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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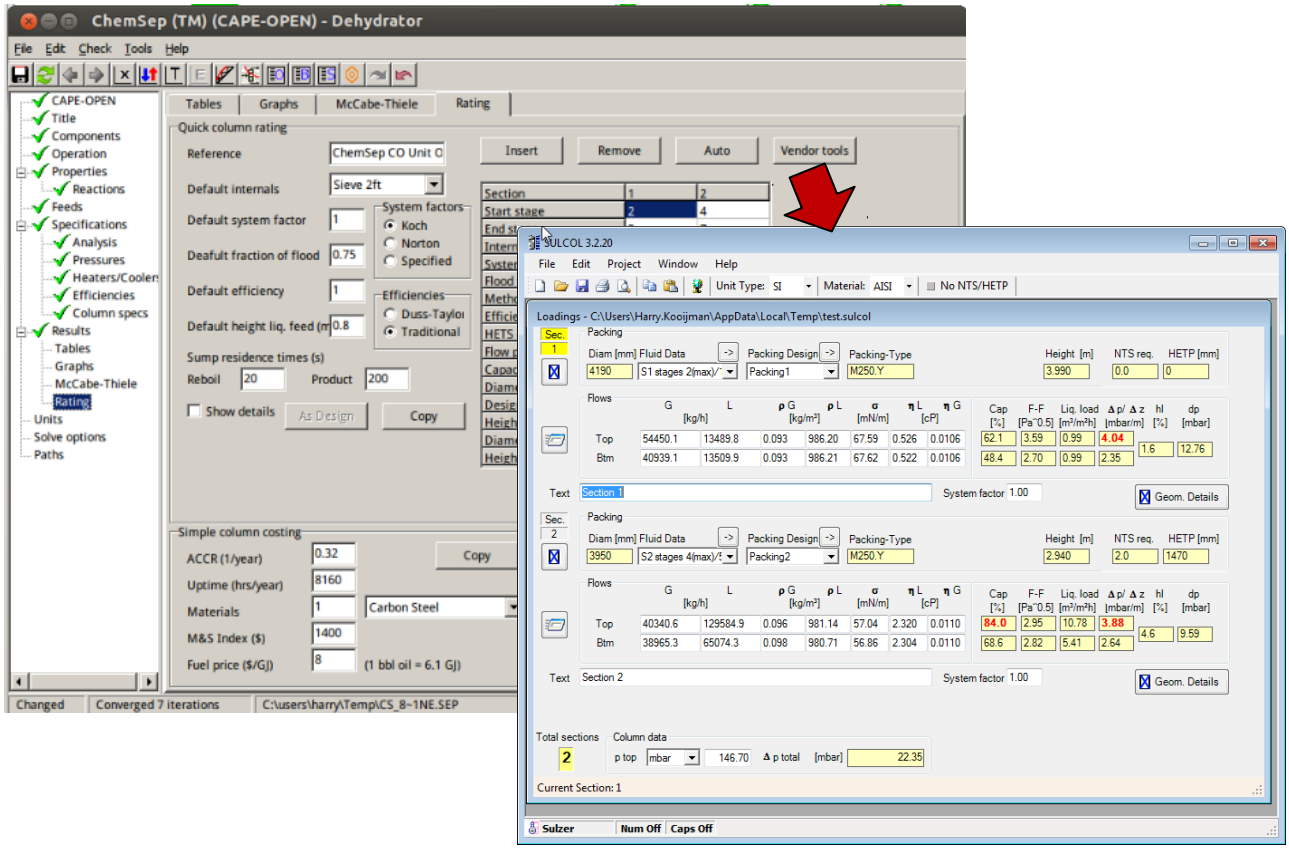
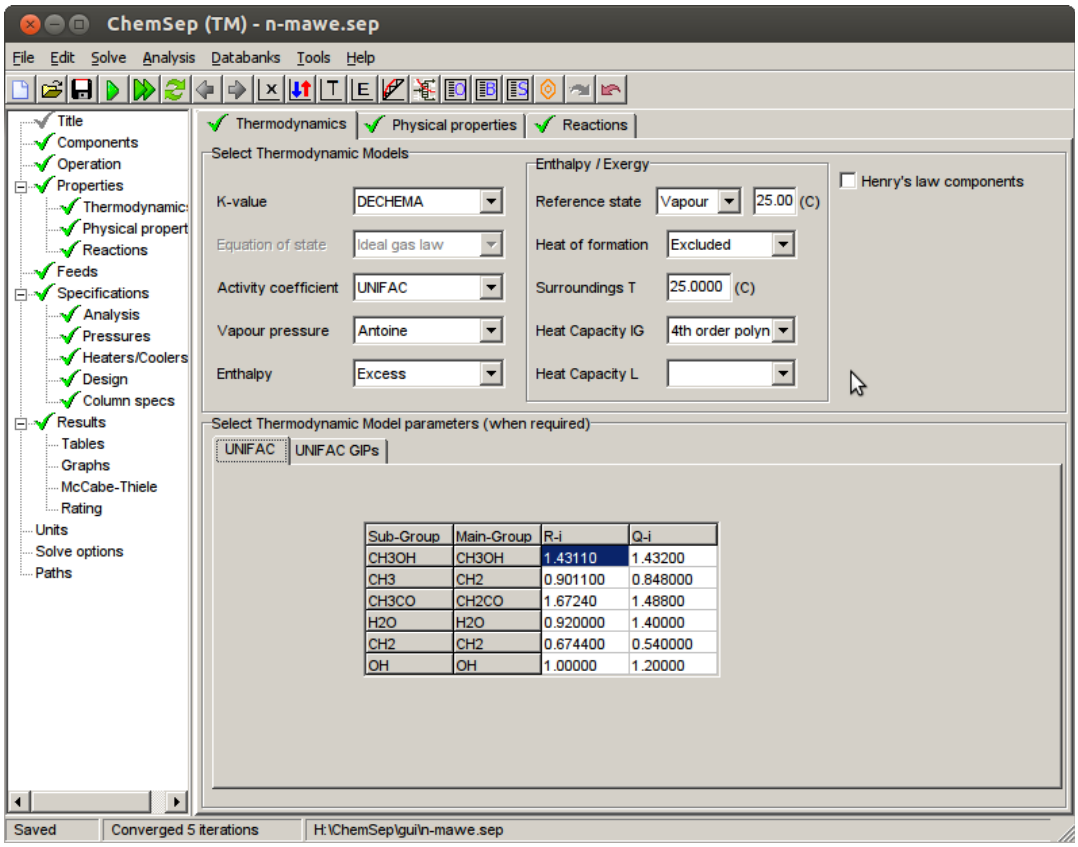
ChemSep Lite is available for free from http://chemsep.com.

