DDB

Version 2022

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

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 Software package names change

The software package has been renamed from “DDBSP” to “DDB”. The software is divided in application modules (like DDB Access Package, Predict Mix, …) and database modules (like AZD, VLE).

Also, some applications have been renamed:

- “Artist” has become “Predict Pure”
- “LEAR” has become “Literature”
- “Predict” has become “Predict Mix”
- “PCP Equation Fit” has become “Regression Pure”
- “RecPar” has become “Regression Mix”

3 New component management

The component management has changed.

With this release a new application called *Components* to search for components and edit (private) components is introduced.

The component data is now organized differently. A migration of existing private data is required. When the *Components* application is started and private component data has to be migrated, then the *DDB Migration Tool* is called to perform the migration.

All data but Antoine parameters (see parameter database) and group assignments (see GC-models parameter) are managed by the *Components* application.

Public component data cannot be modified. Only the override of several properties is possible. During the migration, an existing PRIVATE.PCP is converted to value overrides. After the migration, the PRIVATE.PCP must no longer be edited manually.

For further details have a look at the *Components* documentation.

4 Simulator interface

The simulator interface does now support aspenONE® 11, 12 and 12.1. The 64-bit DDB software does not support aspenONE® version 10 or earlier.

The simulator interface does now support PRO/II™ 2020 and 2021.

The simulator interface for UniSim® Design and Simulis® Thermodynamics does now also support the prediction of ACT, AZD, CPE, HE, SLE.

5 Regression Mix

Fitting with Simulis® Thermodynamics can now also use ACT, AZD, CPE, HE, SLE data.

Fitting with aspenONE® for the models NRTL, UNIQUAC, Wilson is possible.

6 Miscellaneous

As usual this release contains general bugfixes and performance improvements.

7 Dortmund Data Bank Progress

7.1 Overall Statistics

The Dortmund Data Bank 2022 contains more than 53,900 new data sets and more than 363,000 new data points. Data from approximately 3,200 sources have been added.

	2021			2022			Absolute Gain		Relative Gain	
DDB	Sets	Points	Refs	Sets	Points	Refs	Sets	Points	Sets	Points
AAE	5800	78000	350	5940	80400	350	+140	+2400	2.41 %	3.08 %
ACM	2050	11600	90	2050	11700	90	+0	+100	0.00 %	0.86 %
ACT	121450	121400	1470	125050	125000	1480	+3600	+3600	2.96 %	2.97 %
AZD	60150	60100	8900	60550	60500	8980	+400	+400	0.67 %	0.67 %
CPE	7400	86300	860	7650	88900	890	+250	+2600	3.38 %	3.01 %
CRI	3550	24300	1080	4250	25100	1100	+700	+800	19.72 %	3.29 %
EGLE	4450	27900	400	4750	29800	410	+300	+1900	6.74 %	6.81 %
ELE	14650	185900	1990	14950	189400	2020	+300	+3500	2.05 %	1.88 %
ESLE	48050	334000	8020	50000	343500	8310	+1950	+9500	4.06 %	2.84 %
GLE	28750	141500	2800	30600	148900	2900	+1850	+7400	6.43 %	5.23 %
HE	24450	358400	3450	24750	361300	3490	+300	+2900	1.23 %	0.81 %
HPV	47450	400500	5180	48800	410200	5310	+1350	+9700	2.85 %	2.42 %
LLE	38250	356700	5730	39850	370000	5920	+1600	+13300	4.18 %	3.73 %
PCP	358000	2215300	44620	373800	2279900	46350	+15800	+64600	4.41 %	2.92 %
POLYMER	22800	244200	1930	23250	251900	1970	+450	+7700	1.97 %	3.15 %
POW	15050	15000	640	15200	15200	640	+150	+200	1.00 %	1.33 %
SLE	78800	681200	9820	86750	749300	10540	+7950	+68100	10.09 %	10.00 %
VE	85850	961900	8520	88200	989500	8700	+2350	+27600	2.74 %	2.87 %
VLE	42400	614300	8320	43050	623100	8420	+650	+8800	1.53 %	1.43 %
ECND	14050	155700	1230	15000	164600	1340	+950	+8900	6.76 %	5.72 %
GHD	5700	39900	970	6150	42500	1030	+450	+2600	7.89 %	6.52 %
MDEC	8150	74900	990	8500	77900	1010	+350	+3000	4.29 %	4.01 %
MFLP	1020	7300	170	1100	8000	190	+80	+700	7.84 %	9.59 %
MPVT	21300	348300	1520	22300	364000	1590	+1000	+15700	4.69 %	4.51 %
MSFT	9500	100400	1070	10100	105800	1130	+600	+5400	6.32 %	5.38 %
MSOS	33100	380000	2780	35250	404100	2910	+2150	+24100	6.50 %	6.34 %
MTCN	5600	51500	460	5750	53200	480	+150	+1700	2.68 %	3.30 %
VIS	63450	655500	5310	66700	689800	5540	+3250	+34300	5.12 %	5.23 %
X other	53450	533400	6030	62250	596700	6640	+8800	+63300	16.46 %	11.87 %
Total	**1212900**	**9131300**	**87170**	**1266800**	**9494300**	**90400**	**+53900**	**+363000**	**4.44 %**	**3.98 %**

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.

7.2 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+	153250	463400	50100
PCP-VIS	47800	381600	6350
PCP-HCP+	55550	589700	14100
PCP-PVT+	107450	764800	17500
PCP-ENTH	21250	84200	7550
PCP-SFT	8850	42000	3350
PCP-Other	10100	50100	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