

What's New in ChemSep™ 7.2

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In this document we identify and describe the most important new features in **ChemSep** in release 7.2. The following features are discussed:

1. **New: writing of Group Contribution information to the sep-file** 2
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ChemSep Lite is available for free from <http://chemsep.com>.

The screenshot shows the ChemSep software interface. The main window is titled 'ChemSep (TM) (CAPE-OPEN) - Dehydrator'. It has a menu bar (File, Edit, Check, Tools, Help) and a toolbar. The left sidebar contains a tree view with categories like 'CAPE-OPEN', 'Title', 'Components', 'Operation', 'Properties', 'Reactions', 'Feeds', 'Specifications', 'Analysis', 'Pressures', 'Heaters/Coolers', 'Efficiencies', 'Column specs', 'Results', 'Tables', 'Graphs', 'McCabe-Thiele', 'Rating', 'Units', 'Solve options', and 'Paths'. The 'Rating' panel is active, showing 'Quick column rating' options for Reference, Default internals, Default system factor, Default fraction of flood, Default efficiency, and Sump residence times. A red arrow points to the 'Export' button in the 'Rating' panel. A smaller window titled 'SULCOL 3.2.20' is overlaid, showing a table of flow data and packing parameters for two sections.

Sec	Packing	Diam [mm]	Fluid Data	Packing Design	Packing-Type	Height [m]	NTS req.	HETP [mm]
1	4190	S1 stages 2(max)/2	Packing1	M250.Y	3.990	0.0	0	
Flows								
	G	L	ρ G	ρ L	σ	η L	η G	G
	Cap [%]	F-F [Pa ^{0.5}]	Liq. load [m ³ /m ² h]	$\Delta p / \Delta z$ [mbar/m]	hl [%]	dp [mbar]		
Top	54450.1	13489.8	0.093	986.20	67.59	0.526	0.0106	62.1
Btm	40939.1	13509.9	0.093	986.21	67.62	0.522	0.0106	48.4
Text Section 1 System factor 1.00 [X] Geom. Details								
2	3950	S2 stages 4(max)/2	Packing2	M250.Y	2.940	2.0	1470	
Flows								
	G	L	ρ G	ρ L	σ	η L	η G	G
	Cap [%]	F-F [Pa ^{0.5}]	Liq. load [m ³ /m ² h]	$\Delta p / \Delta z$ [mbar/m]	hl [%]	dp [mbar]		
Top	40340.6	129584.9	0.096	981.14	57.04	2.320	0.0110	84.0
Btm	38965.3	65074.3	0.098	980.71	56.86	2.304	0.0110	68.6
Text Section 2 System factor 1.00 [X] Geom. Details								
Total sections		Column data						
2	p top	mbar	146.70	Δp total	mbar	22.35		

ChemSep Rating Panel with export to Sulzer chemtech tool 'SuCol'

New: writing of Group Contribution information to the sep-file

In older versions of *ChemSep* the Group Contribution (GC) information for UNIFAC, modified-UNIFAC, ASOG, PPR78, and PSRK methods was read only during run-time from various library files (with the IPD extension). This forced people to always use the standard determined Group contribution Interaction Parameters (GIP's). In some specific applications this may be too restrictive, as slightly adjusted GIPs can provide much better fits. In the new version the groups are automatically determined (from the component information) and the GC data and GIPs are loaded from the libraries such that the values used at run-time may be altered where desired. For example for Methanol/Acetone/Water/Etanol mixture the following input panels are visible:

The screenshot shows the ChemSep (TM) - n-mawe.sep software interface. The main window displays the 'Thermodynamic Models' section with various settings for K-value, Equation of state, Activity coefficient, Vapour pressure, and Enthalpy. Below this, the 'Select Thermodynamic Model parameters (when required)' section is active, showing a table of UNIFAC GIPs.

