# What's New in ChemSep™ 6.5

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In this document we identify and describe the most important new features in **ChemSep**. (Some of our users will note that some of the features described here actually made it into intermediate releases such as 6.31.)

1.  Updated: Mass transfer coefficient, and pressure drop models

2.  New: Packed column sizing methods

3.  Improved: Modeling columns at Total Reflux

4.  New: Option for piecewise linear pressure profile

5.  Updated: API SRK model and other improvements for thermodynamic properties

6.  Updated: Pure Component Databank

7.  New: CAPE-OPEN 1.1 Interface

8.  New: Cut and paste column columns of data

9.  New: Flooding comparison plot for packed columns

10. New: Capacity plot for packed columns

11. New: GPDC diagrams for packed columns

12. New: Getting more from the McCabe-Thiele diagram

13. New: Convergence methods

14. Improved: Parametric study features

15. New and Improved: Excel export

16. Other important improvements

# Updated: Mass transfer coefficient and pressure drop correlations

*ChemSep* 6.5 includes several new and updated correlations for mass transfer coefficients, interfacial area, and pressure drop. The changes are described below

**Constant Mass Transfer Coefficient**

New in *ChemSep* 6.5 is the option to specify fixed values for the mass transfer coefficients and for the interfacial area as shown in the partial screen shot below:
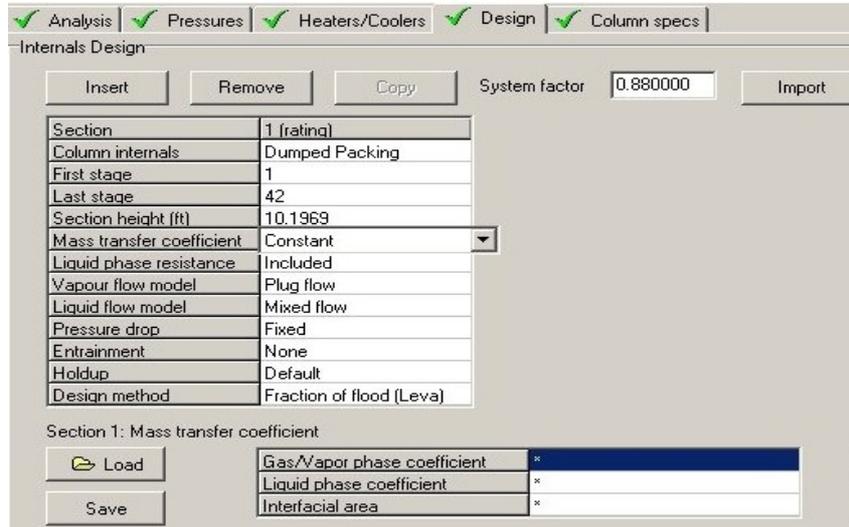


Note that since the coefficients are maintained constant by the program it is important to use the appropriate units (m/s for the mass transfer coefficients and $m^2$ for the area).

This option is used in some of the new convergence methods in *ChemSep* (see other section) but also has value for parameter fitting purposes (tuning mass transfer coefficients that fit plant operating data).

**Scheffe-Weiland correlation for valve trays**

*ChemSep* 6.5 includes the Scheffe-Weiland correlations for mass transfer coefficients and interfacial area on valve trays that were first introduced with *ChemSep* 3, but which had not until now, been included from Version 5 to 6.3.

The Scheffe-Weiland correlations express the mass transfer coefficients and interfacial area per unit tray are for the gas and liquid phases as follows:

$$Sh \text{ or } a = A\, Re_G^{\alpha}\, Re_L^{\beta}\, Sc^{0.5}\, W'^{\gamma}$$

where $Re$ and $Sc$ are the Reynolds and Schmidt numbers of the appropriate phase:

$$Re = \rho\, u_s\, d / \mu \qquad Sc = \mu / (\rho\, D)$$

where $d$ is a characteristic dimension (assumed in the Scheffe-Weiland method to be equal to 1m), $u_s$ is the superficial velocity (m/s) of the appropriate phase, and $W' = W/d$ is the scaled weir height. The numerical constants required for the calculation of the Sherwood numbers are:

$$Gas/vapor: A = 0.93 \quad \alpha = 0.865 \quad \beta = 0.130 \quad \gamma = 0.389$$

$$Liquid: A = 125 \quad \alpha = 0.884 \quad \beta = 0.087 \quad \gamma = 0.051$$

