DDB and DDBSP

Version 2020

Release Notes

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1 Installation notes

1. DDBSP 2020 can be installed in parallel to DDBSP 2019 (and any older version). However, if DDBSP 2019 is uninstalled after the installation of DDBSP 2020, settings like the file type associations will get broken. In that case a repair installation of DDBSP 2020 should solve the problem.
2. An officially supported Microsoft Windows version at release time is required.

2 License management system

The license management system (client and server) has been updated to RLM v14.0 BL2. This solves the problem of an erroneously detected virtual machine when a pen drive is inserted (the problem was introduced with DDBSP 2019).

3 Extended Antoine (Aspen)

The vapor pressure equation “Extended Antoine (Aspen)” is now supported in the VLE and AZD prediction as well as in the binary interaction parameters regression tool (RecPar).

4 Binary interaction parameter regression

The special regression dialog for binary LLE data has been removed. The fit button in the “Dortmund Data Bank” program will now call RecPar with the selected LLE data sets instead. The fitting capabilities have now been incorporated in RecPar (see below).

The following sections describe the changes of the RecPar program.

4.1 New optimization method

- Levenberg-Marquardt
- Combination of Levenberg-Marquardt and simplex Nelder-Mead algorithm

4.2 Improved access to the objective functions

- The objective functions are accessible together with the objective function properties.

4.3 Improvements for cubic equations of state

- Optional delta-phi minimization

4.4 Improvements for LLE data fitting

- Estimate missing phase values
- Improved optimization if only LLE data is used in the regression

4.5 Start parameters dialog

- Display model and equation
- No longer parameter pre-selection in the main window. All parameters can be activated.
- Access to previously fitted parameters has moved to the fit result (see next section).

4.6 Fitted parameters page

- The buttons “Remove” and “Replot” have been replaced by a single button with a drop-down menu.
- The “Replot” feature will now automatically change the model, if required.
- There is a new “Refit” feature which will open the “Start parameters” dialog using the parameters of the selected set as start values.
- The data is now more clearly represented.
- NRTL, UNIQUAC and Wilson parameter sets can now be exported to IK-CAPE PPDX.

4.7 Fitting with Simulis Thermodynamics

- Any Simulis Thermodynamics model which uses binary interaction parameters can be used for fitting.
- Obtained parameters can be saved to a calculator file.

4.8 GUI clean-up

- Removed the intermediate main dialog; data can be added to the fit dialog now.
- The “Temperature Dependency” pre-selection has been removed (see section 4.5 “Start parameters dialog”).
- The “Replot” button has been removed; use the “Replot” menu item of a fitted data set instead.
- The VLE consistency test button has been removed. The consistency test is now performed automatically when VLE data is added. The VLE button “Set weight to 0 for Inconsistent Data” is now available in the popup-menu of the VLE data table.
- In the start parameters dialog the option to revert to the default values has been removed. The “Fit Parameters” button will always open the start parameters dialog with the default values.
- Some further rarely used functionality has been removed as well.

5 Miscellaneous

- General bugfixes and performance improvements
- The Aly-Lee equation is now used per default for the cp ideal calculation.

6 Dortmund Data Bank Progress

6.1 Overall Statistics

The Dortmund Data Bank 2020 contzains more than 48,000 new data sets and more than 440,000 new data points. Data from approximately 2,900 sources have been added.