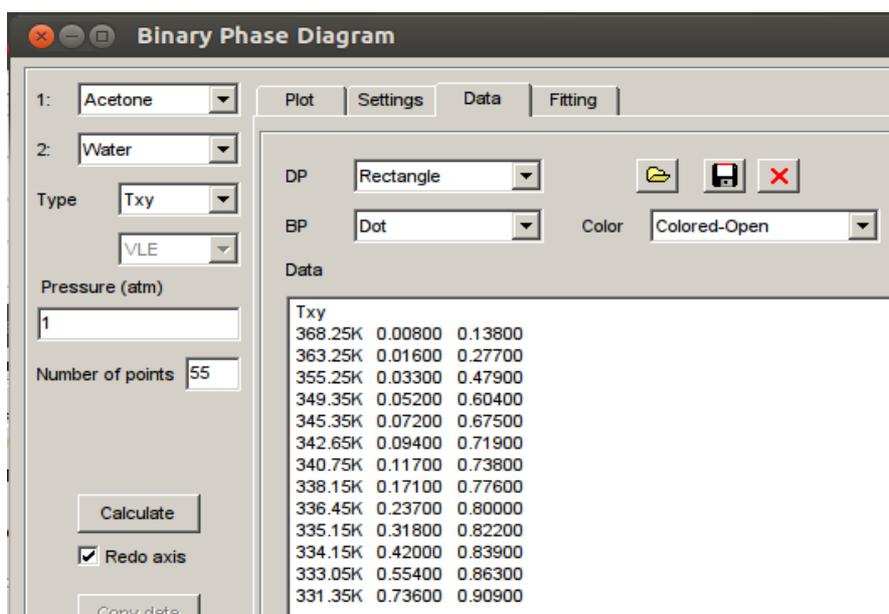
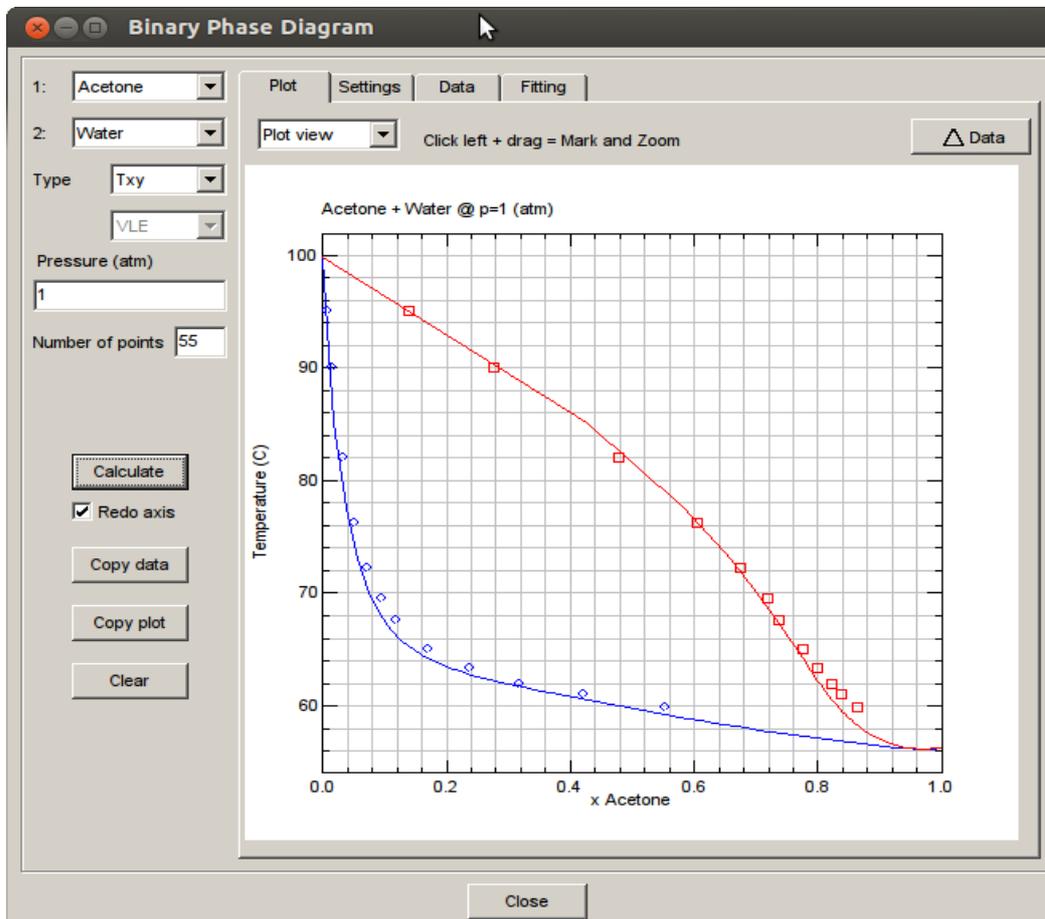
Sub-Group	Main-Group	R-i	Q-i
CH3OH	CH3OH	1.43110	1.43200
CH3	CH2	0.901100	0.848000
CH3CO	CH2CO	1.67240	1.48800
H2O	H2O	0.920000	1.40000
CH2	CH2	0.674400	0.540000
OH	OH	1.00000	1.20000

