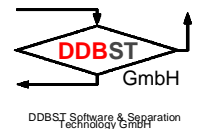


The Dortmund Data Bank (DDB) and the Integrated Software Package DDBSP II

J. Gmehling, K. Fischer, W. Cordes, H. Weinert, J. Rarey, J. Menke

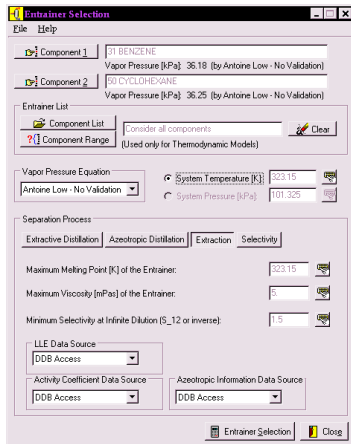


The DDB Software Package

To exploit the vast amount of experimental data from the Dortmund Data Bank for the design and simulation of chemical processes, a sophisticated software package was developed which is used by numerous chemical companies worldwide. As the Windows operating system became generally accepted in chemical industry, DDBST GmbH started to prepare Win9x/NT-versions of the different programs. The current release of the DDB Software Package (DDBSP 2000) offers nearly the full capability of the previous version plus many new features in form of re-engineered Windows software.

Process synthesis - Selection of Solvents for Extractive and Azeotropic Distillation, Extraction, ...

To employ the large number of phase equilibrium data stored in the Dortmund Data Bank for the selection of suitable solvents for azeotropic or extractive distillation a special program was developed.



The table below shows some of the solvents which were selected by this program for the separation of benzene from cyclohexane.

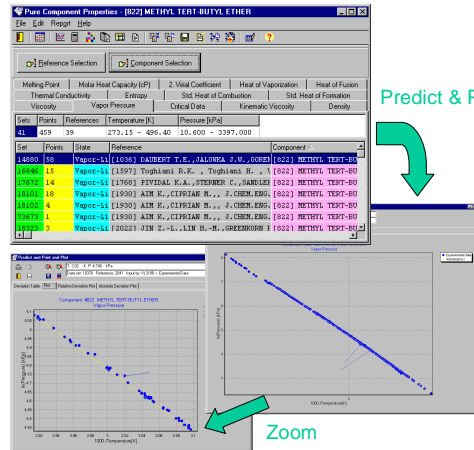
DDB No.	Name	Formula	P _v (kPa)
(1) 01	BENZENE	C6H6	36.18
(2) 09	CYCLOHEXANE	C6H12	36.25

DDB Selective Solvent (Entrainer)	No.	P _v (kPa)	T _m (K)	Viscosity (mPa·s)
470	DIPYRIMETHANE	1.999-000	296.26	1.821
1039	1,4-DIOXANE	1.246-002	336.45	2.382
106	1-METHYL-2-PYRROLIDONE	0.024-002	342.70	1.762
645	THIOUREA	32.38	376.34	0.429
092	1,4-DIOXANE	1.079-002	379.95	n.a.

Instead of utilizing factual data from the DDB it is also possible to employ predictive methods like UNIFAC. Numerous improvements, especially with respect to execution time and the presentation of results were implemented.

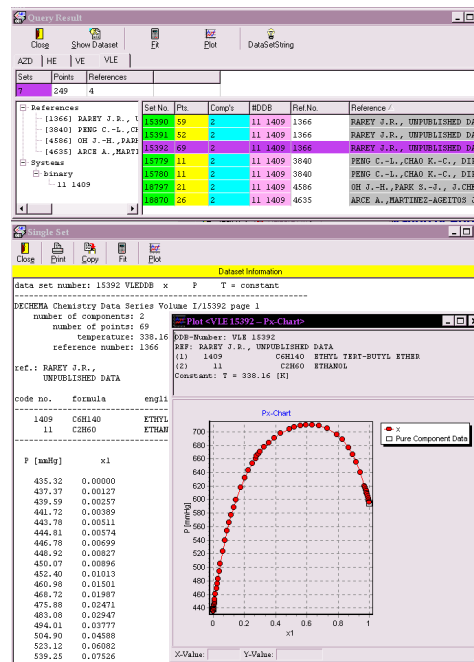
Retrieval, Estimation and Representation of Pure Component Data from DDB

The program *PureComponentProperties* is the graphical user interface of the DDB Pure Component Data Base. Besides giving access to more than 110000 data sets it features tabular and graphical data representation as well as comparison to theoretical correlations.



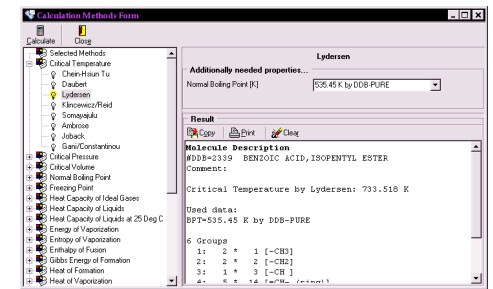
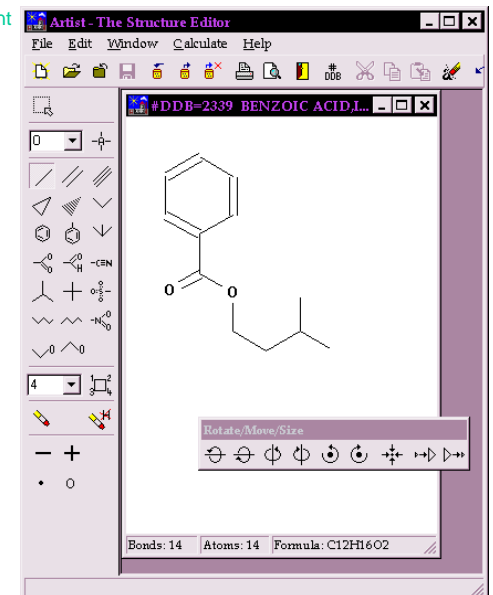
Retrieval, Estimation and Representation of Mixture Data from DDB

In the previous version of DDBSP, each mixture data bank has its own retrieval program. The newly developed Windows-version integrates all mixture data banks under one user interface. The different data sets are conveniently displayed in a treeview. Furthermore improved graphical representations are included. Future versions will utilize standard hierarchical data base servers for the DDB and employ an extended and unified format for data storage.



ARTIST - Property Estimation from Molecular Structure

Artist can be used to draw molecular structures or retrieve structures from a data base of more than 13000 components. Molecules can be automatically fragmented into structural groups for a large number of different group contribution methods. A multitude of different thermophysical and transport properties can be directly estimated at the click of the mouse-button. The graphical editor and the property estimation screen are shown below:



Construction of Residual Curves

Residual and boundary curves (or planes) can be constructed and displayed for inert or reactive systems with the help of the program *ResidualCurves*:

