DDBST
DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

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DDBSP 2016
Aspen Plus, PRO/II and UniSim Interface

Verifying Physical Property Parameters Prior to Process Simulation

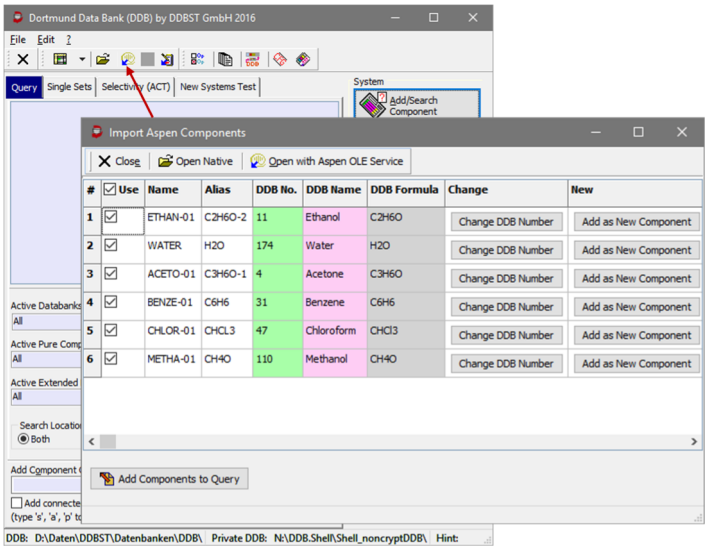
Accurate and verified physical property parameters are a prerequisite for the reliable simulation of chemical processes. Due to the importance of distillation processes this is especially true for parameters used to predict the vapor-liquid equilibrium behavior of liquid mixtures.

In order to verify these parameters against experimental data in the DDB, interfaces to Aspen Plus©, PRO/II© and UniSim© have been implemented in the DDB software package for the following properties:

	VLE	HPV	γ^{∞}	LLE	h^E	c_P^E $c_{P,mix}$	v^E v_{mix}	P^S	c_P^{id}	$c_{P\,L,V,S}$
Aspen Plus©	x	x	x	x	x	x	x	x	x	x
PRO/II©, UniSim©	x	x		x						

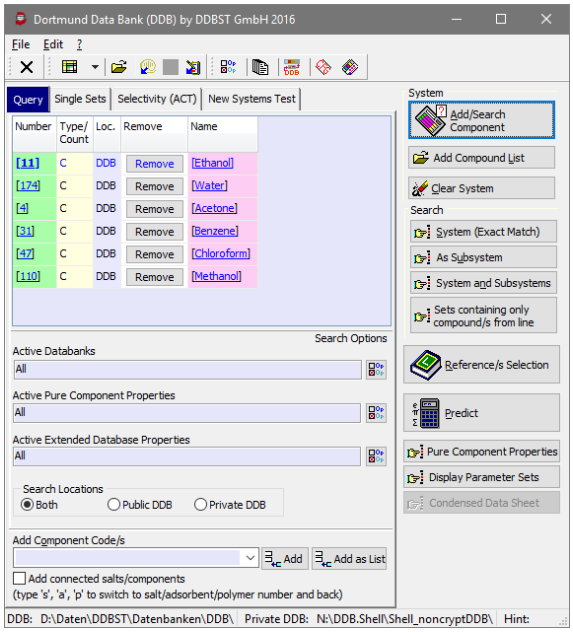
The list of properties will be extended to further data types. The typical workflow consists in case of Aspen Plus © of the following steps:

Start the program “Dortmund Data Bank” and select the Aspen-button to import the list of components from a simulation project (.bkp, .apw).

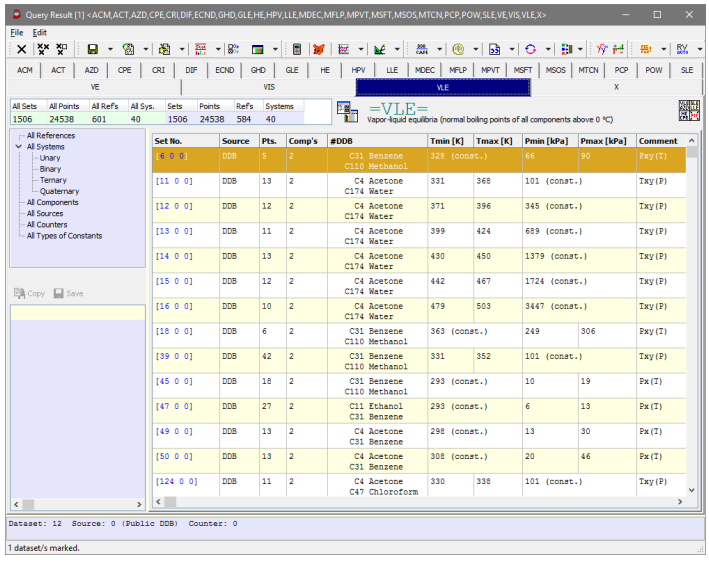


DDBSP is able to identify many components in the Aspen data bank. Manual identification or addition to the private DDB is mostly only required in case of user components.

The list of components can be added to the query:



“System and Subsystems” will yield all unary, binary, … systems in the DDB. The individual subsystems can be conveniently selected in the tree view on the left hand side of the query result dialog. In the next step, several data sets for a system of interest can be selected and data estimation is performed using the “Predict”-button (here for the case of isobaric data for the system acetone – water at 101.3 kPa).



