DDB and DDBSP Delivery

2015

Changes and new Features

DDBSP - Dortmund Data Bank Software Package

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1 Multiple Bug Fixes and Usability Enhancements

1.1 Improved and Uniform Model Selection in Prediction Forms

The model selection has been altered from an increasingly confusing list of check boxes to a rather simple double list with one list for all available methods and one list for all active models. Models can now be selected and deselected by moving them from the available to the active list and vice versa.

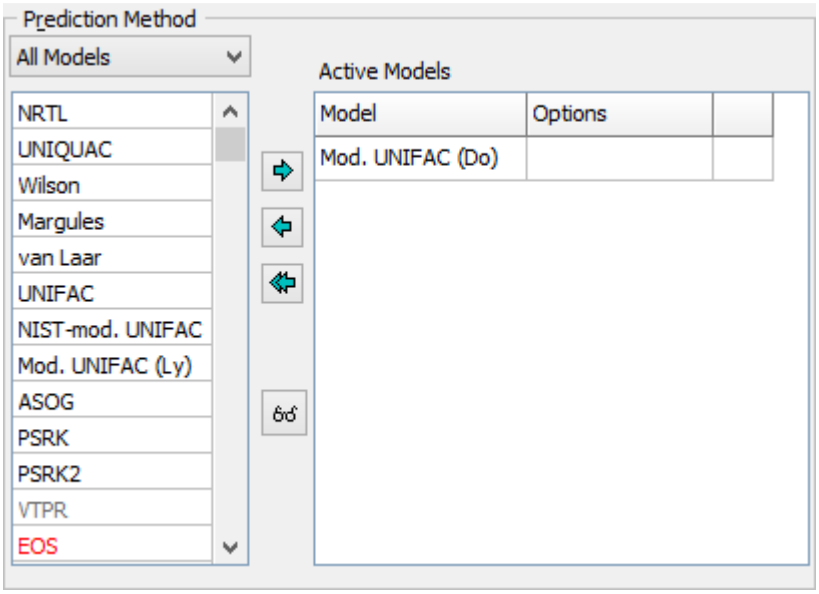


Figure 1: New model selection.

1.2 Diagrams

A function to save all diagrams from a window to a folder has been added. This function automatically generates meaningful file names and stores all diagram in user-defined folder.

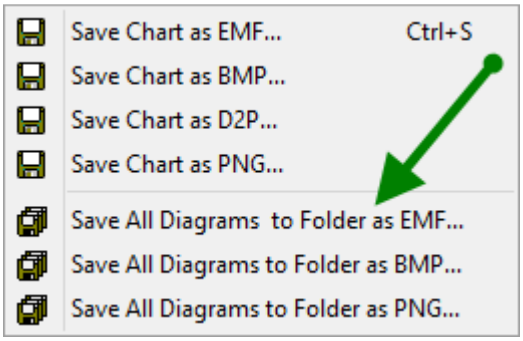


Figure 2: Save all diagrams.

Several options for changing the look of a diagram have been added:

1. Added option to use color gradients for temperature and pressure ranges
2. Configurable fonts (font face and size) for the title and labels or all axes
3. Added option to set background color of chart