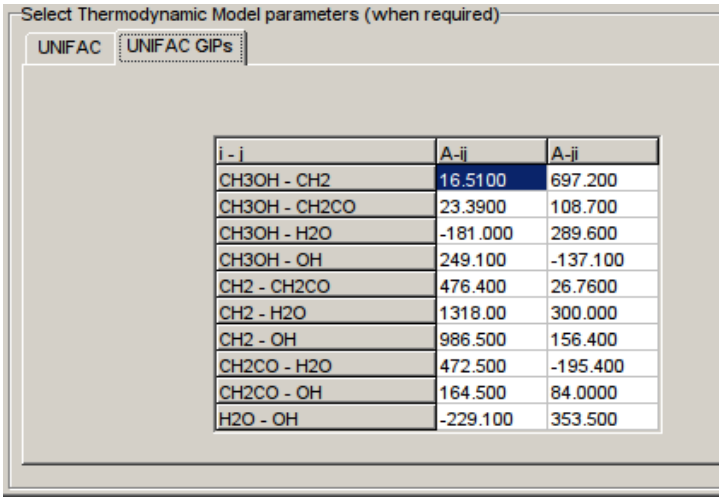


ChemSep Rating Panel with export to Sulzer chemtech tool 'SuCol'

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

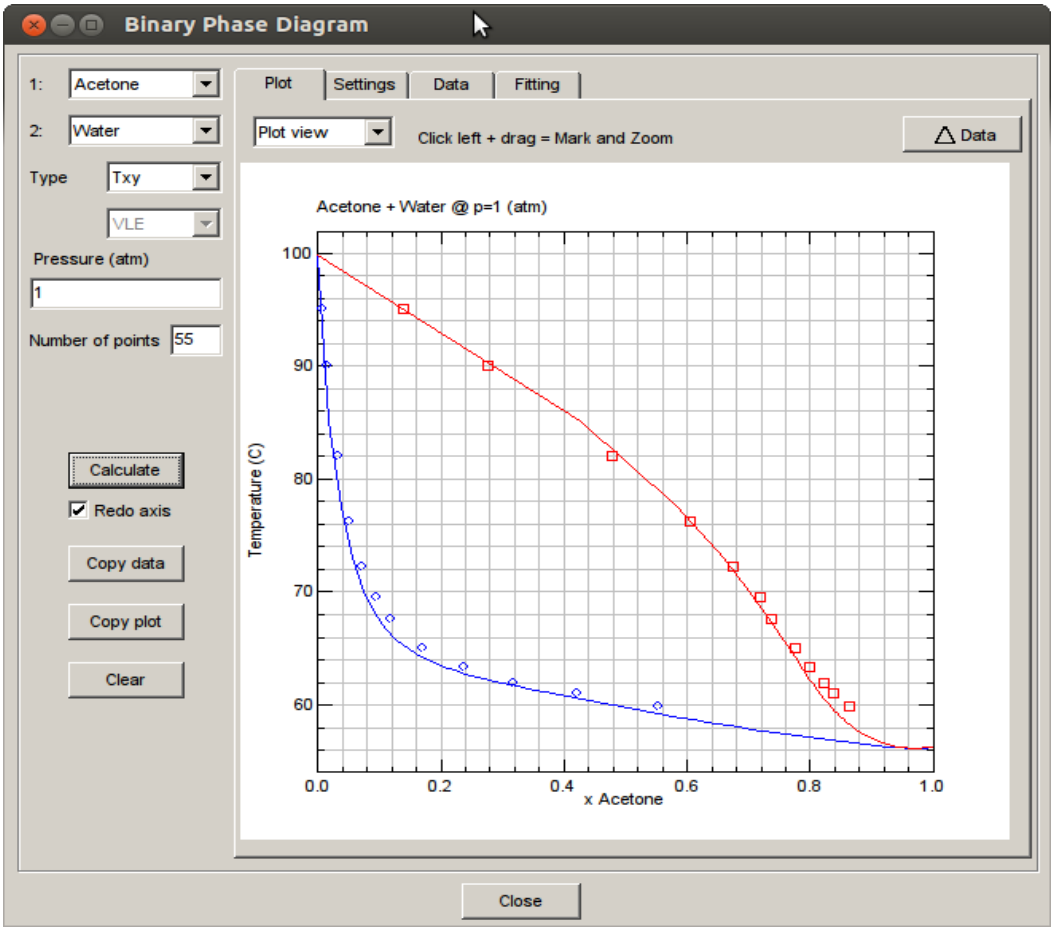
In older versions of *ChemSep* the Group Contribution (GC) information for UNIFAC, modified-UNIFAC, ASOG, PPR78, and PSRK methods was read only during run-time from various library files (with the IPD extension). This forced people to always use the standard determined Group contribution Interaction 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:

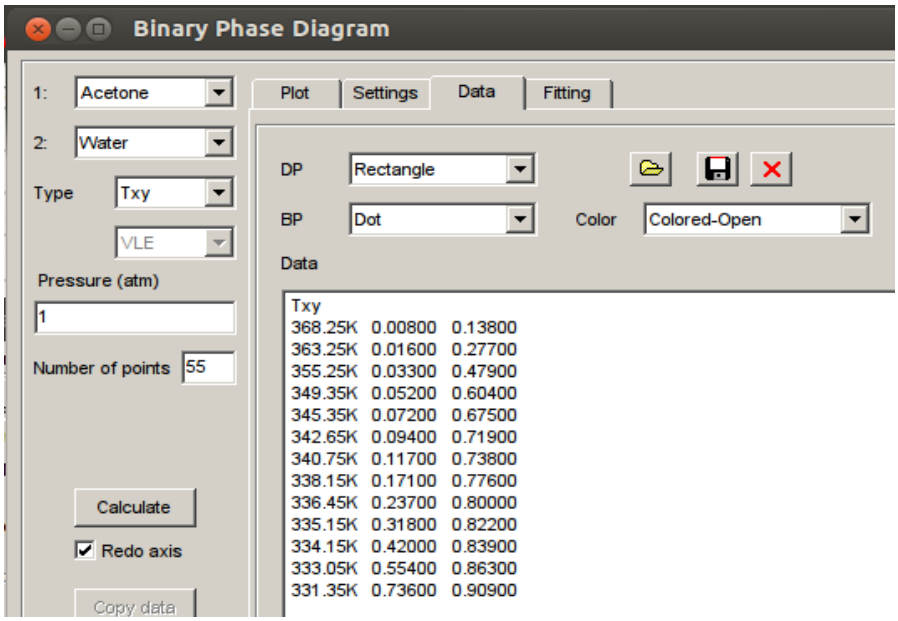




New: fitting of Group Interaction Parameters in GC methods

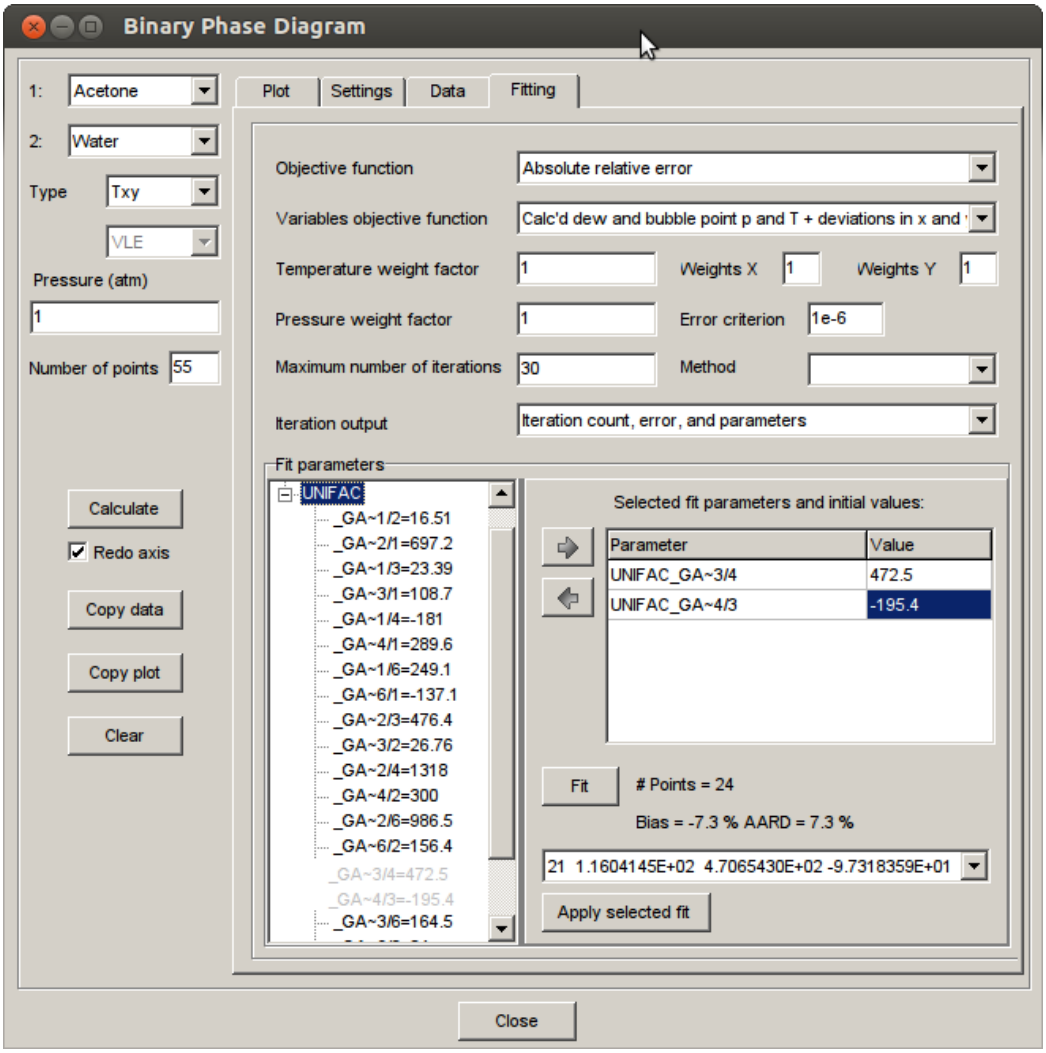
Because the GC data and interaction parameters are stored in the sep-file, they can now also be fitted on the hand of available Vapor-Liquid-Equilibria data. To illustrate this, we use the binary phase diagram option to draw the Txy-diagram for Acetone-Water. We added VLE data at 1 atm in this diagram 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).

