List of Changes from Version 2008 to 2009

Software, Data Banks, and more

DDBST
DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

Contents

Software Changes....2
Artist – Property Prediction....2
Search for Components with Specified Properties....2
Interface for ProSim Software....3
New Models for Kow Predictions....3
New Vapor Pressure Method of Moller/Rarey/Ramjugernath....3
Added Sublimation Pressure Calculation by Myrdal/Yalkowsky, Rarey/Nannoolal and Moller methods....4
Group Contribution Prediction of Surface Charge Density Profiles for COSMO-RS models....4
Water Solubility Prediction with modified UNIFAC....4
Water Solubility Prediction by Moller Method....5
Mixture Calculations....5
Interfaces to Process Simulator Software....5
AspenTech....5
New models....5
Improved VTPR Volume Translation....5
Prediction of VLE by Equation of State....6
Some Minor Improvements....6
Diagrams....6
Pure Component Equations Fit....7
UNIFAC Prediction Software....8
License Management....8
Test DDB Installation Tool....9
Data Banks....10
Data Bank Growth from 2008 to 2009....10
Data Bank Growth from 2007 to 2009....11
Other Important Issues....13
GPA Data Bank Release....13
GPA Data Bank Explorer....13
Rigorous 3-Phase Flash....13
Mixture Properties....13
Thermophysical Property Estimation....14
Maximizing your GPA Research Investment....14
DDB Online Calculations....15
DDB Online Search....15

Software Changes

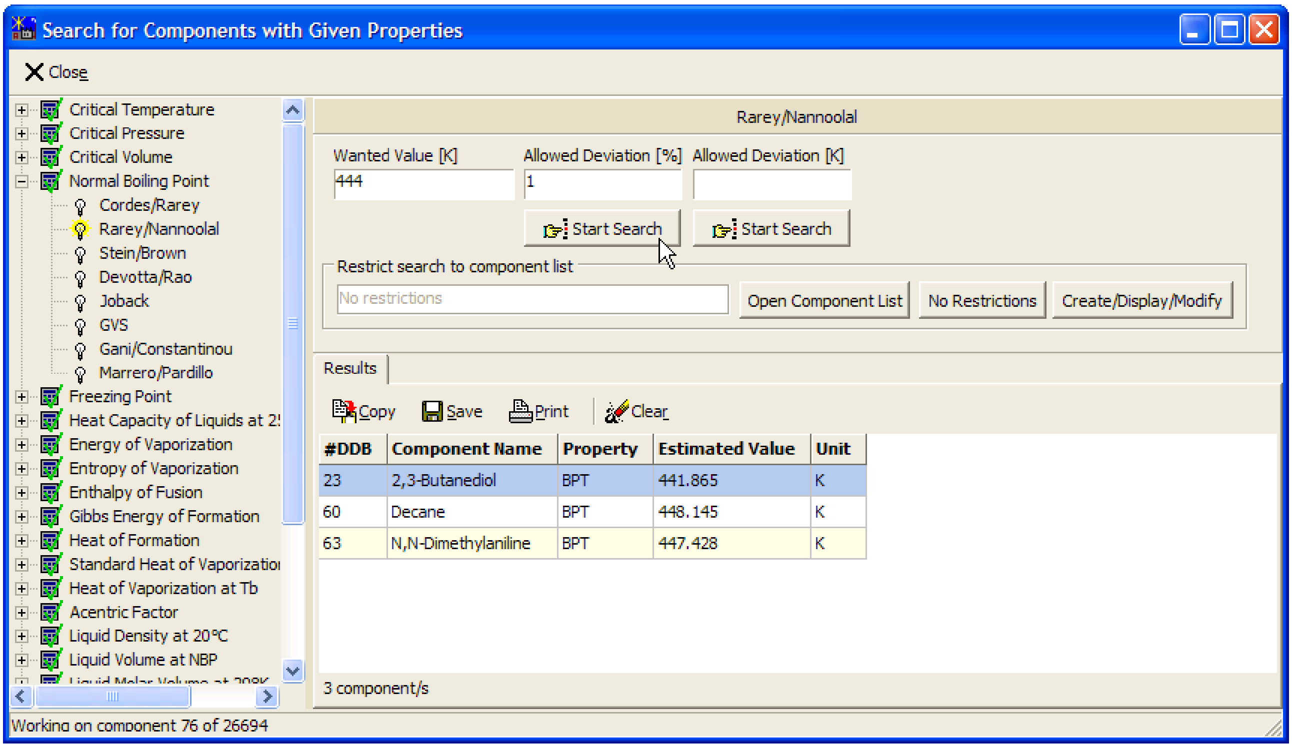
Artist – Property Prediction

Search for Components with Specified Properties

This new function uses the predictive methods in Artist to find molecules with a specified property. This could be, for example, a normal boiling point around 444 K with a maximum deviation of one percent or 5 K. A normal boiling point search of 444 K with the Rarey/Nannoolal method will find e. g. n-Decane, N,N-Dimethyl-Aniline, Phenol and lots of other components. A search for a critical temperature of 555 K with the Gani/Constantinou[1] method which will find Heptane, Cyclohexane, 3-Pentanone among other components.

