

What's New in *ChemSep*[™] 6.8

January 2011
(Updated March 2011)

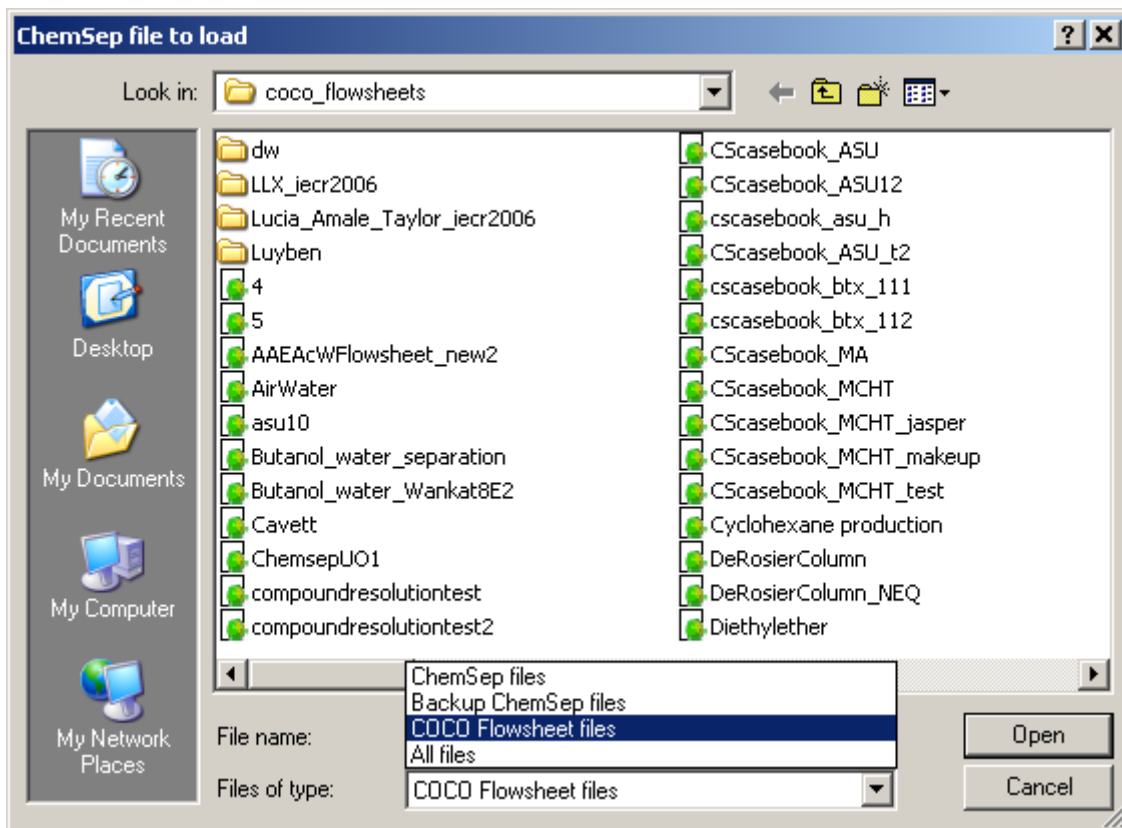
Harry Kooijman and Ross Taylor

In this document we identify and describe the most important new features in *ChemSep*.

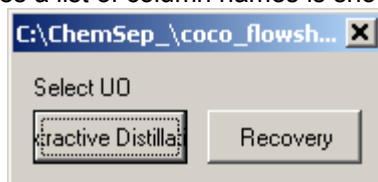
1. **New: GUI can directly load ChemSep columns from COCO flowsheet files**
2. **New: One-Click Tables**
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8. **New: Lambda plot**
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New: Load ChemSep Columns Residing in COCO Flowsheet Files

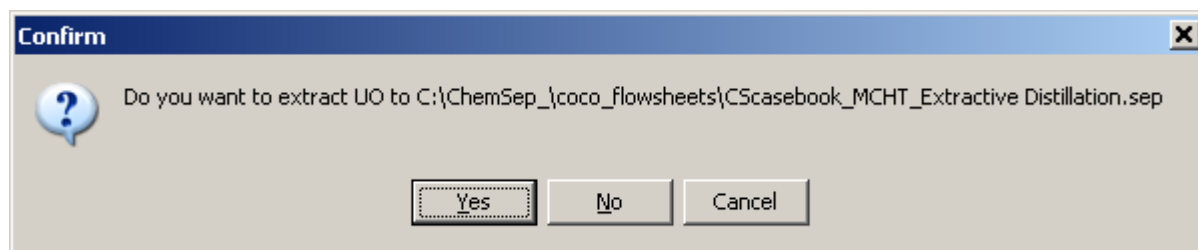
In Version 6.6 we allow direct loading of any ChemSep column from COCO flowsheet files! To see this click on the *File* menu and select *COCO Flowsheet files* from the list of file types:



If multiple columns reside in the FSD files a list of column names is shown for the user to select.



Click on the button corresponding to the desired unit operation to bring up this message:

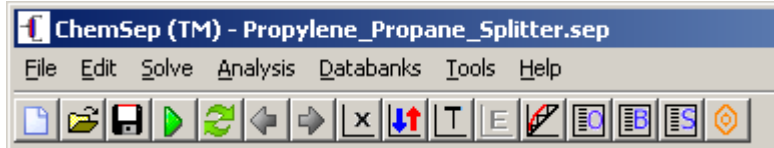


Click on Yes (assuming that having got this far you really did intend to load the column from the fsd file).

The columns are loaded in stand-alone mode i.e. they are saved as sep-files residing outside the flowsheet. This allows the user not only to inspect results but also to solve these columns - but then using ChemSep internal property routines.