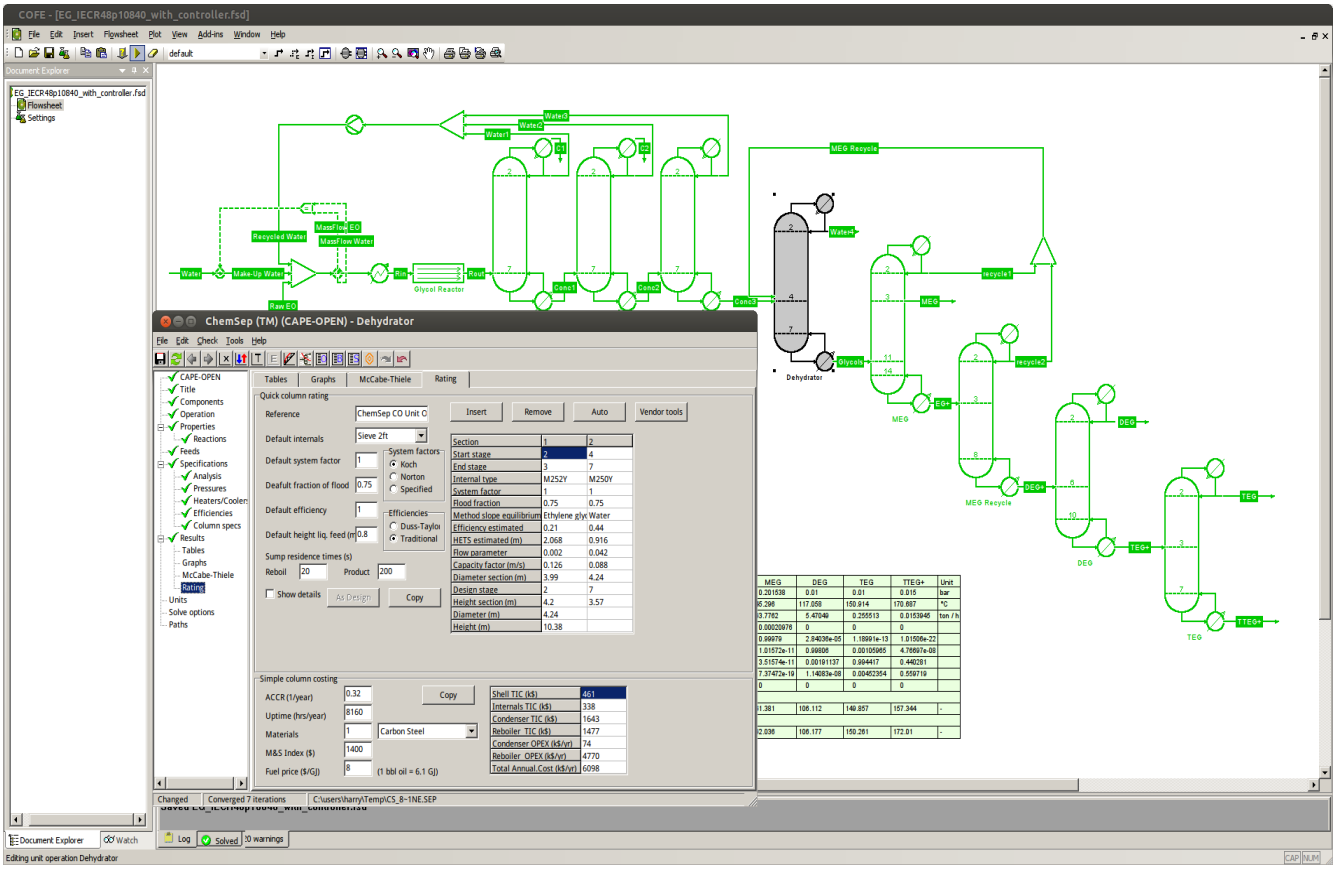


One of the fitted parameters is very close, the other is about half the library value. Pressing the [Apply selected fit] button allows to immediately use these new parameters (the user is prompted whether he wants to