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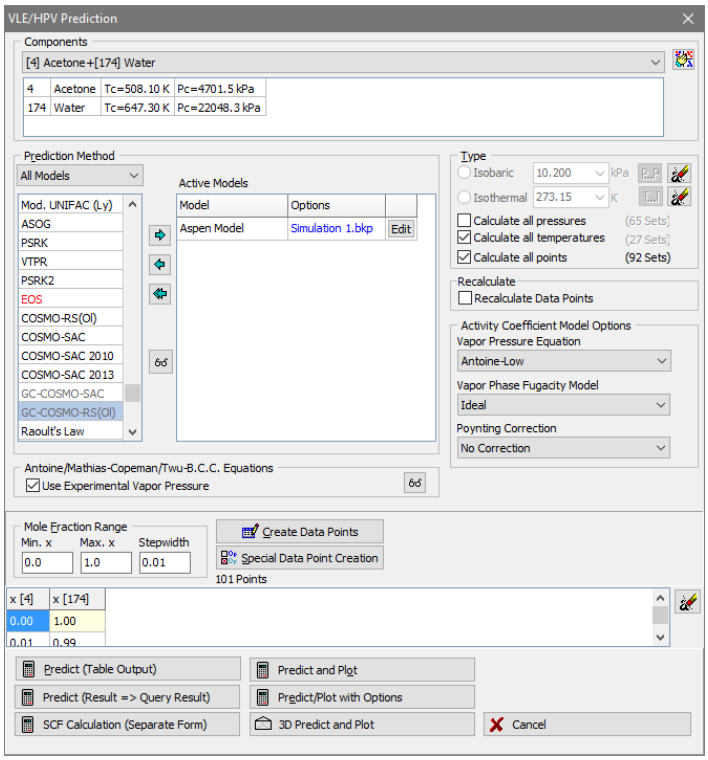
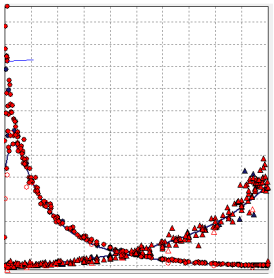
The "VLE/HPV Prediction" dialog offers a large variety of options. In the example on the left side the thermo package as defined in the Aspen project was selected. Note, that DDBSP remembers both the name of the Aspen project selected previously and the component cross-identification between DDB and Aspen.

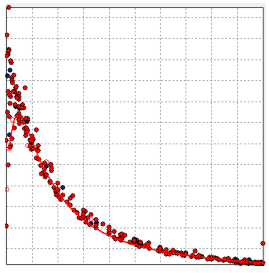
A typical first step is to use "Predict and Plot", which will automatically generate several graphical representations of the data and the estimated or calculated results.



Several typical plots are shown below. When moving the mouse cursor, a connecting line snaps to the next data point or curve and the numerical values, literature source, ... are displayed. It is possible to zoom into any part of the plot, remove data sets from the diagram and export data or graphics to other programs.

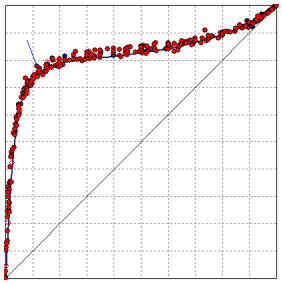


Activity coefficients vs. liquid composition

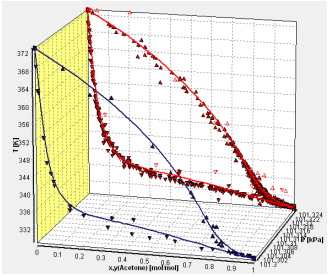


Separation factor vs. liquid composition

Numerous 2D and 3D representations of the data are available including pressure, vapor phase composition, activity coefficients, K-factors or separation factors as function of liquid mole or mass fraction. In the case of acetone-water, Aspen Plus (UNIQUAC using VLE-IG parameters) gives a good description of the experimental data.



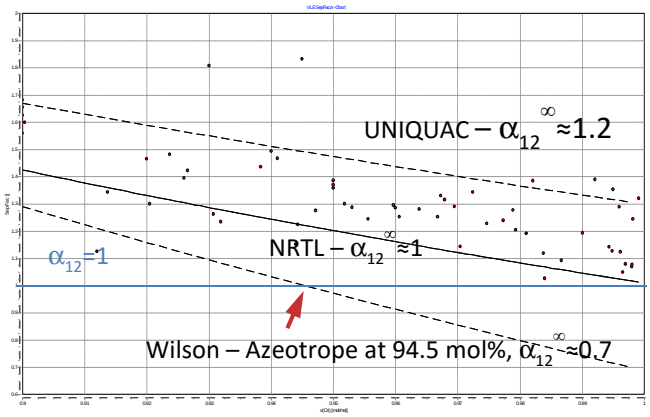
Vapor composition vs. liquid composition



Temperature vs. liquid composition and pressure

However, often the most important concentration range is that at high acetone content, where the separation factor approaches values a little above unity. If acetone of high purity is the desired distillate, nearly all separation effort lies in the top of the column where the separation factor is unfavorable. In this case, the correct description of the concentration range between 90 and 100 mol% of acetone is crucial. It is always stressed by simulator companies that the physical property parameters supplied should be used with care and may not be applicable in every case.

The following plots show this area with experimental data and calculations via Aspen Plus using different models using VLE-IG parameters.



The correct separation factor at infinite dilution is probably close to 1.16 based on activity coefficients at infinite dilution. Both the Wilson and NRTL parameter sets would lead to very unrealistic results in case of pure acetone as distillate. In other situations though, the parameters may be perfectly adequate.

The functionality described here is available as part of the Mixture Predict Add-On of DDBSP.

DDBSP thanks Aspen Tech, Schneider Electric Software and Honeywell for providing the required information and recommendations as well as co-workers of the University of Oldenburg for valuable feedback.