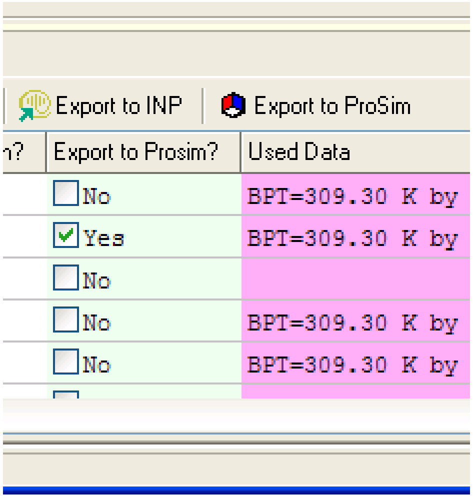
Components with specified properties can be used for process synthesis in separation processes where entrainers with a minimum normal boiling point are needed. One source of information is the Dortmund Data Bank where DDBST already introduced a search for components with specified properties a few years ago. This limits the results to components with available experimental data.

The new approach now opens the door to find components which never have been measured.



1 Constantinou L., Gani R., "New Group Contribution Method for Estimating Properties of Pure Compounds", AIChE J., 40(10), 1697-1710, 1994

Interface for ProSim Software



Artist now allows the export of some predicted properties in a XML-based file format which then can be read in the ProSim[2] Simulis software. The supported properties are currently only critical data, normal boiling point, heat of formation and melting temperature. Further properties will be added in the near future.

ProSim is a leading independent European chemical engineering software company delivering process simulation software and consulting services to the oil, gas, chemical and other processing industries worldwide.

New Models for K_{ow} Predictions

Artist now supports the original UNIFAC[3] and mod. UNIFAC (Dortmund)[4] and also the COSMO-RS(Ol)[5] model for the prediction of Octanol-Water partition coefficients. All three models estimate activity coefficients just like the original K_{OW} UNIFAC method but have a broader range of applicability.

It still has to be remembered that K_{OW} UNIFAC has been explicitly developed for this single purpose and therefore often delivers better results than the three other models.

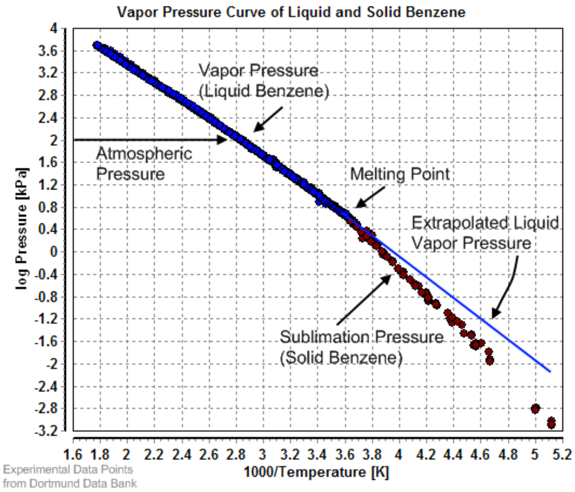
New Vapor Pressure Method of Moller/Rarey/Ramjugernath

The authors have written in their abstract[6]:

“The model represents both a significant improvement and extension of the original method developed by Nannoolal et al.[7] The method was developed with the aid of the Dortmund Data Bank, which contains over 180 000 data points for both solid and liquid vapor pressure (2007). Group parameters were regressed to a training set of nearly 114000 data points for more than 2330 compounds. As in the case of the method of Nannoolal et al. the new model only requires knowledge about the molecular structure and a single vapor pressure point in order to generate the vapour pressure curve. In the absence of experimental data it is possible to predict the normal boiling point by a method developed earlier by Nannoolal et al. The relative error in pressure was found to be 5.0% (113888 data points for 2332 compounds) which compares favorably with the previous model (6.6% for 111757 data points and 2207 compounds).”

2 http://www.prosim.net/ (ProSim Web Site)
3 Wittig R., Lohmann J., Gmehling J., "Vapor-Liquid Equilibria by UNIFAC Group Contribution. 6. Revision and Extension", Ind.Eng.Chem.Res., 42(1), 183-188, 2003
4 Jakob A., Grensemann H., Lohmann J., Gmehling J., "Further Development of Modified UNIFAC (Dortmund): Revision and Extension 5", Ind.Eng.Chem.Res., 45(23), 7924-7933, 2006
5 Grensemann H., Gmehling J., "Performance of a Conductor-Like Screening Model for Real Solvents Model in Comparison to Classical Group Contribution Methods", Ind.Eng.Chem.Res., 44(5), 1610-1624, 2005
6 Moller B., Rarey J., Ramjugernath D., "Estimation of the vapour pressure of non-electrolyte organic compounds via group contributions and group interactions ", J.Mol.Liq., 143(1), 52-63, 2008
7 Nannoolal Y., Rarey J., Ramjugernath D., "Estimation of pure component properties: Part 3. Estimation of the vapor pressure of non-electrolyte organic compounds via group contributions and group interactions", Fluid Phase Equilib., 269(1-2), 117-133, 2008

Added Sublimation Pressure Calculation by Myrdal/Yalkowsky, Rarey/Nannoolal and Moller methods

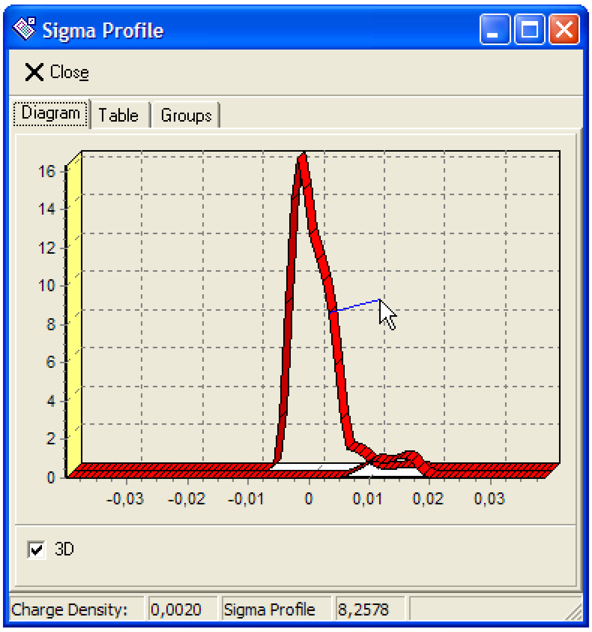


The sublimation pressure can be derived from an extrapolated (then hypothetical) liquid vapor pressure if the melting point and the heat of melting are known.

$$\ln P^s_{solid} = \ln P^s_{liquid} - \frac{\Delta H_m}{R}\left(\frac{1}{T} - \frac{1}{T_m}\right)$$

Artist now uses all three models to estimate a liquid vapor pressure below and corrects this pressure by the given equation.

Group Contribution Prediction of Surface Charge Density Profiles for COSMO-RS models



Artist now supports the creation of σ profiles for COSMO-RS(Ol)[8] and COSMO-SAC by two new group contribution methods developed in the work group of Prof. Gmehling.

Artist display the profile in a diagram and a table which can be stored in a format usable by DDB software.

Water Solubility Prediction with modified UNIFAC

Water solubilities of alkanes, alkenes, and cyclolkanes are normally predicted poorly by modified UNIFAC because of the needed extremely high values of the activity coefficients to describe wide miscibility gaps.

Jakob et al.[9] show a method that converts the standard activity predicts by an empirical equation.

The following equation has been used.

$$\log c_i^{w,s} = A \cdot \log\left(\frac{55.56}{\gamma^{\infty}_{organic\,compound\,in\,water}(298.15\,K)}\right) + B \cdot T + C\left[\frac{mol}{l}\right]$$

The values for A, B, and C are

Component Type	A	B	C
Alkanes	1.104	0.0042	-2.817

8 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

9 Jakob A., Grensemann H., Lohmann J., Gmehling J., "Further Development of Modified UNIFAC (Dortmund): Revision and Extension 5", Ind.Eng.Chem.Res., 45(23), 7924-7933, 2006

Alkenes	1.523	0.00603	-3.0418
Cycloalkanes	1.3326	0.0006427	-3.676

Parameters have been fitted for components with carbons numbers from five to ten, solubilities have been available in the temperature range from 273.15 K to 373.15 K. The parameters for Alkanes are directly taken from Jakob et al., the parameters for alkenes and cycloalkanes have been regressed to experimental data from the Dortmund Data Bank by Prof. Gmehling. These parameters are not yet published.

This method can be used only for a very limited number of components: Alkanes, Cycloalkanes, and Alkenes with carbon numbers from four to ten. No other atoms must be present and only a single double-bond can be present.