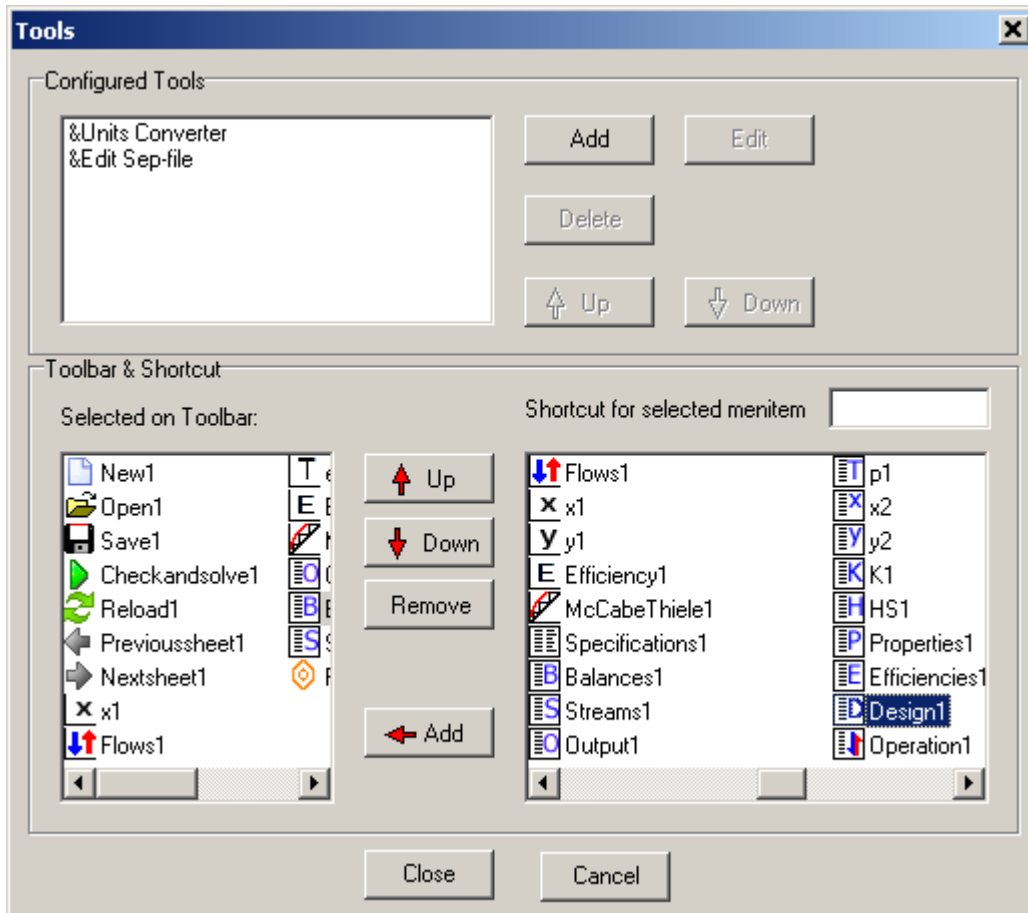
New: “One-Click” Tables

ChemSep 6.7 includes new “buttons” that allow you to view tables with just one click. The screenshot below shows the button bar with some of the newly available buttons (those that are available after the program is installed). From left to right the buttons show: New file, Open file, Save current file, Run current file, Reload currently open file, Previous Input/Output Panel, Next input/output panel, Liquid mole fraction profiles, Vapor and liquid flow profiles, Temperature profile, Efficiency profile (which appears here in grey because this was an equilibrium stage simulation), McCabe-Thiele diagram.



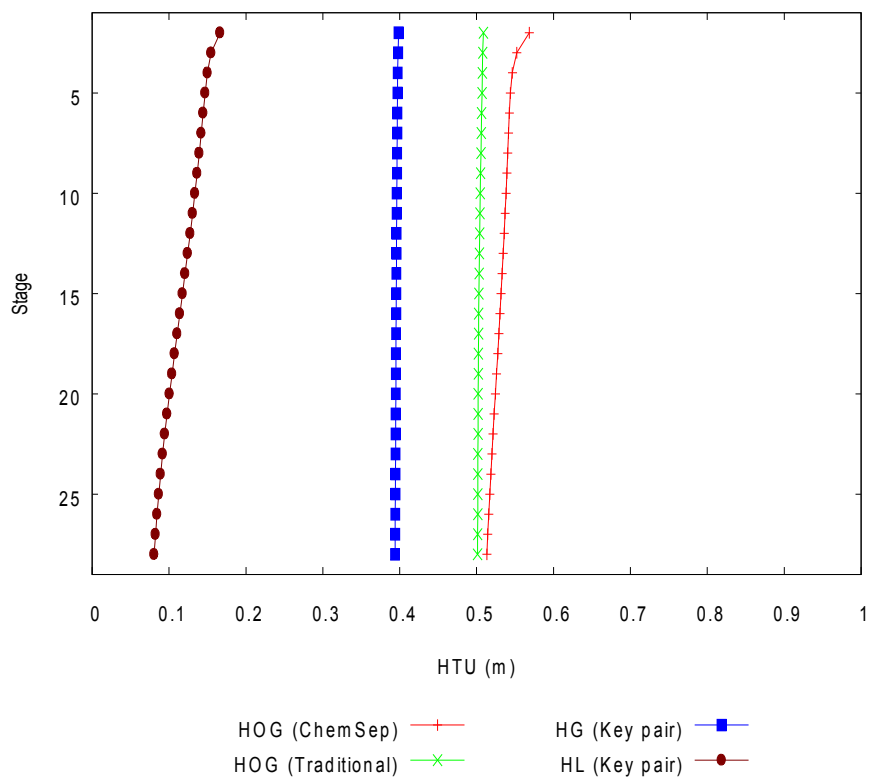
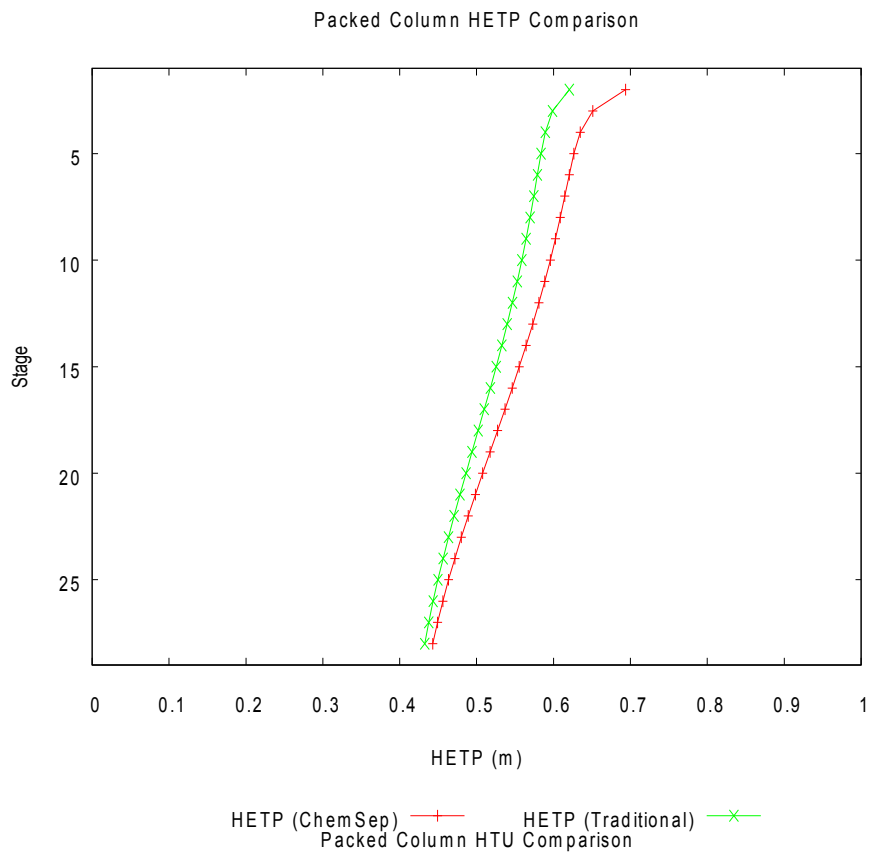
Additional symbols can be installed on the button bar representing nearly all of the tables that are defined in *ChemSep*.

To add (or remove) buttons click on **Tools** and then on **Configure Tools** to bring up the window shown below. The lower left half of this panel shows the buttons that have been selected to appear on the button bar. The list on the lower right half shows available buttons. Buttons can be selected, removed, and their order changed using the grey buttons in the lower center section.



New: HETP and HTU comparison plots for packed columns

New to Version 6.7: two new plots that compare HETP and HTU values. Examples and an explanation follow.



The **traditional method used to predict the HETP of a packed column** is to use the equation below

$$HETP = H_{OG} \frac{\ln \lambda}{\lambda - 1}$$

where H_{OG} is the overall Height of a Transfer Unit and is obtained from

$$H_{OG} = H_G + \lambda H_L$$

with H_G and H_L the Heights of Transfer Units of the gas/vapor and liquid phases respectively and $\lambda = mV/L$ is the stripping factor. These quantities are defined by:

$$H_G = u_G / k_G a' \quad H_L = u_L / k_L a'$$

where u_G and u_L are the superficial velocities of the respective phases, k_G and k_L are the mass transfer coefficients of the vapor and liquid phases (units m/s), and a' is the interfacial area density (units m^2/m^3).

These equations allow the prediction of the HETP from empirical correlations of mass transfer coefficients. Examples of such correlations include the well known correlations, of Onda et al, Bravo, Rocha & Fair, and of Billet & Schultes (and there are many more).

The all important second equation that allows the calculation of the overall Height of a Transfer Unit is a rearrangement of the well known additivity of resistances formula:

$$\frac{1}{K_{OG}} = \frac{1}{k_G} + \frac{c_i^G}{c_i^L} \frac{m}{k_L}$$

where m is the slope of the equilibrium line and where c_i is the molar density.

The formula above for the addition of the inverse mass transfer coefficients and the heights of transfer units apply only to binary systems; for multicomponent mixtures the equations are more complicated and involve matrix generalizations. Worse, **for systems of more than two components there is no unique way to define an overall mass transfer coefficient** (see pages 150 and 151 of Taylor & Krishna, 1993). For these reasons the multicomponent forms of these equations are rarely used; instead, an approximate value for the HETP is found by using the binary equations above with the properties of the key components. It is these approximate values for the HETPs and HTUs that are shown as HETP (Traditional), HOG (Traditional), HG (Key pair), and HL (Key pair).

Also shown in these plots are the HETP (ChemSep) and the HOG (ChemSep). The latter quantity is calculated from the following equations:

$$H_{OG} = Z / \epsilon$$

where Z is the height of packing and ϵ is the Baur efficiency (for which a separate plot is available) and is defined as:

$$\epsilon = \frac{\sqrt{\sum_{i=1}^c \Delta(y_{i,L})^2}}{\sqrt{\sum_{i=1}^c \Delta(y_i^*)^2}}$$

The Baur efficiency is the ratio of the length of the actual composition profile to the length of the profile for a corresponding equilibrium stage. For a mixture in which all the numbers (and heights) of transfer units are the same and for which the liquid phase resistance is negligible it can be shown that the Baur efficiency is given by:

$$\epsilon = N_{OG} = N_G$$

New: Pseudo Streams

New in Version 6.7 are so-called pseudo streams. These virtual product streams may represent any internal stream and, when used in a CAPE OPEN flowsheet environment, can be connected to other unit operations. However, they are not *real* product streams in that they are not included in the column material balance.

To define a pseudo product stream add one (or more) sidestreams to the column:

Configuration

Operation:

Condenser:

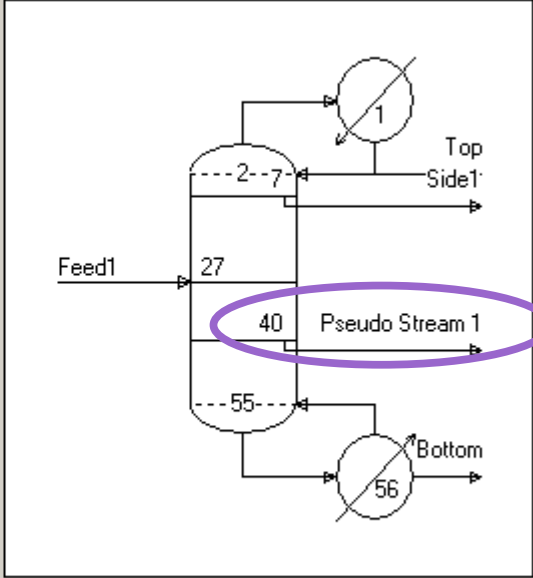
Reboiler:

Number of stages (e.g. 10)

Feed stage(s) (e.g. 5,7)

Sidestream stage(s) (e.g. 2,9)

Pumparound(s) (e.g. 6>8, 9>1)



and then define the sidestream:

Sidestreams

Sidestream:	1	
Name	Side1	Pseudo Stream
Stage	7	40
Phase	Liquid	Pseudo Liquid
Type	Total flow	Flow ratio
Flow ratio (-)		1.00000
Flowrate [kmol/s]:	0.0285123	

Note that the name appears on the flow diagram must first be entered as the stream name on the sidestream panel.

The phase must be selected as either *Pseudo Liquid* or *Pseudo Vapour*. To obtain a pseudo product with the same flow rate as the actual internal stream select *Flow ratio* as the stream specification type and type in 1.0 on the line below as shown above.