	2019			2020			Absolute Gain		Relative Gain	
DDB	Sets	Points	Refs	Sets	Points	Refs	Sets	Points	Sets	Points
AAE	5000	64700	300	5400	71000	320	+400	+6300	8.00 %	9.74 %
ACM	2000	11300	80	2000	11400	90	+0	+100	0.00 %	0.88 %
ACT	112300	112300	1430	115350	115300	1450	+3050	+3000	2.72 %	2.67 %
AZD	58900	58900	8660	59500	59500	8760	+600	+600	1.02 %	1.02 %
CPE	7100	83300	830	7250	84800	840	+150	+1500	2.11 %	1.80 %
CRI	3450	23700	1040	3500	24000	1050	+50	+300	1.45 %	1.27 %
EGLE	4150	25800	360	4350	27300	380	+200	+1500	4.82 %	5.81 %
ELE	14150	177900	1900	14450	183100	1950	+300	+5200	2.12 %	2.92 %
ESLE	44500	307800	7430	46150	320500	7710	+1650	+12700	3.71 %	4.13 %
GLE	26600	128300	2590	27950	136000	2710	+1350	+7700	5.08 %	6.00 %
HE	23900	349900	3390	24150	354500	3410	+250	+4600	1.05 %	1.31 %
HPV	44600	379300	4890	46150	391300	5050	+1550	+12000	3.48 %	3.16 %
LLE	35450	328900	5360	36900	345600	5560	+1450	+16700	4.09 %	5.08 %
PCP	331650	2071700	41370	343100	2150400	42850	+11450	+78700	3.45 %	3.80 %
POLYMER	21950	230400	1830	22350	236600	1870	+400	+6200	1.82 %	2.69 %
POW	15000	15000	630	15050	15000	630	+50	+0	0.33 %	0.00 %
SLE	68650	573100	8800	74000	629900	9300	+5350	+56800	7.79 %	9.91 %
VE	80900	903100	8110	84100	942700	8360	+3200	+39600	3.96 %	4.38 %
VLE	40500	588300	8040	41450	601000	8170	+950	+12700	2.35 %	2.16 %
ECND	11750	124700	1020	13000	144700	1140	+1250	+20000	10.64 %	16.04 %
GHD	5150	36300	890	5500	38500	940	+350	+2200	6.80 %	6.06 %
MDEC	7850	71800	930	8050	73800	970	+200	+2000	2.55 %	2.79 %
MFLP	730	6000	140	810	6400	150	+80	+400	10.96 %	6.67 %
MPVT	17850	298400	1330	19600	322900	1430	+1750	+24500	9.80 %	8.21 %
MSFT	7950	86000	910	8850	94500	1000	+900	+8500	11.32 %	9.88 %
MSOS	27200	321100	2400	30700	354100	2630	+3500	+33000	12.87 %	10.28 %
MTCN	4950	43800	380	5350	48800	410	+400	+5000	8.08 %	11.42 %
VIS	55350	571300	4720	59500	611900	5020	+4150	+40600	7.50 %	7.11 %
X other	46100	460200	4890	51350	512400	5480	+5250	+52200	11.39 %	11.34 %
Total	**1113900**	**8323900**	**81190**	**1162500**	**8765400**	**84170**	**+48600**	**+441500**	**+4.36 %**	**+5.30 %**

Disclaimer: Numbers presented may differ 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.

6.2 Pure Component Properties Data Bank Parts

The PCP parts are defined as shown in the following table:

Partial DDB	Data Sets	Data Points	Components
PCP-VAP+	136100	431300	43500
PCP-VIS	46000	366000	5950
PCP-HCP+	49100	540500	12350
PCP-PVT+	101150	729800	15950
PCP-ENTH	19700	79300	6750
PCP-SFT	8550	40700	3250
PCP-Other	9700	48600	2100

The packages contain these properties:

PCP-VAP+: Vapor Pressure, Critical Data, Triple Point, Melting Point, Heat of Vaporization, Heat of Fusion, Boiling Point, Heat of Sublimation, Standard Heat of Vaporization, Standard Heat of Melting, Standard Heat of Sublimation, Freezing Point (Supercooled Liquid to Crystal/Solid only), Decomposition Temperature, Heat of Crystallization, Hypothetical Vapor Pressure (often pS(VL) of Solid Compounds)
PCP-VIS+: Dynamic Viscosity, Kinematic Viscosity, Thermal Conductivity
PCP-HCP+: Molar Heat Capacity (cP), Heat of Vaporization, Heat of Fusion, Mass Heat Capacity, Enthalpy (H0), Enthalpy (H298), Enthalpy (H-H298/T), Enthalpy (H-H0/T), Transition Temperature, Heat of Transition, Molar Heat Capacity (cV), Mass Heat Capacity (cV), Ideal Gas Heat Capacity, Molar Saturation Heat Capacity, Heat of Sublimation, Entropy of Vaporization, Entropy of Fusion, Entropy of Transition, Entropy of Formation, Mass Saturation Heat Capacity, Gibbs Energy of Sublimation, Entropy of Sublimation, Standard Heat of Vaporization, Standard Heat of Melting, Standard Heat of Sublimation, Heat of Crystallization
PCP-PVT+: Density. Virial Coefficients, Volume, P-v-T, Speed of Sound, Virial Coefficients (Berlin form), Thermal Expansion Coefficient, Compressibility (isothermal), Compressibility (isentropic), Compressibility Factor (isothermal), Compressibility Factor (isentropic), Joule-Thomson Coefficient (isenthalpic dT/dP), Compressibility (adiabatic)
PCP-ENTH: Entropy, Std. Heat of Combustion, Std. Heat of Formation, Gibbs Energy of Form./T, Gibbs Energy of Form., G function (G-G0)/T, Enthalpy (H298/T), Gibbs Energy, Gibbs Energy (G-G0), Gibbs Energy (G-G298), Enthalpy, Entropy (S-S0), Entropy (S-S298), G function (G-G298)/T
PCP-SFT: Surface Tension
PCP-Other: Dielectric Constant, Diffusion Coefficient, Flash Point, Dipole Moment, Molar Polarization