Water Solubility Prediction by Moller Method

This method is not yet published and will be part of the Ph. D. thesis of Bruce Moller. The method is a group contribution method which estimates activity coefficients at infinite dilution of components solved in Water. This is a very specialized method allowing a much better description of this property as modified UNIFAC will ever be able to. In addition, this method predicts solubilities for a much wider range of components.

Mixture Calculations

Interfaces to Process Simulator Software

AspenTech

The interface with the AspenTech[10] simulator (especially support of different Aspen versions) has been improved. Some limited functionality has already been available in the 2008 version and this is now updated for newer AspenTech simulator versions and extended by new functions supporting a lot of new properties.

New models

Three new models can be used to predict Octanol-Water partition coefficients. These are the models original UNIFAC, modified UNIFAC, and COSMO-RS(Ol).

Improved VTPR Volume Translation

The prediction of the liquid volumes resp. densities is one of the advantages of VTPR[11] (**V**olume-**T**ranslated-**P**eng-**R**obinson) compared to PSRK (**P**redictive **S**oave-**R**edlich-**K**wong). The DDB has now stored 841 volume translation constants directly obtained from the difference between volumes calculated by the Peng-Robinson equation of state and volumes calculated by the DIPPR 105 equation with parameters obtained from direct regression of density data from the pure component

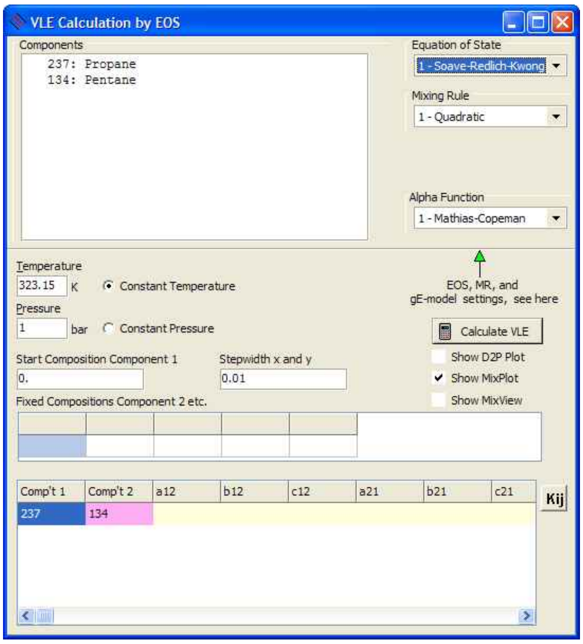
10 http://www.aspentech.com/

11 Ahlers J., Gmehling J., "Development of an universal group contribution equation of state. I. Prediction of liquid densities for pure compounds with a volume translated Peng-Robinson equation of state", Fluid Phase Equilib., 191, 177-188, 2001

properties data bank. This improves the prediction of liquid volumes significantly compared to calculations with the volume translation constant estimated from critical data and the acentric factor.

Prediction of VLE by Equation of State

Vapor-liquid equilibria (VLE) can now be predicted by equation of states (EOS, supported equation of states are Redlich-Kwong, Soave-Redlich-Kwong, and Peng-Robinson) and mixing rules (MR, supported mixing rules are quadratic, several g^E mixing rules, and Panagiotopoulos/Reid). The calculation of VLE with equation of state mixing rule parameters has long been available in a stand-alone software tools (called GenPar) which is mainly used to regress these parameters. This calculation routine has now been integrated in the standard mixture calculation software and make the EOS-MR available without switching to a separate software.