This is a close-up view of the 'Select Thermodynamic Model parameters (when required)' section, specifically the 'UNIFAC GIPs' tab. It displays a table of interaction parameters for various component pairs.

i - j	A-ij	A-ij
CH3OH - CH2	16.5100	697.200
CH3OH - CH2CO	23.3900	108.700
CH3OH - H2O	-181.000	289.600
CH3OH - OH	249.100	-137.100
CH2 - CH2CO	476.400	26.7600
CH2 - H2O	1318.00	300.000
CH2 - OH	986.500	156.400
CH2CO - H2O	472.500	-195.400
CH2CO - OH	164.500	84.0000
H2O - OH	-229.100	353.500

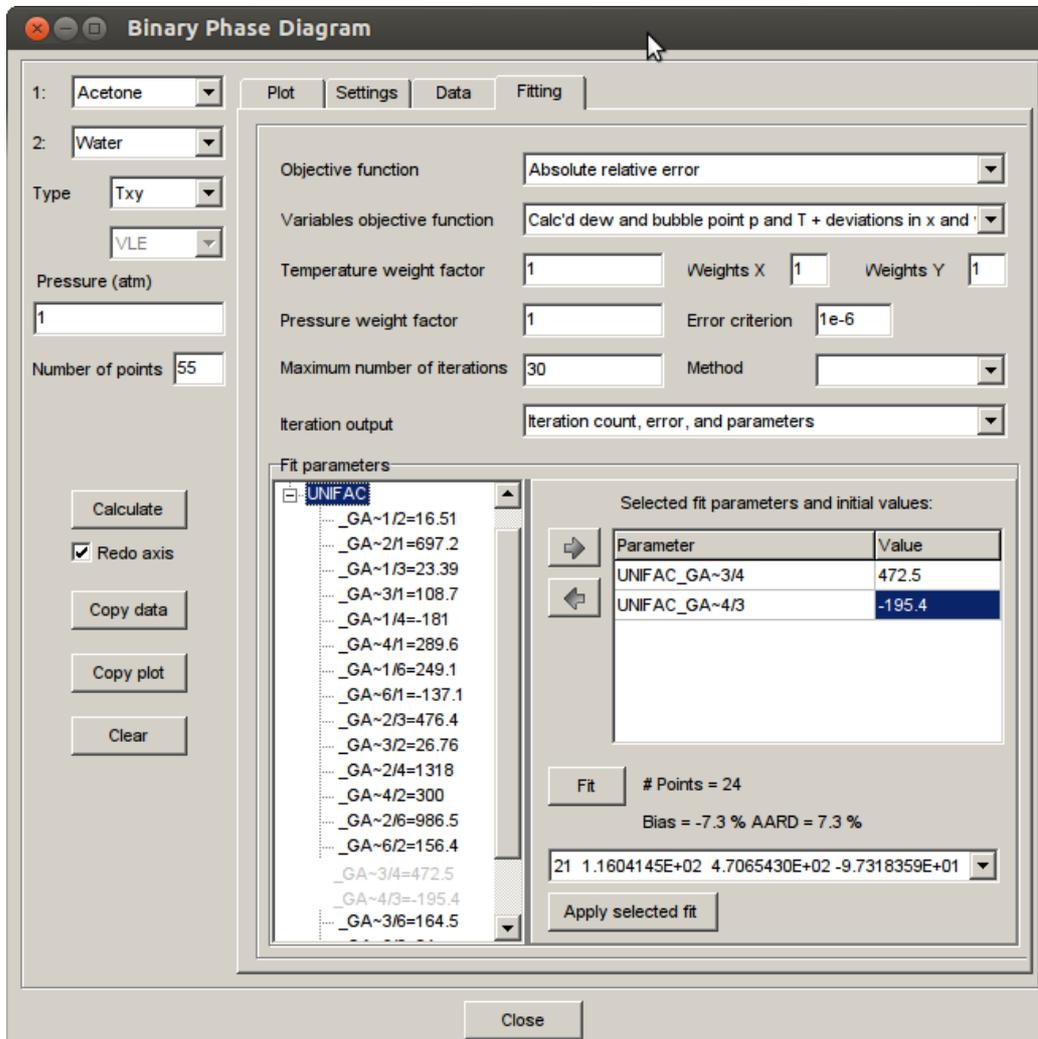
New: fitting of Group Interaction Parameters in GC methods

Because the GC data and interaction parameters are stored in the sep-file, they can now also be fitted on the hand of available Vapor-Liquid-Equilibria data. To illustrate this, we use the binary phase diagram option to draw the Txy-diagram for Acetone-Water. We added VLE data at 1 atm in this diagram from W. Reinders, C.H. de Minjer, *Recl.Trav.Chim.Pays-Bas* **66** (1947) pp. 573-604 by entering this on the data panel:



(see <http://www.ddbst.com/en/EED/VLE/VLE%20Acetone%3BWater.php>).

On the fitting panel we see the GUI already determined the datapoints and we only need to select the group interactions we want to refit. Here we selected the the groups for the keton (3) and Water (4).



One of the fitted parameters is very close, the other is about half the library value. Pressing the [Apply selected fit] button allows to immediately use these new parameters (the user is prompted whether he wants to update the diagram to visualize the improvements). In this case there is not much change.

New Rating Panel

The new ChemSep now has a simplified rating panel with which a column design is made. It can handle trayed and packed columns using different tray and packing types with different tray spacings and specific packing area's. The design automatically assigns different sections in the column from feed and draw locations. The resulting column is then designed with a different diameter for each section, where there is also height allocated for feeds, distributors, and column swages as well as a bottom sump to provide reboiler and product holdup. As such, the rating panel allows users to interchange column internals in a quick manner to minimize column cost on the hand of a simple TAC-type cost estimate.

For example, the dehydrator column in the MEG flowsheet looks like:

The screenshot displays the ChemSep (TM) (CAPE-OPEN) - Dehydrator interface. The main window shows a process flowsheet with a distillation column and associated vessels. The 'Rating' panel is open, showing the following data:

Section	1	2
Sieve size	2	4
Start stage	3	7
End stage	3	7
Internal type	M252Y	M250Y
System factor	1	1
Flood fraction	0.75	0.75
Method slope equilibrium	Ethylene glycol/Water	
Efficiency estimated	0.21	0.44
WEIS estimated (m)	2.068	0.916
Flow parameter	0.002	0.042
Capacity factor (m/s)	0.126	0.088
Diameter section (m)	3.99	4.24
Design stage	2	7
Height section (m)	4.2	3.57
Diameter (m)	4.24	
Height (m)	10.38	

MEG	DEG	TEG	TTEG+	Unit
0.201938	0.01	0.01	0.019	bar
0.206	117.058	160.814	170.807	°C
0.7762	5.47540	0.205513	0.0153045	ton/h
0.00020978	0	0	0	
0.99979	2.8420e-20	1.18991e-13	1.01506e-22	
1.01572e-11	0.30009	0.00105669	4.76697e-09	
3.51574e-11	0.00101137	0.004617	0.440281	
7.37472e-19	1.14602e-09	0.00402354	0.559719	
0	0	0	0	
1.381	108.112	148.857	157.344	
0.036	106.177	150.261	172.01	