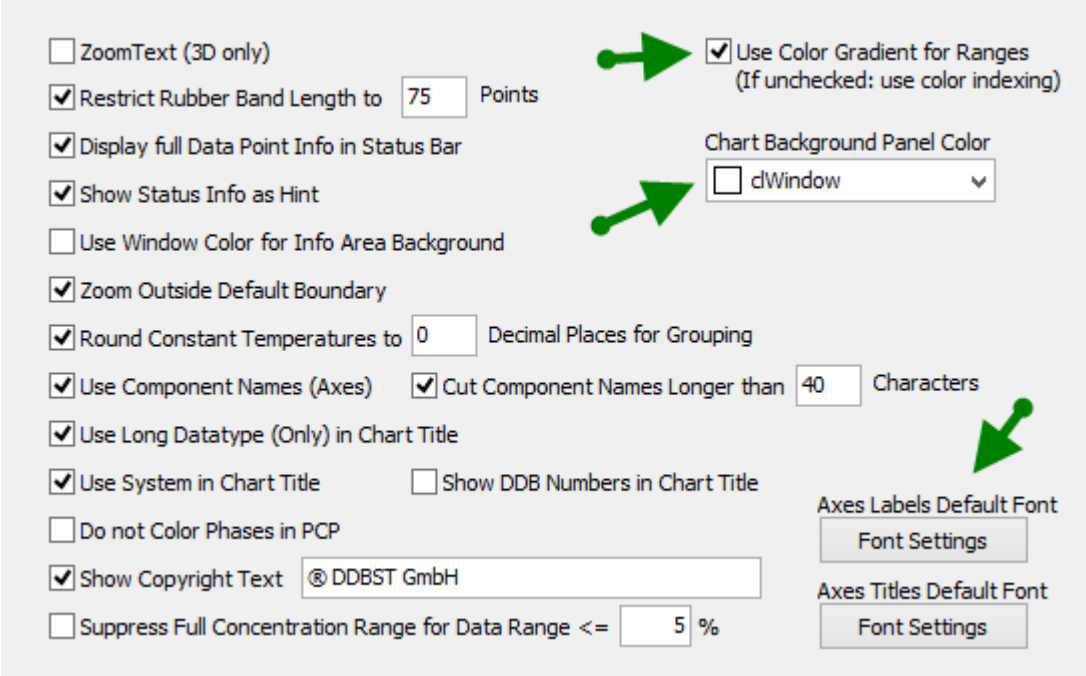


Figure 3: New plot settings

2 Enhanced Predictions

2.1 Enhanced Calculation Speed

1. Many calculation routines have been moved from external separate programs to internal code resulting in a distinct increase in calculation speed.
2. An impressive enhancement has been achieved for isobaric VLE phase equilibrium calculations. This accelerates the isobaric calculations in the tools for simultaneous regression (“RecPar”), residual curves, contour lines and search for azeotropes (“ResidueCurves”) and anywhere else where VLEs are calculated.
3. The entrainer selection for “Azeotropic Distillation” is also much quicker now because some external FORTRAN based tools have been replaced by internal code so that slow program calls aren't necessary anymore.

2.2 New Model

NIST-modified UNIFAC[1] is now implemented and can be used to predict multiple properties. The model is closely related to modified UNIFAC (Dortmund) using the same mathematics but different interaction parameters and a different group assignment scheme.

2.3 Prediction of Vapor-Liquid Equilibria

The EOS "model" available in the VLE prediction dialog now allows specifying the equation of state, mixing rule, g^E-model and alpha-function as well as k_{ij} parameters and valid temperature range. Project files from GenPar as well as parameters stored in the parameter DDB can also be loaded clicking the k_{ij} button.

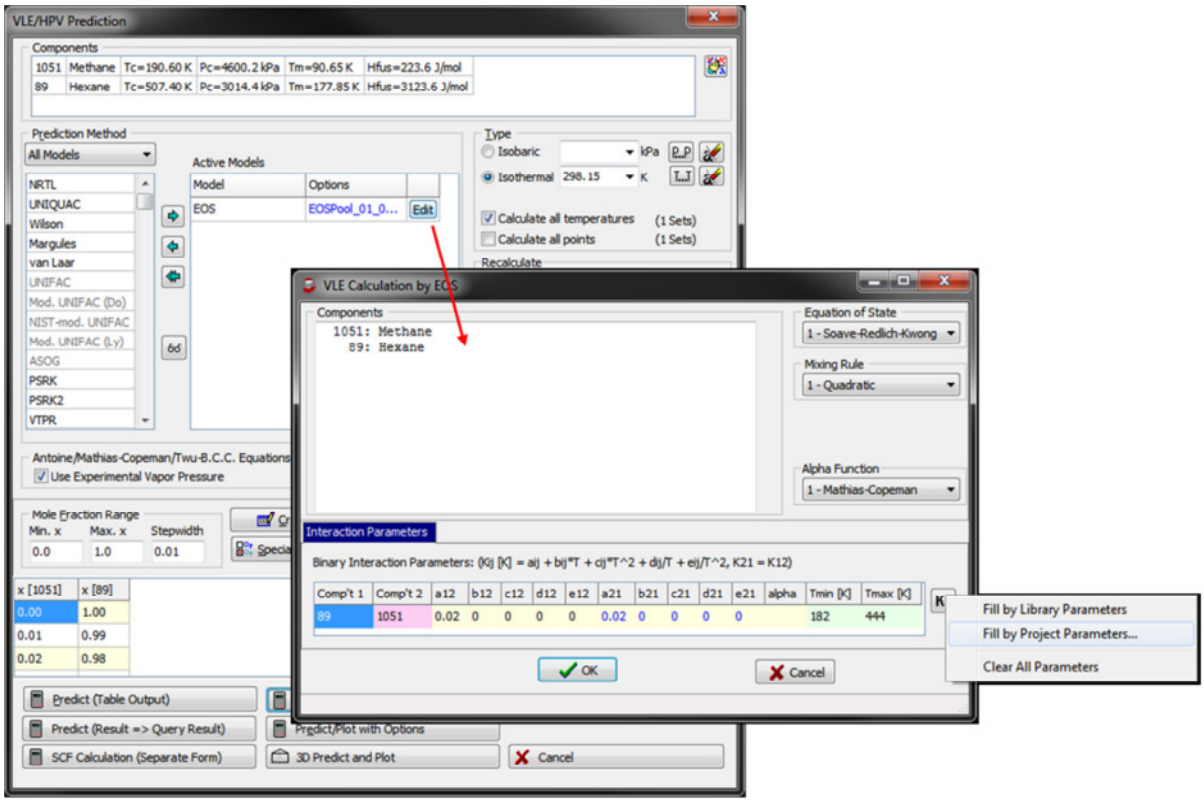


Figure 4: EOS options in the VLE prediction dialog.

The prediction itself is performed as usual.

1 Kang J.W., Diky V., Frenkel M., "New modified UNIFAC parameters using critically evaluated phase equilibrium data", Fluid Phase Equilib., 388, 128-141, 2015

2.4 Prediction of Excess Heat Capacities

The prediction of excess heat capacities with a variety of activity coefficient models like UNIFAC and derivatives and also some COSMO-based models is available in the 2015 version of DDBSP.

2.5 Prediction of Gas Solubilities

The prediction of gas solubilities is now possible with a variety of activity coefficient models like UNIFAC and derivatives.

2.6 Prediction of Azeotropic Points in Multicomponent Mixtures

Additional models like PSRK and VTPR, COSMO-based models and also the new NIST-modified UNIFAC model have been added to the completely redesigned prediction tool.

2.7 Excess Volume Prediction

A volume correction for PSRK similar to the one used in VTPR has been adopted. The volume correction parameters have to be ordered separately; only the values for our 30 demo components will be freely available.

2.8 Salt Solubility Prediction

The model LIFAC is now available.