update the diagram to visualize the improvements). In this case there is not much change.

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.

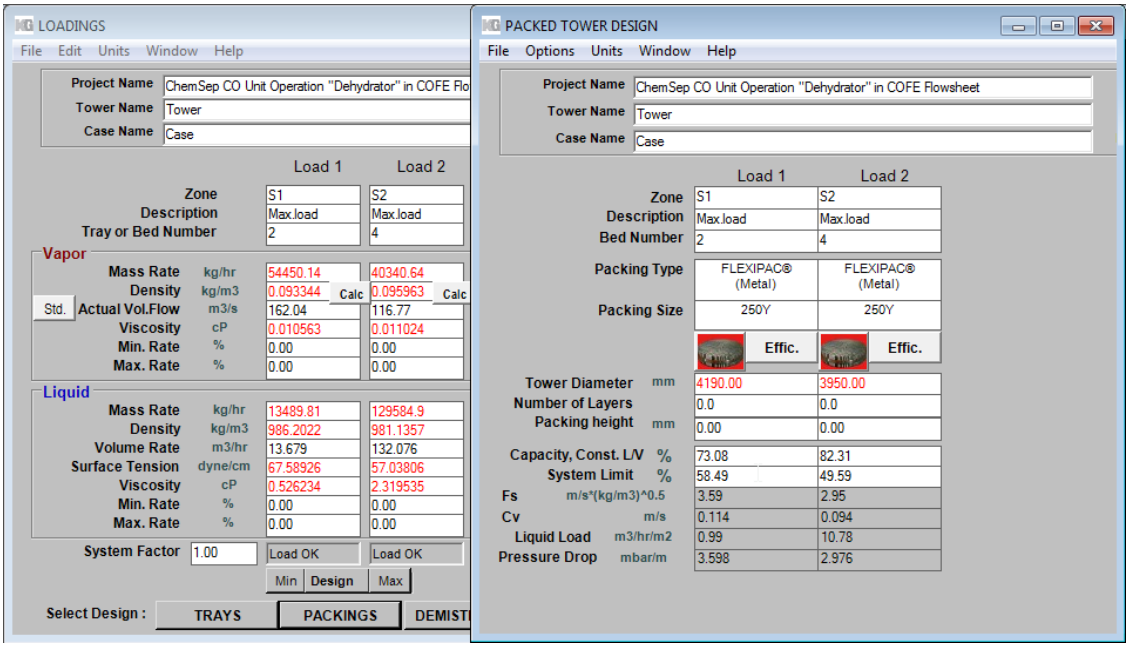
For exampled, the dehydrator column in the MEG flowsheet looks like:



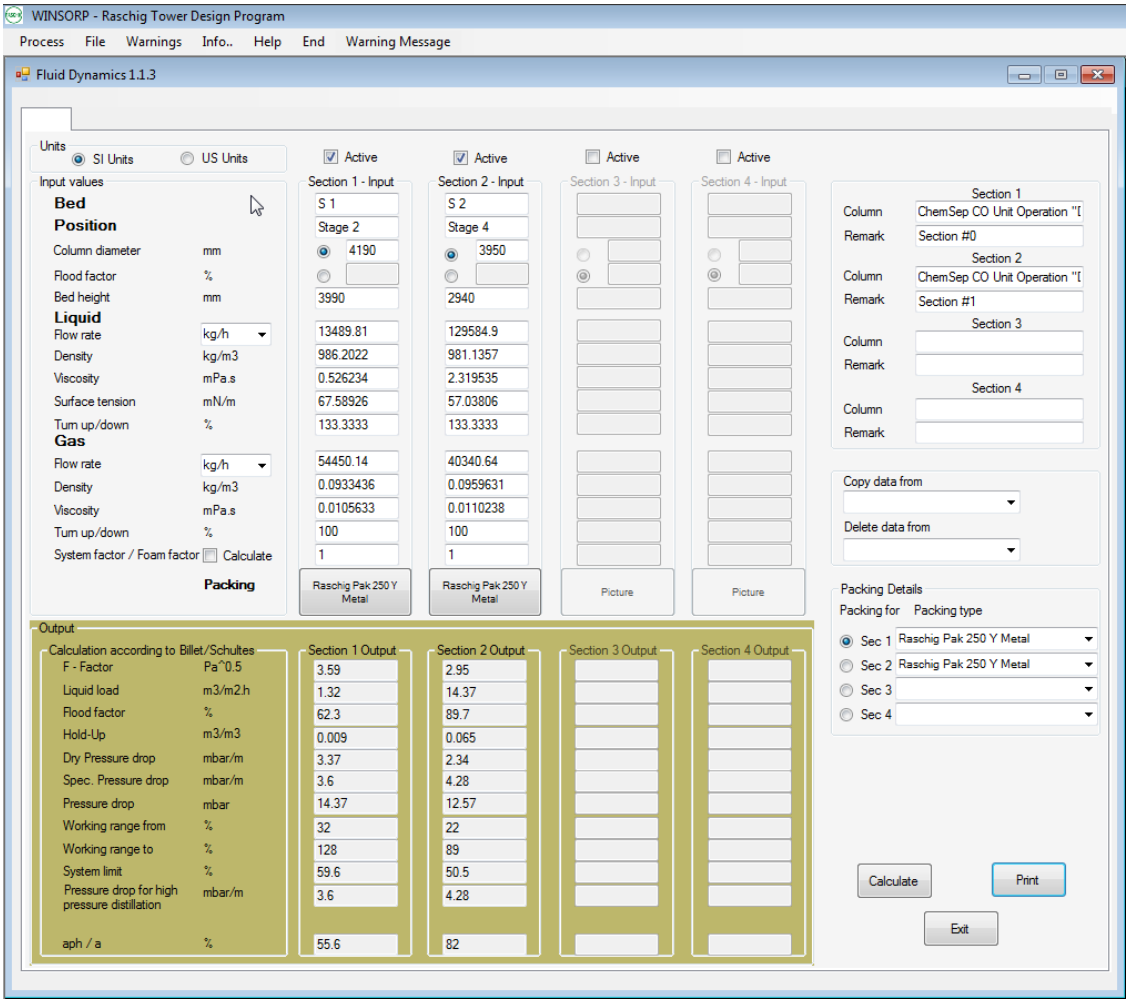
The rating is done by capacities calculated on the Wallis model. Of course, for industrial designs the rating tool of the tray/packing vendor should be used. In ChemSep we have made this easier by allowing an export to the vendor tools. Currently three tools are supported:

- '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.