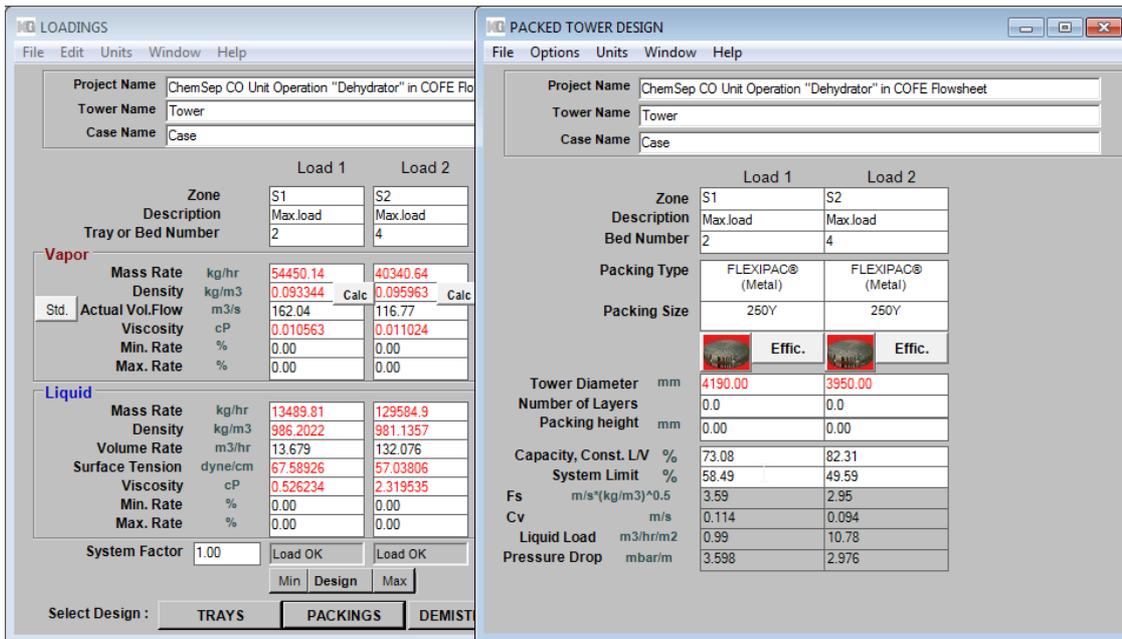
The 'Simple column costing' table is also visible:

ACCR (1/year)	0.32	Shell TIC (k\$)	461
Uptime (hrs/year)	8160	Internals TIC (k\$)	338
Materials	1	Condenser TIC (k\$)	1643
M&S Index (\$)	1400	Reboiler TIC (k\$)	1477
Fuel price (\$/GJ)	8	Condenser OPEX (k\$/yr)	74
		Reboiler OPEX (k\$/yr)	4770
		Total Annual Cost (k\$/yr)	6098

