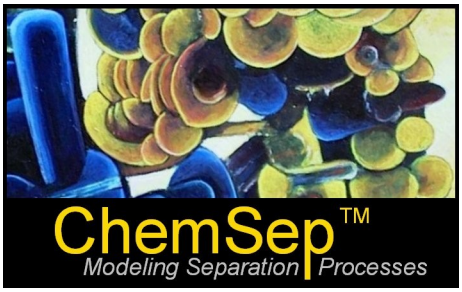


What's New in ChemSep 6.3

Harry Kooijman and Ross Taylor

ChemSep 6.3 has many new features and very many more minor upgrades and small improvements that, by and large, are invisible to most users. In this document we identify and describe the most important new features in ***ChemSep***™

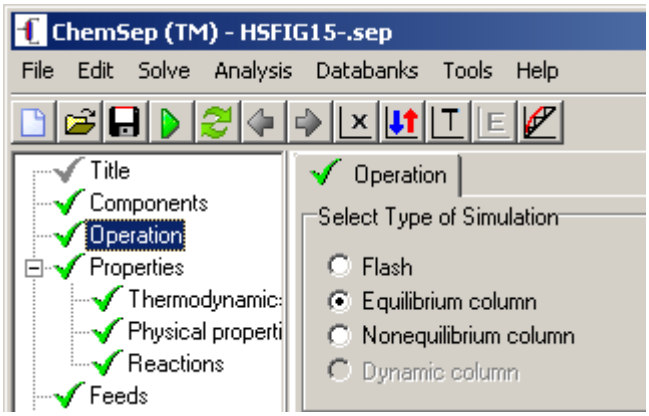
1. New: Equilibrium Stage Model and Efficiency Calculation *and* internals design
2. New: CAPE-OPEN Interface
3. New: Models for the System factor
4. New: Billet and Schultes (1999) models for packed column performance
5. New: Proprietary model for packed column performance developed by Raschig Gmbh.
6. New: Packed Column Design methods
7. New: Efficiency Derating
8. Improved: Packings Database
9. Improved: Operation limits plot
10. Improved: Output tables

The new models for the System Factor are described in a separate tutorial.

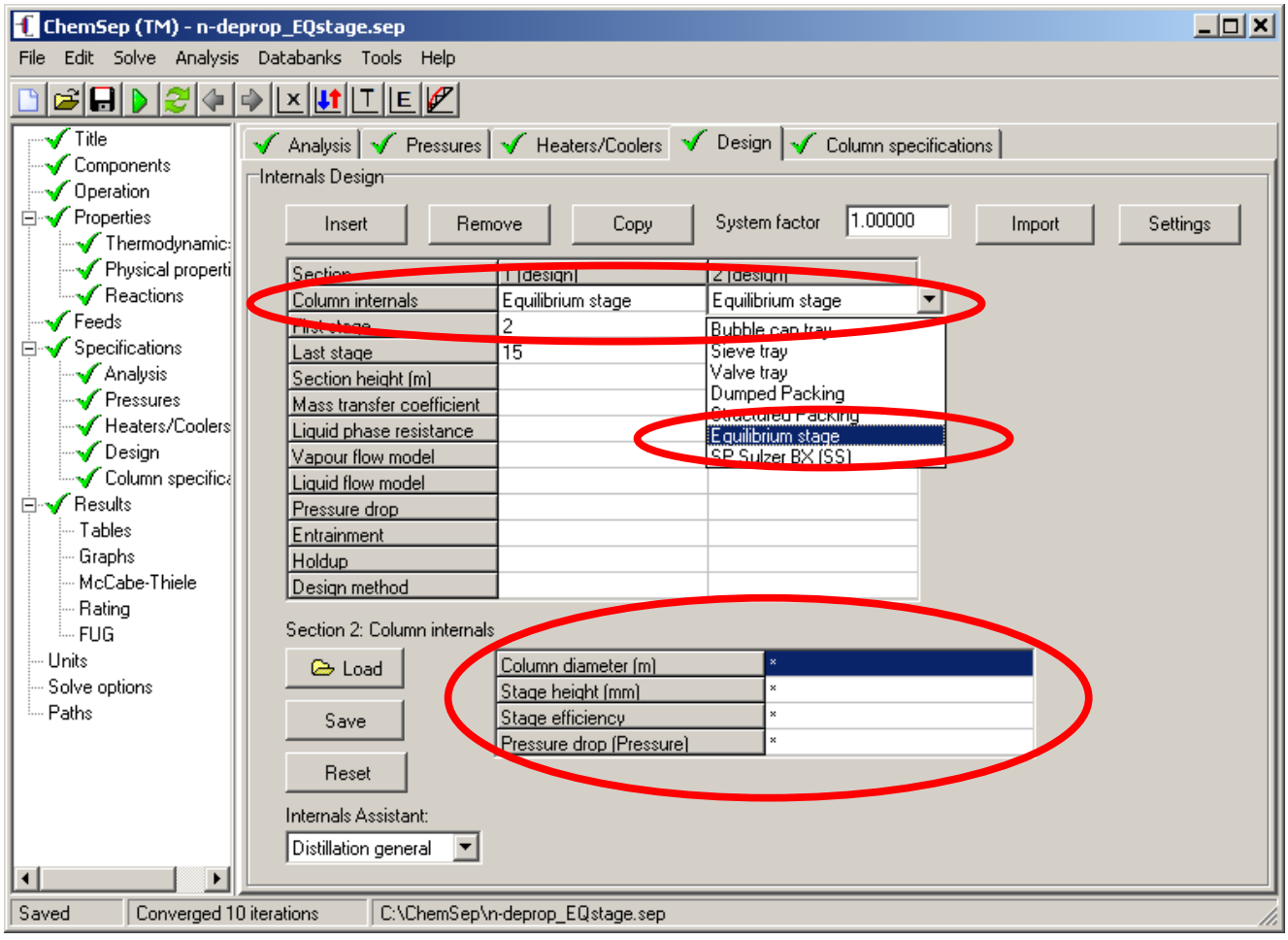
New: Equilibrium Stage Mass Transfer Model with Internals Design!

ChemSep now includes no less than 3 ways to model columns using the classical equilibrium stage model.

The first and most obvious way to choose the equilibrium stage model is on the *Operation* panel as shown below.

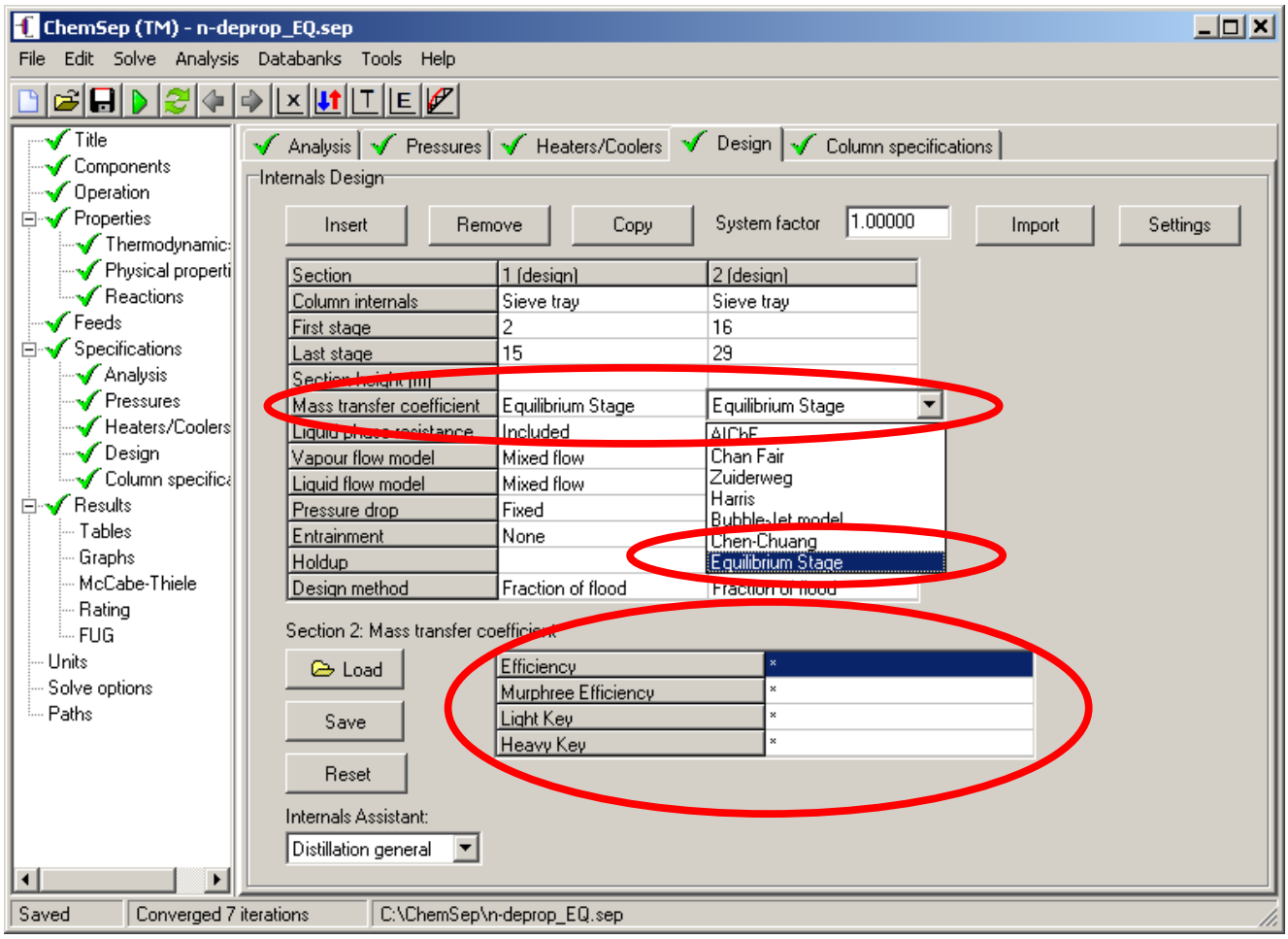


It may come as something of a surprise to many *ChemSep* users that the equilibrium stage model also is available after selecting the ***Nonequilibrium*** *model* on the above panel. In fact, the second method of selecting the equilibrium stage model, via the ***Design*** panel as shown below has always been part of *ChemSep*.