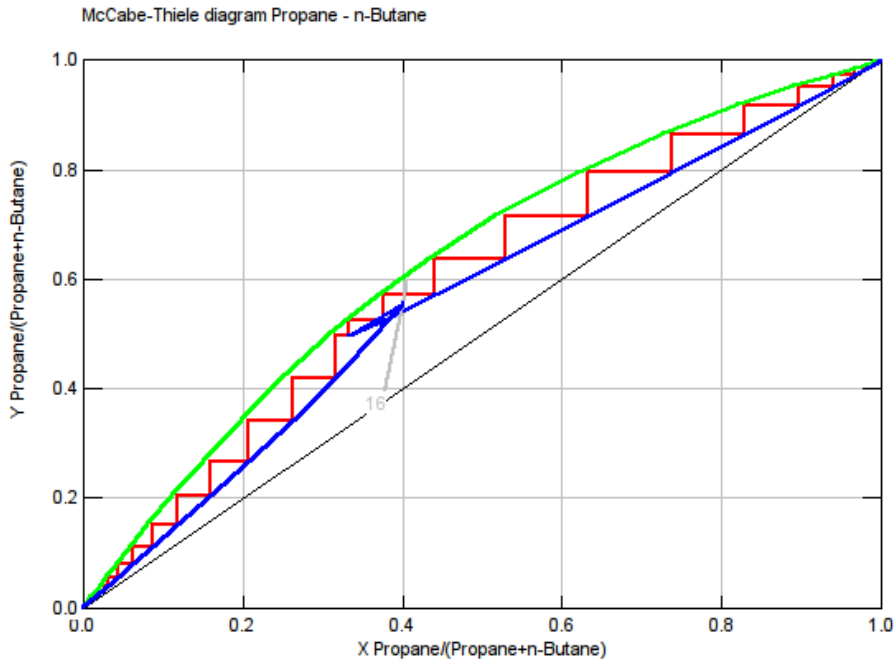
Export to Koch-Glitsch tool 'KG-Tower'



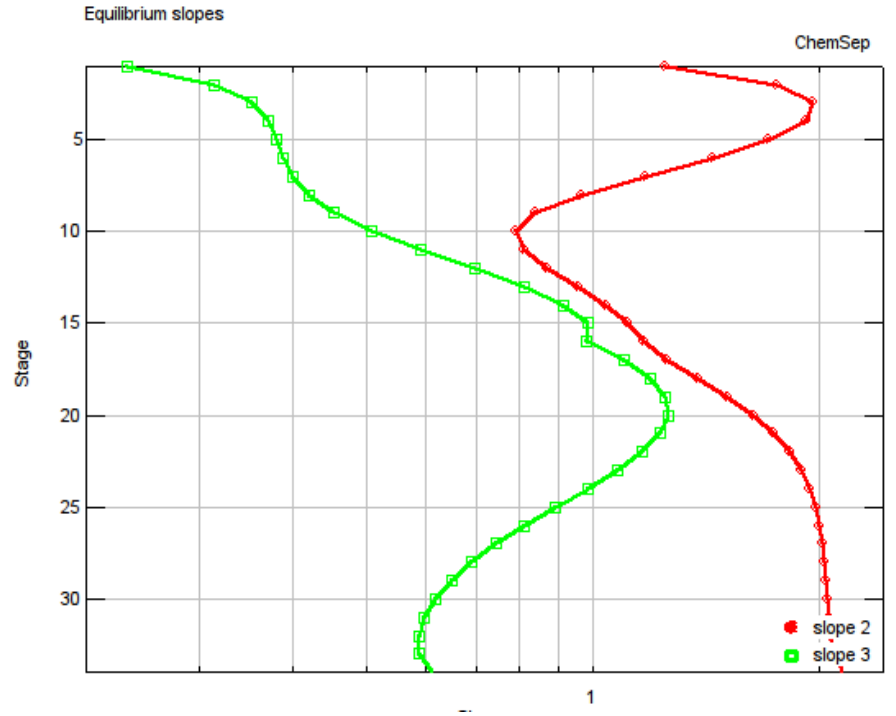
Export to Raschig GmbH tool 'Winsorp'

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.