DDB and DDBSP

Delivery 2019

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

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1 Installation Notes

1. If any updates for DDBSP 2018 are installed and DDBSP 2018 is uninstalled before the updates are uninstalled then the uninstall of the updates will fail. In that case install DDBSP 2018 again and uninstall the updates and the original application in the right order.
2. DDBSP 2019 can be installed in parallel to DDBSP 2018 (and any older version). However, if DDBSP 2018 is uninstalled after the installation of DDBSP 2019 then settings like the file type associations will get broken. In that case a repair installation of DDBSP 2019 should solve the problem.

2 COSMO calculations

2.1 Changes in COSMO-RS(OL) calculation

A model inconsistency for systems with more than two components was solved. New equations for $r_i^{\#}$ and $q_i^{\#}$ were implemented which reproduce the old results for binary systems and give consistent results for higher systems.

Old equations:

$$r_i^{\#} = (1 - x_i) \sum_{j \neq i} \frac{r_j}{x_j}$$

$$q_i^{\#} = (1 - x_i) \sum_{j \neq i} \frac{q_j}{x_j}$$

New equations:

$$r_i^{\#} = \frac{\sum_{j \neq i} x_j r_j}{\sum_{j \neq i} x_j}$$

$$q_i^{\#} = \frac{\sum_{j \neq i} x_j q_j}{\sum_{j \neq i} x_j}$$

2.2 GC-COSMO calculation available

The models GC-COSMO-RS(Ol)[1] and GC-COSMO-SAC[2] are now available for calculations. They allow the calculation of systems with components with no sigma profile. In these cases intermediate sigma profiles are estimated on basis of a group contribution method. The parameters of this method were fitted with the help of already existing sigma profiles for both COSMO-methods.

GC-COSMO is available for the properties ACT, ACM, AZD, CPE, GLE, HE, LLE, MFLP and VLE.

1 Mu T., Rarey J., Gmehling J., "Group Contribution Prediction of Surface Charge Density Profiles for COSMO-RS(Ol)", AIChE J., 53(12), 3231-3240, 2007

2 Mu T., Rarey J., Gmehling J., "Group Contribution Prediction of Surface Charge Density Distribution of Molecules for COSMO-SAC", AIChE J., 55(12), 3298-3300, 2009

3 Gamma-phi vapor phase model

The vapor phase association model[3] (VPA) is now available for calculations. Dimerization, tetramerization and hexamerization (e.g. in case of HF) are supported.

To consolidate the results with VPA the Marek-Standart vapor phase model does no longer use a special cross dimerization term for the component pair “Formic acid”-“Acetic acid”.

4 Predictive EOS

For TP flash calculations the Peneloux correction for PSRK is now optionally available.

5 Entrainer Selection

The “Absorption (Extended)” option is now available. It adds new features to the solvent selection for absorption processes. It can search for solvent mixtures and can use molality-based Henry coefficients. Additionally, it uses a sophisticated selection criterion for the performance evaluation of the solvents, which consists of the selectivity, the capacity and the solvent loss.

6 Simulator Interface

The mapping between the aspenONE®[4] and the DDB components has been updated. Now more than 14500 components can be automatically assigned.

7 Miscellaneous

- **Similarity Search**
  The “Similarity Search” can be opened from the “Component Selection” with contains only a rudimentary selection criterion for the molecular size. The user can freely define criteria from the group list at the right bottom of the menu for components which should be found.
- General bugfixes and performance improvements

3 Gmehling J., Kolbe B., Kleiber M., Rarey J., “Chemical Thermodynamics for Process Simulation”, Wiley-VCH, 573-590, 2012

4 aspenOne is a registered trademark of Aspen Technology, Inc., Burlington, MA.

8 Dortmund Data Bank Progress

8.1 Overall Statistics

The Dortmund Data Bank 2019 has more than 57000 new data sets and more than 435000 new data points. Data from more than 3300 sources have been added.

	2018			2019			Absolute Gain		Relative Gain	
DDB	Sets	Points	Refs	Sets	Points	Refs	Sets	Points	Sets	Points
AAE	5000	64000	290	5040	64700	300	+40	+700	0.80 %	1.09 %
ACM	1900	11000	80	2000	11300	85	+100	+300	5.26 %	2.73 %
ACT	103100	103100	1400	112300	112300	1430	+9200	+9200	8.92 %	8.92 %
AZD	58300	58300	8550	58900	58900	8660	+600	+600	1.03 %	1.03 %
CPE	6950	80700	790	7100	83300	830	+150	+2600	2.16 %	3.22 %
CRI	3400	23300	1010	3450	23700	1040	+50	+400	1.47 %	1.72 %
EGLE	3950	24500	330	4150	25800	360	+200	+1300	5.06 %	5.31 %
ELE	13800	173500	1850	14150	177900	1900	+350	+4400	2.54 %	2.54 %
ESLE	42950	296200	7120	44500	307800	7430	+1550	+11600	3.61 %	3.92 %
GLE	25950	124400	2500	26600	128300	2590	+650	+3900	2.50 %	3.14 %
HE	23650	346900	3350	23900	349900	3390	+250	+3000	1.06 %	0.86 %
HPV	42600	365400	4710	44600	379300	4890	+2000	+13900	4.69 %	3.80 %
LLE	34000	309300	5170	35450	328900	5360	+1450	+19600	4.26 %	6.34 %
PCP	317650	2001400	39760	331650	2071700	41370	+14000	+70300	4.41 %	3.51 %
POLYMER	21400	223100	1780	21950	230400	1830	+550	+7300	2.57 %	3.27 %
POW	14850	14800	610	15000	15000	630	+150	+200	1.01 %	1.35 %
SLE	64850	539400	8360	68650	573100	8800	+3800	+33700	5.86 %	6.25 %
VE	79100	884300	7940	80900	903100	8110	+1800	+18800	2.28 %	2.13 %
VLE	39500	575600	7900	40500	588300	8040	+1000	+12700	2.53 %	2.21 %
ECND	10550	110800	920	11750	124700	1020	+1200	+13900	11.37 %	12.55 %
GHD	4750	34200	820	5150	36300	890	+400	+2100	8.42 %	6.14 %
MDEC	7550	69500	890	7850	71800	930	+300	+2300	3.97 %	3.31 %
MFLP	690	5800	120	730	6000	140	+40	+200	5.80 %	3.45 %
MPVT	16000	274700	1210	17800	298400	1330	+1800	+23700	11.25 %	8.63 %
MSFT	7000	76700	820	7950	86000	910	+950	+9300	13.57 %	12.13 %
MSOS	24100	288000	2140	27200	321100	2400	+3100	+33100	12.86 %	11.49 %
MTCN	4850	42800	370	4950	43800	380	+100	+1000	2.06 %	2.34 %
VIS	50150	523300	4340	55350	571300	4720	+5200	+48000	10.37 %	9.17 %
X other	38050	353700	4190	46100	460200	4890	+8050	+106500	21.16 %	30.11 %
Total	**1056500**	**7883900**	**77880**	**1113800**	**8323700**	**81190**	**+57400**	**+440000**	**+5.43 %**	**+5.58 %**

Disclaimer: The numbers presented here may be different 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+	130700	419400	42000
PCP-VIS	44700	349900	5800
PCP-HCP+	47000	517200	11750
PCP-PVT+	97950	705400	15500
PCP-ENTH	19200	75900	6600
PCP-SFT	8350	39500	3200
PCP-Other	9400	45400	2000

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