Here we see that an equilibrium stage can be selected as a possible **Column internal** in the same way that sieve trays, structured packing and so on can be selected. In fact, it is possible to model a column with a mixture of equilibrium stages together with sieve trays, valve trays, and packed sections should that be desired. The bottom part of the design panel lists the design parameters that may be specified for the equilibrium stage internal. **Note that none of these design parameters are calculated by the program**. The default value of the stage efficiency is 1; the default value of the other three parameters is 0.

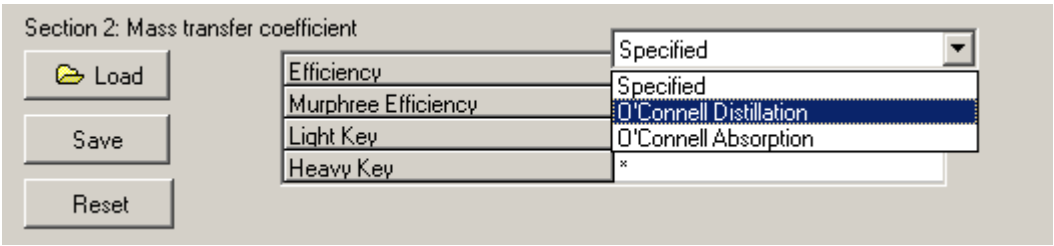
The third (and the only new) **way of selecting the equilibrium stage model is as a mass transfer coefficient model for any of the column internals** (EXCEPT the equilibrium stage model)**!** The screen shot below shows the equilibrium stage mass transfer model selected for a column fitted with **sieve trays**.



There is a very important difference between the equilibrium stage model as a column internal and as a mass transfer coefficient model. If selected as a mass transfer model it is necessary first to select the type of internal **and, as noted above, that internal cannot be the equilibrium stage model**.

Note the parameters section in the bottom part of the panel shown above (and it compare to the corresponding section shown above for the equilibrium stage internal. There are some similarities, but the equilibrium stage mass transfer model parameters do not include the diameter and stage height, although it does appear that both options have the efficiency in common.

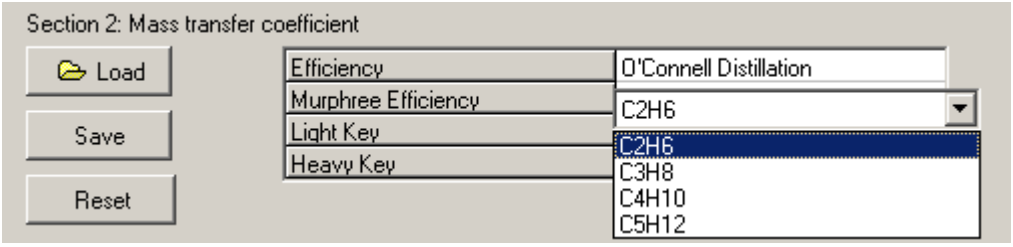
Click in the white space to right of *Efficiency* and you will see a drop down list appear:



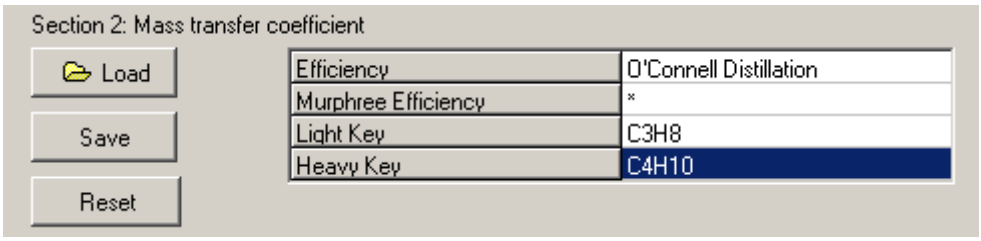
We see that for the equilibrium stage mass transfer model we may specify the efficiency (as also was the case for the equilibrium stage internal). We may also choose to calculate the efficiency using one of two O'Connell correlations: that for distillation or the one for absorption! These options are not available for either of the other two methods of selecting the equilibrium stage model.

If we elect to specify the tray efficiency then its value must be entered on line 2 of this section.

If we select either of the O'Connell methods then we need not enter anything on line 2 (it will be ignored if we do). In this case, however, we must select the light and heavy key components. Click in the white cell to the right of **Light Key** to see a list of compounds:

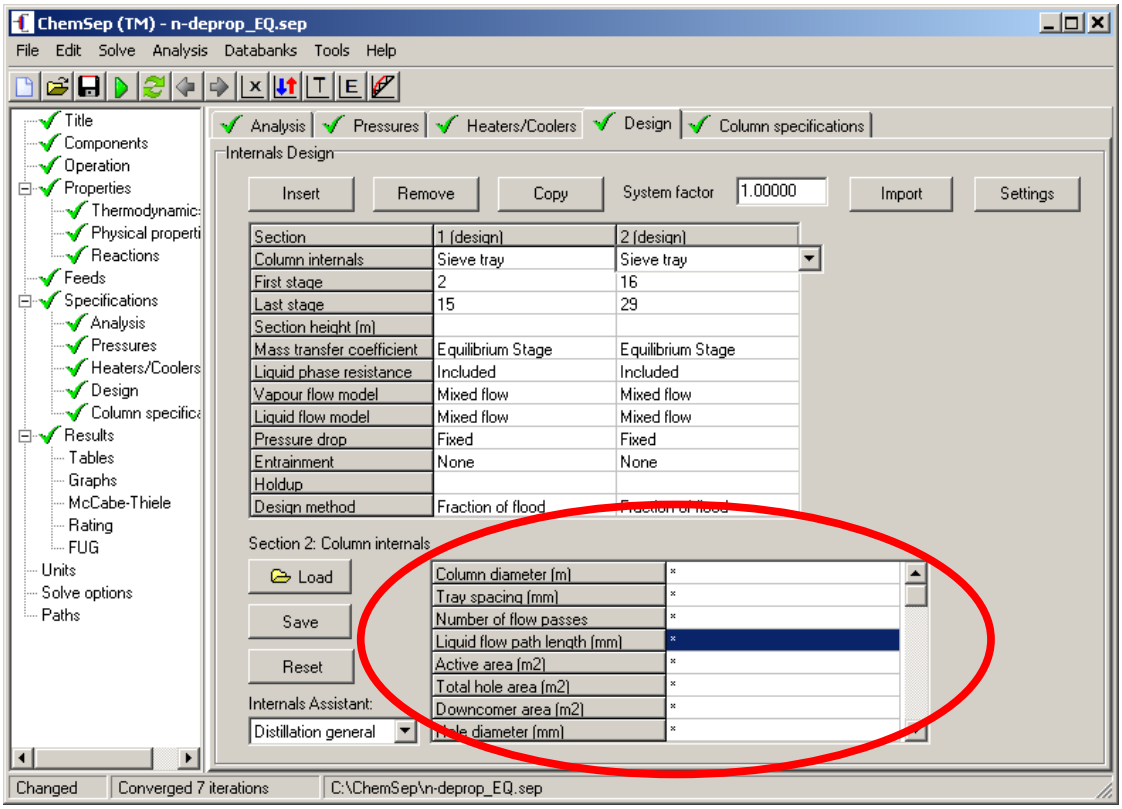


Select the light key from the list that appears. Repeat this action to select the heavy key in the white cell below. For the example shown here this part of the design panel now looks like this:



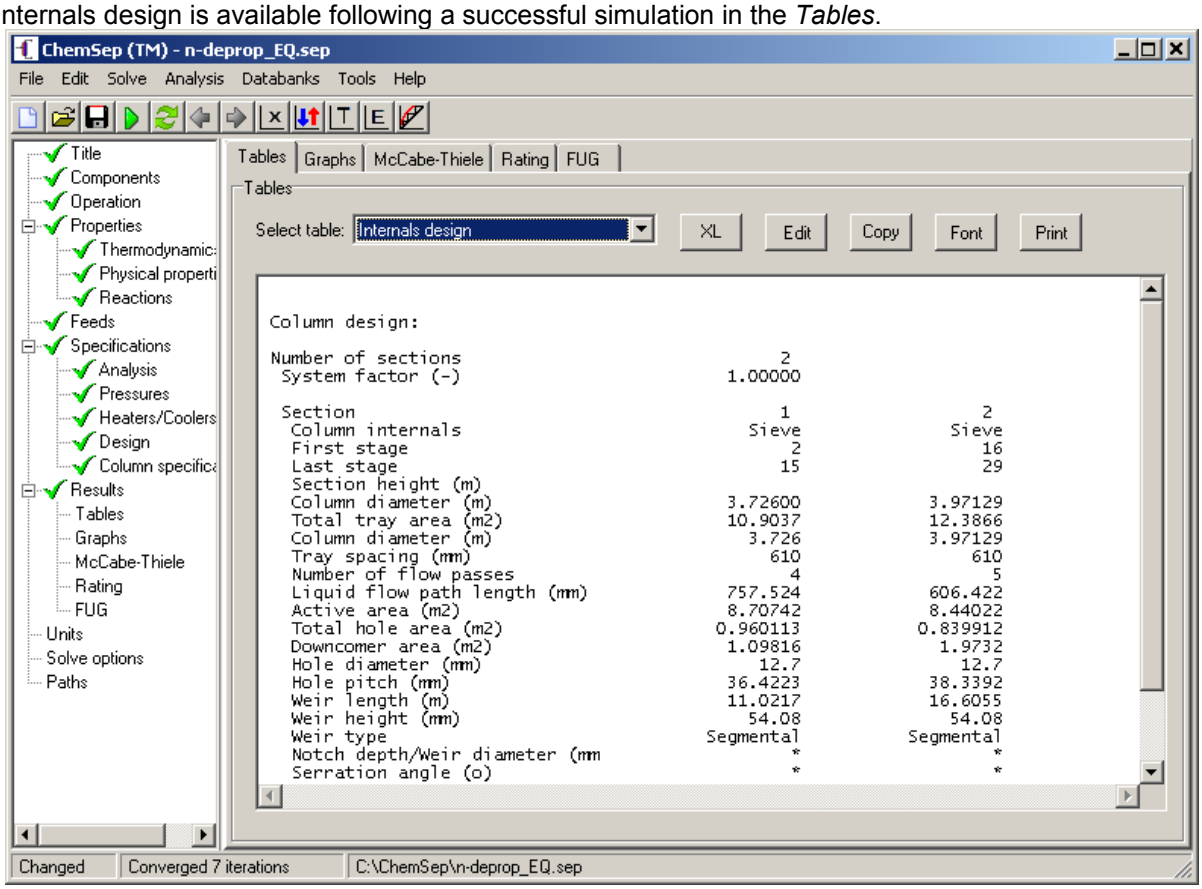
If the key compounds are not specified then *ChemSep* will estimate the O'Connell efficiency for all possible binary pairs in the mixture and then compute the average value of all of these efficiencies to use in the simulation!

Click on the column internal to see the equipment design section at the bottom of the panel:

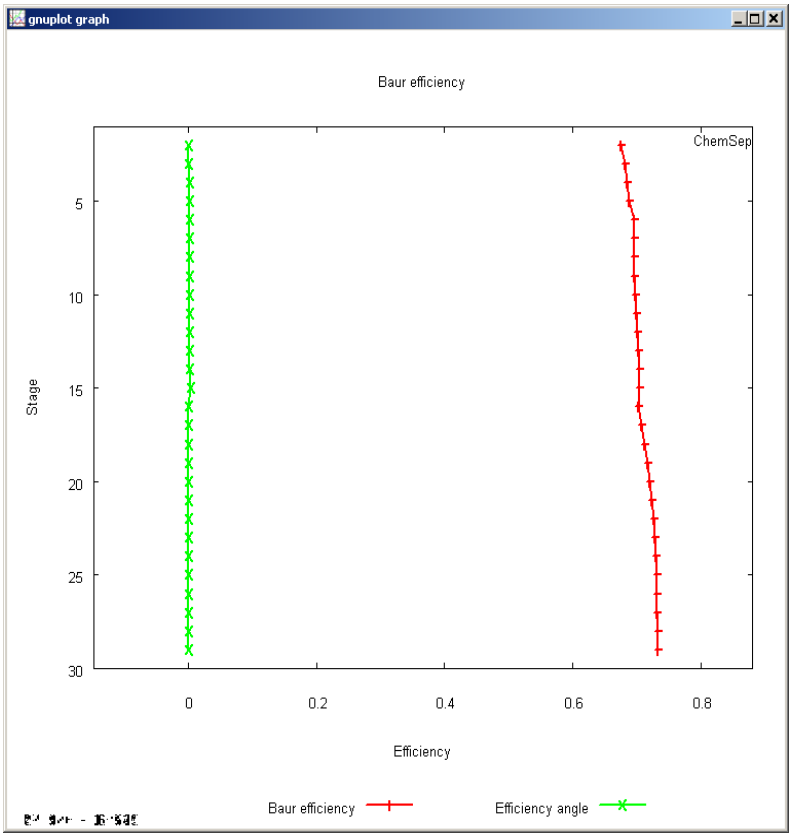


If we leave this section empty (as is the case here) then *ChemSep* will carry out tray (or packed column) sizing calculations. These equipment sizing calculations are not done for the equilibrium stage internal (because *ChemSep* does not then know what kind of column section – tray or packing – to design).

The internals design is available following a successful simulation in the *Tables*.



The estimated efficiencies are also available either in a table or as shown below:



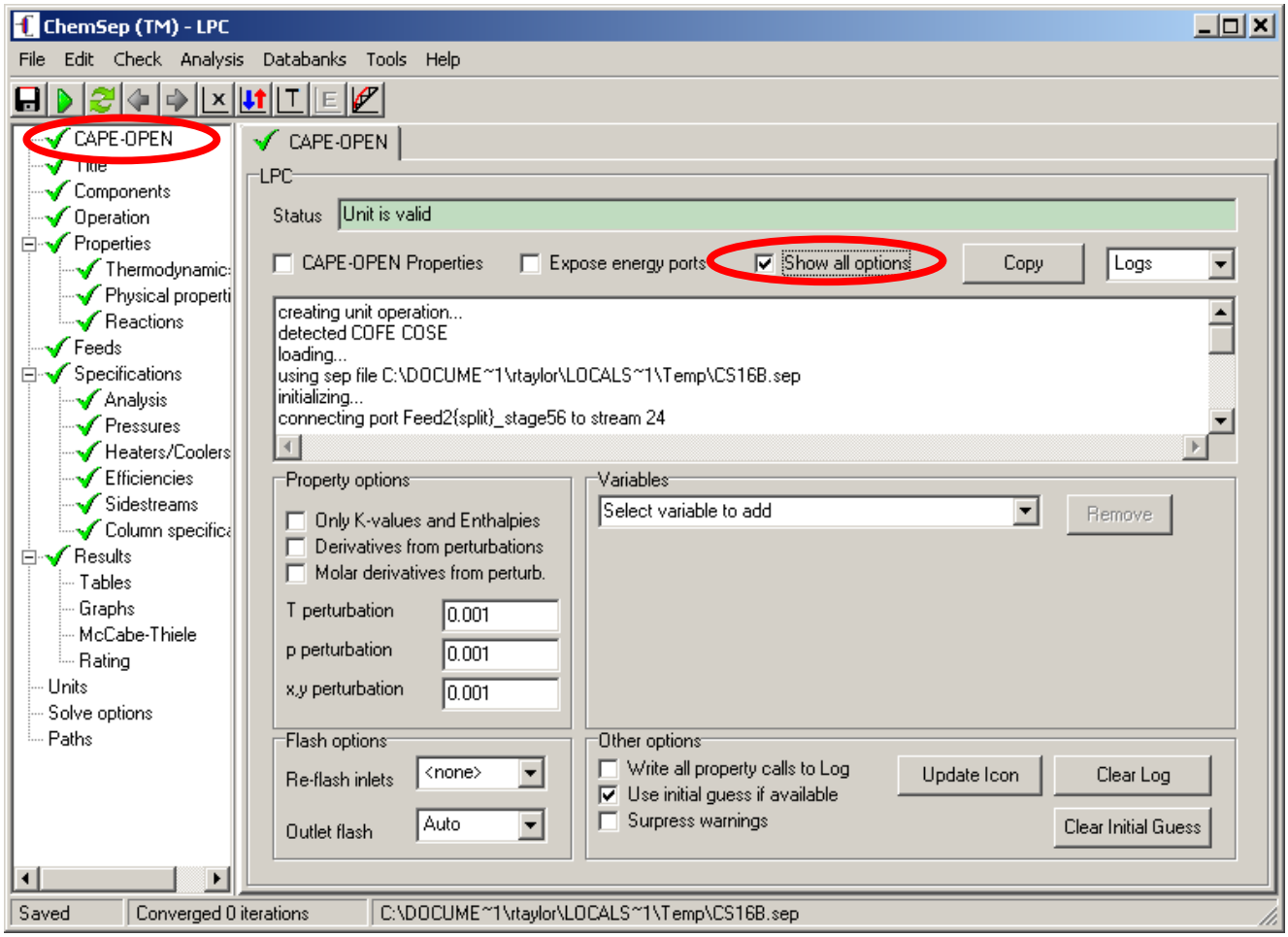
The Baur efficiency shown here is the same as the Murphree stage efficiency in this case (the reasons for this are discussed in our tutorial on efficiencies).