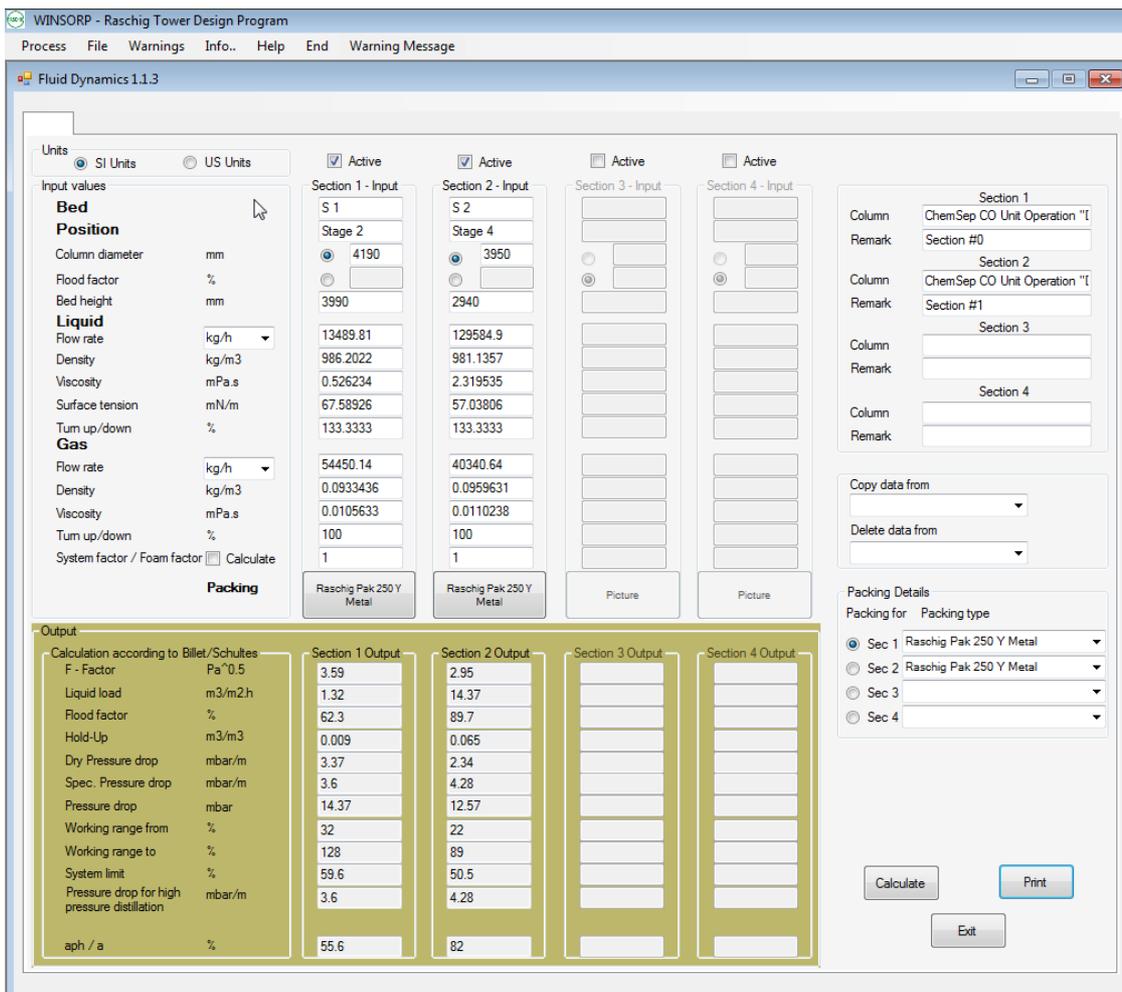
The rating is done by capacities calculated on the Wallis model. Of course, for industrial designs the rating tool of the tray/packing vendor should be used. In ChemSep we have made this easier by allowing an export to the vendor tools. Currently three tools are supported:

- 'KG-Tower', by Koch-Glitsch
- 'SolCol', by Sulzer chemtech
- 'Winsorp', by Raschig GmbH

On page 1 you can see the export to SulCol. The export to KG-Tower and WinSorp are shown below.



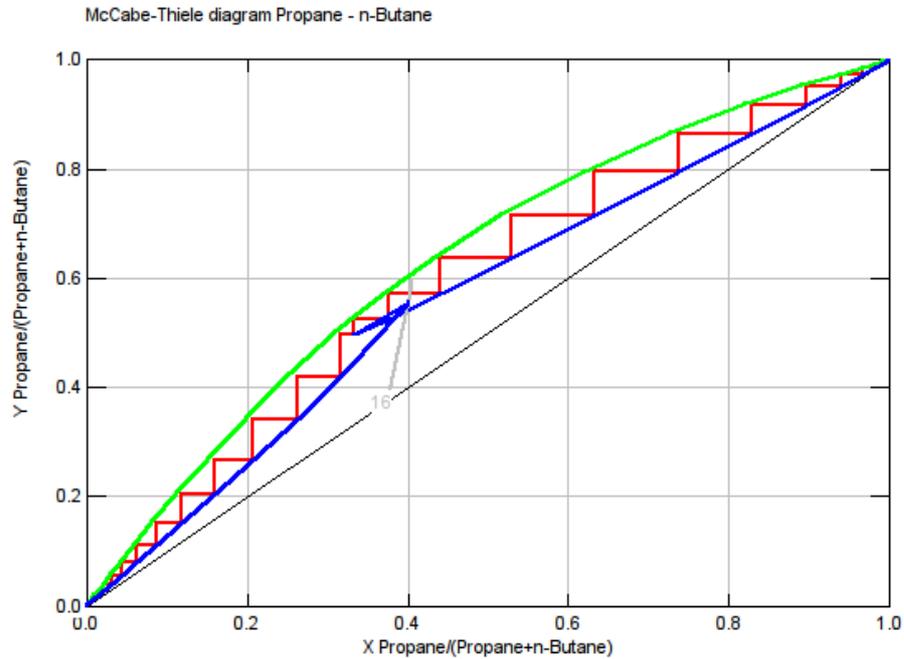
Export to Koch-Glitsch tool 'KG-Tower'



