What's New in *ChemSep*™ 8.2

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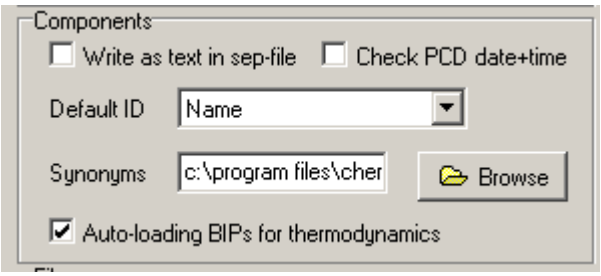
Harry Kooijman and Ross Taylor

The following features were added:

- Automatic loading of thermodynamic model parameters while loading components / changing models thereby simplifying the setting up a new simulation or CAPE-OPEN Property Package (COPP)
- A new property diagram option that can show any physical property as function of temperature, pressure, or composition
- Expander and compressor operations (as well as other flash types that include entropy)
- Use of multiple condensers / reboilers for Dividing Wall Columns (DWC)
- Calculation of Total Annualized Cost on flowsheet level

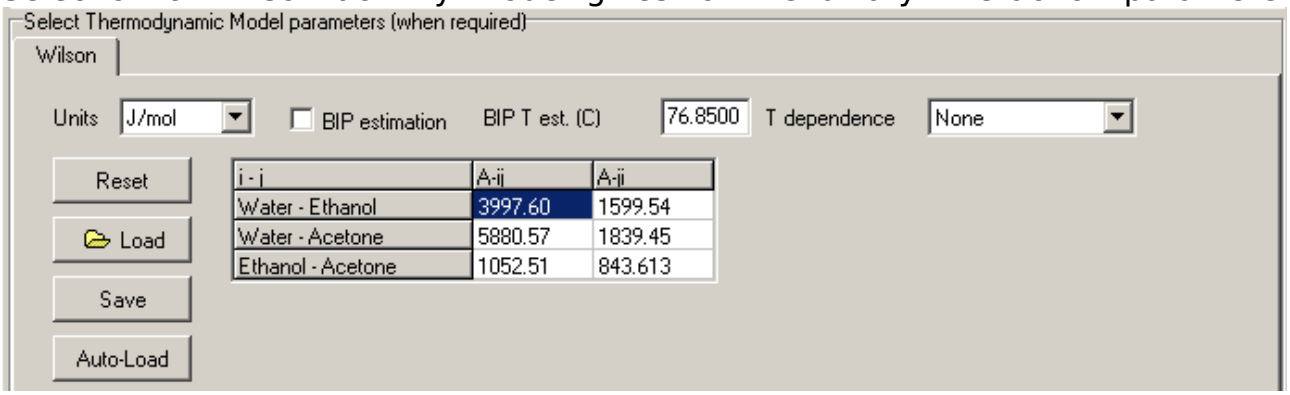
Automated Loading of Model Parameters

To facilitate a quicker setup of a new simulation, we added the automated loading of Binary Interaction Parameters (BIPs) for activity coefficient models, Equations of State, and Group Contribution methods. It is activated by default in the new version 8v2 but can optionally be switched off with the check box in the Components panel under Tools & Interface Settings:



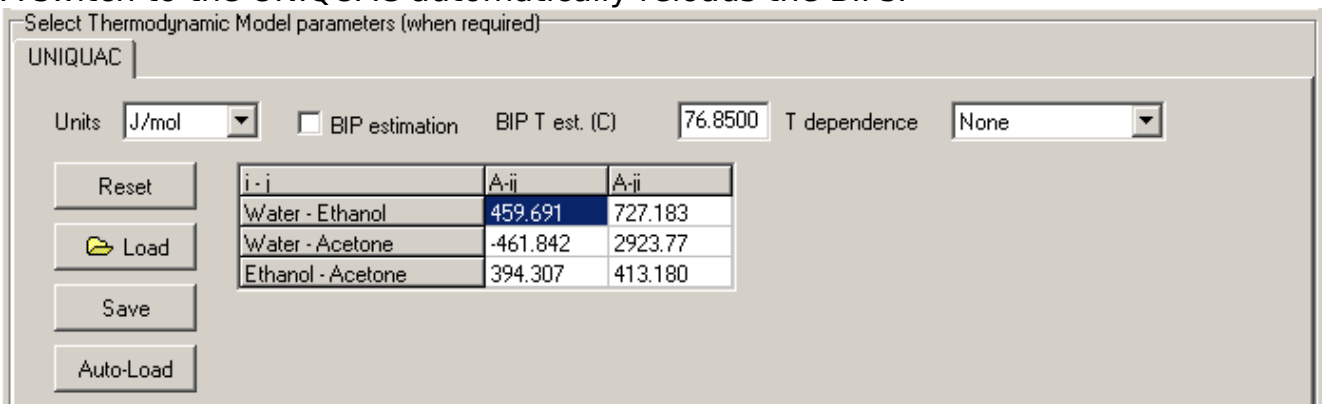
Settings are loaded from the configuration file chemsep.cnf that each user has in the C:\users\user.name\Application Data\ChemSep folder. When we now load Water, Ethanol, and Acetone as components and select DECHEMA as K-value model, a switch in activity coefficient model automatically reloads the respective BIPs for these components from the appropriate libraries.

