DDB and DDBSP

Version 2021

Release Notes

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1 Installation notes

1. The current DDBSP release can be installed in parallel to any previous DDBSP 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.
2. An officially supported Microsoft Windows version at release time is required.

2 DDB format has changed

With this release the DDB database file format has changed. The new files are not backwards compatible with the previous format.

In order to use private (experimental) data with the current software the data has to be upgraded to the new format. To perform a data upgrade run the program *Edit Mixture Data*. It will directly offer to perform a data conversion if private data in the old format is present. Although the conversion will make a backup of all converted files, we recommend to make a backup-copy of the private DDB folder before starting the conversion. After the conversion the backup files will be present in a ZIP archive in the private DDB folder. If an error occurs during the conversion, then a roll-back will be performed.

It is no longer possible to store data sets as QR data files. Now QRX data files are used. However, it is still possible to read QR data files which were generated with a previous release.

3 Mixture parameter fitting

In the query result of the *Dortmund Data Bank* program there is now a newly introduced *Fit* (calculator icon) drop-down menu to perform mixture parameter regressions. It replaces the *RecPar* drop-down menu which is no longer available.

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

The following sections describe the changes of the RecPar program.

3.1 New fit for ternary LLE data

- Uses a Levenberg-Marquardt, a Simplex Nelder-Mead or a combination fit.
- Uses an isoactivity or concentration fit criteria.

3.2 New fit for ternary VLE data

- Uses a Simplex Nelder-Mead fit.
- Fitting of more VLE Data types is possible.
- Fit can use up to six criteria dependent on the data type.

3.3 Integration of the DCDS fit

- The DCDS fit was integrated in RecPar for g^E models. Different VLE settings can be used.

4 New Predict program

The *Predictive EOS* program has been renamed to *Predict*. The program also contains the functionality of the programs *Activity Coefficient at Infinite Dilution* and *UNIFAC*. It also contains the predict functionality of GenPar.

4.1 Supported models

Predict supports the calculation of different thermodynamic phase behaviors and values with the following models: PSRK, PSRK2, VTPR, EOS, UNIFAC and Mod. UNIFAC (Do.).

4.2 Supported prediction properties

Predict can calculate different VLE behaviors. It also calculates the solubilities for different kinds of equilibria. The prediction of activities under different conditions is possible. Predict also supports the calculation of different excess properties.

5 Integration of the Bondi method in Artist

A new method on basis of Bondi was implemented to calculate R and Q values for molecules and molecule fragments.

6 Integration of COSMO models in Calculate X3

COSMO-RS(Ol), COSMO-SAC, COSMO-SAC 2010 and COSMO-SAC 2013 were implemented in Calculate X3.

7 Miscellaneous

- The license management system (client and server) has been updated to RLM v14.1 BL3.
- GC2gE does now support COSMO-SAC 2010/2013.
- In the *Groups* section of the components editor it is now possible to run an automatic group assignment.
- General bugfixes and performance improvements

8 Dortmund Data Bank Progress

8.1 Overall Statistics

The Dortmund Data Bank 2021 contains more than 50,000 new data sets and more than 365,000 new data points. Data from approximately 3,000 sources have been added.

	2020			2021			Absolute Gain		Relative Gain	
DDB	Sets	Points	Refs	Sets	Points	Refs	Sets	Points	Sets	Points
AAE	5350	71000	320	5850	78000	350	+500	+7000	9,35 %	9,86 %
ACM	2000	11400	80	2050	11600	90	+50	+200	2,50 %	1,75 %
ACT	115350	115300	1450	121450	121400	1470	+6100	+6100	5,29 %	5,29 %
AZD	59500	59500	8760	60150	60100	8900	+650	+600	1,09 %	1,01 %
CPE	7250	84800	840	7400	86300	860	+150	+1500	2,07 %	1,77 %
CRI	3500	24000	1050	3550	24300	1080	+50	+300	1,43 %	1,25 %
EGLE	4350	27300	380	4450	27900	400	+100	+600	2,30 %	2,20 %
ELE	14450	183100	1950	14650	185900	1990	+200	+2800	1,38 %	1,53 %
ESLE	46150	320500	7710	48050	334000	8020	+1900	+13500	4,12 %	4,21 %
GLE	27950	136000	2710	28750	141500	2800	+800	+5500	2,86 %	4,04 %
HE	24150	354500	3410	24450	358400	3450	+300	+3900	1,24 %	1,10 %
HPV	46150	391300	5050	47450	400500	5180	+1300	+9200	2,82 %	2,35 %
LLE	36900	345600	5560	38250	356700	5730	+1350	+11100	3,66 %	3,21 %
PCP	343100	2150400	42850	358000	2215300	44620	+14900	+64900	4,34 %	3,02 %
POLYMER	22350	236600	1870	22800	244200	1930	+450	+7600	2,01 %	3,21 %
POW	15050	15000	630	15050	15000	640	+0	+0	0,00 %	0,00 %
SLE	74000	629900	9300	78800	681200	9820	+4800	+51300	6,49 %	8,14 %
VE	84100	942700	8360	85850	961900	8520	+1750	+19200	2,08 %	2,04 %
VLE	41400	601000	8170	42400	614300	8320	+1000	+13300	2,42 %	2,21 %
ECND	13000	144700	1140	14050	155700	1230	+1050	+11000	8,08 %	7,60 %
GHD	5500	38500	940	5700	39900	970	+200	+1400	3,64 %	3,64 %
MDEC	8050	73800	970	8150	74900	990	+100	+1100	1,24 %	1,49 %
MFLP	810	6400	150	1020	7300	170	+210	+900	25,93 %	14,06 %
MPVT	19600	322900	1430	21300	348300	1520	+1700	+25400	8,67 %	7,87 %
MSFT	8850	94500	1000	9500	100400	1070	+650	+5900	7,34 %	6,24 %
MSOS	30700	354100	2630	33100	380000	2780	+2400	+25900	7,82 %	7,31 %
MTCN	5350	48800	410	5600	51500	460	+250	+2700	4,67 %	5,53 %
VIS	59500	611900	5020	63450	655500	5310	+3950	+43600	6,64 %	7,13 %
X other	51350	512400	5480	53450	533400	6030	+2100	+21000	4,09 %	4,10 %
Total	**1162500**	**8765400**	**84170**	**1212900**	**9131300**	**87170**	**+50400**	**+365900**	**4,34 %**	**4,17 %**

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.

8.2 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+	144150	446700	46400
PCP-VIS	46950	373000	6150
PCP-HCP+	51500	563200	12950
PCP-PVT+	105000	750000	16900
PCP-ENTH	20500	81900	7150
PCP-SFT	8700	41300	3300
PCP-Other	9900	49100	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 (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