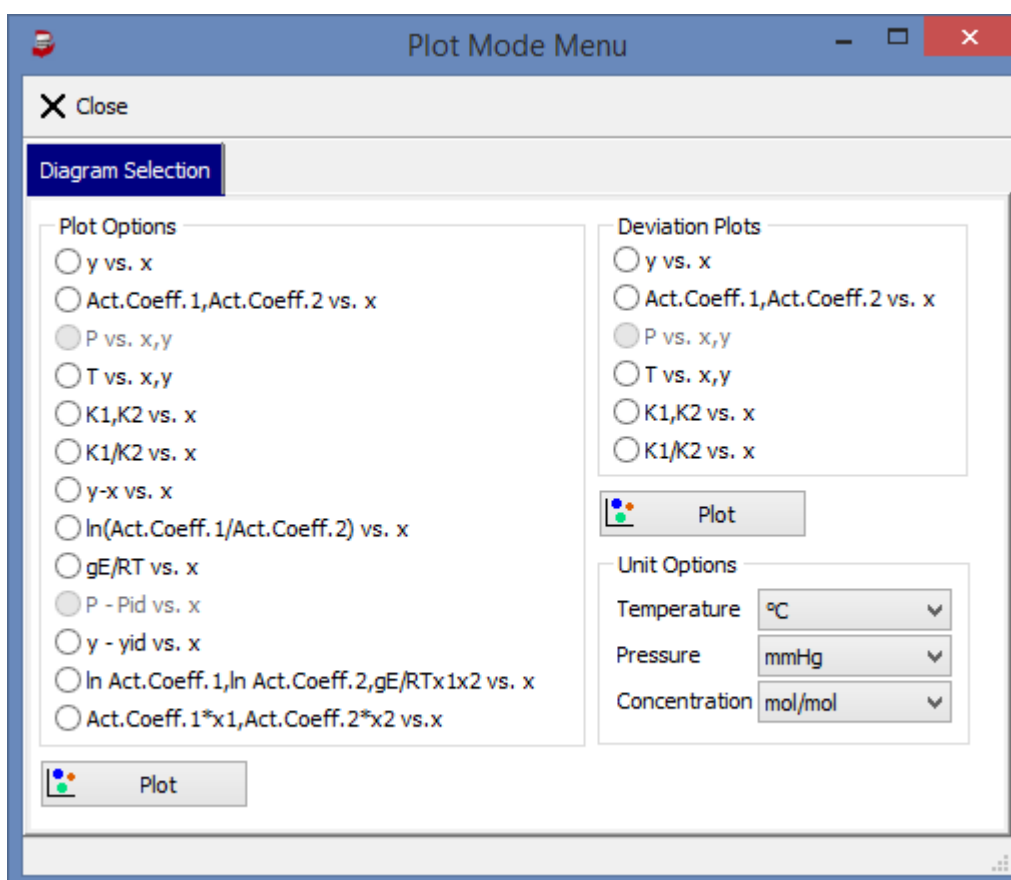
6.3 GC2gE – Regression of g^E model parameters to data from predictions

Pasting or typing activity coefficients is now possible. This offers the opportunity to use activity coefficients from models not (yet) implemented in the software.

An option to use Levenberg-Marquardt (LM) fit algorithm in combination with Simplex-Nelder-Mead (SNM) has also been added. LM uses derivations and is normally much quicker than SNM but is also not that reliable and robust.