Note: the design options do not have to be the same in all column sections.

New: CAPE-OPEN Interface

ChemSep 6.3 has been CAPE-OPEN compliant for a log time. What is new with version 6.3 is the interface between the external program (this would be a flowsheet simulation program such as COCO – see www.cocosimulator.org) and *ChemSep*. The CAPE-OPEN interface now is part of the *ChemSep* interface itself.

If *ChemSep* has been called from a CAPE-OPEN simulator the CAPE-OPEN panel in *ChemSep* is visible:

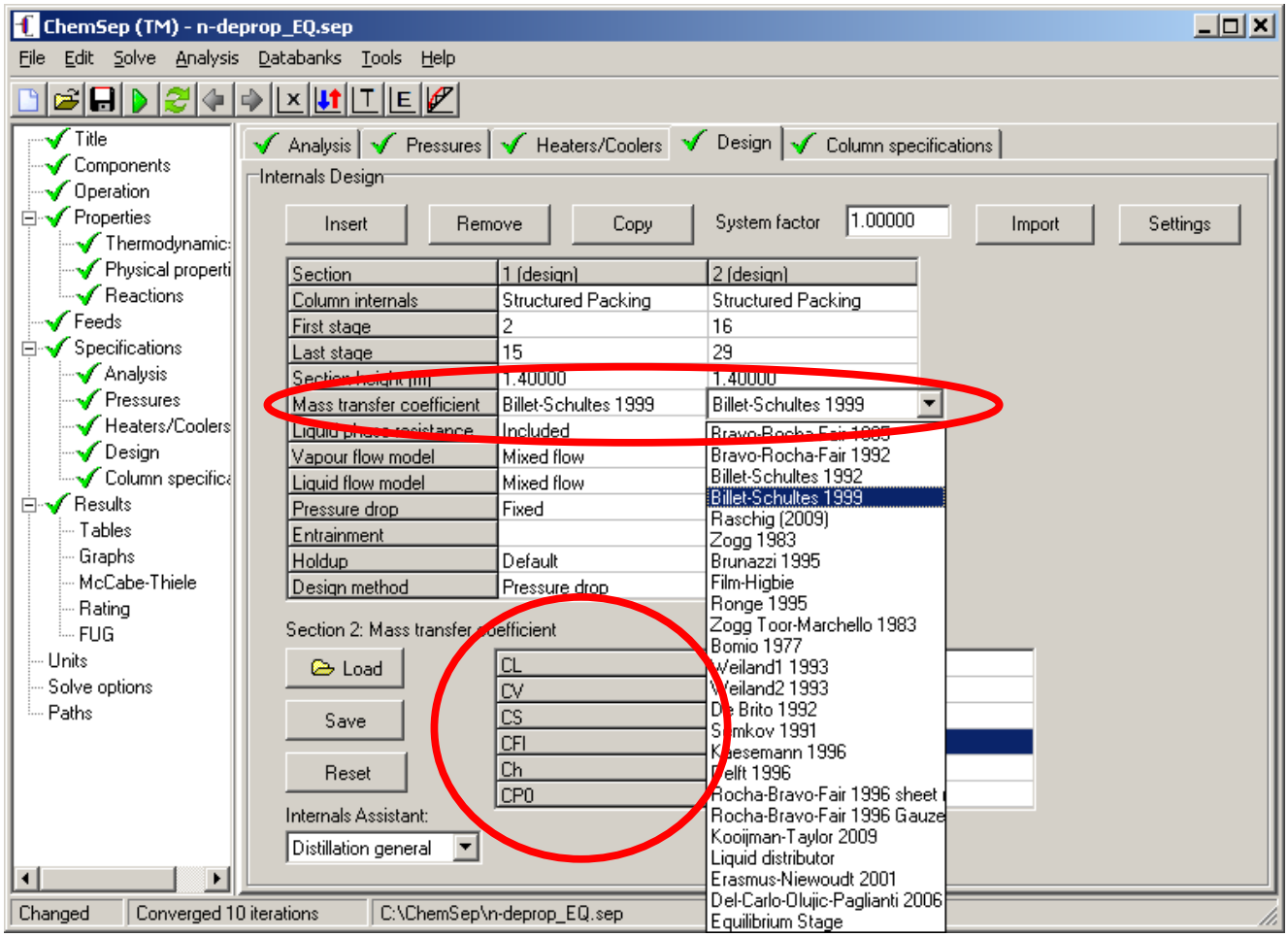


The lower half of this panel usually is hidden from view, becoming visible when the *Show all options* is checked (highlighted in the rightmost of the red ovals above).

New: Correlations for Packed Column Performance

ChemSep 6.3 includes two new models for estimating mass transfer coefficients and pressure drop in packed columns. These are the model of Billet and Schultes (1999) and a proprietary model developed at Raschig Gmbh and included in ChemSep with their permission.

To select either of these models click on the mass transfer coefficient model selection for a packed column section:



The Billet and Schultes (1999) model requires a number of parameters to be entered in the lower part of the Design panel (visible after selecting the Billet and Schultes model or by clicking again in the mass transfer coefficient cell). Parameters for some packings are available in the original paper by Billet and Schultes as well as in some standard textbooks (e..g Separation Process Principles by J.D. Seader and E.J. Henley, Wiley New York 2002).

Important notes:

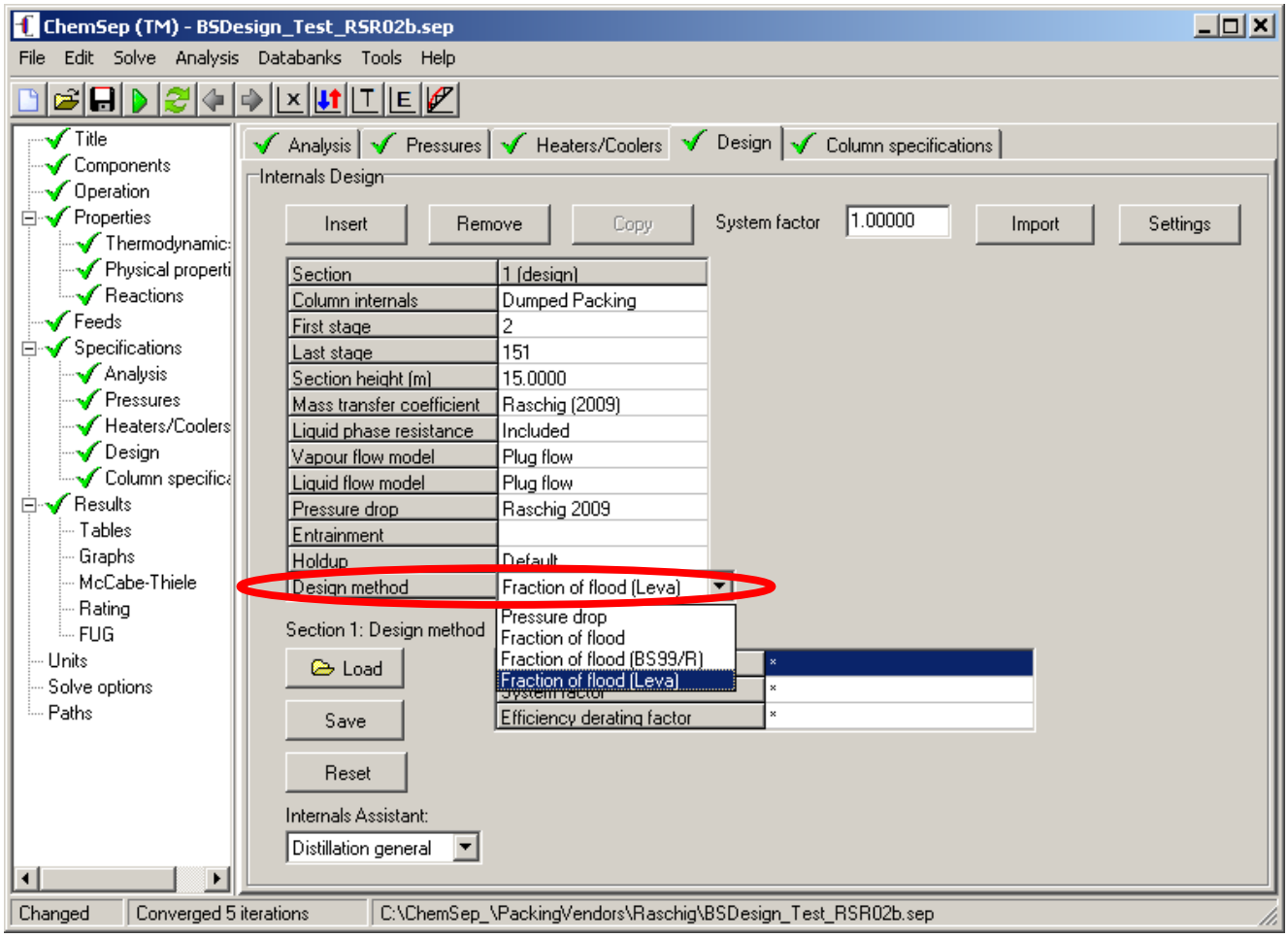
1. The parameters for the Billet and Schultes model must be entered separately for each column section for which the model is selected.

2. *ChemSep* does not require the Billet and Schultes model to be selected for both mass transfer and pressure drop (although one may certainly do so). The model parameters must be entered separately for the pressure drop model.

