

DDB

Version 2024

Release Notes



DDBST

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Software & Separation
Technology

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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 License Server

The web server does now support HTTPS.

A login is now required to access the web interface.

3 New File Format

Files with the extension *.ddbpr* are used for component lists and Regression Mix projects.

4 Multiple GC Matrix Versions

For the models UNIFAC, Mod. UNIFAC (Do.), PSRK, and VTPR it is now possible to use multiple matrix versions at the same time.

5 Dortmund Data Bank

- main window clean-up
- the T/P unit in the query result is now taken from the *Mixture Properties* unit setting
- improved composition unit selection
- X-derived data is no longer displayed in separate query result pages

6 Mixture Plot

The components in the binary VLE plot are now sorted by T_c , T_b , or component numbers.

Swapping the component order is now possible.

7 Predict Pure

Multiple parallel instances of the *Group assignments* window are now possible.

The user can now modify the *Fedors* groups.

8 Entrainer Selection

- added support for PSRK and VTPR to the classic separation processes
- added support for UNIFAC-MCM and PSRK-MCM
- extended support for component lists

9 Mixture Prediction

- improved parameter selection for EOS models
- added support for AZD prediction with external models
- the v^E prediction does now support further external models

10 Regression Mix

- added support for loading start values for EOS models from the Parameter DDB
- the components are now sorted by T_c , T_b , or component numbers
- added a graphical fit progress

11 Miscellaneous

The simulator interface does now support aspenOne™ v14.

As usual, this release contains general bugfixes and performance improvements.

12 Dortmund Data Bank Progress

12.1 Overall Statistics

The Dortmund Data Bank 2024 contains more than 68,900 new data sets and more than 375,300 new data points.

DDB	2023		2024		Absolute Gain		Relative Gain	
	Sets	Points	Sets	Points	Sets	Points	Sets	Points
AAE	6150	86000	6350	88700	200	2700	3.25 %	3.14 %
ACM	2450	13400	2750	14600	300	1200	12.24 %	8.96 %
ACT	126750	126700	128150	128100	1400	1400	1.10 %	1.10 %
AZD	61300	61300	61800	61800	500	500	0.82 %	0.82 %
CPE	7850	91700	8250	95000	400	3300	5.10 %	3.60 %
CRI	4300	25600	4350	25800	50	200	1.16 %	0.78 %
EGLE	4900	30700	5000	31400	100	700	2.04 %	2.28 %
ELE	15100	191800	15500	195900	400	4100	2.65 %	2.14 %
ESLE	52000	355400	53400	364500	1400	9100	2.69 %	2.56 %
GLE	31300	153100	31650	155300	350	2200	1.12 %	1.44 %
HE	24900	364000	25350	366200	450	2200	1.81 %	0.60 %
HPV	50200	420600	51700	430400	1500	9800	2.99 %	2.33 %
LLE	40950	380500	41800	386900	850	6400	2.08 %	1.68 %
PCP	390800	2351900	423150	2428900	32350	77000	8.28 %	3.27 %
POLYMER	23750	258300	24250	269100	500	10800	2.11 %	4.18 %
POW	15350	15300	15350	15300	0	0	0.00 %	0.00 %
SLE	92800	805000	97000	842100	4200	37100	4.53 %	4.61 %
VE	90200	1015500	91650	1030500	1450	15000	1.61 %	1.48 %
VLE	43800	633100	44750	642600	950	9500	2.17 %	1.50 %
ECND	16850	182100	21300	225400	4450	43300	26.41 %	23.78 %
GHD	6550	45400	6850	47100	300	1700	4.58 %	3.74 %
MDEC	8650	79400	8750	80300	100	900	1.16 %	1.13 %
MFLP	1440	9700	1530	10100	90	400	6.25 %	4.12 %
MPVT	23100	390800	24700	409800	1600	19000	6.93 %	4.86 %
MSFT	10800	112200	11550	118900	750	6700	6.94 %	5.97 %
MSOS	38600	439100	41400	464700	2800	25600	7.25 %	5.83 %
MTCN	6000	56700	6350	59700	350	3000	5.83 %	5.29 %
VIS	71050	735100	74700	770300	3650	35200	5.14 %	4.79 %
X other	66800	626900	75050	679900	8250	53000	12.35 %	8.45 %
Total	1320800	9898600	1389700	10273900	68900	375300	5.22 %	3.79 %

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.

12.2 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+	179050	508700	63800
PCP-VIS	49600	397300	6750
PCP-HCP+	74700	650200	20250
PCP-PVT+	113000	811600	18800
PCP-ENTH	23650	87900	8450
PCP-SFT	9250	44100	3500
PCP-Other	10550	53100	2300

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