The interfacial area per unit tray area is obtained from an correlation of the same general form with

$$Relative\ interfacial\ area: A = 0.27 \quad \alpha = 0.375 \quad \beta = 0.247 \quad \gamma = 0.515$$

**Updated: Onda and Bravo & Fair correlations for random packings**

*ChemSep* 6.5 includes a new option for the Onda and for the Bravo & Fair correlations for random packings that permits the user to specify a characteristic dimension to be used in the correlation that is different from the nominal packing size specified by the packing manufacturer. Now, either of these correlations is selected you will see a new section appear below the main table on the design panel as shown below:
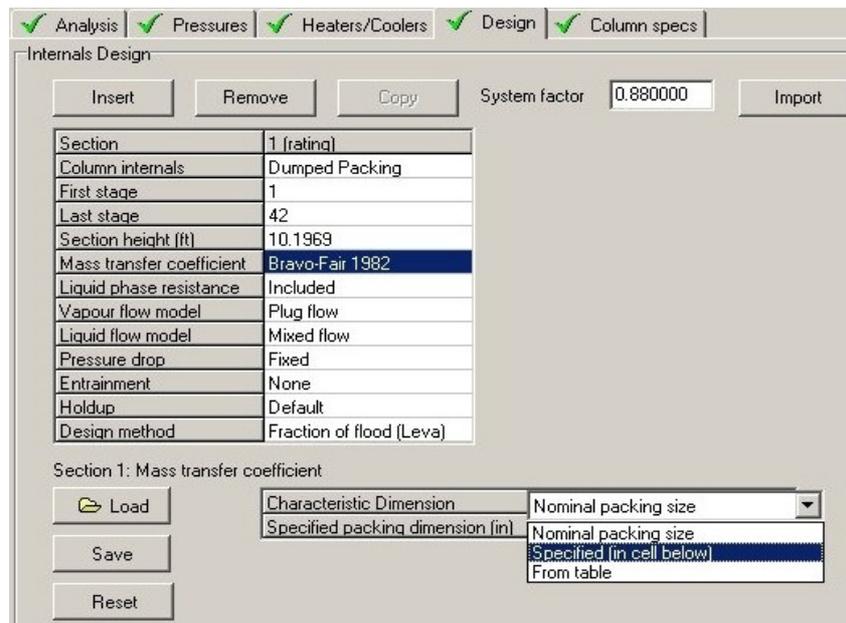


The options for specifying the characteristic dimension are also shown in this screen shot; they are:

1. Nominal packing size – in which *ChemSep* simply uses the dimension already supplied
2. Specified (in cell below) – in this case (and **only** in this case) the user must enter a value in the second (and last) cell in this mini-table
3. From table – in which case *ChemSep* reads a file that contains predefined values of the characteristic dimension.

**Note that the user is not required to select any of these options. In the event that no option is selected *ChemSep* will simply use the nominal packing size that was loaded when the packing was selected.**

**The packing dimension file is named PackSize.par and must be located in the \chemsep\ild folder**. It is a plain text file that can be edited with any text editor (e.g. Notepad, but not Word). The first few lines of the file supplied with *ChemSep* look like this:

```
# Column 2 = Characteristic dimenision
#
# IMPORTANT: First 31 characters are reserved
#           for the packing identifier.
#           dimension may start in col 32
#
Nutter No. 1                    0.0305
Nutter No. 1.5                  0.0406
Nutter No. 2                    0.0508
```

The # sign signifies a comment and there can be any number of these at the top of the file. The first 31 characters on each subsequent line are reserved for the **short name used by ChemSep to identify packings**.

If you wish to add new packings to this file and don't know what the short name is, click on the packing internals line on the design panel and look for the name in the table that will appear in the bottom part of the design tab sheet. The packing dimension (in m) starts in column 32. In the event that no dimension is listed for the selected packing the characteristic dimension will be set to the nominal packing size.
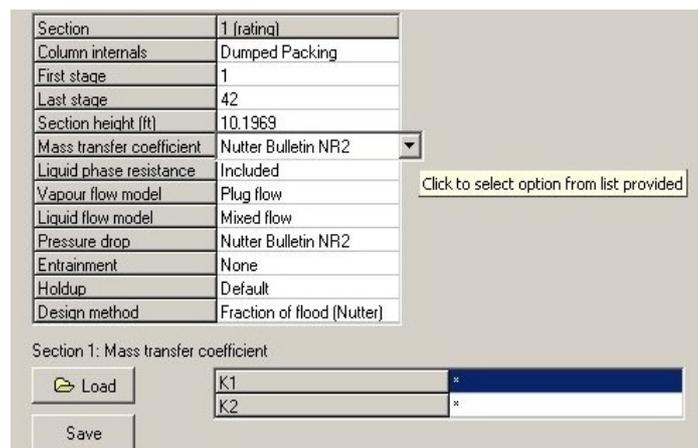
**New: Nutter correlations for Nutter rings**

New in *ChemSep 6.5* is are performance correlations for Nutter rings from the Nutter Bulletin NR-2.