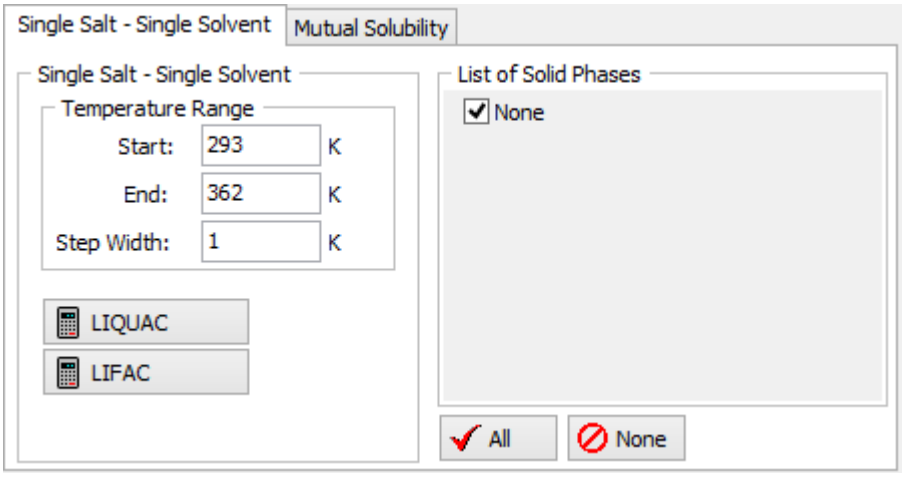


Figure 5: Solubility calculation dialog for a single salt – single solvent system.

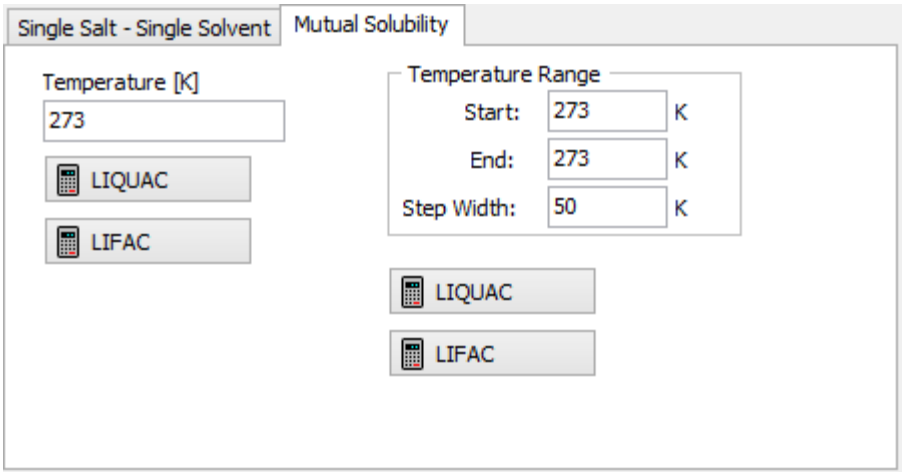


Figure 6: Mutual solubility calculation dialog.

2.9 101 Points Limit Lifted

The 101 points limit for predicting vapor-liquid and solid-liquid equilibria, heats of mixing, excess heat capacities, mixture viscosities and activity coefficients is removed. This is especially important for data sets with ternary and higher mixtures.

3 Predictive EOS

The prediction of excess enthalpies is now available within the Predictive EOS package.

4 Enhanced Interfaces to Commercial Simulator Software

4.1 Calculation with UniSim Design

Version 2015 supports UniSim Design as additional commercial simulator software using a COM interface. The features are:

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

An installation of UniSim Design is automatically detected. After the successful identification of the components in a UniSim Design case file which can be opened from here,

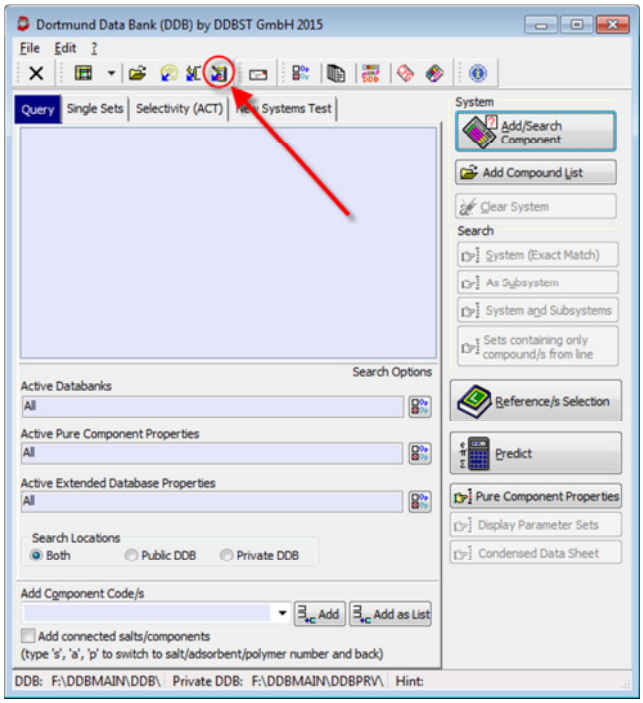


Figure 7: The Dortmund Data Bank program.

the simulator thermodynamics is displayed as “USD Model” in the VLE prediction dialog.