Pseudo streams flows and conditions are summarized on the stream table

Stream	Feed1	Top	Bottom	Side1	Pseudo Str
Stage	27	1	56	7	10
Pressure (psig)	10.0000	9.90000	9.90000	9.90000	9.90000
Vapour fraction (-)	0.000000	0.000000	0.000000	0.000000	0.000000
Temperature (oF)	164.000	123.000	269.450	207.763	264.359
Enthalpy (J/kmol)	-2.869E+07	-2.944E+07	-1.959E+07	-2.307E+07	-1.996E+07
Entropy (J/kmol/K)	-67340.5	-82526.2	-44591.2	-64172.4	-46330.1

but, as noted above, are not included in the column material balances:

Mass and Energy Balances			
Stream / Apparatus	Mass (kmol/s)	Energy (J/s)	Exergy (J/s)
Feed1	0.0766893	-2.200E+06	-660934
Top	-6.000E-08	1.76661	0.290304
Bottom	-0.0481769	944136	303630
Side1	-0.0285123	657894	112368
Qcondenser		-5.180E+06	-408947
Qreboiler		5.7786E+06	1.5252E+06
Balance	-1.862E-09	0.000000	871380

New: Combined feed fractions in output tables

Now included in the stream tables are the combined feed fractions in each stream.

The screenshot shows the ChemSep (TM) interface with the 'Tables' tab selected. The 'Streams' table is displayed, showing various properties for three streams: Feed1, Top, and Bottom. The 'Combined feed fractions (-)' section is highlighted with a purple oval.

Stream	Feed1	Top	Bottom
Stage	90	1	150
Pressure (kPa)	2027.00	1931.00	2069.00
Vapour fraction (-)	0.000000	0.000000	0.000000
Temperature (K)	325.000	320.178	331.235
Enthalpy (J/kmol)	-1.221E+07	-1.277E+07	-1.158E+07
Entropy (J/kmol/K)	-54395.0	-60953.8	-55658.4
Mole flows (kmol/h)			
Propylene	163.300	157.797	5.50341
Propane	108.900	5.29975	103.600
Total molar flow	272.200	163.096	109.104
Mole fractions (-)			
Propylene	0.599926	0.967505	0.0504420
Propane	0.400074	0.0324946	0.949558
Mass flows (kg/s)			
Propylene	1.90878	1.84445	0.0643282
Propane	1.33393	0.0649176	1.26902
Total mass flow	3.24272	1.90937	1.33335
Mass fractions (-)			
Propylene	0.588637	0.966001	0.0482458
Propane	0.411363	0.0339995	0.951754
Combined feed fractions (-)			
Propylene	1.000000	0.966299	0.0337012
Propane	1.000000	0.0486662	0.951334

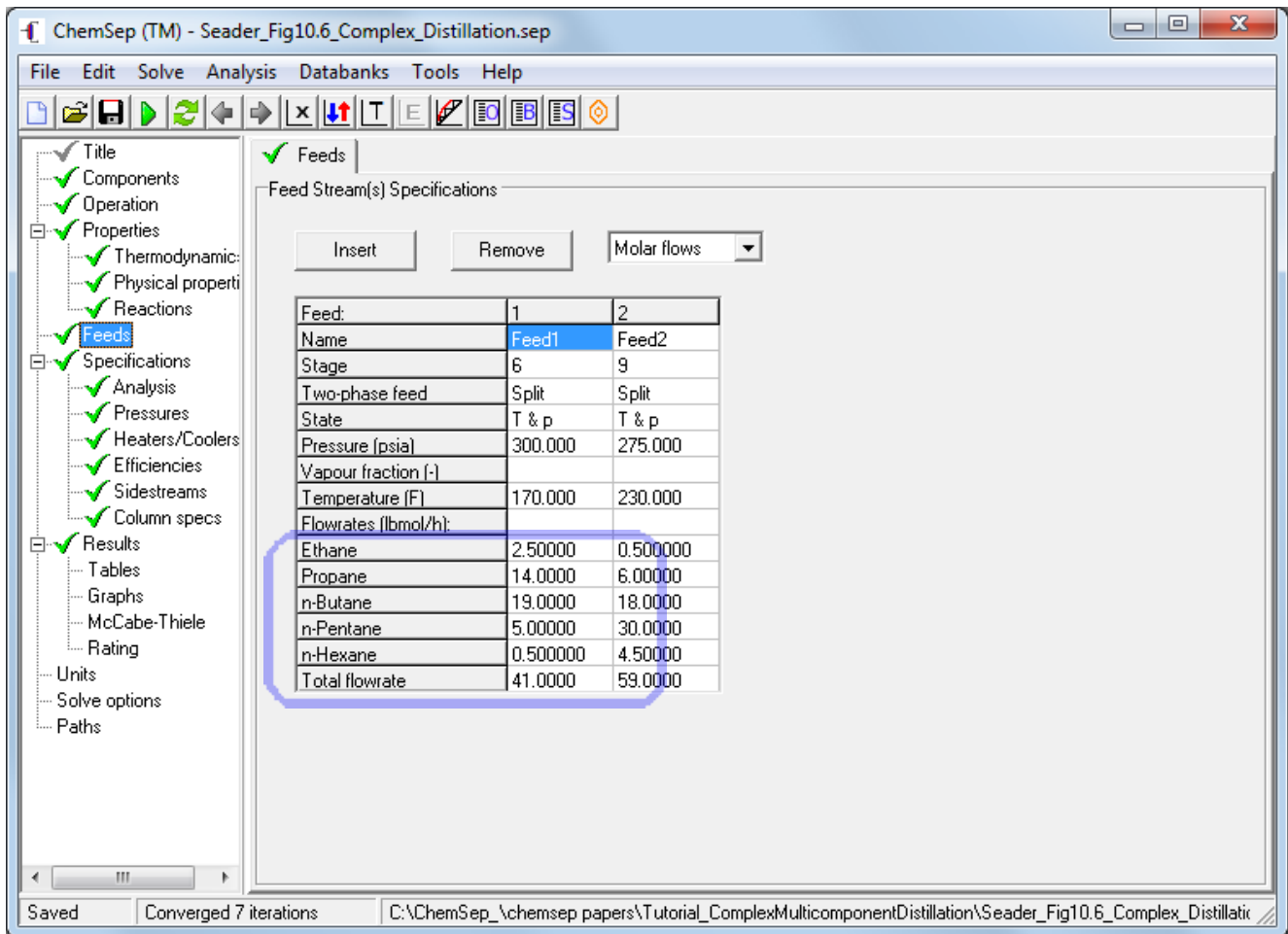
The combined feed fraction of any compound i in stream j is defined as:

$$\text{Combined Feed Fraction of compound } i \text{ in stream } j = \frac{\text{Molar flow of compound } i \text{ in stream } j}{\text{Molar flow of compound } i \text{ in all feeds}}$$

This quantity helps one see where a particular compound leaves a column.