Selection of Wilson activity model gives for the binary interaction parameters:



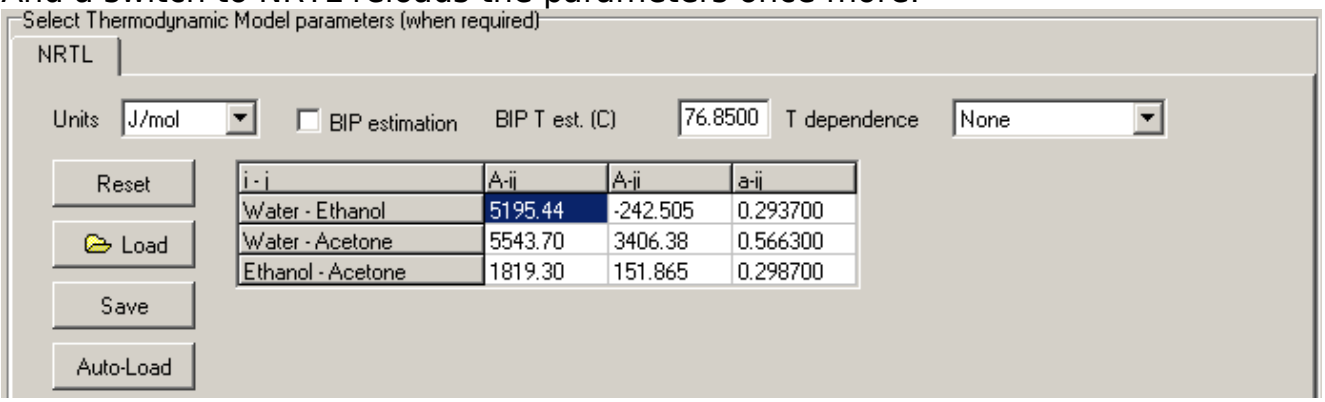
i - j	A-ij	A-ji
Water - Ethanol	3997.60	1599.54
Water - Acetone	5880.57	1839.45
Ethanol - Acetone	1052.51	843.613

A switch to the UNIQUAC automatically reloads the BIPs:



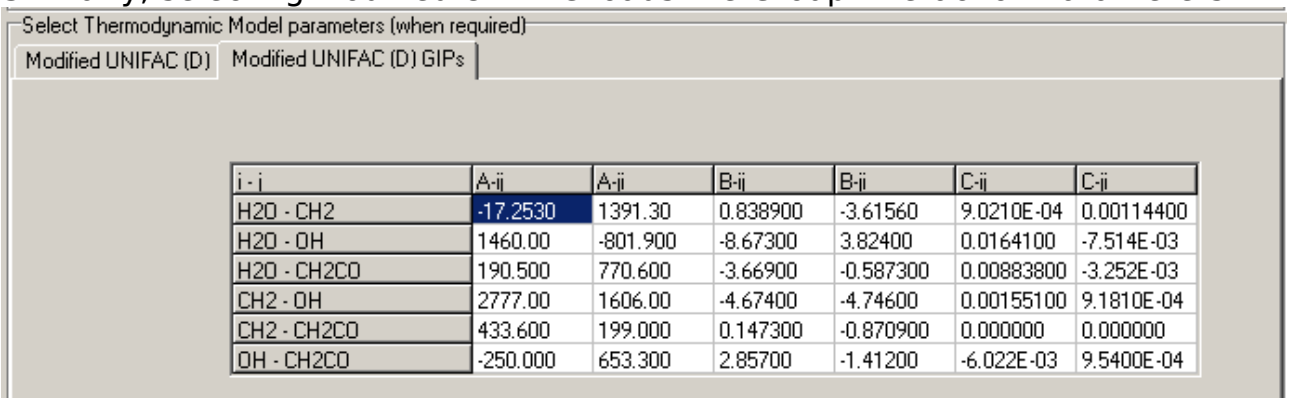
i - j	A-ij	A-ji
Water - Ethanol	459.691	727.183
Water - Acetone	-461.842	2923.77
Ethanol - Acetone	394.307	413.180

And a switch to NRTL reloads the parameters once more:



i - j	A-ij	A-ji	a-ij
Water - Ethanol	5195.44	-242.505	0.293700
Water - Acetone	5543.70	3406.38	0.566300
Ethanol - Acetone	1819.30	151.865	0.298700

Similarly, selecting Modified UNIFAC loads the Group Interaction Parameters:

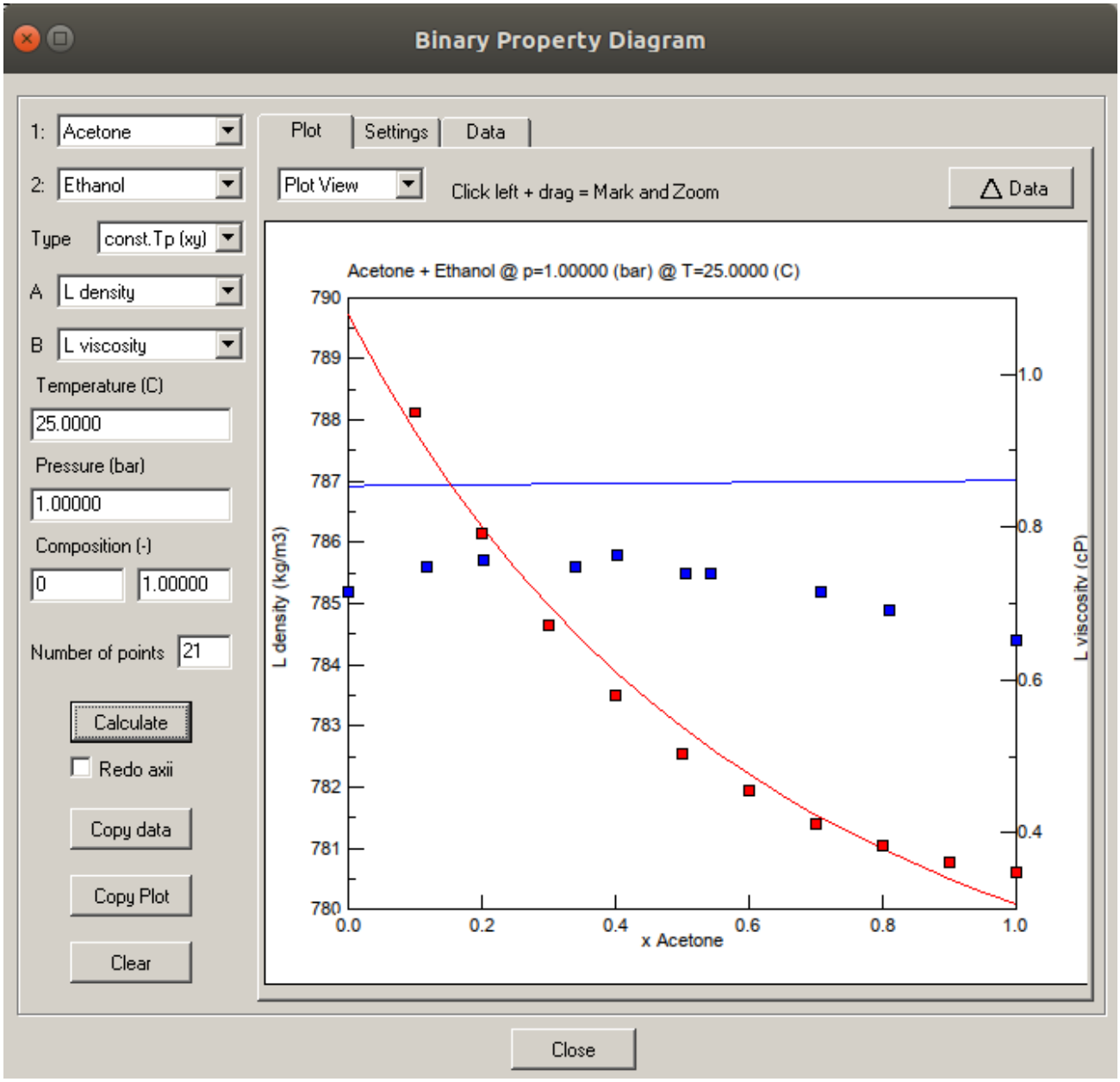


i - j	A-ij	A-ji	B-ij	B-ji	C-ij	C-ji
H2O - CH2	-17.2530	1391.30	0.838900	-3.61560	9.0210E-04	0.00114400
H2O - OH	1460.00	-801.900	-8.67300	3.82400	0.0164100	-7.514E-03
H2O - CH2CO	190.500	770.600	-3.66900	-0.587300	0.00883800	-3.252E-03
CH2 - OH	2777.00	1606.00	-4.67400	-4.74600	0.00155100	9.1810E-04
CH2 - CH2CO	433.600	199.000	0.147300	-0.870900	0.000000	0.000000
OH - CH2CO	-250.000	653.300	2.85700	-1.41200	-6.022E-03	9.5400E-04

(note that the GIPs are always loaded automatically irrespective of the checkbox)

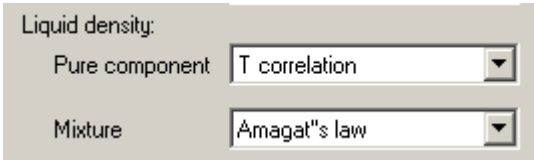
Binary Property Diagrams

To validate the modeling of physical properties we added the ability to generate a physical property diagram which allow a quick model comparison with available experimental data. One or two properties can be compared in one go. For example, plotting both the liquid density and viscosity for the Acetone/Ethanol system as function of composition is simple:



Clicking the property selection box for property A or B shows the list of available physical and thermodynamic properties that can be displayed: Vapor or liquid molar mass, density, viscosity, thermal conductivity, and heat capacity or the surface tension. Thermodynamic properties such as K-values, activity coefficients, fugacity coefficients, vapor pressures, Henry coefficient, volumes, enthalpies, and entropies also can be plotted. The plot can be done at constant {T,p} over a specified composition range, or at constant composition over a

specifed temperature or pressure range. Alternatively, the properties can be computed at VLE conditions at a fixed p or T. Note that to get the liquid densities accurate for this system, we need to select the component density to predicted from the pure component T correlation model and the Mixture model to Amagat's law:



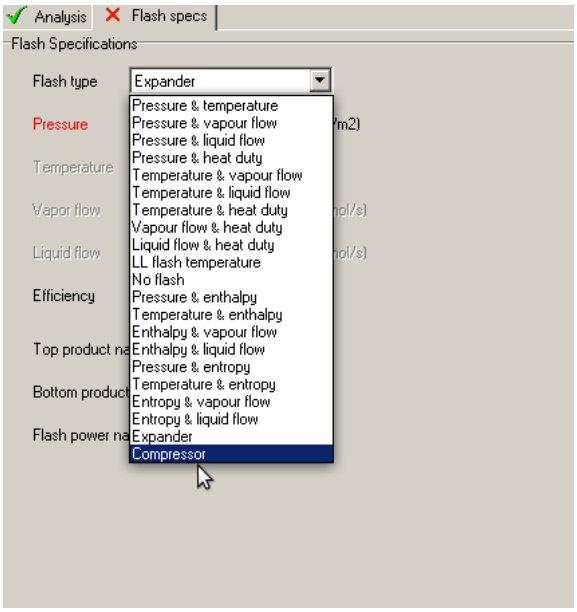
The data points shown in the diagram come from the literature. The data were entered in the comments panel of the sep-file as follows:

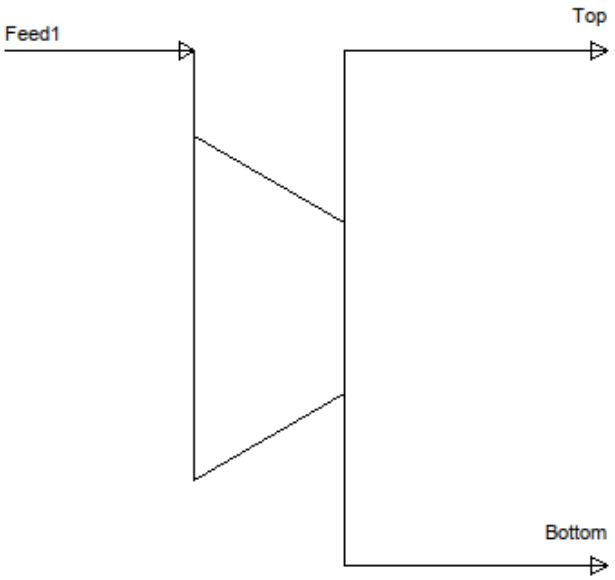
```
# I.-C.Wei, R.L. Rowley, J.Chem.Eng.Data, 29(3), 332-335, 1984
# 1 Acetone 2 Ethanol T=298.15K P=101.325kPa
# X Liq.Density
xA
0.0000  785.2
0.1163  785.6
0.2030  785.7
0.3396  785.6
0.4016  785.8
0.5058  785.5
0.5437  785.5
0.7084  785.2
0.8097  784.9
1.0000  784.4
~

# J. B. Irving, "Viscosity of binary liquid mixtures, a survey of mixture equations",
# NEL Report 630, National Eng Lab, East Kilbride, UK, 1977.
# X Liq.Viscosity
xB
1.000           0.349
0.900           0.362
0.800           0.383
0.700           0.412
0.600           0.455
0.500           0.504
0.400           0.579
0.300           0.671
0.200           0.792
0.100           0.950
0.000           1.180
```

This facilities easy import using the file button on the "data" panel. Note that there are two sets, one for property A which is the liquid density (in blue, using the left axis). This is indicated by the keyword "xA". The data for the second property B is liquid viscosity (in red, using right axis) and starts with the keyword "xB" (indicated there will be pairs of mole fractions and viscosities). Data sets are separated by "~".
After selecting the right order of the components and the temperature and pressure, values are computed and plotted by clicking the [Calculate] button. Adjustment to the axis were made on the "settings" panel. The color and property of the lines and symbols can be selected on that panel as well. When done, the diagram can be copied to be pasted in a text or presentation.

Expander & Compressors

The range of flash operations available in ChemSep has been extended to now include expanders and compressors as to be able to make use of ChemSep to perform flash calculations for the isentropic type of operations in flowsheets. These type of unit operations typically operate in the single (gas) phase regions and so do not separate phases. However, since ChemSep flash calculations always report two-phases, we need both a vapor and a liquid product stream:



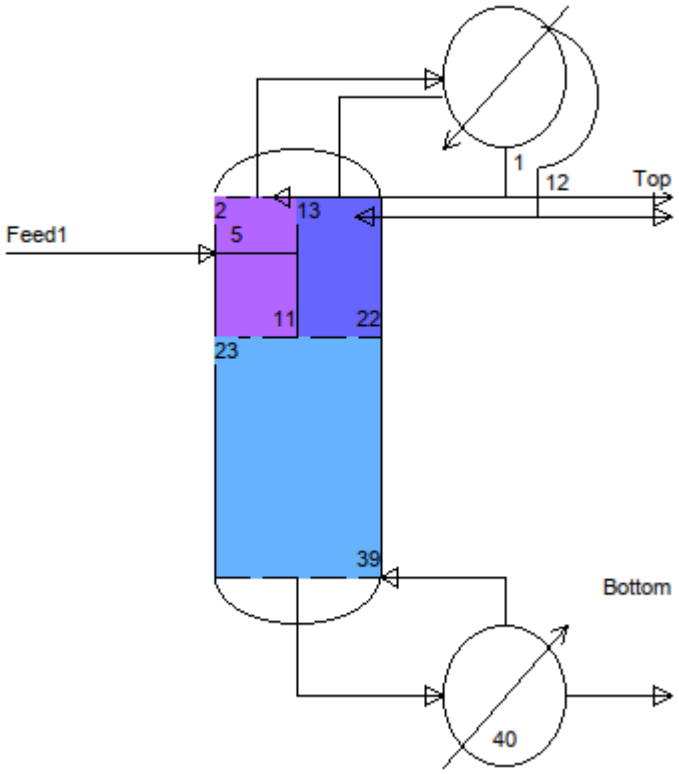


For example we can now compute the resulting temperature and physical properties for a 50-50mol% gas mixture of Acetone-Ethanol of 100 C that is compressed with a 75% isentropic efficiency from 1.1 to 2.0 bar:

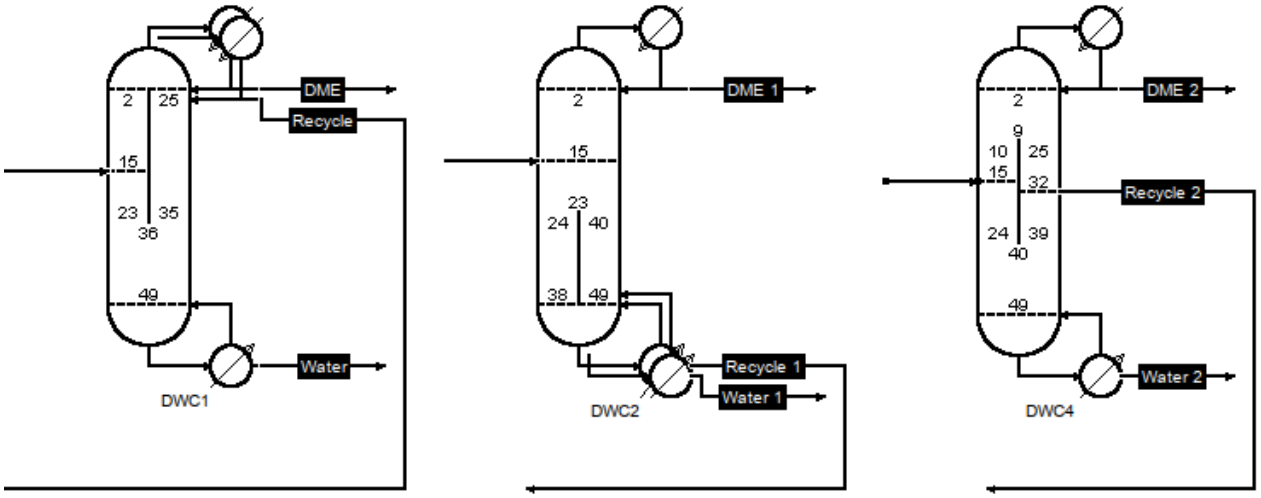
Stream	Feed1	Top	Bottom
Pressure (bar)	1.1	2.0	2.0
Vapour fraction (-)	1.0	1.0	0.0
Temperature (C)	100.0	131.0	131.0
Enthalpy (kJ/kmol)	5706	8329	0.0
Entropy (J/kmol/K)	21854	23511	-40440
Total molar flow (mol/s)	1000.0	1000.0 0.0	
Total mass flow (kg/s)	52.1	52.1	0.0
Vapour std.vol.flow (NCMD)	1.94e+6	1.94e+6	
Mole flows (mol/s)			
Acetone	500.0	500.0	0.0
Ethanol	500.0	500.0	0.0
Vapour:			
Mole weight (kg/kmol)	52.07	52.07	
Density (kg/m3)	1.846	3.1	
Std.density (kg/m3)	2.198	2.1981	
Viscosity (cP)	0.01026	0.01109	
Heat capacity (J/kmol/K)	82163	87116	
Thermal cond. (J/s/m/K)	0.02020	0.02351	