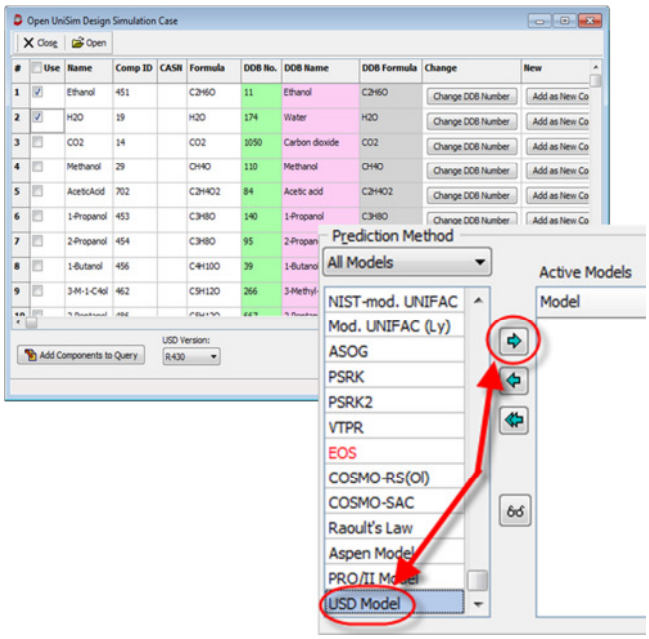


Figure 8: Component identification and model selection.

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

If the mouse is over the *USD Model* field in the *Active Models* area then some additional

information is displayed.

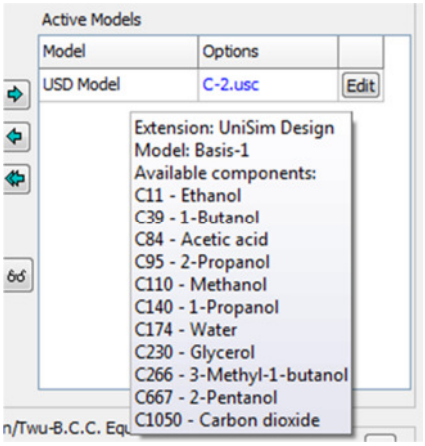


Figure 9: Model options in the VLE prediction dialog.

Use the *Edit* button next to the displayed file name to select a different fluid package or file for the calculation.

5 RecPar – Simultaneous Correlation

Our previous main tool RecVal/3 for fitting g^E model parameters is no longer distributed. RecPar as successor is able to handle former RecVal projects and adds several new features.

5.1 Loading RecVal/3 Projects

RecPar now can load RecVal/3 projects and read all settings and information from these files in order to create a RecPar project. This function may have some difficulties if RecVal/3 projects aren't complete because, for example, experimental data aren't included.

5.2 Reduced Number of Dialogs

Some formerly independent dialogs, especially the dialogs for storing fitted parameters and the window showing the fit progress, have been docked in the main RecPar window.