Some Minor Improvements

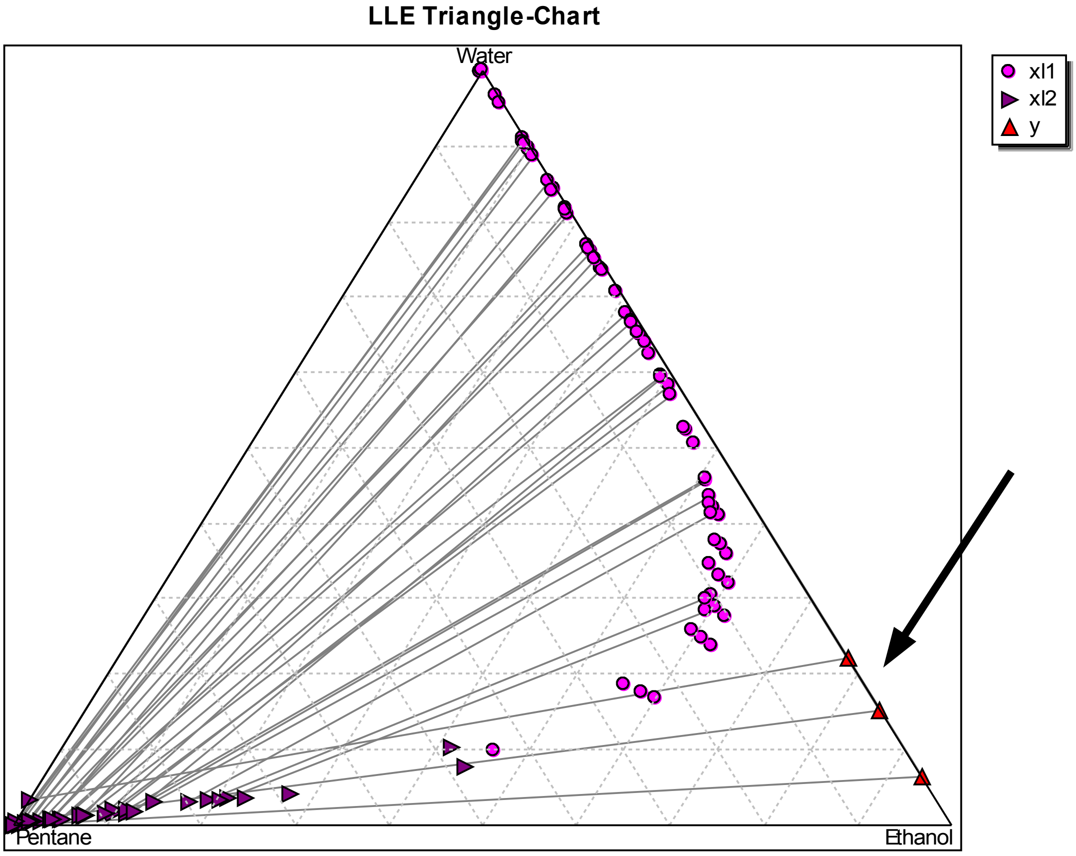
These improvements include:

1. Added function to use gas solubility data sets for fitting g^E model interaction parameters. Gas solubility data are often convertible to standard Ptxy data which then can be used directly to obtain activity coefficients necessary for the regression of g^E model (NRTL, Wilson, UNIQUAC) parameters.
2. Improved support for managing g^E model interaction parameters obtained from LLE data. This effects mainly the storage and export of g^E model parameters with LLE-specific temperature dependencies.
3. LLE data sets can now be recalculated. In older software only the entire range of compositions have been calculated which didn't allow matching exactly the data points from experimental data sets. The new feature now allows a direct comparison of predicted and experimental data points.

Diagrams

1. If marked sets can't be shown together in one diagram because they are of different shape, contain different properties, or can't be converted into a single format the old software only displayed the first matching sets. Now the remaining sets are processed again and put into new pages until all data sets are processed.

2. In LLE ternary and quaternary diagram also data sets of binary (or ternary) subsystem are



displayed if the first marked data set is the full-system data set.

3. Some new plots for vapor-liquid equilibria of electrolyte containing mixture, solid-liquid equilibria, volumes and densities of mixtures, and vapor-liquid equilibria added.

Pure Component Equations Fit

Several PPDS (Physical Property Data Service) equations have been added. These equation offer an alternative to the well-known DIPPR equations and are sometimes better suited for the given properties.

PPDS 15 $c_p = R\left(\frac{A}{\tau} + C\tau + D\tau^2 + E\tau^3 + F\tau^4\right)$ with $\tau = 1 - \frac{T}{T_c}$ for liquid heat capacity

PPDS 2 $C_P = R\left(B + (C-B)y^2\left[1 + (y-1)\left(D + Ey + Fy^2 + Gy^3\right)\right]\right)$ with $y = \frac{T}{A+T}$ for ideal gas heat capacity

PPDS 12 $H_{Vap} = RT_c\left(A\tau^{\frac{1}{3}} + B\tau^{\frac{2}{3}} + C\tau + D\tau^2 + E\tau^6\right)$ with $\tau = 1 - \frac{T}{T_c}$ for heat of vaporization

PPDS 8 $\lambda = A\left(1 + B\tau^{\frac{1}{3}} + C\tau^{\frac{2}{3}} + D\tau\right)$ with $\tau = 1 - \frac{T}{T_c}$ for liquid thermal conductivity

PPDS 3 $\lambda = \frac{\sqrt{T_r}}{A + \frac{B}{T_r} + \frac{C}{T_r^2} + \frac{D}{T_r^3}}$ with $T_r = \frac{T}{T_c}$ for vapor thermal conductivity

UNIFAC Prediction Software

The stand-alone UNIFAC prediction software has been updated, extended and improved by many different aspects. It now fully supports the latest published version of original UNIFAC and modified UNIFAC (Dortmund), it has a way better handling of compositions allowing many different calculation modes and the user interface has improved a lot. It is now fully integrated in the DDB software package including the standard editors for components and group interaction parameters. It now also allows using the parameters from the UNIFAC consortium (as an additional option). A short manual (PDF, approx. 364 KB) is available for download.