ChemSep 6.3 also includes proprietary models for mass transfer and pressure drop developed by Raschig Gmbh. Parameters for this model are loaded automatically at run-time if they are available. It is important to note that parameters for the Raschig correlations are available primarily for packings manufactured by Raschig Gmbh.

New: Packed Column Design Methods

ChemSep has always included two different methods for sizing packed columns. These are described in *The ChemSep Book* (see www.chemsep.com\book) and in the technical section of the *ChemSep* help system. Version 6.3 introduces two new packed column sizing method. Click on the *Design Method* to see a list of possible design methods:



The new methods are:

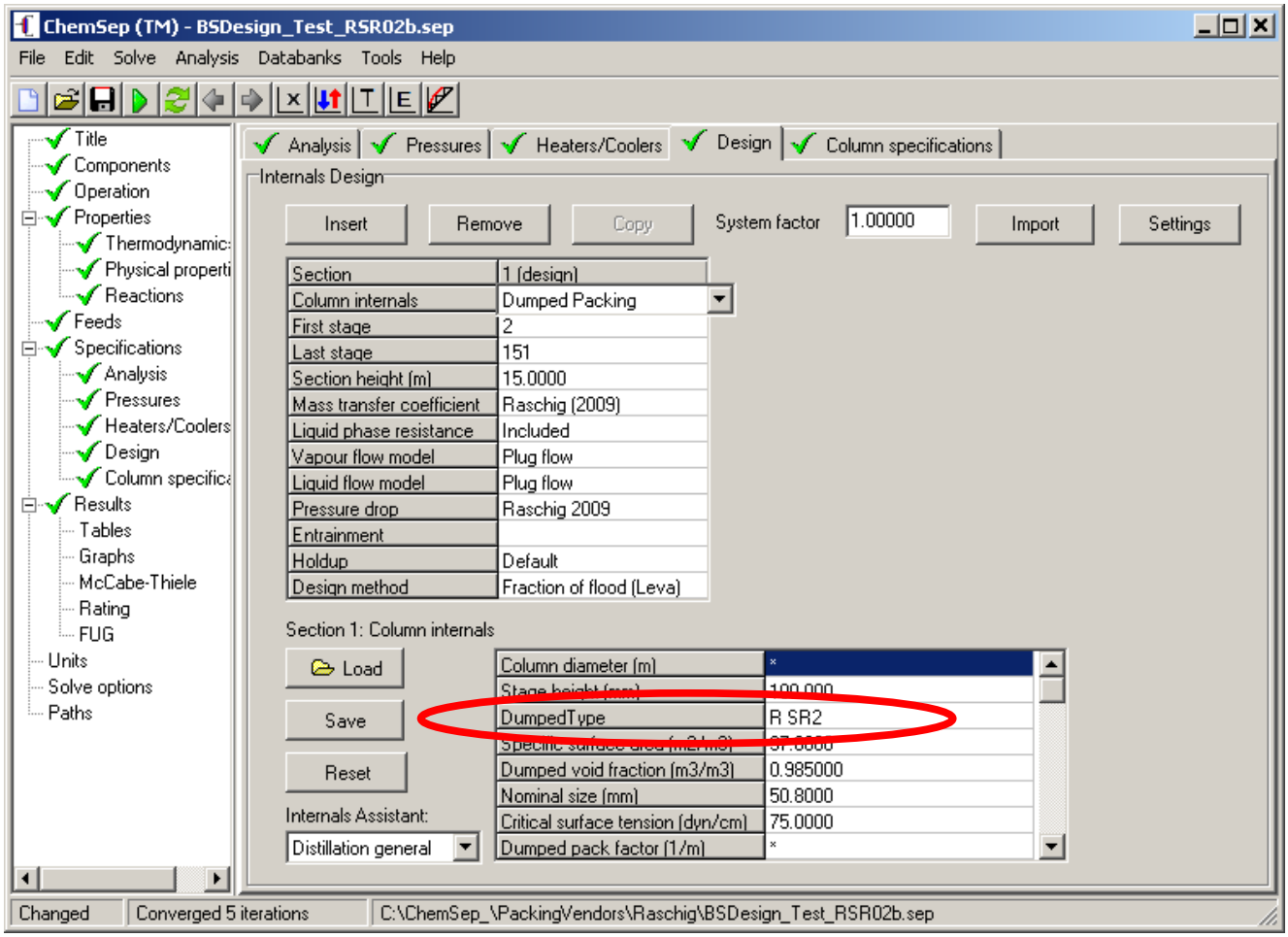
- Fraction of Flood (BS99/R)
- Fraction of Flood (Leva)

In the first of these two methods the diameter is calculated using the flooding velocity calculated from either the method of Billet and Schultes (1999) or from the Raschig model. Note that if this option is selected then the BS99 method will be used if the Billet and Schultes method was chosen as the pressure drop model; the Raschig method will be used to calculate the flooding velocity if that method is selected to calculate the pressure drop. The Raschig model can also be used to calculate the flooding velocity if some method other than either of these two models was selected for the pressure drop!

The Leva design method uses the well-known Leva version of the GPDC to estimate the flooding velocity. Note that the original design by fraction of flooding method in *ChemSep* may also employ the Leva method if that model was selected as the pressure drop model. However, the way in which the calculations are done differs from the new (in *ChemSep*) method discussed here.

Improved: Packing Database

The files containing packing parameters have been revised as part of our ongoing work towards developing a validated set of design methods and correlations.



We now use a short name to identify the packing as shown inside the red oval in the image above. A few examples are:

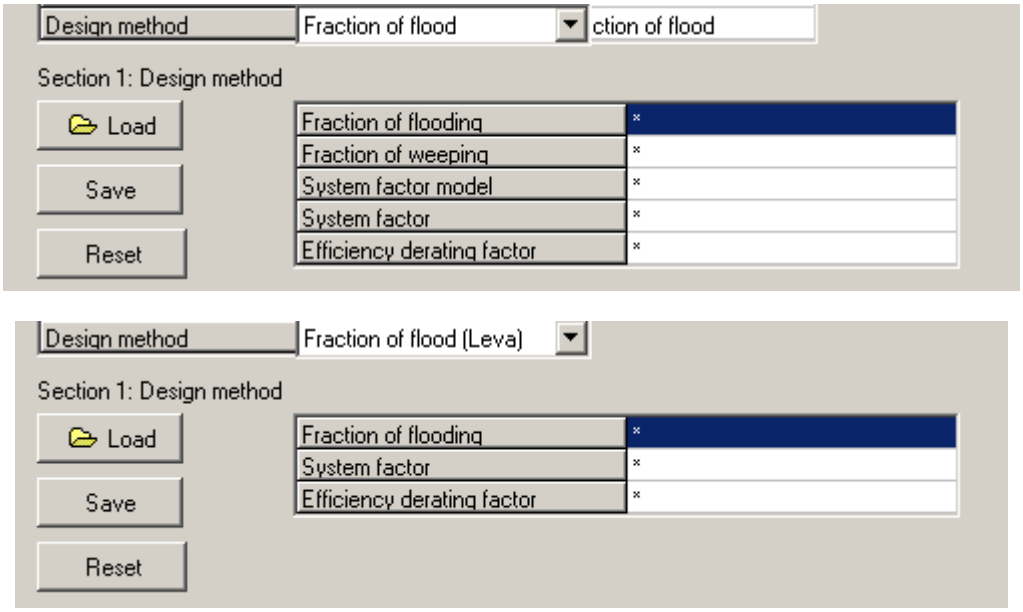
Vendor Name	*ChemSep* Name
Raschig SuperRings No. 2	R SR2
Sulzer Mellapak 250.X	S M250X
Koch-Glitcsh IMTP 40	KG IMTP40
Montz B1-200	M B1-200

These short names are used by some of the new correlations and design methods. For this reason, **if you use *ChemSep* to model packed columns it is essential that you reload the packing parameters** so that the correct short name will be written to the simulation case file.

New: Efficiency Derating

ChemSep 6.3 includes for the first time the ability to apply safety factors to stage efficiencies and mass transfer coefficients.

To enter a derating factor click in a cell for the internals design method as shown in the two views of part of the design panel that appear below.