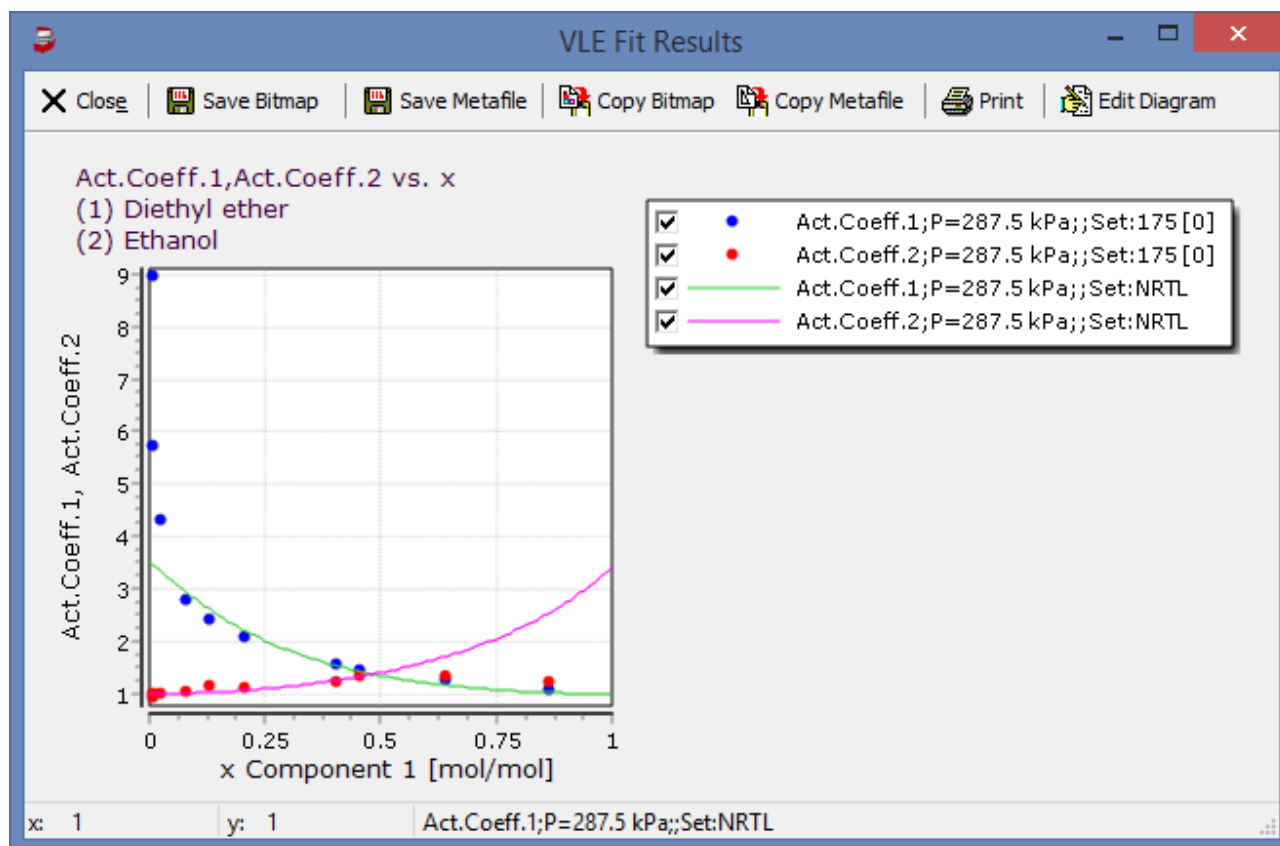
6.4 Fitting single VLE or HPV sets has been redesigned

A new design with a new functionality has been implemented for the diagrams making it easier to customize the output and also make it easier to use the diagram in reports.

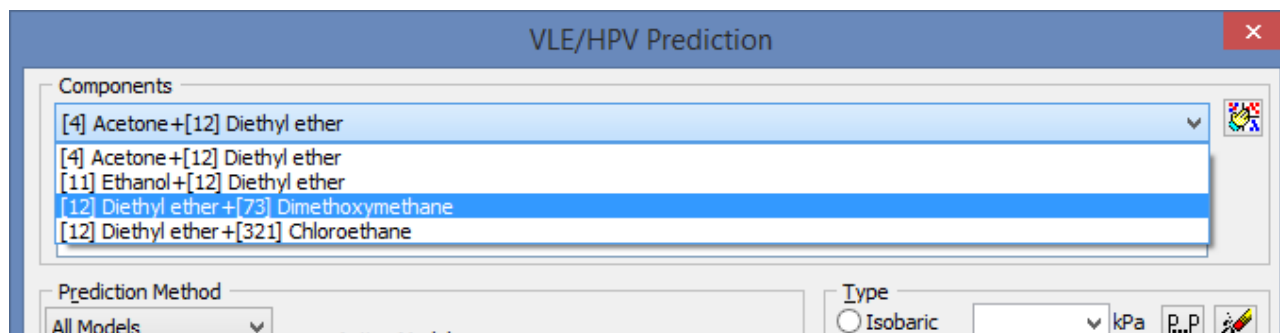


All the settings and display options are still available but the diagram output is now made with our standard chart