DWCs with extra Condensers and Reboilers

Extractive distillation processes can be simplified when the extractive column is combined with the solvent recovery into one column shell by using a dividing wall. Frequently this provides also significant economic benefits. An example of such an operation looks like this:



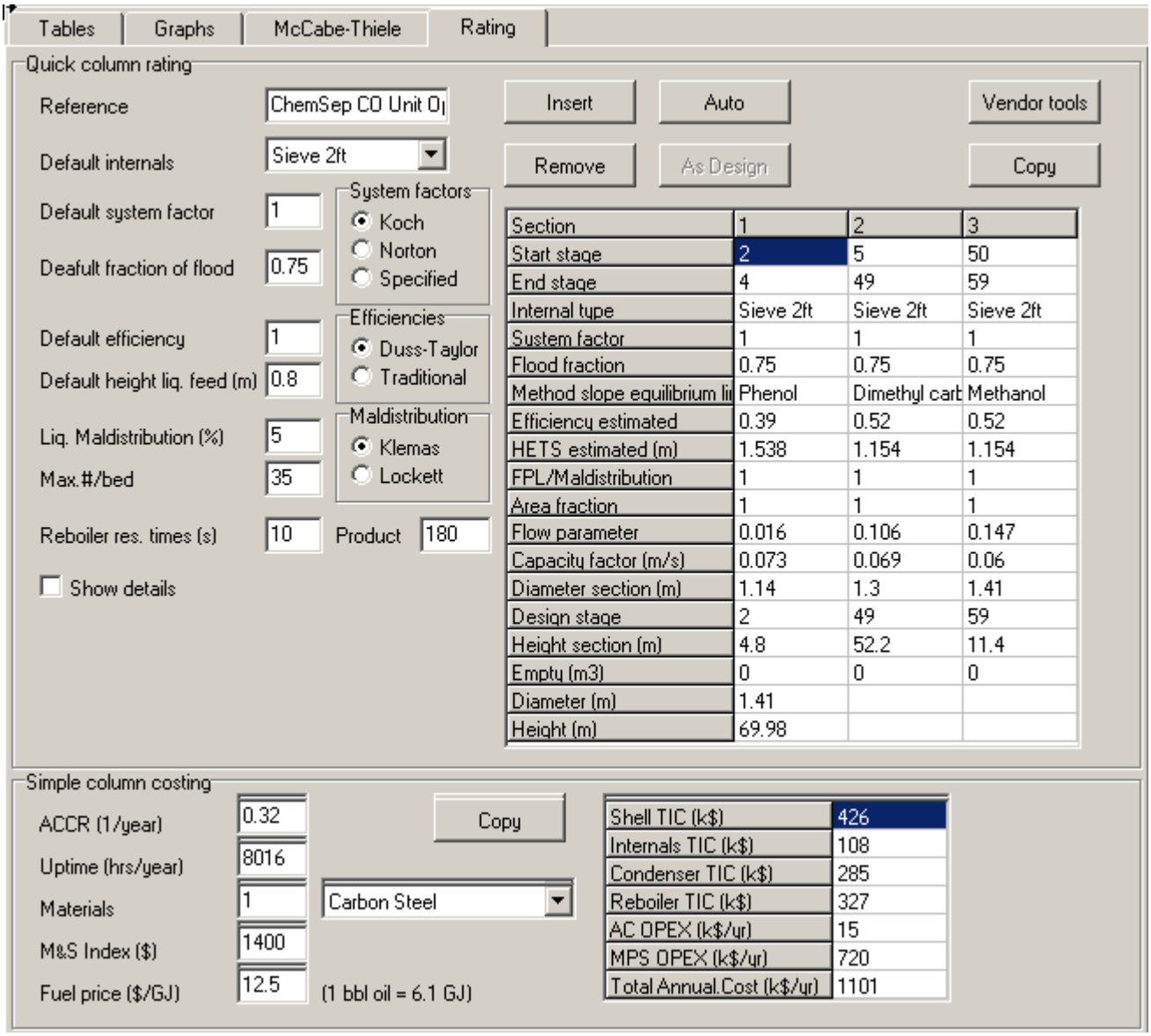
Note that in COCO flowsheets the wall and stage configurations are visualized on the column icons e.g. as seen below for various DWC arrangement for the separation of the ternary DiMethylEther / Water / Methanol mixture:



where the Methanol is recycled to the reactor inlet. Each extra condenser and extra reboiler gives the column an extra product stream and set of specifications.