Efficiency derating works by multiplying the efficiency or mass transfer coefficient by a "safety factor". For example, if an efficiency model is used (as discussed above) the value of efficiency used in the simulation is

$$E_{used} = E_{estimated} \times DeratingFactor$$

If a mass transfer coefficient model is selected then

$$[ka]_{used} = [ka]_{estimated} \times DeratingFactor$$

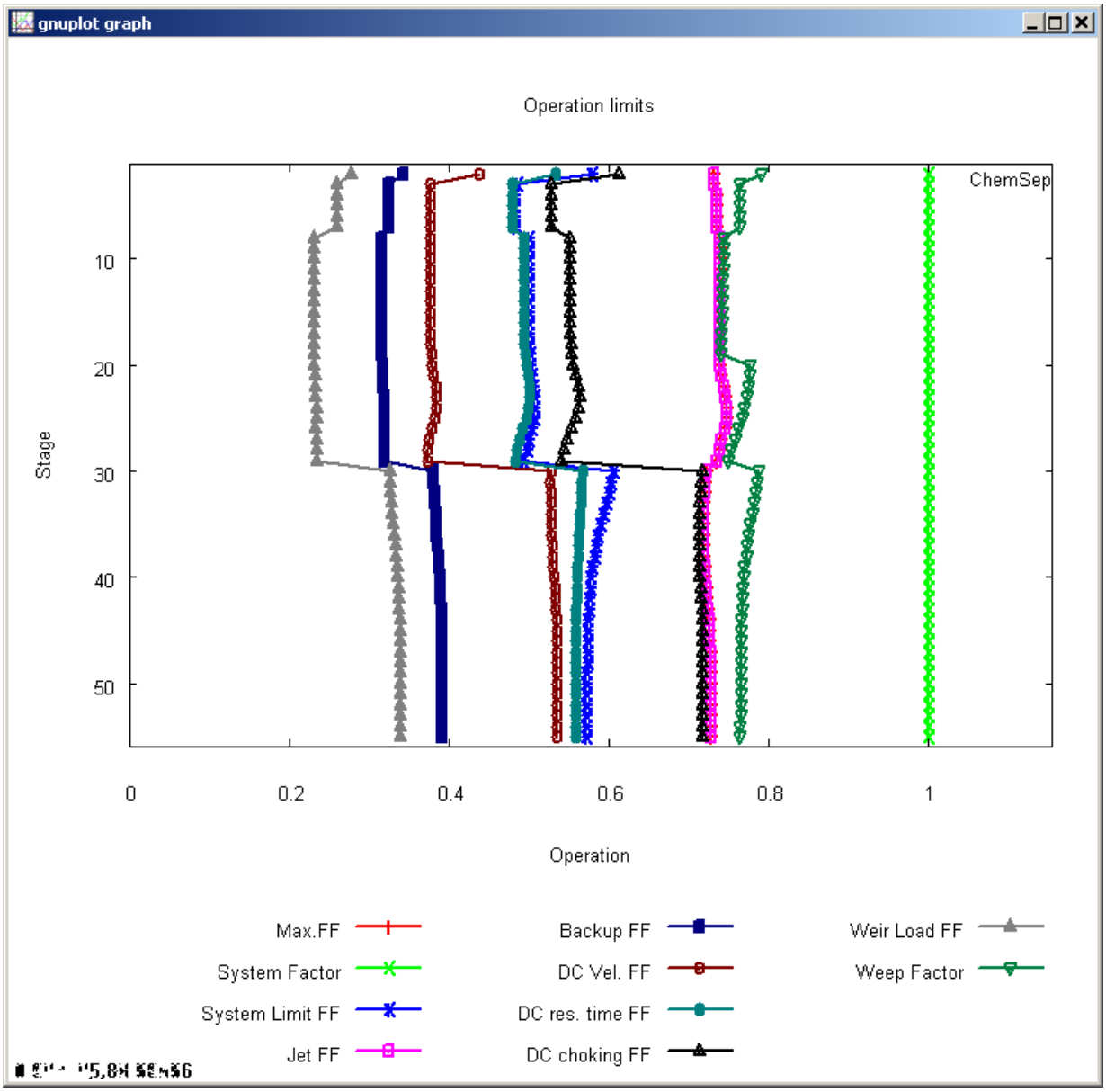
where $[ka]$ is the product of the mass transfer coefficient and interfacial area.

The default value of the *Derating Factor* is 1.

It is possible to specify values of the *Derating Factor* that exceed 1; caution must be exercised in interpreting the results from such a simulation (assuming that the calculation works – something that becomes increasingly less likely as the *Derating Factor* increases in value).

Improved: Plot (and Table) of Operation Limits

The Operation Limits plot provided by *ChemSep* 6.3 provides much more information than it did in earlier versions of the program. The example below is for a column with 54 valve trays (FF stands for fraction of flooding).



The many different lines on this diagram are described briefly below:

The **Max FF** is the largest of the various flooding factors and is shown in red. Often, as is the case here, it is not visible in the above plot; being entirely hidden behind one of the other flood factors.

System Factor – also known as the foaming or derating factor. This parameter was either specified or calculated from a model as discussed in a separate tutorial.

The **System Limit**, or Ultimate Capacity is given by the smaller of C_1 and C_2 where

$$C_1 = 0.445\,(1-F)\,(\sigma/(\rho_L-\rho_V))^{0.25} - 1.45\mathrm{u}_L$$

$$C_2 = 0.356\,(1-F)\,(\sigma/(\rho_L-\rho_V))^{0.25}$$

where u_L is the superficial liquid velocity in m/s and where

$$F = \frac{1}{\left(1 + 1.4\left(\rho_L - \frac{\rho_V}{\rho_V}\right)^{0.25}\right)}$$

The surface tension should be in dyne/cm and the density in kg/m^3 when using the above equations. For considerable discussion of this concept see Stupin and Kister (*Trans. IChemE.*, **81A**, 136-146, 2003). For a brief introduction see *Separation Process Principles* (2nd Ed.) by J.D. Seader and E.J. Henley (Wiley, 2006 p218).

The *Jet Flood Fraction of Flooding* (**Jet FF**) - also known as *Entrainment Flooding*. - is calculated from

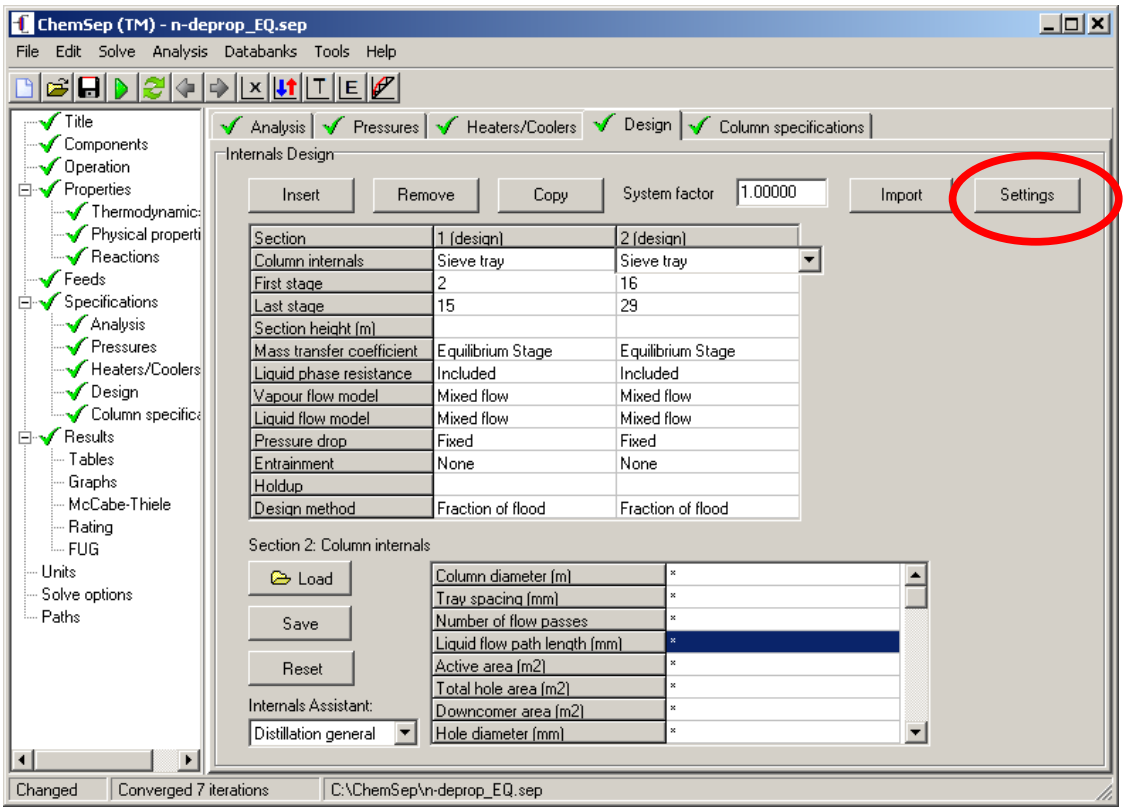
$$FF_{Jet} = u_V / u_F$$

where u_V is the superficial vapor velocity and u_F is the (estimated) flooding velocity.