New: Undo/Redo

New in Version 6.8 is a complete *Undo/Redo* facility. Any change to input can be reversed up to the point at which the file was last saved. It is, perhaps, easier to demonstrate this feature rather than try to explain how it works. Consider this input screen from a file modeling a complex distillation column.



We will now change the flow rates of feed 1. The numbers in the illustration below are purely for illustrative purposes and have no significance in the problem at hand.

Feed:	1	2
Name	Feed1	Feed2
Stage	6	9
Two-phase feed	Split	Split
State	T & p	T & p
Pressure (psia)	300.000	275.000
Vapour fraction (-)		
Temperature (F)	170.000	230.000
Flowrates (lbmol/h):		
Ethane	1.00000	0.500000
Propane	2.00000	6.00000
n-Butane	3.00000	18.0000
n-Pentane	4.00000	30.0000
n-Hexane	5.00000	4.50000
Total flowrate	15.0000	59.0000

We now decide that it was a mistake to have changed these flows and we want to recover the old values. To do so we use *Ctrl-Z* once to get:

Feed:	1	2
Name	Feed1	Feed2
Stage	6	9
Two-phase feed	Split	Split
State	T & p	T & p
Pressure (psia)	300.000	275.000
Vapour fraction (-)		
Temperature (F)	170.000	230.000
Flowrates (lbmol/h):		
Ethane	1.00000	0.500000
Propane	2.00000	6.00000
n-Butane	3.00000	18.0000
n-Pentane	4.00000	30.0000
n-Hexane	0.500000	4.50000
Total flowrate	10.5000	59.0000

Notice that the flow rate of n-Hexane in Feed 1 has reverted to the old value of 0.5 lbmol/h. Use *Ctrl-Z* a second time:

Feed:	1	2
Name	Feed1	Feed2
Stage	6	9
Two-phase feed	Split	Split
State	T & p	T & p
Pressure (psia)	300.000	275.000
Vapour fraction (-)		
Temperature (F)	170.000	230.000
Flowrates (lbmol/h):		
Ethane	1.00000	0.500000
Propane	2.00000	6.00000
n-Butane	3.00000	18.0000
n-Pentane	5.00000	30.0000
n-Hexane	0.500000	4.50000
Total flowrate	11.5000	59.0000

and a third:

Feed:	1	2
Name	Feed1	Feed2
Stage	6	9
Two-phase feed	Split	Split
State	T & p	T & p
Pressure (psia)	300.000	275.000
Vapour fraction (-)		
Temperature (F)	170.000	230.000
Flowrates (lbmol/h):		
Ethane	1.00000	0.500000
Propane	2.00000	6.00000
n-Butane	19.0000	18.0000
n-Pentane	5.00000	30.0000
n-Hexane	0.500000	4.50000
Total flowrate	27.5000	59.0000

Using *Ctrl-Z* two more times and we will recover the original set of component feed flows.

Feed:	1	2
Name	Feed1	Feed2
Stage	6	9
Two-phase feed	Split	Split
State	T & p	T & p
Pressure (psia)	300.000	275.000
Vapour fraction (-)		
Temperature (F)	170.000	230.000
Flowrates (lbmol/h):		
Ethane	2.50000	0.500000
Propane	14.0000	6.00000
n-Butane	19.0000	18.0000
n-Pentane	5.00000	30.0000
n-Hexane	0.500000	4.50000
Total flowrate	41.0000	59.0000

Now, suppose that we decide that the first of the feed flow changes was, in fact, correct. If he use *Ctrl-Y* we will reverse the last *Undo* as shown below:

Feed:	1	2
Name	Feed1	Feed2
Stage	6	9
Two-phase feed	Split	Split
State	T & p	T & p
Pressure (psia)	300.000	275.000
Vapour fraction (-)		
Temperature (F)	170.000	230.000
Flowrates (lbmol/h):		
Ethane	1.00000	0.500000
Propane	14.0000	6.00000
n-Butane	19.0000	18.0000
n-Pentane	5.00000	30.0000
n-Hexane	0.500000	4.50000
Total flowrate	39.5000	59.0000

Undo and *Redo* can be used to reverse (and re-reverse) any change to the input including, for example, specifications as shown below. Before:

Top specification Reflux flow rate = 150.000 (lbmol/h)

Change to:

Top specification Reflux ratio = 10.0000 (-)

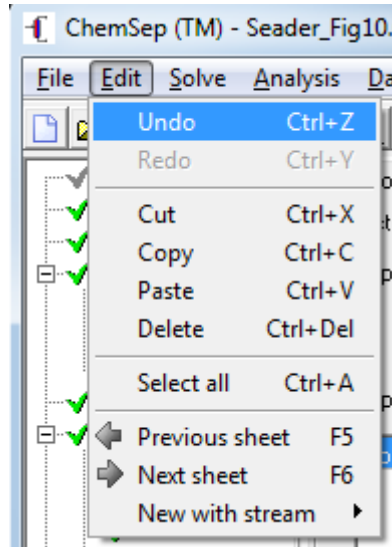
Reverse the change with *Ctrl-Z* (twice because the first use enters the default value):

Top specification Reflux flow rate = 150.000 (lbmol/h)

Redo the change with *Ctrl-Y* (twice):

Top specification Reflux ratio = 10.0000 (-)

Undo and Redo are also available from the *Edit* menu:



New: Physical Property Models

In a famous paper published in 1972 Soave presented a modification of the Redlich-Kwong Equation of State:

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)}$$

where

$$a = a(T_c)\alpha$$

$$a(T_c) = \frac{\Omega_A RT_c^2}{P_c}$$

$$\Omega_A = 0.42747 \quad \Omega_B = 0.08664$$

$$\sqrt{\alpha} = 1 + (0.480 + 1.57\omega - 0.176\omega^2)(1 - \sqrt{T_r})$$

$$b = \frac{\Omega_B RT_c}{P_c}$$

The Peng-Robinson Equation of State (EOS) is a modification of the concepts pioneered by Soave with a view towards improving the estimates of liquid density provided by the basic EOS.

The Peng-Robinson EOS is:

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)}$$

with the parameters given by the same equations as for the SRK EOS with the following differences:

$$\sqrt{\alpha} = 1 + (0.37464 + 1.5422\omega - 0.26992\omega^2)(1 - \sqrt{T_r})$$

$$\Omega_A = 0.45724 \quad \Omega_B = 0.07880$$

For mixtures the parameters are obtained from the following simple "mixing rules":

$$a = \sum_{i=1}^c \sum_{j=1}^c x_i x_j a_{i,j}$$

$$b = \sum_{i=1}^c x_i b_i$$

where

$$a_{i,j} = \sqrt{a_i a_j} (1 - k_{i,j})$$

$k_{i,j}$ is the binary interaction parameter for the i-j pair of compounds.

