

DDB

Version 2023

Release Notes



DDBST - Dortmund Data Bank Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Phone: +49 441 361819 0

support@ddbst.com

www.ddbst.com

Contents

1	Installation notes	3
2	Migration of private Firebird databases	3
3	Components	3
4	Entrainer Selection.....	3
5	Flash Point Estimation	3
6	Regression Mix	3
7	Regression Pure	3
8	Miscellaneous	4
9	Dortmund Data Bank Progress	5
9.1	Overall Statistics	5
9.2	Pure Component Properties Data Bank Parts.....	6

1 Installation notes

The current software release is provided as 64-bit version and can be installed in parallel to any previous release. However, if a previous release is uninstalled after the installation of the current release, then settings like the file type associations will get broken. In that case a repair installation of the current release should solve the problem.

An officially supported Microsoft Windows version at release time is required.

2 Migration of private Firebird databases

The DDB software does now use Firebird 4 databases.

Private databases created with Firebird 2.5 (which was used in DDB 2022) have to be upgraded to Firebird 4 before they can be used in the DDB 2023 software. Start the *DDB Components* application for a one-time check. If private data has to be migrated, then the *DDB Migration Tool* is called to perform the migration.

3 Components

In the *DDB Components* application a page does now contain a data sheet in addition to an optional search result area. It is possible to open a new page using a tab context menu. When the last page is closed, then the whole application closes.

In the data sheet there is now an additional category for additional component numbers. The context menu allows the user to clone a substance. And there is a new option called “Show all data fields”.

Please have a look at the *DDB Components* documentation for further details.

4 Entrainer Selection

The *DDB Entrainer Selection* has been reworked. Different processes (Extractive Distillation, Azeotropic Distillation and Selectivity) were combined in the “Distillation Process” menu. All “Entrainer Preselection” functions were included for overview reasons in this menu. Some of the previous functions are now accessible with *DDB Components*.

The functions of the “Extraction” Process were integrated in “LLE Extraction (Extended)” and are now labeled as “Extraction (LLE)”.

The “Absorption” and “Absorption (Extended)” processes and all its functions were combined in the “Absorption” dialogue.

5 Flash Point Estimation

The integrated components editor has been removed. Now the standard DDB applications are used to modify components data which are required for the flash point estimation.

6 Regression Mix

Fitting of Henry constants is now supported.

7 Regression Pure

The Modified Rackett equation was added as an additional option to correlate liquid saturated densities.

An additional simultaneous fit for some vapor pressure equations has been added which combines the fit of vapor pressures and heat of vaporizations.

8 Miscellaneous

The simulator interface does now support PRO/II™ 2023.

As usual this release contains general bugfixes and performance improvements.

9 Dortmund Data Bank Progress

9.1 Overall Statistics

The Dortmund Data Bank 2023 contains more than 54,000 new data sets and more than 404,300 new data points.

DDB	2022			2023			Absolute Gain		Relative Gain	
	Sets	Points	Refs	Sets	Points	Refs	Sets	Points	Sets	Points
AAE	5900	80400	350	6150	86000	380	+250	+5600	4.24 %	6.97 %
ACM	2050	11700	80	2450	13400	110	+400	+1700	19.51 %	14.53 %
ACT	125050	125000	1480	126750	126700	1560	+1700	+1700	1.36 %	1.36 %
AZD	60550	60500	8980	61300	61300	9510	+750	+800	1.24 %	1.32 %
CPE	7650	88900	890	7850	91700	960	+200	+2800	2.61 %	3.15 %
CRI	4250	25100	1100	4300	25600	1200	+50	+500	1.18 %	1.99 %
EGLE	4750	29800	410	4900	30700	470	+150	+900	3.16 %	3.02 %
ELE	14950	189400	2020	15100	191800	2150	+150	+2400	1.00 %	1.27 %
ESLE	50000	343500	8310	52000	355400	9810	+2000	+11900	4.00 %	3.46 %
GLE	30600	148900	2900	31300	153100	3140	+700	+4200	2.29 %	2.82 %
HE	24750	361300	3490	24900	364000	3640	+150	+2700	0.61 %	0.75 %
HPV	48800	410200	5310	50200	420600	5690	+1400	+10400	2.87 %	2.54 %
LLE	39850	370000	5920	40950	380500	6320	+1100	+10500	2.76 %	2.84 %
PCP	373800	2279900	46350	390800	2351900	51380	+17000	+72000	4.55 %	3.16 %
POLYMER	23250	251900	1970	23750	258300	2020	+500	+6400	2.15 %	2.54 %
POW	15200	15200	640	15350	15300	670	+150	+100	0.99 %	0.66 %
SLE	86750	749300	10540	92800	805000	12430	+6050	+55700	6.97 %	7.43 %
VE	88200	989500	8700	90200	1015500	9270	+2000	+26000	2.27 %	2.63 %
VLE	43000	623100	8420	43800	633100	8930	+800	+10000	1.86 %	1.60 %
ECND	15000	164600	1340	16850	182100	1560	+1850	+17500	12.33 %	10.63 %
GHD	6150	42500	1030	6550	45400	1120	+400	+2900	6.50 %	6.82 %
MDEC	8500	77900	1010	8650	79400	1080	+150	+1500	1.76 %	1.93 %
MFLP	1100	8000	190	1440	9700	230	+340	+1700	30.91 %	21.25 %
MPVT	22350	364000	1590	23100	390800	1760	+750	+26800	3.36 %	7.36 %
MSFT	10100	105800	1130	10800	112200	1230	+700	+6400	6.93 %	6.05 %
MSOS	35250	404100	2910	38600	439100	3130	+3350	+35000	9.50 %	8.66 %
MTCN	5750	53200	480	6000	56700	550	+250	+3500	4.35 %	6.58 %
VIS	66700	689800	5540	71050	735100	6080	+4350	+45300	6.52 %	6.57 %
X other	62250	596700	6640	66800	626900	7270	+4550	+30200	7.31 %	5.06 %
Total	1266800	9494300	90400	1320800	9898600	94180	54000	+404300	4.26 %	4.26 %

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.

9.2 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+	163100	482100	50100
PCP-VIS	48900	392800	6350
PCP-HCP+	59900	616000	14100
PCP-PVT+	110350	796100	17500
PCP-ENTH	22450	86400	7550
PCP-SFT	9100	43200	3350
PCP-Other	10250	51700	2150

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 (c_p), 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 (c_v), Mass Heat Capacity (c_v), 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