

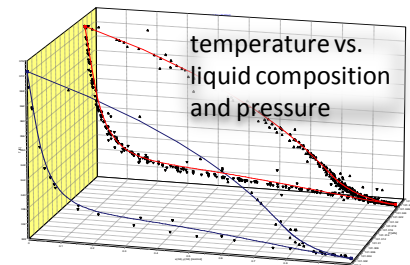
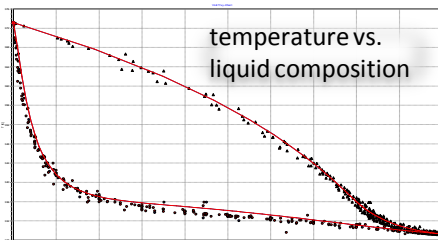
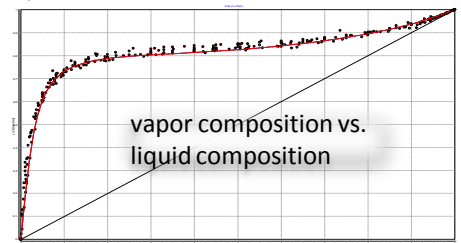
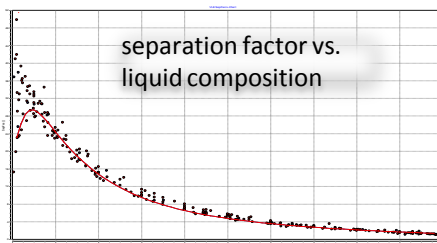
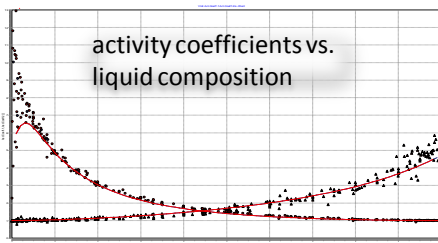
The “VLE/HPV Prediction” dialog offers a large variety of options. In the example on the left side the thermo package as defined in the Aspen project was selected.

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.

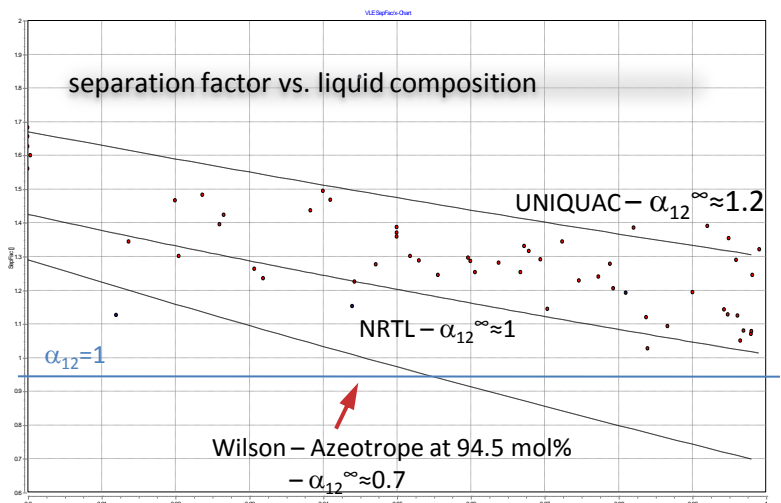
Numerous 2D and 3D representations of the data are available including pressure, vapor phase composition, activity coefficients, K-factors or separation factors as function of liquid mole or mass fraction. In the case of acetone-water, Aspen Plus (UNIFAC using VLE-IG parameters) gives a good description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



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.



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