License Management

The license management has been thoroughly reengineered. This includes a change of the license management software vendor. DDBST now uses the Reprise License Manager (RLM) from Reprise Software, Inc.

- The license server installation does not require a valid license anymore. A new or updated license can be activated without re-installing the license server.
- The license upgrade for single user licenses is possible without administrative user rights. This gives the standard user the ability to update the license without contacting software administrators.
- A local workstation license can be used in combination with a server license which is useful if some licensed data or programs are single-user licenses and only accessible on the specific workstation whereas the other more limited licenses can be used from different workstation in the network.
- Permanent licenses can be combined with time-limited licenses. This feature is used to combine e. g. a yearly license for some products with an unlimited license for other products or for providing demonstration version with even a shorter time frame than one year.
- Single user and site licenses do not require a license server installation. The old license system always needed a two-step installation of the standard software and the license server. This is not necessary anymore for single-user licenses and for site licenses with an unlimited number of licenses. The license manager is included in the standard software in these two cases. A license server setup is only necessary for multiple licenses in a network.
- License server communication ports can be configured by the administrator. This feature is important in networks with restricted access to some network services. The limitations are mainly implemented through firewalls blocking all unneeded ports.
- A BIOS update will no longer invalidate the license. The old licenses system used some BIOS information for identifying the machine it is running on. Since there are some machines with occasional updates (especially some notebooks) of the BIOS the DDB license server ceased to work. The new license management system now relies only on hardware specific details which will (probably) never change.

Test DDB Installation Tool

DDBST now delivers a new test tool with its normal software. This test software can be used to identify problems with installations and gives valuable hints how to resolve such errors.

Typical errors that can be identified can be

- errors in the DDB folder structure. The folder structure will be normally correct after an installation but might get corrupted by wrong entries in the DDB configuration tool.
- access problems. These can occur if an administrator has installed the software but a user with very limited access rights tries to use the software.
- installation problems. These are mainly write errors so that some parts of software or data files haven't been installed properly or problems with the registration of DDB software components in Windows.
- licensing problems. A time-limited license might be expired or the license server might not be accessible because of network problems.
- corrupted data banks. Data banks might become unreadable by hard disk failures or because of wrong data bank encoding (DDBST delivers the data banks with a customer specific encoding).

Data Banks

Data Bank Growth from 2008 to 2009

	Current State 2009			2008			Gain			Percentage		
Databank	Sets	Points	References	Sets	Points	References	Sets	Points	References	Sets	Points	References
AAE	3576	43122	194	3576	43122	194	0	0	0	0.00%	0.00%	0.00%
ACM	1409	9209	54	1107	6849	40	302	2360	14	27.28%	34.46%	35.00%
ACT	53838	53838	1023	50853	50853	884	2985	2985	139	5.87%	5.87%	15.72%
AZD	50904	50904	7254	50200	50200	7141	704	704	113	1.40%	1.40%	1.58%
CPE	3025	33010	374	2872	31481	352	153	1529	22	5.33%	4.86%	6.25%
CRI	1858	14666	512	1674	13589	427	184	1077	85	10.99%	7.93%	19.91%
EGLE	1444	7920	108	1358	7346	103	86	574	5	6.33%	7.81%	4.85%
ELE	7496	93019	981	6872	85568	920	624	7451	61	9.08%	8.71%	6.63%
ESLE	26894	182687	4361	23808	163407	3760	3086	19280	601	12.96%	11.80%	15.98%
GLE	18565	79627	1587	18249	77979	1538	316	1648	49	1.73%	2.11%	3.19%
HE	19261	282489	2758	18607	275674	2696	654	6815	62	3.51%	2.47%	2.30%
HPV	28408	247473	3166	26975	234716	3029	1433	12757	137	5.31%	5.44%	4.52%
LLE	19575	156108	3009	18546	144887	2776	1029	11221	233	5.55%	7.74%	8.39%
PCP	178755	1204889	23115	169843	1156120	21896	8912	48769	1219	5.25%	4.22%	5.57%
POLYMER	16916	161218	1370	15832	145811	1257	1084	15407	113	6.85%	10.57%	8.99%
POW	7739	7737	314	7720	7718	311	19	19	3	0.25%	0.25%	0.96%
SLE	28580	241391	3559	23677	203989	2881	4903	37402	678	20.71%	18.34%	23.53%
VE	36739	438706	4081	32996	397253	3701	3743	41453	380	11.34%	10.43%	10.27%
VLE	29476	428404	6245	28167	409525	6106	1309	18879	139	4.65%	4.61%	2.28%
Sum	**534458**	**3736417**		**502932**	**3506087**		**31526**	**230330**		**6.27%**	**6.57%**	

.