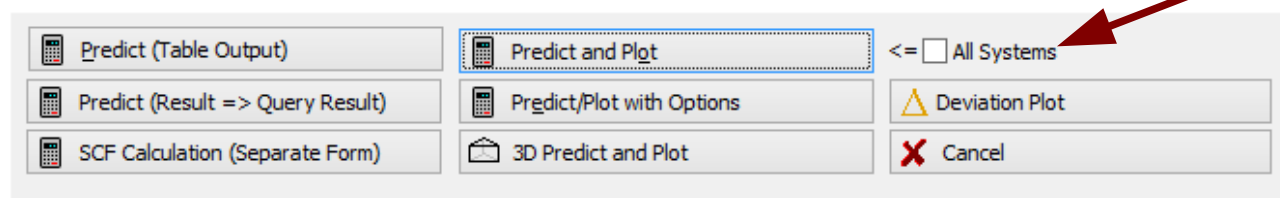
component.



6.5 VLE predictions: Allow prediction of multiple systems in one step



The dialog now contains a control with all available systems and a check box where this batch mode can be



switched on and off.

6.6 LLE prediction enhancements

1. The prediction can now use EOS mixing rule parameters fitted with GenPar/RecPar.
2. If the user does not specify a pressure value, then the calculation with simulator thermodynamics does now use a VLLE calculation instead of a TP-flash calculation.

6.7 Simulator prediction enhancements

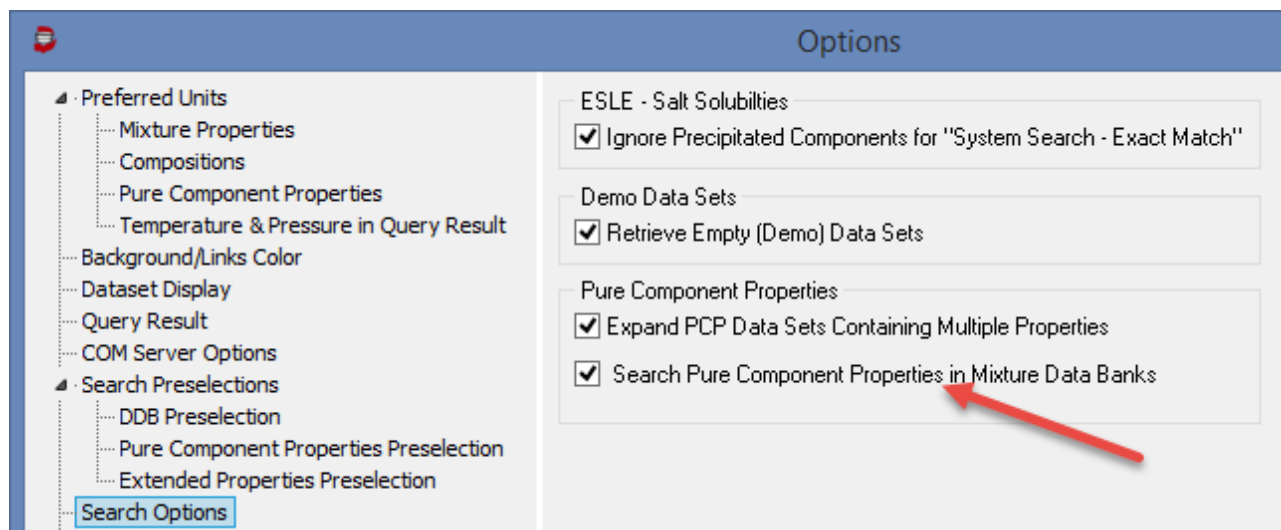
The simulators PRO/II 9.4 and UniSim Design R440 are now supported.

7 Dortmund Data Bank

7.1 Search for pure component points in several mixture data banks

Several mixture data banks contain pure component points (mole fraction $x=1$. ^{mol/mol}). These are boiling points from the VLE data banks, melting temperatures from the SLE data bank, saturated densities from the VE data bank, and heat capacities from the CPE data bank.

Some of these points have also been added to the pure component data bank (PCPDDB) but by far not all. The Dortmund Data Bank retrieval program now optionally



