DDBST
Dortmund Data Bank
Software & Separation
Technology

Aspen Plus, PRO/II, UniSim and Simulis Interface 2025

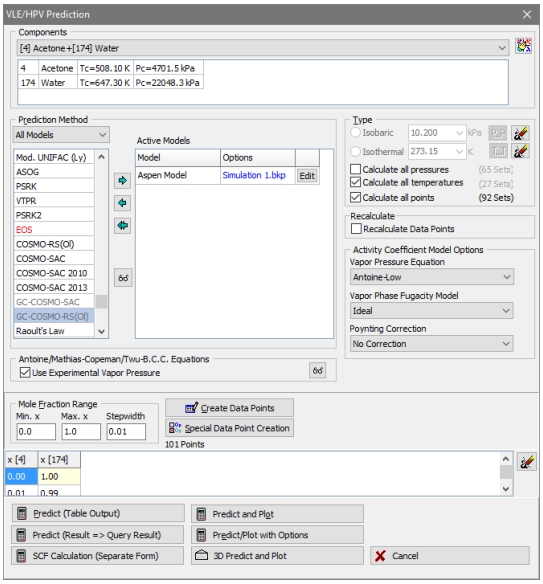
Verifying Physical Property Parameters Prior to Process Simulation

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, interfaces to the following process simulators have been implemented in the DDB software package.

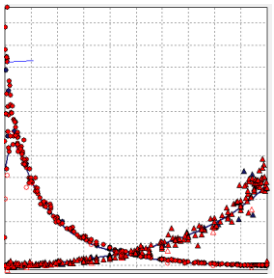
	VLE	HPV	γ^{∞}	LLE	h^E	c_P^E $c_{P,mix}$	v^E v_{mix}	P^S	c_P^{id}	$c_{P,L,V,S}$
Aspen Plus©	x	x	x	x	x	x	x	x	x	x
AVEVA™ Process Simulation	x	x	x	x	x	x	x			
PRO/II©	x	x		x						
UniSim©	x	x		x	x	x				
Simulis Thermodynamics©	x	x	x	x	x	x	x			

Information about parameter fitting capabilities with simulator thermodynamics can be found in the Regression Mix documentation.

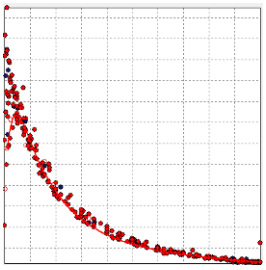
The "VLE/HPV Prediction" dialog offers a large variety of options. In the following example, the thermo package as defined in the Aspen project was selected. A typical first step is to use "Predict and Plot", which will automatically generate several graphical representations of the data and the estimated or calculated results.



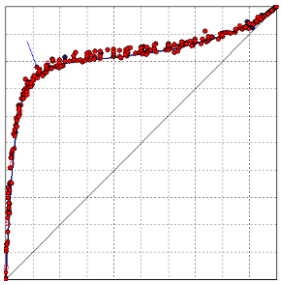
Numerous 2D and 3D representations of the data are available including pressure, vapor phase composition, activity coefficients, K-factors or separation factors as function of liquid mole or mass fraction. In case of acetone-water, Aspen Plus (UNIQUAC using VLE-IG parameters) gives a good description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



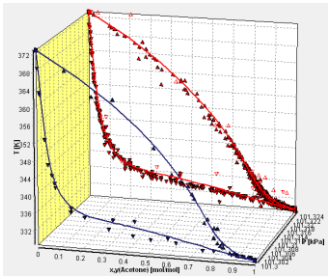
Activity coefficients vs. liquid composition



Separation factor vs. liquid composition

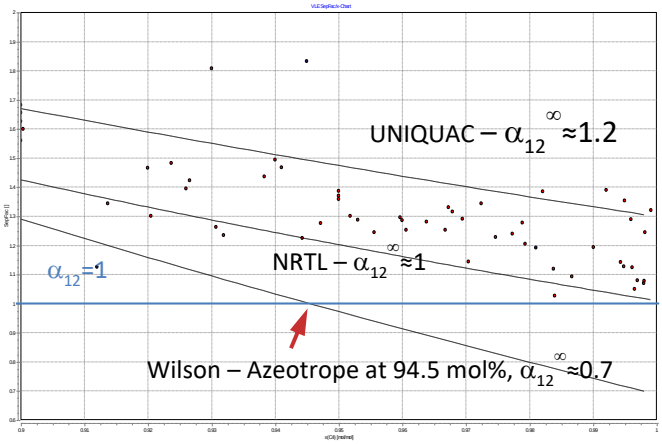


Vapor composition vs. liquid composition



Temperature vs. liquid composition and pressure

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. The following plot shows 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. Changes and errors are possible regarding all information.

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DDBST GmbH
HRB Oldenburg 2521
TAX ID: DE 117483996

Board of Executive Directors:
Dr. Andreas Grybat, Dr. Sven Horstmann,
Dr. Christian Ihmels, Dr. Bastian Schmid

Oldenburgische Landesbank AG
Account: 142 61648 00
Bank Code: 280 200 50
SWIFT-BIC: OLBO DE H2
IBAN: DE46 2802 0050 1426 1648 00