Correlations are available for pressure drop:



and for mass transfer coefficients



The Nutter correlation for pressure drop is available only for Nutter rings 1, 1.5 and 2. In the event that the model is selected for other packing sizes the program will stop with an appropriate warning.

The mass transfer model for Nutter rings as described in the Nutter Bulletin NR2 is incomplete. Two parameters named K1 and K2 in the bulletin were never made public by Nutter. Thus, in order to use this model the user must provide values for both of these coefficients. Note that because the Nutter correlation is for heights of transfer units larger values of K1 and K2 signify poorer mass transfer performance.

Despite the lack of published values for K1 and K2 we have found the model useful for fitting performance data in columns filled with Nutter rings.

**Updated: Raschig correlation for packed columns**

The proprietary Raschig correlation in *ChemSep* has been updated in Version 6.5 and now includes a correction for pressure drop at high pressures. The correction is not applied automatically; rather it must be selected by the user. **It is important to note that the Raschig correlation has been tuned to column data at all pressure ranges including at high pressures.**

# New: Packed column sizing methods

*ChemSep* 6.5 includes several updated methods for estimating the diameter of a packed column. The methods are selected from the usual list on the *Design* tab sheet, which now appears as shown below:
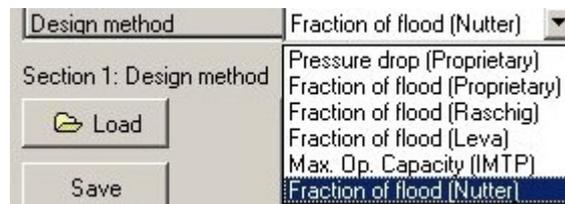


The methods are as follows:

1.  A proprietary method based on the pressure drop

2.  A proprietary method based on a specified fraction of flood

3.  A method that uses the Raschig correlation (if applicable) or the Billet and Schultes correlation (also of applicable) and the specified fraction of flood.

4.  A method that uses the Leva correlation for flooding

5.  A method that uses the fraction of the maximum capacity as defined for IMTP packings only.

6.  A method that used the flooding correlation from the Nutter Bulletin NR-2 (only for Nutter rings).
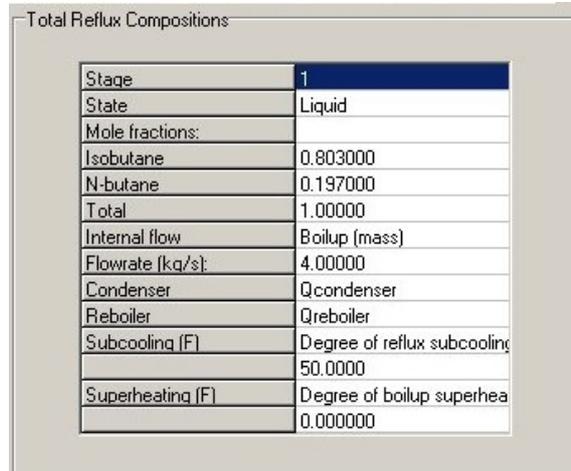
Methods 5 and 6 are entirely new with this version.

The default value of the fraction of flood is 0.75.

The default value of the fraction of maximum capacity of IMTP packing is 0.9. The maximum capacity is calculated from the curve fits of the capacity curves published by Koch-Glitsch or by Norton.

# Improved: Modeling columns at Total Reflux

Total reflux is only used for some experimental studies since there is no (or negligible) material loss from the column. To the best of our knowledge *ChemSep* is the only column simulation tool that includes a special feature for modeling total reflux operations. Version 6.5 introduces an improved *Total reflux* specification panel shown below.



The various items in this panel are shown below.

| Line | Description |
|------|-------------|
| Stage | Enter the number of the stage for which the mole fractions below belong. |
| State | Select (from a list) whether the mole fractions are for a liquid or vapor stream |
| Mole fractions | On the lines that follow enter the mole fractions of the designated stream |
| Total | This line shows the sum of the component mole fractions (type a 1 to normalize) |
| Internal flow | Select the internal flow to be specified from: Reflux or Boilup (in mass or molar units) |
| Flowrate | Specify the internal flow rate (in mass or molar units as selected on the line above) |
| Condenser | Name of the condenser |
| Reboiler | Name of the reboiler |
| Subcooling | Choose to specify the condenser temperature or the degree of condensate subcooling |
|  | Enter here the value of the temperature (or temperature difference) selected above |
| Superheating | Choose to specify the reboiler temperature or the degree of boilup superheating |
|  | Enter here the value of the temperature (or temperature difference) selected above |

The features that are new in Version 6.5 are the ability to specify mass flows (as an alternative to molar flows and to be able to set the condenser and/or the reboiler temperature (as an alternative to the degree of subcooling and superheating).

# New: Piecewise linear pressure profile

*ChemSep* 6.5 permits columns pressure to be given a piecewise linear profile. This new option is available on the *Pressure* panel.

Click on the column pressure line to bring up the list of options that includes *Specified pressure profile* as shown in the partial screen shot below.



Click on the Insert button to insert as many stages for which pressures are to be specified. Type in the stage numbers and the values of the pressures on those stages. You may give each specified pressure a name if desired (in other words, it is perfectly OK to leave empty the name column).

The pressure on stages not listed will be given values obtained by linear interpolation between the specified pressures. It is always necessary with this option to specify the pressure of the top stage of the column (this will be stage 2 if a condenser is present).

# New: ChemSep CAPE-OPEN Version 1.1 Thermodynamic Interface

*ChemSep 6.5* now offers two versions of the CAPE-OPEN thermodynamic standard; Version 1.0 and Version 1.1. This allows *ChemSep* to communicate with software systems that do not have a CAPE-OPEN thermodynamic interface standard version 1.0

# Updated: SRK Equation of State

*ChemSep* 6.5 now includes the Gray correlation for interaction parameters for the SRK Equation of State (*VLE Predictions for Multicomponent H2 Systems with Cubic Equations of State*, R.D. Gray, J.L. Heidman, R.D. Springer, and C. Tsonopoulos, Proc. 64th Annual Convention of the Gas Processors Association, pp289-298).

In its *Technical Data Book* the American Petroleum Institute (API) recommends methods for estimating physical and thermodynamic models for mixtures that are typically encountered in the petroleum industry. The API technical data book has long recommended a modified version of the SRK equation of state for estimating K-values and enthalpies. In *ChemSep 6.5* the API model has been upgraded to reflect the version of the SRK EOS described in the 8th edition of the book published in 2006. Pure component parameters for many compounds as well as interaction parameters (taken from the data book) are included in a new versions of the *ChemSep* databanks. Also included in *ChemSep 6.5* is an option to use the API correlation to estimate interaction parameters for binary pairs that are not included in the tables in the *API Technical Data Book*.

*If you have created your own databanks for use with ChemSep you will need to update your databank(s) so that they include the API parameters. Contact the authors for further information.*

# Updated: Pure Component Databank

The databank that is supplied with *ChemSep* has been updated to accommodate the parameters needed for the updated version of the SRK equation of state as recommended by the API (see above). As a result of the change to the databank *ChemSep* will display a warning message that the databank has changed for every affected component every time a simulation done with an older version of *ChemSep* is loaded into the new version.