In total the Dortmund Data Bank contains in 2009 **31526** new data sets and **230330** new data points. This is an increase of 6.27 % in data sets resp. 6.57 % in data points. This amount of new data sets and points is comparable to the data bank growth from 2007 to 2008.

Data Bank Growth from 2007 to 2009

	Current State 2009			2007			Gain			Percentage		
Databank	Sets	Points	References	Sets	Points	References	Sets	Points	References	Sets	Points	References
AAE	3576	43122	194	3547	42662	191	29	460	3	0.82%	1.08%	1.57%
ACM	1409	9209	54	1107	6849	40	302	2360	14	27.28%	34.46%	35.00%
ACT	53838	53838	1023	48324	48324	861	5514	5514	162	11.41%	11.41%	18.82%
AZD	50904	50904	7254	49568	49568	7031	1336	1336	223	2.70%	2.70%	3.17%
CPE	3025	33010	374	2245	25407	331	780	7603	43	34.74%	29.92%	12.99%
CRI	1858	14666	512	1379	11526	374	479	3140	138	34.74%	27.24%	36.90%
EGLE	1444	7920	108	1223	6843	95	221	1077	13	18.07%	15.74%	13.68%
ELE	7496	93019	981	6354	79030	832	1142	13989	149	17.97%	17.70%	17.91%
ESLE	26894	182687	4361	19067	134408	2867	7827	48279	1494	41.05%	35.92%	52.11%
GLE	18565	79627	1587	17711	75899	1491	854	3728	96	4.82%	4.91%	6.44%
HE	19261	282489	2758	18111	268584	2638	1150	13905	120	6.35%	5.18%	4.55%
HPV	28408	247473	3166	25915	225694	2910	2493	21779	256	9.62%	9.65%	8.80%
LLE	19575	156108	3009	17332	133399	2573	2243	22709	436	12.94%	17.02%	16.95%
PCP	178755	1204889	23115	159295	1095043	20564	19460	109846	2551	12.22%	10.03%	12.41%
POLYMER	16916	161218	1370	15832	145811	1257	1084	15407	113	6.85%	10.57%	8.99%
POW	7739	7737	314	7667	7665	307	72	72	7	0.94%	0.94%	2.28%
SLE	28580	241391	3559	19587	164751	2321	8993	76640	1238	45.91%	46.52%	53.34%
VE	36739	438706	4081	29484	353101	3318	7255	85605	763	24.61%	24.24%	23.00%
VLE	29476	428404	6245	27142	396857	5998	2334	31547	247	8.60%	7.95%	4.12%
Sum	**534458**	**3736417**		**470890**	**3271421**		**63568**	**464996**		**13.50%**	**14.21%**	

Short terms: 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, EGLE: Gas solubilities in electrolyte-containing mixtures, ELE: Vapor-liquid equilibria of electrolyte-containing mixture, ESLE: Salt solubilities, GLE: Gas solubilities (gas-liquid equilibria), HE: Heats of mixing, HPV: Vapor-liquid equilibria (at least one component has a normal boiling point below 0°C), LLE: Liquid-liquid equilibria (miscibility gaps), 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, VLE: Vapor-liquid equilibria (all components with a normal boiling point above 0°C).

In total the Dortmund Data Bank contains in 2009 **63568** new data sets and **464996** new data points. This is an increase of 13.50 % in data sets resp. 14.21 % in data points.

A big step forward this year is the integration of all the data from the GPA research reports and technical publications (see chapter below for more details). Several of these data are not part of the standard data banks listed above but are only distributed through the GPA specific version).

Starting with the GPA version DDBST now provides a full coverage of all available data sets in the Dortmund Data Bank to every customer. The non-licensed data sets, of course, don't contain the experimental values but they give the information that there are data available for a specific system and property. An even more up-to-date overview can be obtained through our new online DDB search system.