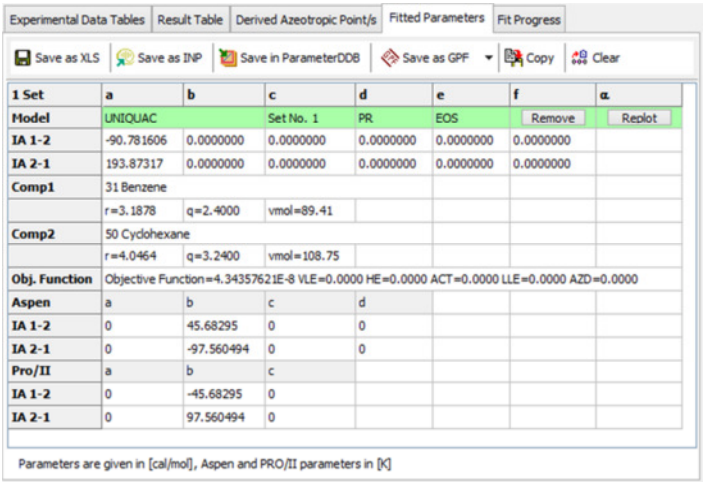


Figure 10: Docked form for fitted parameters.

6 New Vapor Pressure Equation in PCPEquationFit

PVExpansion: $P = \exp\left(A + \frac{B}{T} + C\ln(T) + DT + ET^2 + \frac{F}{T^2} + GT^6 + \frac{H}{T^4}\right)$

7 New Data Bank for Flash Points of Mixtures

A new data bank containing mainly mixture flash points but also some explosion limits, fire points and similar safety-related properties is now available.

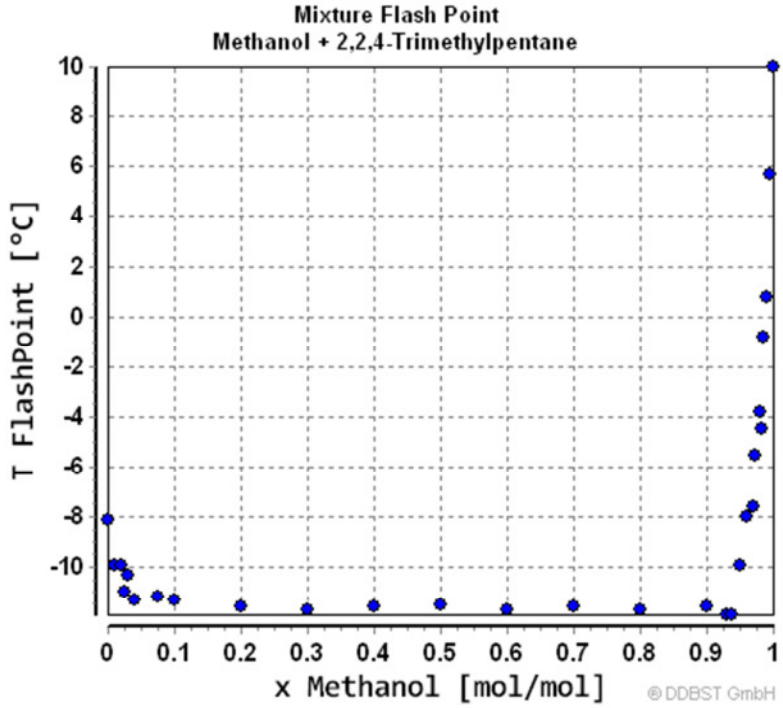
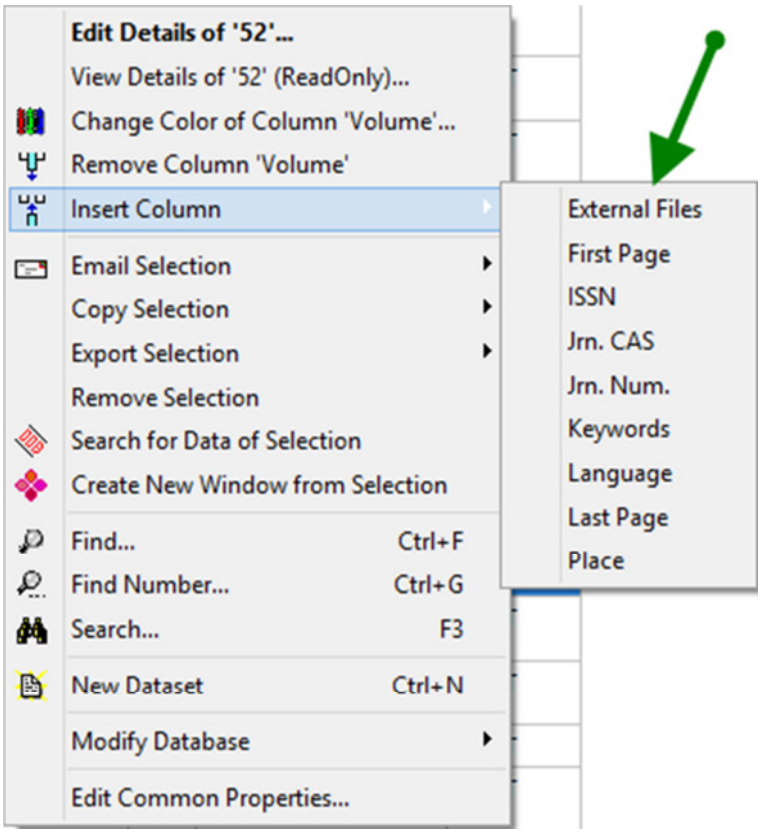