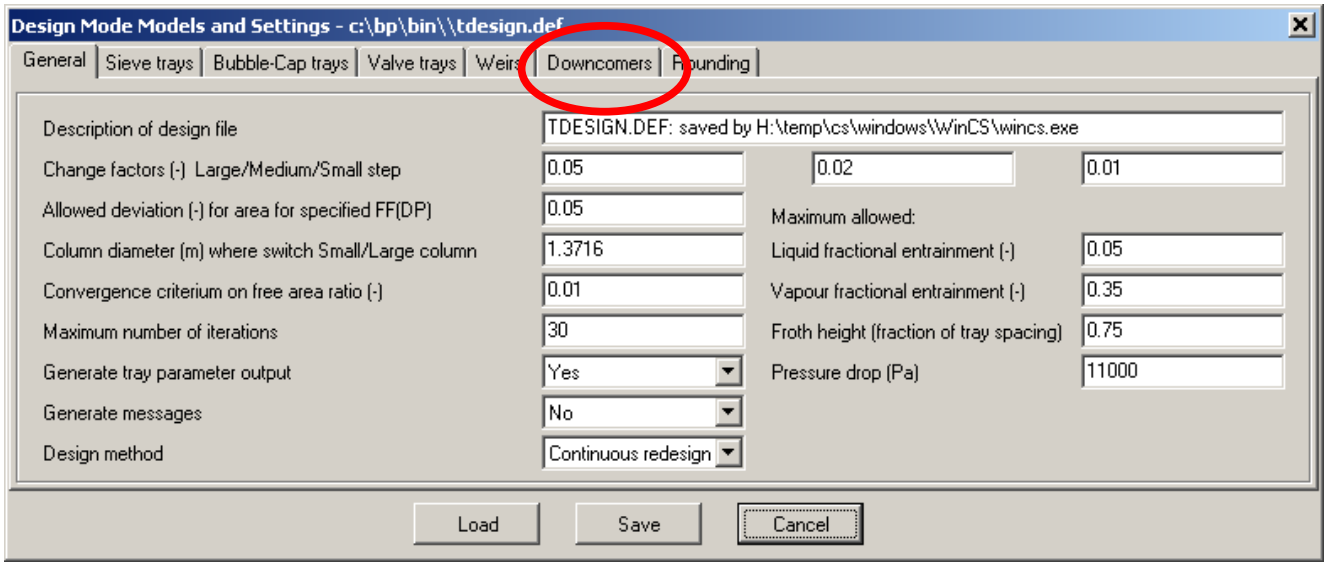
The *Downcomer Residence Time Flood Factor* (**DC res time FF**) is calculated from:

$$Time_{DC} = \frac{Minimum\ Residence\ Time}{Downcomer\ Residence\ time}$$

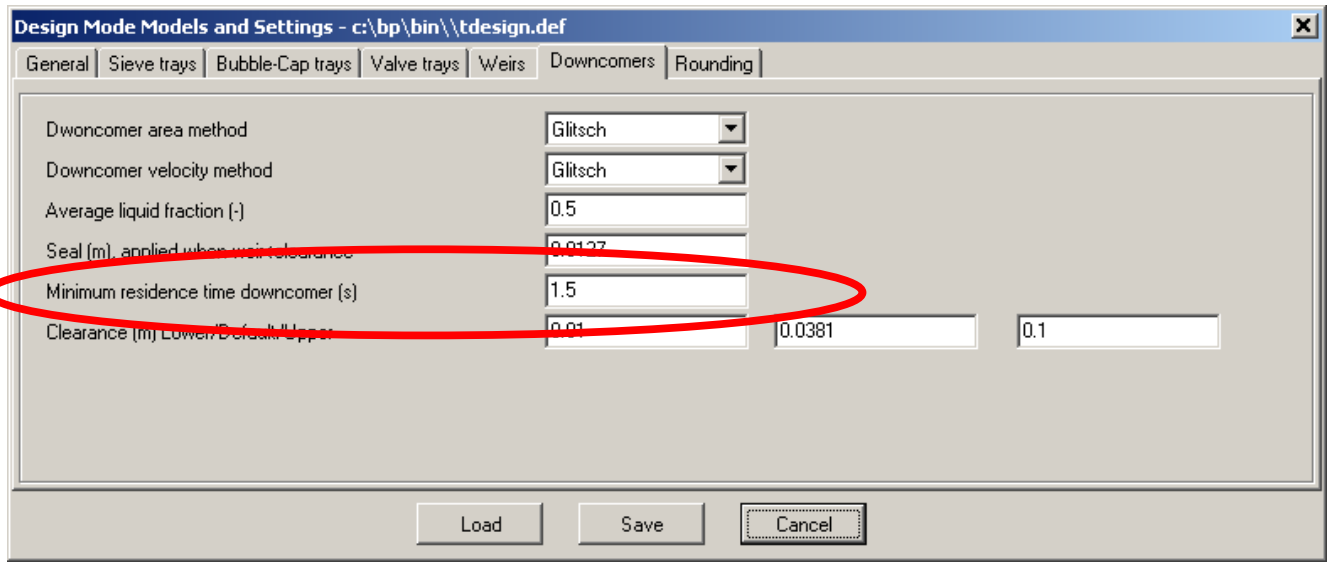
The *Minimum Residence Time* is specified in *ChemSep* and can be changed by the user. First locate the *Settings* button on the *Design* panel:



Click on this button to bring up the *Design Settings* in a separate window:



Click on the *Downcomers* tab (circled in red in the image above). The Minimum residence time can be set in the cell shown circled in the image below. The default value shown above is based on guidelines in *Distillation Design* by H.Z. Kister (McGraw-Hill, 1992, p291) noting further that the figure shown here is for clear liquid (as distinct from the lower density froth). For trays with very low flows the default value is probably too high.

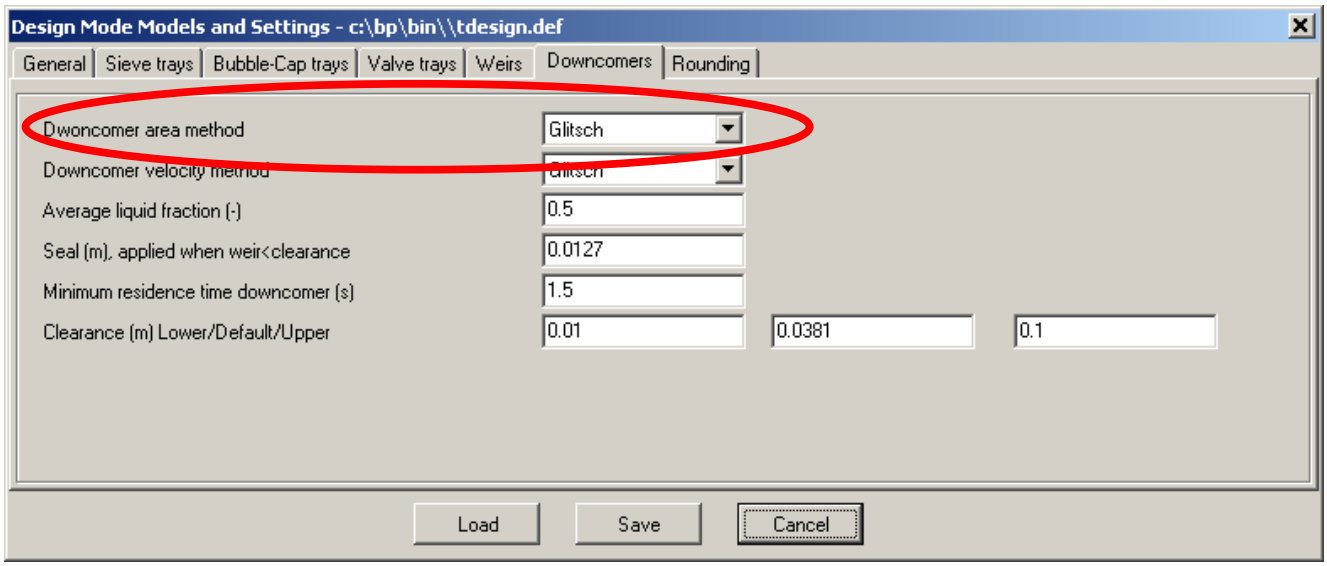


Downcomer backup flooding occurs when the height of aerated liquid in the downcomer exceeds the tray spacing. The **Backup FF** in the above plot is the ratio of the actual height to the calculated backup. The calculation of this height is described in *Distillation Design* by H.Z. Kister (McGraw-Hill, New York, 1992, p 283).

The *Downcomer Velocity Flood Factor* (**DC Vel FF**) is calculated from one of two ways. If the *Downcomer Area method* (see image below) is *Glitsch* then

$$FF_{DC\,backup} = \frac{Q_L}{A_d\, u_{L,DC,Glitsch}}$$

where $u_{L,DC,Glitsch}$ is the downcomer velocity calculated from the Glitsch method.



On the other hand, if the *Downcomer Area method* is *Koch* then

$$FF_{DC\,backup} = \frac{A_{d,Koch}}{A_{d,Actual}}$$

Liquid will backup onto the tray if the downcomer is not large enough. The Downcomer Choke Fraction of Flood (**DC Choking FF**) is estimated from:

$$FF_{DC\,Choke} = \begin{Bmatrix} 0.9\,(h_f - h_w)\,L_w / A_d & if\ h_f > h_w \\ 1 & if\ h_f \le h_w \end{Bmatrix}$$

where h_f is the froth height, h_w is the weir height, L_w is the weir length, and A_d is the cross sectional area of the downcomer.