The warning is displayed because we think it advisable to let you know that there have been changes to the databank that could, under some circumstances, affect the results of your simulations with *ChemSep*. (Note that once the simulation has been done again with the updated databank those messages will not recur.) Nevertheless, it can be quite tiresome to have to deal with many separate warnings, all saying the same thing (this can especially annoying if *ChemSep* is used with a flowhsheeting program like COCO (www.cocosimulator.org). **To skip the warning messages** click on *Tools*, then on *Interface Settings* to bring up this panel:
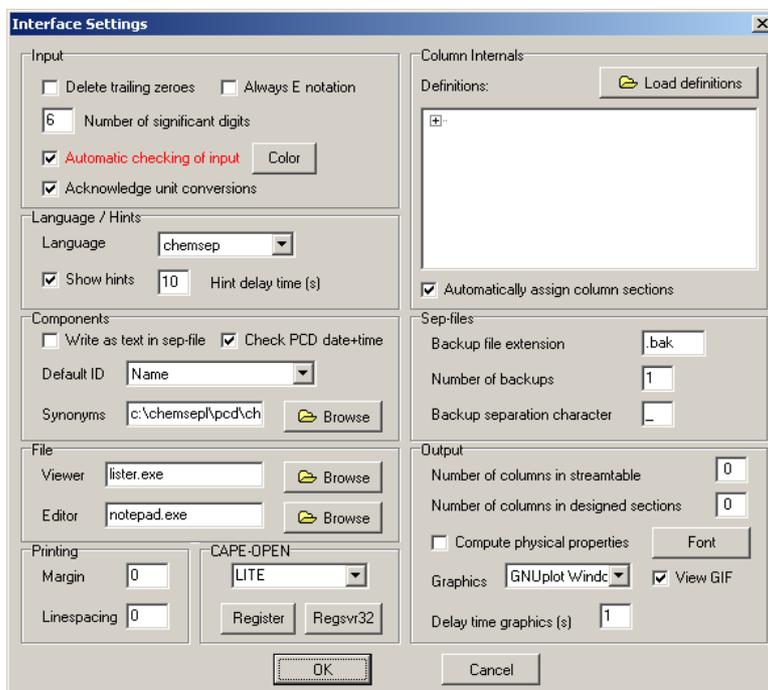


Note the check in the box labeled *Check PCD date+time*. **To skip the warning messages remove the check mark**. Then click on OK; click on *Tools*, then on *Save settings* and overwrite the file *chemsep.cnf*.

# New: Cut and paste columns of data

It is now possible to paste entire columns of data in certain sections of the *ChemSep* interface. Data contained in a column in, for example, Microsoft Excel, may now be copied and pasted as a column in *ChemSep*. The sequence is illustrated below:

In the first image we see part of the feed panel for a reboiled absorber (the example actually comes from a textbook by C.D. Holland). The values for the component flows have not yet been specified.
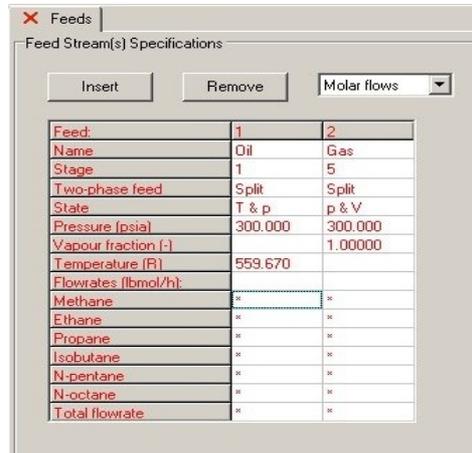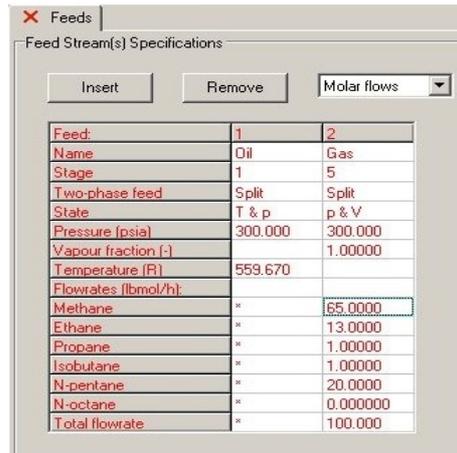


The next step is to switch (in this particular case) to Excel where we find a table of the feed flow rates (in the appropriate units):



Highlight the cells to be copied (as shown here), hold *Ctrl-C* and switch pack to ChemSep.

Select the cell in *ChemSep* to receive the first cell in the Excel block and press *Ctrl-V* to see:

| Feed: | 1 | 2 |
|---|---|---|
| Name | Oil | Gas |
| Stage | 1 | 5 |
| Two-phase feed | Split | Split |
| State | T & p | p & V |
| Pressure (psia) | 300.000 | 300.000 |
| Vapour fraction (-) | | 1.00000 |
| Temperature (R) | 559.670 | |
| Flowrates (lbmol/h): | | |
| Methane | × | 65.0000 |
| Ethane | × | 13.0000 |
| Propane | × | 1.00000 |
| Isobutane | × | 1.00000 |
| N-pentane | × | 20.0000 |
| N-octane | × | 0.000000 |
| Total flowrate | × | 100.000 |

Repeat this step for column 1 (if desired).