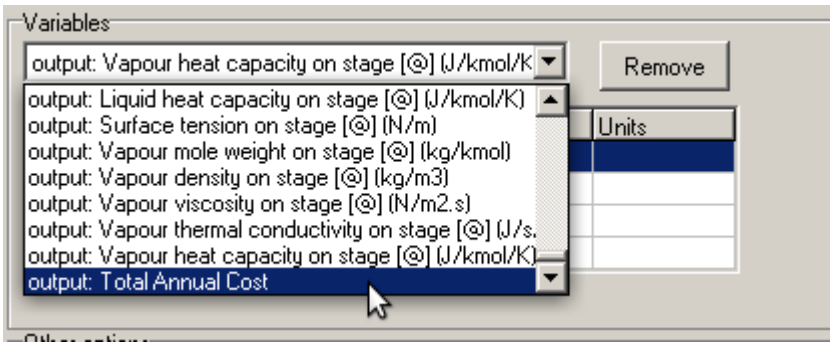
Calculation of Total Annualized Cost

The *Rating* panel in ChemSep includes improved cost calculation accounting for different levels of heating and/or cooling. That is, the different steam levels for reboilers and refrigerants for the condenser. The key parameters to computes the Total Annualized Cost (TAC) are calculated based on the uptime, cost index, general fuel price and materials of construction, all of which can defined as shown below:

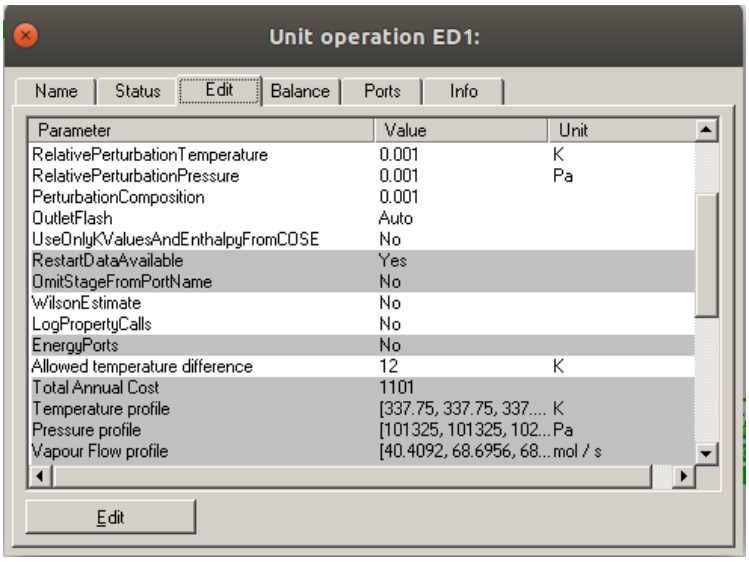


The resulting TAC can now also can used in the Parametric Studies to plot the cost as function of the reflux ratio, or any operating parameters e.g. the column pressure, or the column configuration e.g. the number of stages.

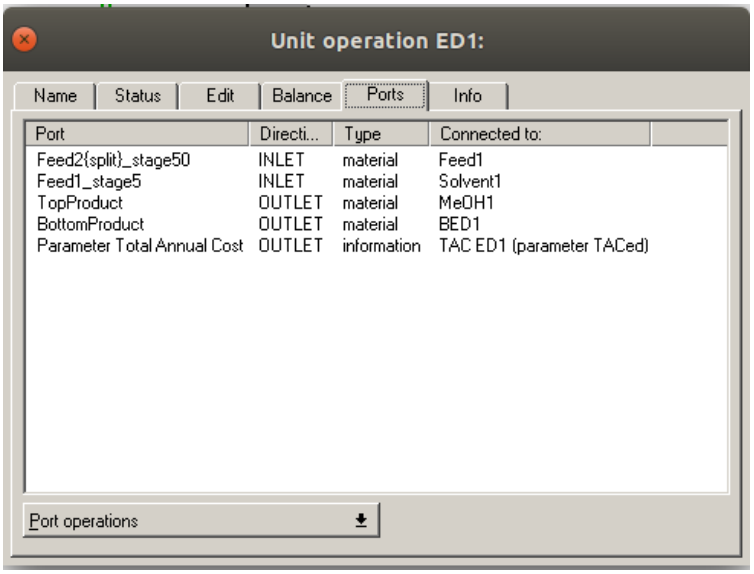
The TAC can also be selected as a CAPE-OPEN parameter and exported to a flowsheet. To do this select the CAPE-OPEN panel and assign the TAC as output parameter:



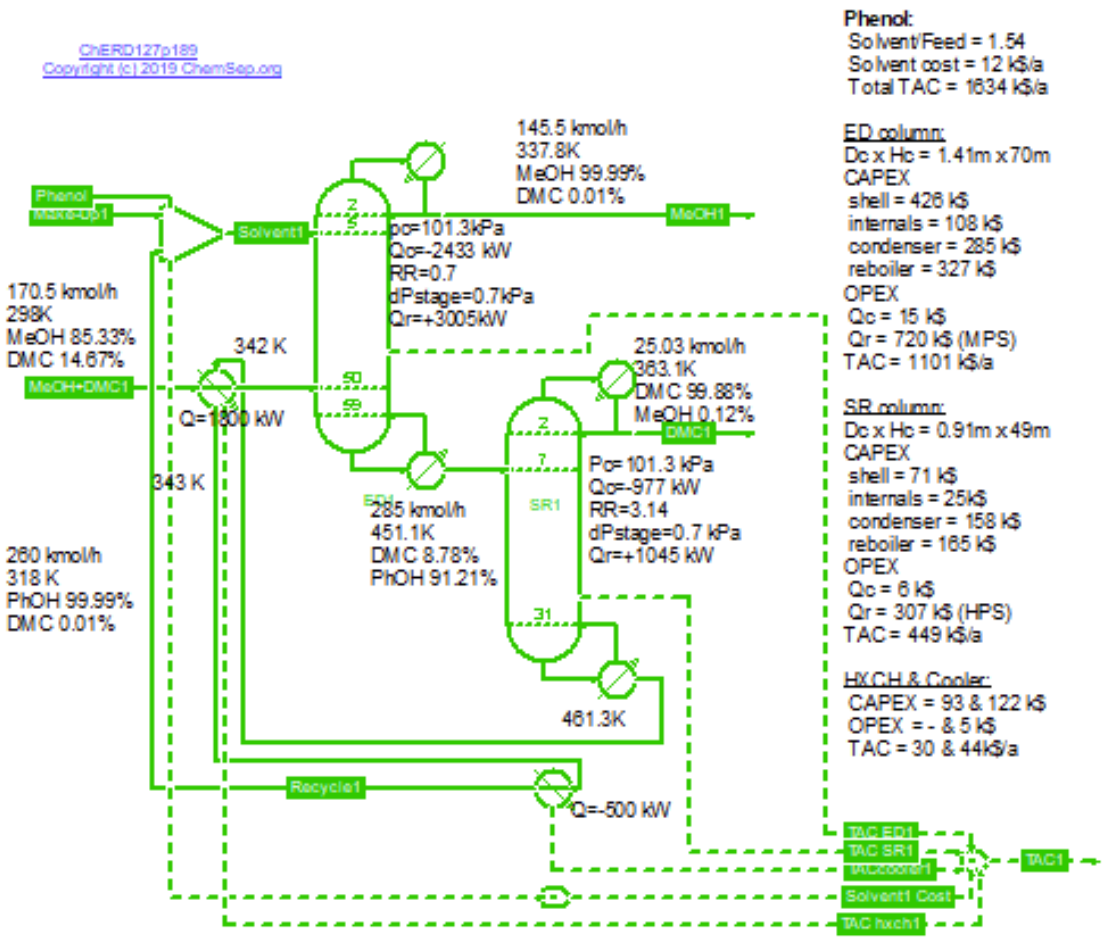
After which the TAC becomes visible as CAPE-OPEN parameter:



Now we can add an additional (information) port which we assign to the TAC:



On the flowsheet we add an information stream and hook it up to the TAC port. In that manner we can add all the TAC's for the various pieces of equipment in a flowsheet and compute an overall TAC, see the example for the Extractive Distillation of the azeotropic DMC/Methanol mixtures on our web site: http://chemsep.org/downloads/data/MeOH-DMC_ChERD127p189.fsd



Note that we computed the TAC values for the heat exchangers by using sub-flowsheets as to maintain readability.

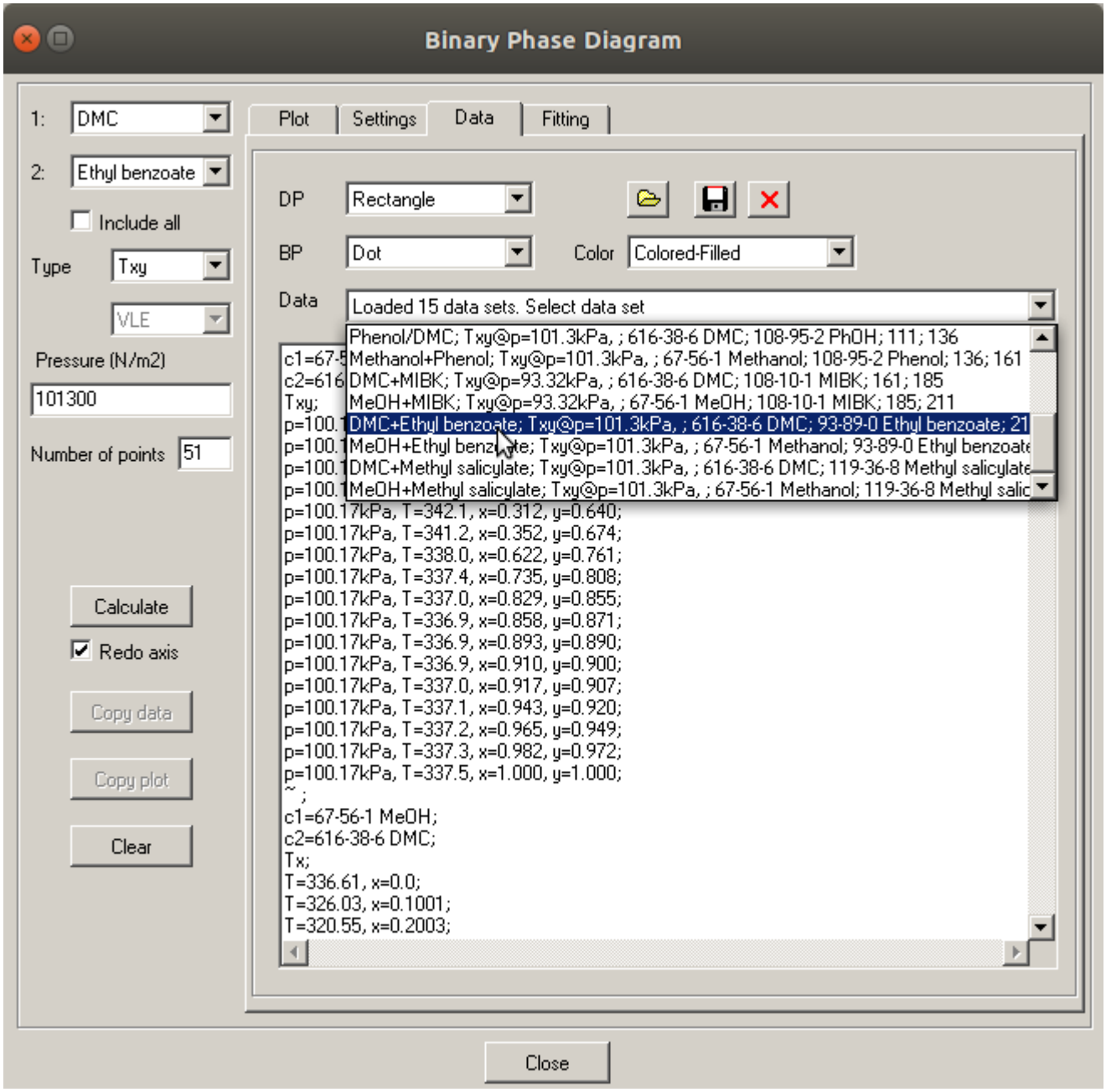
Fitting multiple VLE data sets

When VLE data is entered in multiple sets on the comments section and separated with ~, then these multiple data sets can also be automatically imported on the data panel of the binary phase diagram. The keywords c1= and c2= followed by the CAS numbers of the respective compounds enables the simultaneous fitting of systems with different components:

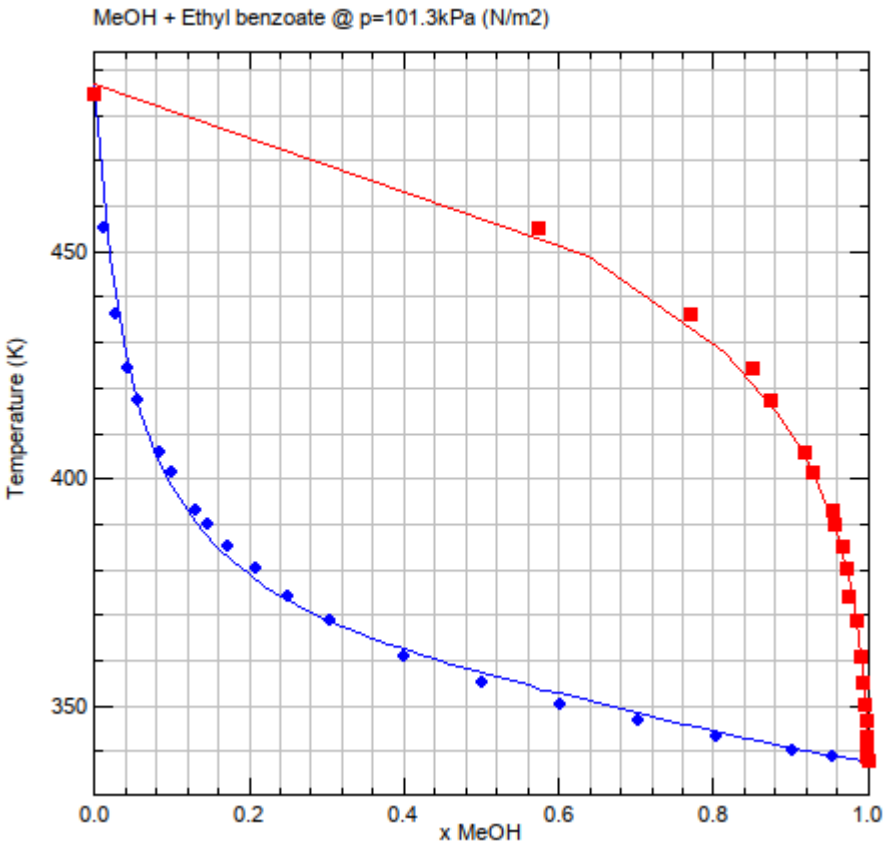
```
ref=ChERD127p189
c1=616-38-6
c2=119-36-8
title=DMC + Methyl salicylate
Txy@p=101.3kPa
494.3   0       0
463.3   0.043   0.522
455.7   0.06    0.62
448.6   0.077   0.693
441.9   0.096   0.753
438.7   0.106   0.778
433.3   0.125   0.816
420.2   0.183   0.888
412.1   0.231   0.921
406.3   0.273   0.94
402.0   0.309   0.952
395.4   0.374   0.967
390.4   0.433   0.976
382.7   0.547   0.986
375.0   0.696   0.994
373.9   0.72    0.994
371.4   0.77    0.996
368.9   0.828   0.997
366.8   0.886   0.998
365.4   0.934   0.999
363.1   1       1
~

ref=ChERD127p189
c1=67-56-1
c2=119-36-8
title=MeOH + Methyl salicylate
Txy@p=101.3kPa
494.3   0       0
427.5   0.024   0.832
402.2   0.052   0.925
391.3   0.072   0.947
375.3   0.128   0.978
371.1   0.156   0.98
365.5   0.204   0.987
361.1   0.264   0.99
357.5   0.336   0.992
355.2   0.396   0.994
352.2   0.472   0.995
351.4   0.496   0.996
350.2   0.532   0.996
348.7   0.58    0.997
346.5   0.656   0.998
345.1   0.708   0.998
342.6   0.8     0.998
342.2   0.816   0.998
339.6   0.92    0.999
338.7   0.952   0.999
337.8   1       1
~
```

Note that the keywords Txy and pxy indicate the type of VLE data. They are followed by the conditions at which the data were measured; e.g. Txy@p=101.3kPa states that the measurements were obtained at a constant pressure of one atmosphere. For measurements at equal pressure we use, for example, pxy@T=30C to indicate data measured at 30 degrees Celcius. Note that the units of measure are optional and in the above data the default temperature units was set to Kelvin. To enable the selection of a data-set we need to assign a title. It is possible to enter dozens of data-sets, which facilitates the fitting of group interaction parameters. Optional keywords are “ref=” and “url=” that in the future will be used to enable linking to original sources and documentation.

After all the data sets were entered and imported, each individual data sets can be selected for plotting by using the data pull down menu on the data panel:



After the selection of the data the VLE can be computed and plotted by pressing the Calculate button:



Clicking the right mouse button enables changing the graph settings directly without having to switch to the settings panel. We can plot Txy or pxy for multiple conditions but only for one system of compounds. However, it is possible to export a plot to file and to then import it again over plot with a different system. For this we need to ensure the T or p ranges are set to cover the same range so as to ensure that the axes properly align.

Miscellaneous Updates

Version 8.2 includes many small improvements such as:

- PPR78 equation of state
- Improved prediction methods for petroleum fractions
- Bug fixes in the automated assignment of key compounds for the McCabe-Thiele diagrams
- Bug fixes in the parametric study
- Bug fixes liquid Cp & viscosity errors for supercritical compounds
- Bug fixes for handling Group Contribution Methods

Availability

As always, *ChemSep* Lite is available free from http://chemsep.com.