Volume Translation for Liquid Density

It has long been recognized that the liquid density predicted by the SRK and PR equations of state are inadequate for process engineering work (this despite the fact that both models are capable of excellent predictions of vapor-liquid phase equilibrium). The idea of correcting the liquid phase densities was first proposed long ago. In the so-called "volume translation" methods the volume is calculated as follows:

$$V = V_{EOS} - c_{EOS}$$

where V_{EOS} is the volume computed from the original equation of state (i.e. the unmodified SRK or PR models) and c_{EOS} is the volume translation parameter for that particular EOS **and** compound. Several methods of calculating the volume shift parameter have been proposed. *ChemSep 6.8* includes the pioneering method of Peneloux and a generic approach.

Peneloux proposed the following correlations for the volume shift parameter:

$$c_{PR} = -0.50033 \frac{RT^c}{P_c} (0.25969 - z_{Ra})$$

$$c_{SRK} = -0.40768 \frac{RT^c}{P_c} (0.29441 - z_{Ra})$$

where z_{Ra} is the Rackett parameter, values of which have been published for many compounds. In case the Rackett parameter is not known, it can be estimated from correlations or set equal to the critical compressibility to which it is often very nearly equal.

ChemSep also includes a generic approach to volume translation in which we compute the shift parameter from:

$$c_{EOS} = V - V_{EOS}$$

where V is the pure component molar volume. The pure component volume needed for this calculation may be obtained from data or can be estimated from an alternative method for predicting pure compound volumes. In ChemSep the pure component density is estimated for each compound at a reduced temperature of 0.7 from the method selected to estimate pure component liquid densities. The default choice (when no selection is made) is an accurate correlation of pure component density data.

For mixtures the volume translation parameter is calculated from:

$$c = \sum_{i=1}^c x_i c_i$$

The Rackett Models for Liquid Density

The well known Rackett method as modified by Spencer and Danner is as follows:

$$V_{sat} = \frac{RT_c}{P_c} F_z$$
$$F_z = Z_{Ra}^{1+(1-T_r)^{2.7}}$$

The Rackett equation has been extended for mixtures as follows:

$$V_{sat} = R \sum_{i=1}^c x_i \frac{T_{c_i}}{P_{c_i}} F_z$$

In order to calculate the function F_z we must select a method of estimating the critical temperature of the mixture and the mixture Rackett parameter. Since there are several ways to estimate mixture critical properties there are, necessarily, several ways to use the Rackett equation for mixtures (all of which give the same results when applied to pure compounds). Three different mixing rules now are available in ChemSep: those in the DIPPR handbook (which is the version that was available in earlier versions of ChemSep), the mixing rules of Li et al. as given in PGL5 (page 5.23), and the mixing rules of Chueh and Prausnitz (also as reported on the same page in PGL5).

The mixing rules of Chueh and Prausnitz are:

$$Z_{Ra_m} = \sum_{i=1}^c x_i Z_{Ra_i}$$

$$T_{c_m} = \sum_{i=1}^c \sum_{j=1}^c \phi_i \phi_j T_{c_{i,j}}$$

where

$$\phi_i = \frac{V_{c_i}}{\sum_{j=1}^c x_j V_{c_j}}$$

$$T_{c_{i,j}} = (1 - \kappa_{i,j}) \sqrt{T_{c_i} T_{c_j}}$$

$$(1 - \kappa_{i,j}) = 8 \frac{\sqrt{V_{c_i} V_{c_j}}}{(V_{c_i} + V_{c_j})^{1/3}}$$

The mixing rules of Li et al. are similar to those of Chueh and Prausnitz but with:

$$T_{c_m} = \sum_{i=1}^c \phi_i T_{c_i}$$

and the DIPPR Handbook suggests using:

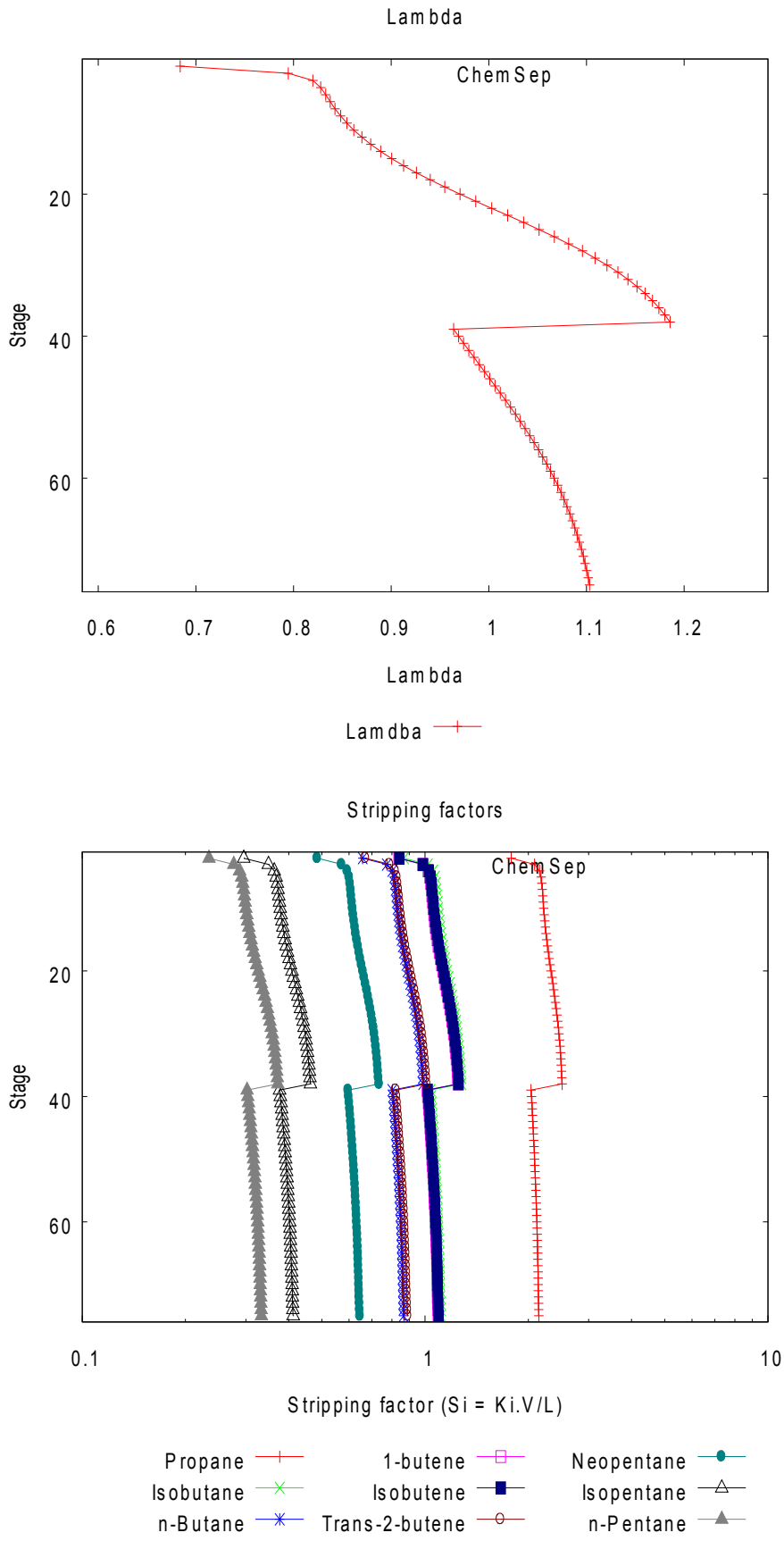
$$T_{c_m} = \sum_{i=1}^c x_i T_{c_i}$$

Liquid Viscosity

ChemSep 6.8 includes a new method for mixture liquid viscosity: The Letsou-Stiel method for mixtures. This method used the same equations as the Letsou-Stiel method for pure compounds (which has always been available in ChemSep) but uses the mixing rules of Li et al discussed above to get the pseudo-critical properties.

New: Lambda plot

New to Version 6.8: The Lambda plot. An example and an explanation follow.



The parameter known as *Lambda* appears in many different distillation calculations and is defined as follows:

$$\lambda = \frac{mV}{L}$$

where *m* is the (local) slope of the equilibrium line. For multicomponent systems the slope of the equilibrium line depends on the choice of the key components (and on whether or not the components are “lumped” together or not. For more discussion of the latter point we refer readers to the discussion of the McCabe-Thiele diagram in *What's New in ChemSep* 6.5.

It will be immediately apparent that the *Lambda* parameter bears a strong relationship to the stripping factors illustrated for the same separation in the second plot above and defined by:

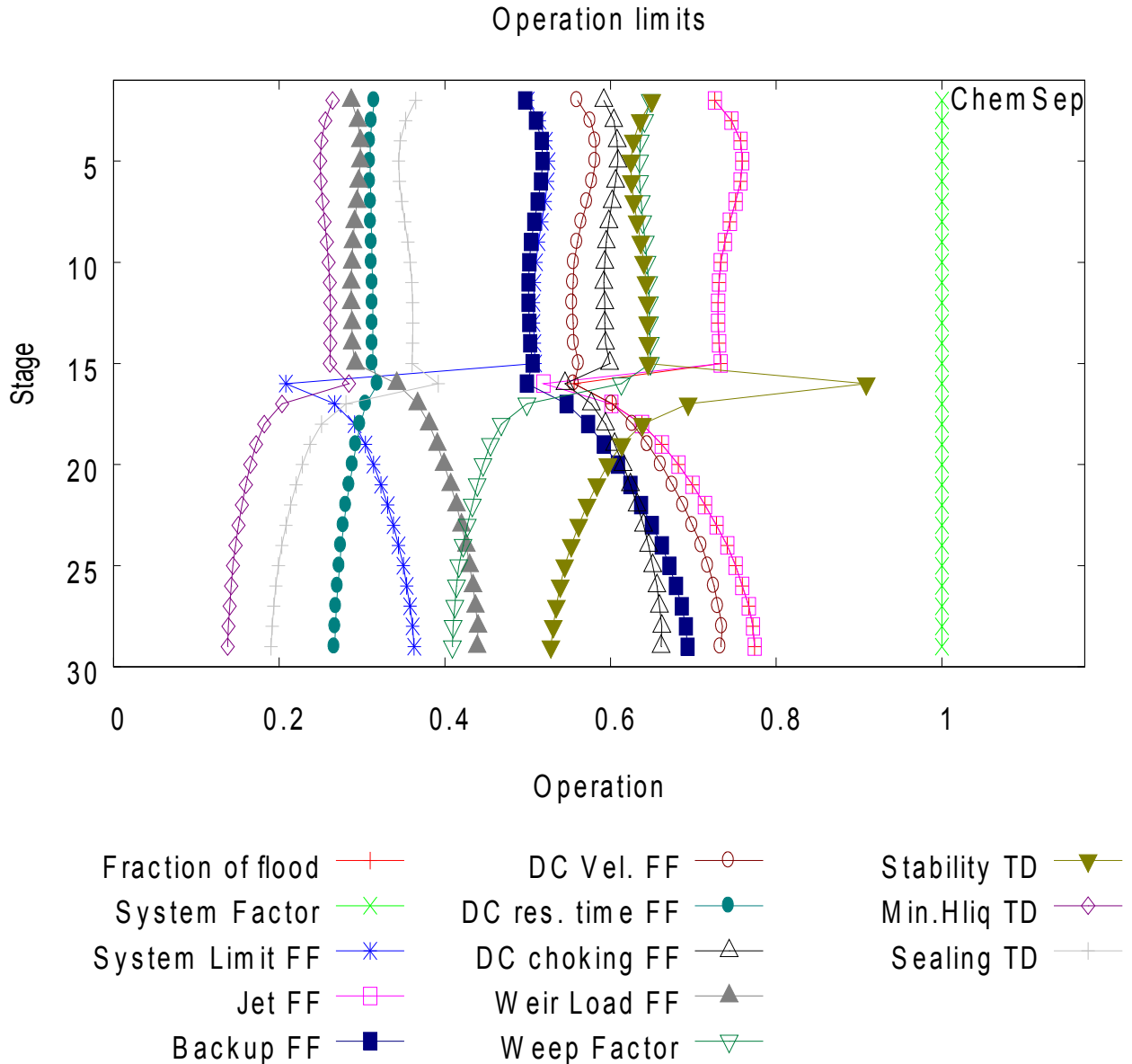
$$S_i = \frac{K_i V}{L}$$

The only difference between these two definitions is that the equilibrium slope is replaced by the K-value. There is, therefore, a stripping factor for each component.