Column pasting is also possible in the stage efficiencies panel (for the equilibrium stage model) and in thermodynamic interaction parameter panel:

Enter Thermodynamic Model Parameters (when required)

Peng-Robinson   Peng-Robinson
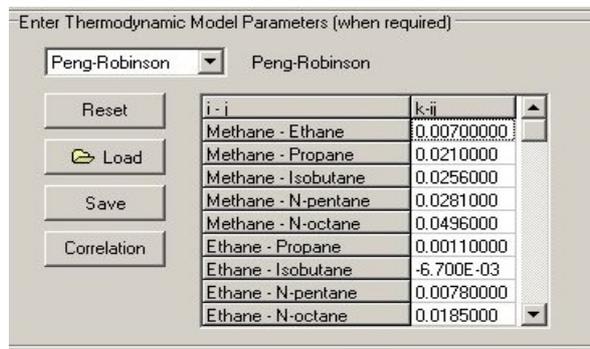
| i - j | k-ij |
|---|---|
| Methane - Ethane | 0.00700000 |
| Methane - Propane | 0.0210000 |
| Methane - Isobutane | 0.0256000 |
| Methane - N-pentane | 0.0281000 |
| Methane - N-octane | 0.0496000 |
| Ethane - Propane | 0.00110000 |
| Ethane - Isobutane | -6.700E-03 |
| Ethane - N-pentane | 0.00780000 |
| Ethane - N-octane | 0.0185000 |

This feature will be very welcome when handling systems with many compounds.

# New: Flooding comparison plot for packed columns

New in *ChemSep* 6.5 is a plot that shows the fraction of flooding for packed columns computed in several different ways. An example appears below:

Packed Column Flooding Comparison
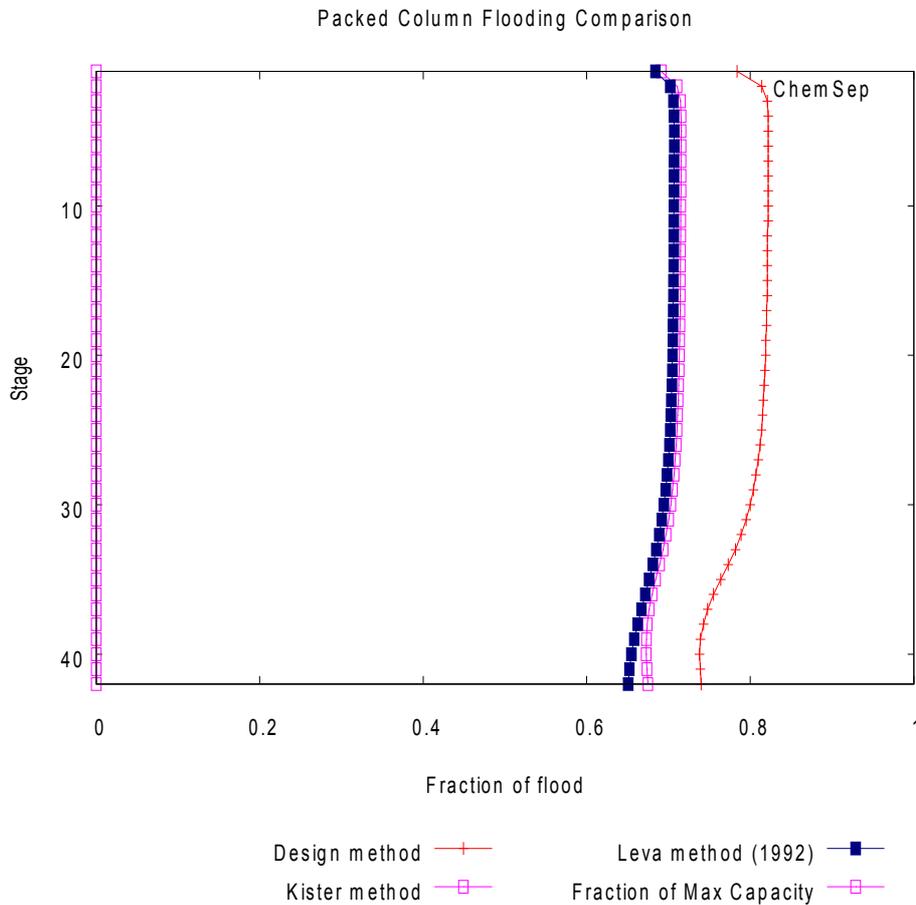


The plot shows the fraction of flood computed using the Leva (1992) method, the method of Kister (using the fit published by Piche in his PhD thesis, University of Laval, 2000), and what we call the *Design method*. The latter is the fraction of flooding computed using the method selected to size the column. If, for example, the Leva method had been used to size the column the plot would show only two flooding profiles that could be distinguished. In the example shown here all three are clearly visible (although two of them are in very close agreement indeed). This means that the column diameter was not estimated using either the Leva or the Kister methods.