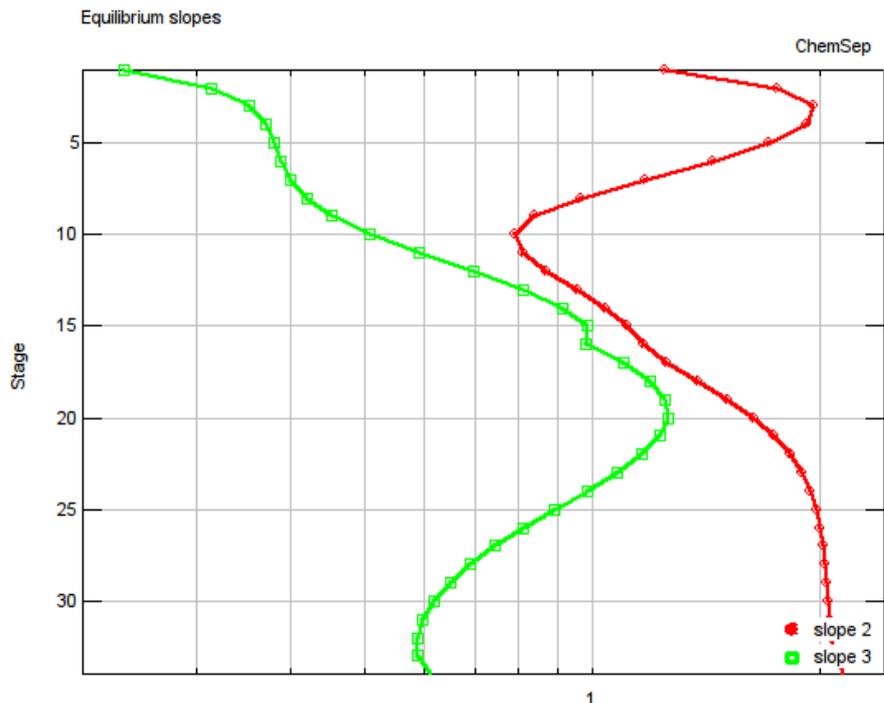
Export to Raschig GmbH tool 'Winsorp'

Equilibrium Slope Calculations and Graphs

The new Chemsep includes the new equilibrium line slope calculation as was put forth by Markus Duss and Ross Taylor in paper 302AB on March 28 at the Spring 2017 AIChE Meeting. The traditional approach for computing tray efficiencies requires a slope of the equilibrium line. This can be the slope from a pseudo-binary McCabe-Thiele diagram, e.g. for a multicomponent Depropanizer:



Or the slopes can be computed rigorously for each component:



The latter has the advantage that the user can select the design component per section (e.g. n-Butane in the rectification and Propane in stripping section).

Various Fixes and New Features

Version 7.2 includes the usual amount of small bug fixes such as:

- proper handling of two product condensers,
- no wrong values for the surface tensions in Pro/II via Cape-Open,
- proper drawing of dual axis diagrams,
- an unzoom option for the graphs,
- second virial coefficients,
- a more robust initialization method.

Another New feature is that the column sizing and cost can also be included in a new results report that can be display while hovering over a column in a converged COCO flowsheet which also displays key component's split factors, top/bottom T&p, duties, and flows.

As before, *ChemSep* Lite is available free from <http://chemsep.com>.