Other Important Issues

GPA Data Bank Release

by EPCON International[12]

The GPA Data Bank, 5th Edition delivers over 37 years of GPA research data for immediate, productive use in process simulation tools. Included is a completely remastered thermophysical property database with all GPA Research Reports and Technical Publications and powerful data fitting, correlation, and phase equilibrium software applications. The GPA Data Bank is now over twice the size of previous versions and includes a significant amount of new VLE data for low-boiling hydrocarbons never before available in previous versions of the GPA Data Bank published by Penn State (1st Ed.-1983, 2nd Ed.-1990, 3rd Ed-1993) and Oklahoma State University (4th Ed.-2000). The GPA Data Bank, 5th Edition was jointly development by EPCON International (developer of the popular API Technical Data Book and Engineer's Aide software) and DDBST (developer of the popular Dortmund Data Bank and co-founder of the UNIFAC consortium). The result is a software that can be widely used by engineers within your organization with direct links to major process simulators to immediately improve your company's gas processing operations.

GPA Data Bank Explorer

The GPA Data Bank Explorer provides electronic access and searching capabilities for all 195 GPA Research Reports and 30 GPA Technical Publications. The 12 software programs are loaded from a convenient Outlook style navigation pane with two categories of software to choose from. The GPA Data Bank Explorer provides all GPA research work in a convenient, intuitive software interface developed over 10 years in the API Technical Data Book software product.

Rigorous 3-Phase Flash

Utilize the advanced 3-phase flash engine provided in the GPA Data Bank to accurately determine the 3rd liquid phase vital for compressor operations and pipeline transportation applications. Developed in cooperation with the API Technical Data Committee - the 3-phase flash outperforms major simulators in 5 key areas for hydrocarbon process system design and operations.

Mixture Properties

The GPA Data Bank with the stored pure component properties and the comprehensive GPA VLE, LLE, and VLLE mixture data is the ideal tool for fitting reliable model parameters. Fit GPA data to gE-models or equations of state, for the development of group contribution methods and for fitting the required interaction parameters for process simulation.

It is especially helpful for the critical examination of model parameters prior to process simulation. For the development of reliable group contribution methods with a broad range of applicability nearly all available information covering a large temperature and the whole concentration range for a variety of compounds very different in size can be used.

12 http://www.epcon.com

Thermophysical Property Estimation

The ARTIST software provides estimation of pure component properties using the molecular structure. It incorporates a large number of different group contribution methods for a multitude of different properties. Using a special coding scheme for molecular structures, ARTIST is able to take into account the chemical neighborhood of the individual groups thus implementing chemical know-how. To ensure the correctness of the algorithm, the program has already been tested for years during the development of the well known UNIFAC and mod. UNIFAC methods. ARTIST utilizes a user-friendly Windows graphical user interface. Results can be copied to the clipboard or automatically sent to Microsoft Excel™ for further processing.

Maximizing your GPA Research Investment

The GPA Data Bank maximizes the benefits of your GPA research investment by directly applying GPA data to the simulation and design of your gas processing operations.

DDB Online Calculations

DDBST has published a variety of free online services for the calculation and prediction of several thermophysical properties. These services includes the calculation of

- Vapor pressures by the Antoine equation
- Liquid densities by the DIPPR 105 equation
- Liquid dynamic viscosities by the Vogel equation
- Surface tensions by the DIPPR 106 equation
- Heats of vaporization by the PPDS 12 equation

The prediction of normal boiling points and vapor pressures by the Rarey/Nannoolal[13], the Moller, the Stein/Brown[14] and the Myrdal/Yalkowsky[15] methods is done in cooperation with the E-AIM project of Prof. Clegg from the University of East Anglia in Norwich/UK.

The prediction of critical data, liquid viscosities, and other properties is implemented through the Joback[16] method. DDBST chose to publish the Joback method as an example for the methods implemented in Artist because it is simple, widely known and widely used. It allows the estimation of several properties but it is also known to be unreliable and of limited quality. The Artist program package contains many newer and better methods.

DDB Online Search

The DDB online search[17] is updated on a regular basis and always gives an overview over the current status of the Dortmund Data Bank. This online search is also updated by new features from time to time. As a result the “DDB Overview” stand-alone Windows program is not updated any more.

13 Nannoolal Y., Rarey J., Ramjugernath D., Cordes W., "Estimation of Pure Component Properties. Part 1. Estimation of the Normal Boiling Point of Non-Electrolyte Organic Compounds via Group Contributions and Group Interactions", Fluid Phase Equilib., 226, 45-63, 2004

14 Stein S.E., Brown R.L., "Estimation of Normal Boiling Points from Group Contributions ", J.Chem.Inf.Comput.Sci., 34, 581-587, 1994

15 Myrdal P.B., Yalkowsky S.H., "Estimating Pure Component Vapor Pressures of Complex Organic Molecules", Ind.Eng.Chem.Res., 36(6), 2494-2499, 1997

16 Joback K.G., Reid R.C., "Estimation of Pure-Component Properties from Group-Contributions", Chem.Eng.Commun., 57, 233-243, 1987

17 http://ddboverview.dortmunddatabank.com/