**The plot above shows a fourth line, the *Fraction of Maximum Capacity*; this quantity is defined only for IMTP packing**; for all other packing the *Fraction of Maximum Capacity* is shown, as is the case here, by a line at zero.

# New: Capacity comparison plot for packed columns

New in *ChemSep* 6.5 is a plot that shows the capacity.
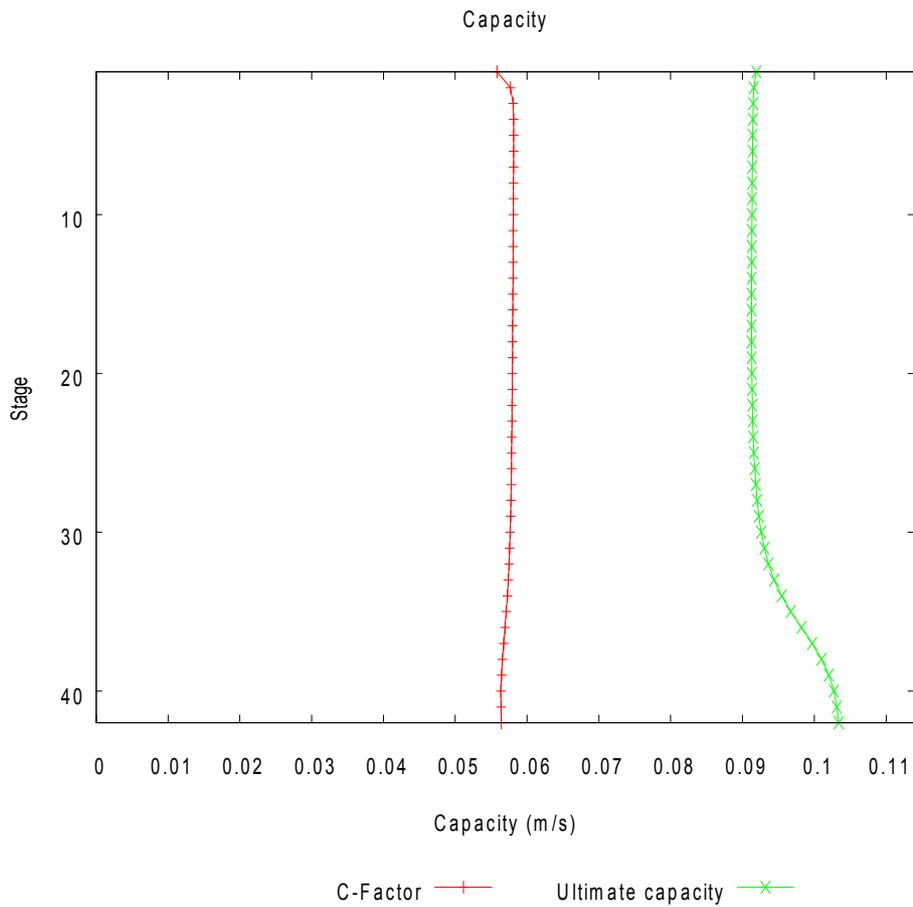


Also shown is the *ultimate capacity* (sometimes referred to as the *System Limit* – see What's New in *ChemSep* 6.3 for a discussion of this concept).

The ratio of these capacities is called the System Limit Fraction of Flood and is displayed in the standard flooding plot.

# New: GPDC plots for packed column design

The Generalized Pressure Drop Correlation (GPDC) has been part of chemical engineering since it was first introduced by Sherwood in 1938. Since then it has undergone a number of revisions and extensions, but it remains an important tool for the packed column designer and in one form or another is included in every major text that covers packed column design. We strongly recommend the following articles for those wanting to know more about the history, use (and misuse) of the GPDC.

> McNulty, K.J., "What's wrong with the GPDC?," Paper presented at the 4th Topical Conference on Separation Science & Technology, AIChE National Meeting, Dallas, TX, 1999.