Figure 11: Mixture flash points for methanol (1) – 2,2,4-trimethylpentane.

8 Literature Management

The links to external files can now be displayed directly in the query result window.



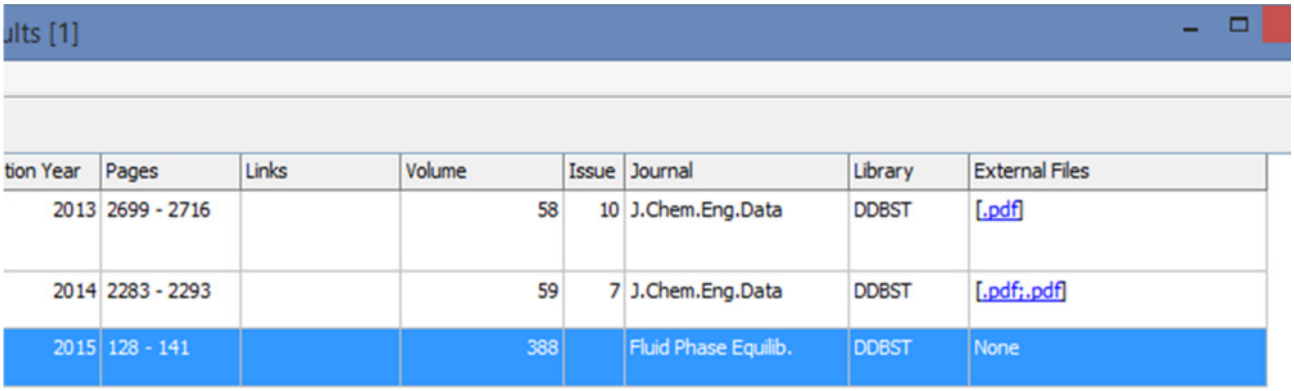


Figure 12: Links to external files in the query result window.

Displaying these links is done in a background thread and it can need some seconds before the links actually appear.

9 Data Bank Progress

The DDB 2015 has around 63,500 new data sets and 497,000 new data points.