For more on the differences between stripping factors and *Lambda* see *Distillation Design* (H.Z. Kister, McGraw-Hill).

New: Tray Stability Plot

ChemSep 6.8 has a new version of the *Operation Limits* plot. An example for a large tray column appears below.



In a paper entitled “Tray Stability at Low Vapor Load” by D. Summers, L. Spiegel, and E. Kolesniko (Proc. *Distillation and Absorption 2010*, p611, I. Chem. E., 2010) defined a tray stability factor by:

$$\eta = \sqrt{\frac{\Delta P_{dry}}{h_{cl}}}$$

The significance of this parameter is that for a tray with a stability factor greater than 0.6 has less than 30% weeping. It is considered that the adverse effect of weeping on tray efficiency will be small if weeping is less than 30%.

We have, therefore defined the *Stability TD* as:

$$TD_{Stability} = 0.7 \frac{W_F}{\eta}$$

where W_F is the weep factor and is given in the plot shown above. We have used the more conservative value of 0.7 rather than the value of 0.6 of Summers et al. in defining this turndown ratio. With this definition weeping should not be a problem if this turndown ratio is less than 1.

In the example shown above the *Stability TD* is always less than 1, showing that the tray efficiency is not adversely affected by weeping.

The *Sealing TD* is defined by:

$$TD_{Seal} = W_F \frac{d_{cl}}{h_{cl}}$$

where d_{cl} is the downcomer clearance.

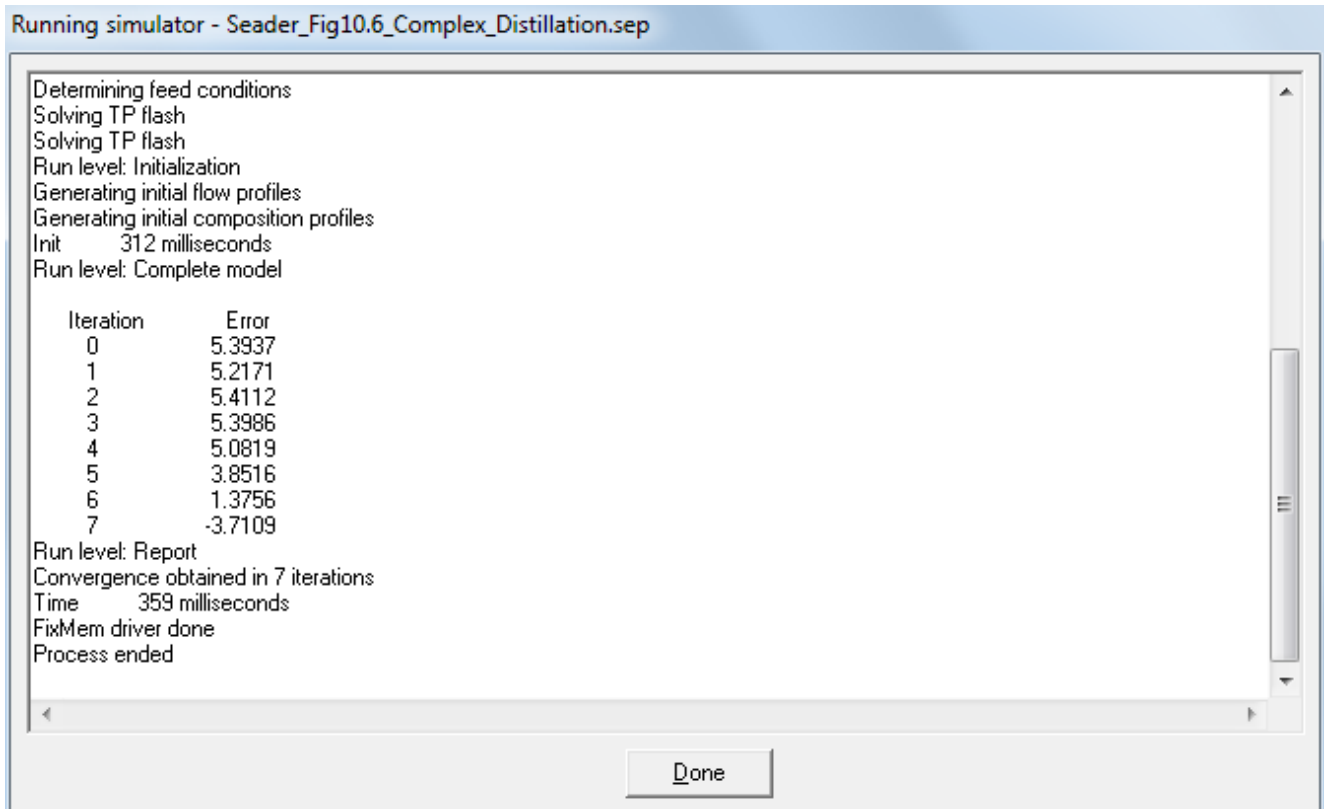
The *Minimum liquid height turndown ratio* is defined by:

$$TD_{h_{l,min}} = \begin{cases} W_F \frac{2d_{hole}}{h_{cl}} & \text{if } 2d_{hole} > d_{bub,max} \\ W_F \frac{2d_{bub,max}}{h_{cl}} & \text{if } 2d_{hole} \leq d_{bub,max} \end{cases}$$

with the maximum bubble size set to 30 mm.

Revised: Display While Calculating

The information displayed while actually carrying out a simulation has been improved. Some of this is simply textual changes to the words printed to the screen, but there is one change that will be more noticeable. The number displayed to indicate the current “error” (the extent to which the model equations are not yet solved) has been revised as shown in the screen image below:



The screenshot shows a window titled "Running simulator - Seader_Fig10.6_Complex_Distillation.sep". The text inside the window is as follows:

```
Determining feed conditions
Solving TP flash
Solving TP flash
Run level: Initialization
Generating initial flow profiles
Generating initial composition profiles
Init      312 milliseconds
Run level: Complete model

  Iteration      Error
    0           5.3937
    1           5.2171
    2           5.4112
    3           5.3986
    4           5.0819
    5           3.8516
    6           1.3756
    7           -3.7109

Run level: Report
Convergence obtained in 7 iterations
Time      359 milliseconds
FixMem driver done
Process ended
```

At the bottom of the window is a button labeled "Done".

The number that represents the error is defined as follows:

$$Error = \log(Norm) - \log(Tolerance)$$

where Norm is the square root of the sum of the squares of the errors in each separate model equation and Tolerance is the (user defined) value to which Norm is compared to determine convergence. It can be seen that last number shown in the image above is negative demonstrating that the simulation has converged to within the specified tolerance.