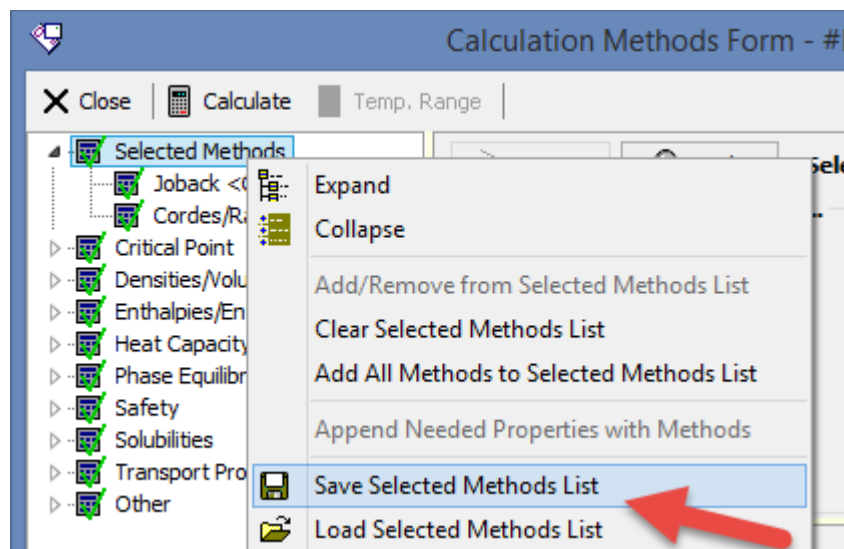
searches these mixture data bank and displays these pure component values from the mixture data banks together with the values from the PCPDDB. This may cause some values to be shown twice if they have been stored already in the PCPDDB.

8 Artist

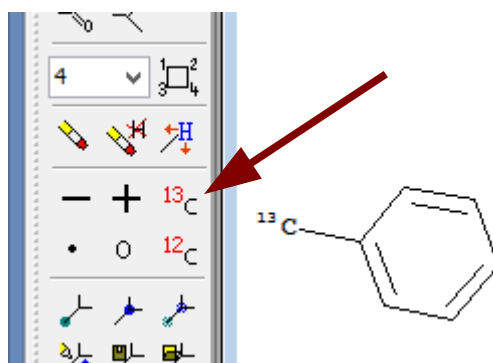
1. Default folder for GC-COSMO results set to private DDB folder which allows using the estimated σ

profile directly.

2. Implement COSTALD^{1,2,3} equation for liquid densities
3. Save and load "Selected Methods" lists



4. Support for Isotopes



5. Temperature range calculation for multiple properties simultaneously.

A temperature can now be specified for a group of properties – as, for example, for all models predicting liquid dynamic viscosities.

1 Hankinson R.W., Thomson G.H., "A New Correlation for Saturated Densities of Liquids and Their Mixtures", *AIChE J.*, 25(4), 653-663, 1979

2 Thomson G.H., Brobst K.R., Hankinson R.W., "An Improved Correlation for Densities of Compressed Liquids and Liquid Mixtures", *AIChE J.*, 28(4), 671-676, 1982

3 Hankinson R.W., Thomson G.H., "Calculate Liquid Densities Accurately", *Hydrocarbon Process.*, 58(9), 277-283, 1979

9 Entrainer Selection

9.1 Extended search of entrainers for LLE Extraction is now available.

The “Liquid-Liquid Extraction (Extended)” program adds many new features to the solvent selection for liquid-liquid extraction, like, for example, the search for solvent mixtures or the use of experimental ternary and quaternary liquid-liquid-equilibria. Additionally, the density difference between the two liquid phases is calculated and the program estimates how difficult it would be to separate all components by distillation after the extraction step.

In comparison to the old program this software package does not only rely on the activity coefficient at infinite dilution for the solvent selection, but it also uses the actual distribution coefficients of the different components between the two liquid phases. The distribution coefficients show a more accurate description of the reality and can be directly used to estimate the value of the solvents for the given separation problems.

Entrainer Selection 2016

File Help

Entrainer Preselection Processes

Extractive Distillation Azeotropic Distillation Extraction Absorption Selectivity **LLE Extraction (Extended)**

System (Experimental Data Bases: 2 Components, Predictive Methods: 2-4 Components)

	DDB Number	Remove?	Component	Formula	Molecular Weight	Diluted?
1	[159]	Remove	Tetrahydrofuran	C4H8O	72.1069	<input type="checkbox"/>
2	[174]	Remove	Water	H2O	18.0153	<input type="checkbox"/>

Basic Settings

Temperature [K] Min. Separator Factor

Pressure [kPa] (only EoS)

Database

Options

Search for Solvent Mixtures
 Calculate User-Defined Mixtures
 Use Weight Fractions for Distribution Coefficients

Weight Factors

Capacity
 Selectivity
 Solvent Loss
 Distillation

Preselected Components

229 components

Use All Components (Ignore List)

Result Table User Defined Mixtures

Respect Viscosity Limit Respect Flammability Limit Only Solvents with LLE
 Max. Viscosity [mPas] Min. Flashpoint. [K] Only Solvents without Homogeneous Azeotrope
 Only Solvents with Viscosities Only Solvents with Flash Points

Public DDB: K:\DDB2016\ Private DDB: K:\DDBPRVLeer\

10 Dortmund Data Bank progress

The Dortmund Data Bank 2016 has around 58000 new data sets and almost 447000 new data points. Data from more than 4200 sources have been added.