	2014			2015			Gain (Absolute)			Gain (Relative)		
Databank	**Sets**	**Points**	**References**	**Sets**	**Points**	**References**	**Sets**	**Points**	**References**	**Sets**	**Points**	**References**
AAE	4,296	53,412	259	4,359	54,006	263	+63	+594	+4	+1.47%	+1.11%	+1.54%
ACM	1,561	9,814	69	1,592	9,955	71	+31	+141	+2	+1.99%	+1.44%	+2.90%
ACT	79,471	79,471	1,306	84,904	84,904	1,346	+5,433	+5,433	+40	+6.84%	+6.84%	+3.06%
AZD	55,212	55,212	8,199	56,088	56,084	8,400	+876	+872	+201	+1.59%	+1.58%	+2.45%
CPE	5,173	58,941	652	5,990	68,405	746	+817	+9,464	+94	+15.79%	+16.06%	+14.42%
CRI	3,031	20,499	941	3,193	21,858	993	+162	+1,359	+52	+5.34%	+6.63%	+5.53%
ECND	5,317	56,923	463	7,186	73,811	640	+1,869	+16,888	+177	+35.15%	+29.67%	+38.23%
EGLE	2,411	13,835	176	2,575	14,856	195	+164	+1,021	+19	+6.80%	+7.38%	+10.80%
ELE	9,969	122,177	1,393	10,840	134,167	1,531	+871	+11,990	+138	+8.74%	+9.81%	+9.91%
ESLE	36,739	253,726	6,758	38,732	268,481	7,260	+1,993	+14,755	+502	+5.42%	+5.82%	+7.43%
GHD	2,819	21,418	495	3,268	24,623	580	+449	+3,205	+85	+15.93%	+14.96%	+17.17%
GLE	21,454	99,444	2,000	22,355	105,952	2,135	+901	+6,508	+135	+4.20%	+6.54%	+6.75%
HE	21,902	323,148	3,190	22,469	332,565	3,266	+567	+9,417	+76	+2.59%	+2.91%	+2.38%
HPV	36,220	309,451	4,106	38,149	325,653	4,357	+1,929	+16,202	+251	+5.33%	+5.24%	+6.11%
LLE	27,820	241,129	4,348	29,489	257,932	4,623	+1,669	+16,803	+275	+6.00%	+6.97%	+6.32%
MDEC	4,758	47,406	575	6,136	57,349	724	+1,378	+9,943	+149	+28.96%	+20.97%	+25.91%
MFLP	**n.a.**	**n.a.**	**n.a.**	**420**	**4,035**	**71**	**+420**	**+4,035**	**+71**	**n.a.**	**n.a.**	**n.a.**
MPVT	8,196	146,660	583	10,846	196,876	851	+2,650	+50,216	+268	+32.33%	+34.24%	+45.97%
MSFT	2,867	37,045	383	4,924	57,531	628	+2,057	+20,486	+245	+71.75%	+55.30%	+63.97%
MSOS	7,450	108,092	906	15,189	192,067	1,471	+7,739	+83,975	+565	+103.88%	+77.69%	+62.36%
MTCN	3,599	31,062	267	4,541	39,987	346	+942	+8,925	+79	+26.17%	+28.73%	+29.59%

PCP	255,335	1,664,967	33,662	270,475	1,750,308	35,844	+15,140	+85,341	+2,182	+5.93%	+5.13%	+6.48%
POLYMER	19,608	197,059	1,623	20,021	203,942	1,661	+413	+6,883	+38	+2.11%	+3.49%	+2.34%
POW	12,034	12,034	548	14,040	14,040	562	+2,006	+2,006	+14	+16.67%	+16.67%	+2.55%
SLE	48,768	402,368	6,680	52,568	433,674	7,529	+3,800	+31,306	+849	+7.79%	+7.78%	+12.71%
VE	63,902	727,196	6,789	67,423	761,729	7,166	+3,521	+34,533	+377	+5.51%	+4.75%	+5.55%
VIS	22,719	260,488	2,473	36,240	389,767	3,466	+1,3521	+129,279	+993	+59.51%	+49.63%	+40.15%
VLE	35,022	513,463	7,425	36,415	531,977	7,650	+1,393	+18,514	+225	+3.98%	+3.61%	+3.03%
X	33,426	340,787	3,129	24,166	237,474	2,652	-9,260	-103,313	-477	-27.70%	-30.32%	-15.24%
Sum	831,079	6,207,227	65,431	894,593	6,704,008	69,915	+63,514	+496,781	+4484	+7.64%	+8.00%	+6.85%

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 – 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.

9.1 Literature Data Bank

The literature data bank contains now 153,750 references. 146,124 references have been stored in 2014 resulting in +7,626 references added from 2014 to 2015. For comparison: 139,298 references have been stored in 2013.

The Dortmund Data Bank contains data from 69,912 references.