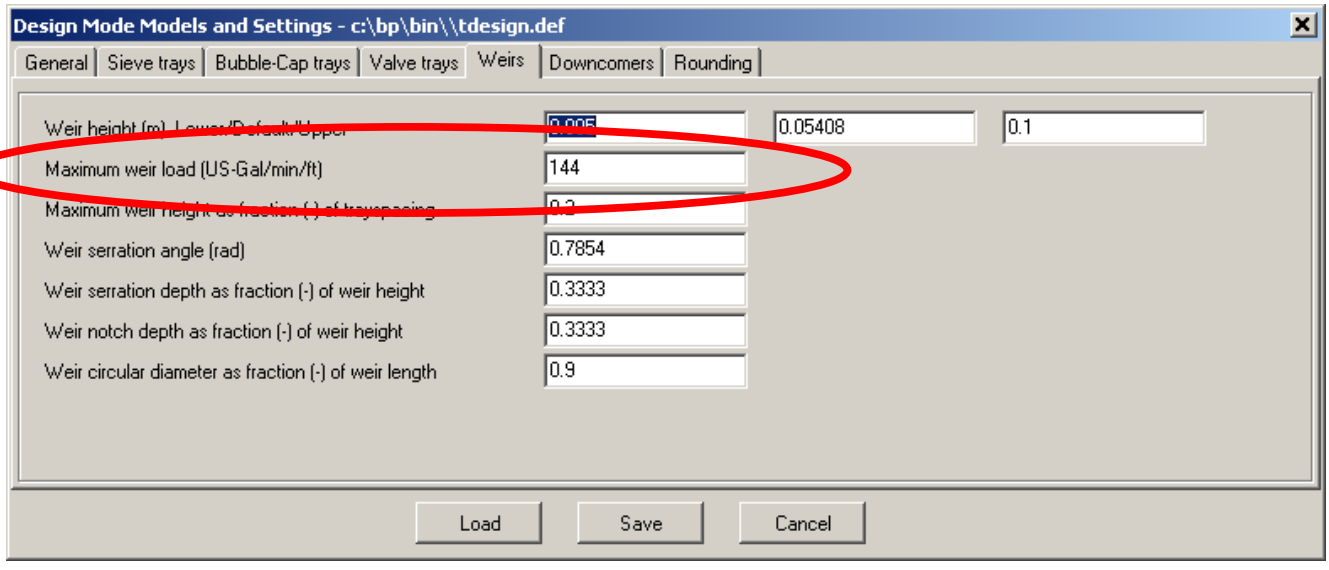
The *Weir Load* is the volumetric liquid flow rate per unit length of weir.

$$Q_{L,W} = Q_L / L_W$$

The **Weir Load FF** is calculated from

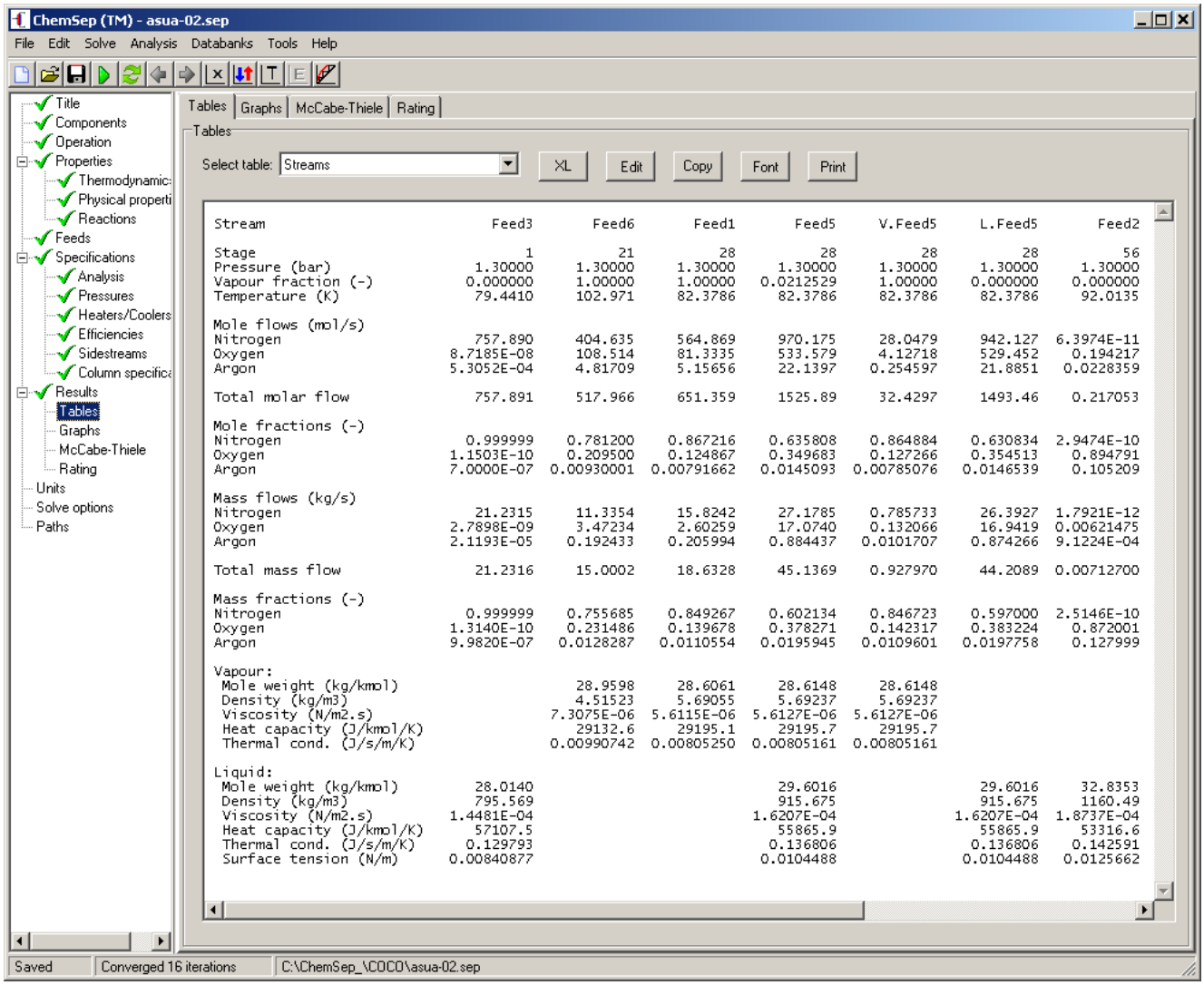
$$FF_{Weir} = Q_{L,W} / Q_{L,W,max}$$

The maximum weir load is set on the *Weirs* tab of the *Design Settings* window:



Improved: Flow and Stream Tables

For two phase feeds, *ChemSep* shows the state of the combined feed and, in separate columns, the flow rate, composition and columns of the vapor and liquid portions of the feed. An example is shown below; note the 3 columns for Feed 5.



Stream	Feed3	Feed6	Feed1	Feed5	V.Feed5	L.Feed5	Feed2
Stage	1	21	28	28	28	28	56
Pressure (bar)	1.30000	1.30000	1.30000	1.30000	1.30000	1.30000	1.30000
Vapour fraction (-)	0.000000	1.00000	1.00000	0.0212529	1.00000	0.000000	0.000000
Temperature (K)	79.4410	102.971	82.3786	82.3786	82.3786	82.3786	92.0135
Mole flows (mol/s)							
Nitrogen	757.890	404.635	564.869	970.175	28.0479	942.127	6.3974E-11
Oxygen	8.7185E-08	108.514	81.3335	533.579	4.12718	529.452	0.194217
Argon	5.3052E-04	4.81709	5.15656	22.1397	0.254597	21.8851	0.0228359
Total molar flow	757.891	517.966	651.359	1525.89	32.4297	1493.46	0.217053
Mole fractions (-)							
Nitrogen	0.999999	0.781200	0.867216	0.635808	0.864884	0.630834	2.9474E-10
Oxygen	1.1503E-10	0.209500	0.124867	0.349683	0.127266	0.354513	0.894791
Argon	7.0000E-07	0.00930001	0.00791662	0.0145093	0.00785076	0.0146539	0.105209
Mass flows (kg/s)							
Nitrogen	21.2315	11.3354	15.8242	27.1785	0.785733	26.3927	1.7921E-12
Oxygen	2.7898E-09	3.47234	2.60259	17.0740	0.132066	16.9419	0.00621475
Argon	2.1193E-05	0.192433	0.205994	0.884437	0.0101707	0.874266	9.1224E-04
Total mass flow	21.2316	15.0002	18.6328	45.1369	0.927970	44.2089	0.00712700
Mass fractions (-)							
Nitrogen	0.999999	0.755685	0.849267	0.602134	0.846723	0.597000	2.5146E-10
Oxygen	1.3140E-10	0.231486	0.139678	0.378271	0.142317	0.383224	0.872001
Argon	9.9820E-07	0.0128287	0.0110554	0.0195945	0.0109601	0.0197758	0.127999
Vapour:							
Mole weight (kg/kmol)		28.9598	28.6061	28.6148	28.6148		
Density (kg/m3)		4.51523	5.69055	5.69237	5.69237		
Viscosity (N/m2.s)		7.3075E-06	5.6115E-06	5.6127E-06	5.6127E-06		
Heat capacity (J/kmol/K)		29132.6	29195.1	29195.7	29195.7		
Thermal cond. (J/s/m/K)		0.00990742	0.00805250	0.00805161	0.00805161		
Liquid:							
Mole weight (kg/kmol)	28.0140			29.6016		29.6016	32.8353
Density (kg/m3)	795.569			915.675		915.675	1160.49
Viscosity (N/m2.s)	1.4481E-04			1.6207E-04		1.6207E-04	1.8737E-04
Heat capacity (J/kmol/K)	57107.5			55865.9		55865.9	53316.6
Thermal cond. (J/s/m/K)	0.129793			0.136806		0.136806	0.142591
Surface tension (N/m)	0.00840877			0.0104488		0.0104488	0.0125662

Improved: Internal Flow Table

ChemSep 6.3 now displays the mass flows (as well as the molar flows) in the output flow table. An example is shown below.