Databank	2015			2016			Absolute Gain			Relative Gain		
	Sets	Points	References	Sets	Points	References	Sets	Points	References	Sets	Points	References
AAE	4359	54006	263	4592	57044	283	+233	+3038	+20	5.35%	5.63%	7.60%
ACM	1592	9955	71	1725	10312	75	+133	+357	+4	8.35%	3.59%	5.63%
ACT	84904	84904	1346	90047	90047	1380	+5143	+5143	+34	6.06%	6.06%	2.53%
AZD	56088	56084	8400	56637	56637	8548	+549	+553	+148	0.98%	0.99%	1.76%
CPE	5990	68405	746	6483	75083	794	+493	+6678	+48	8.23%	9.76%	6.43%
CRI	3193	21858	993	3303	22548	1020	+110	+690	+27	3.45%	3.16%	2.72%
DIF		n.a.		1820	13297	303	+1820	+13297	+303	New Data Bank 2016		
ECND	7186	73811	640	8827	93230	822	+1641	+19419	+182	22.84%	26.31%	28.44%
EGLE	2575	14856	195	2868	16939	222	+293	+2083	+27	11.38%	14.02%	13.85%
ELE	10840	134167	1531	11904	148675	1682	+1064	+14508	+151	9.82%	10.81%	9.86%
ESLE	38732	268481	7260	40469	280257	7592	+1737	+11776	+332	4.48%	4.39%	4.57%
GHD	3268	24623	580	3862	28845	698	+594	+4222	+118	18.18%	17.15%	20.34%
GLE	22355	105952	2135	23018	110360	2221	+663	+4408	+86	2.97%	4.16%	4.03%
HE	22469	332565	3266	22810	337224	3316	+341	+4659	+50	1.52%	1.40%	1.53%
HPV	38149	325653	4357	39925	341370	4554	+1776	+15717	+197	4.66%	4.83%	4.52%
LLE	29489	257932	4623	30824	272370	4831	+1335	+14438	+208	4.53%	5.60%	4.50%
MDEC	6136	57349	724	6762	62846	813	+626	+5497	+89	10.20%	9.59%	12.29%
MFLP	420	4035	71	567	5148	105	+147	+1113	+34	35.00%	27.58%	47.89%
MPVT	10846	196876	851	12804	222746	1026	+1958	+25870	+175	18.05%	13.14%	20.56%
MSFT	4924	57531	628	5691	64957	697	+767	+7426	+69	15.58%	12.91%	10.99%

MSOS	15189	192067	1471	17654	218973	1681	+2465	+26906	+210	16.23%	14.01%	14.28%
MTCN	4541	39987	346	4764	41872	377	+223	+1885	+31	4.91%	4.71%	8.96%
PCP	270475	1750308	35844	286327	1832731	37923	+15852	+82423	+2079	5.86%	4.71%	5.80%
POLYMER	20021	203942	1661	20539	210443	1704	+518	+6501	+43	2.59%	3.19%	2.59%
POW	14040	14040	562	14359	14359	581	+319	+319	+19	2.27%	2.27%	3.38%
SLE	52568	433674	7529	56196	462496	8178	+3628	+28822	+649	6.90%	6.65%	8.62%
VE	67423	761729	7166	71425	801490	7550	+4002	+39761	+384	5.94%	5.22%	5.36%
VIS	36240	389767	3466	40909	435572	3895	+4669	+45805	+429	12.88%	11.75%	12.38%
VLE	36415	531977	7650	37490	547577	7840	+1075	+15600	+190	2.95%	2.93%	2.48%
X	24166	237474	2652	27896	275350	3037	+3730	+37876	+385	15.43%	15.95%	14.52%
Sum	894593	6704008	69915	952497	7150798	74117	+57904	+446790	+4202	6.47%	6.66%	6.01%

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 – VLE: Vapor-liquid equilibria (all components with a normal boiling point above 0°C) – X: Different thermodynamic properties.