> Kister, H.Z.; Scherffius, J.; Afshar, K.;, Abkar, E. "Realistically predict capacity and pressure drop for packed columns," *CEP*, p. 28, July 2007

In the introduction to his article McNulty lists no less than 9 different versions of the GPDC that have appeared over the years; four of which now are available in *ChemSep*. An example is shown below.
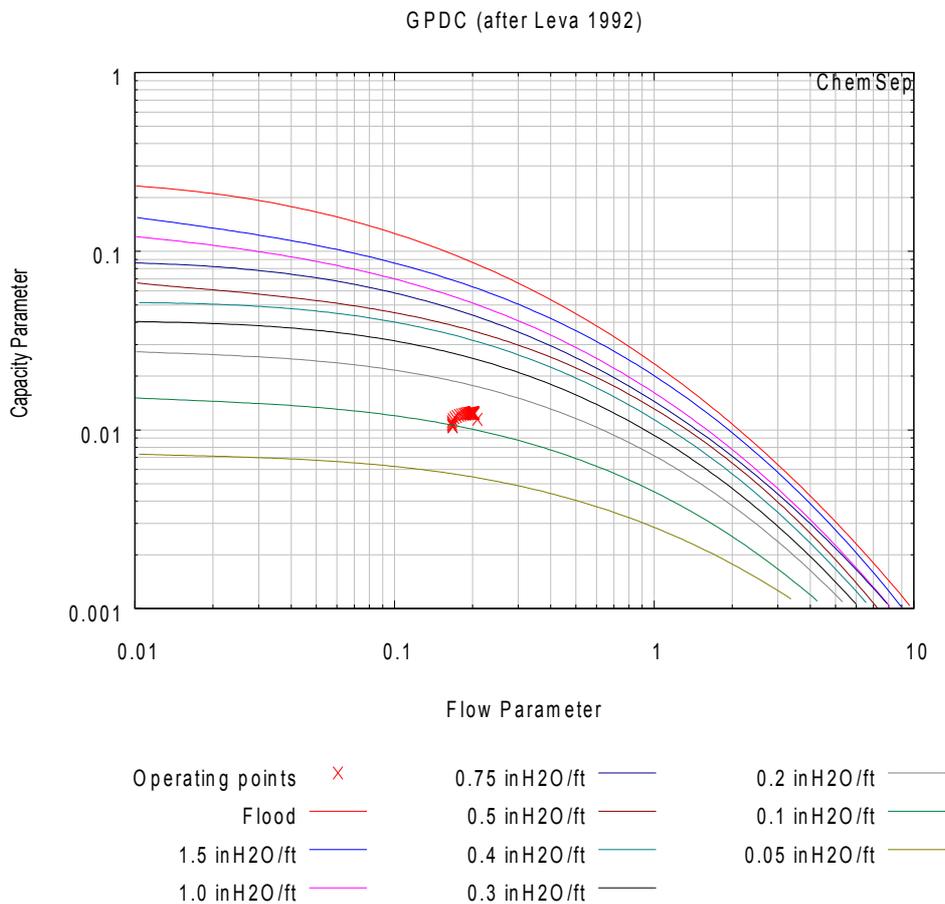


The scattered red points are the operating points for the column that was modeled.

The ordinate in most versions of the GPDC (and all of those now available in ChemSep) is the (dimensionless) Flow Parameter:

$$F_{LV} = \frac{L}{G}\sqrt{\frac{\rho_G}{\rho_L}}$$

The Capacity parameter on the vertical axis differs between GPDC versions as summarized below (from McNulty, 1999) for the versions of the GPDC that now are included as standard plots in *ChemSep*.

1.  GPDC of Leva (1992)

2.  GPDC that appears in the IMTP packing brochure of Norton

3.  GPDC as modified by Strigle and adopted by Kister & Gill

4.  The Kister and Gill version of the GPDC for structured packing.

The abscissa for the GPDC plot of Leva is

$$Y = \frac{0.016}{g} \frac{G^2}{\rho_G} F_p f(\rho_L) f(\mu_L)$$

where $G$ is the gas mass velocity ib lb/h/ft$^2$, $g$ is the acceleration due to gravity capacity in ft/s, $F_p$ is the packing factor in 1/ft, $f(\mu_L)$ is a correction that is a function of the liquid viscosity and $f(\rho_L)$ is a correction that is a function of the liquid density.

The abcissa for the GPDC plots by Strigle and followers is

$$Y = C_s \sqrt{(F_p)} (\mu_L / \rho_L)^{0.05}$$

where $C_s$ is the capacity in ft/s, $F_p$ is the packing factor in 1/ft, $\mu_L$ is the liquid viscosity in cP, and $\rho_L$ is the liquid density in g/cm$^3$.
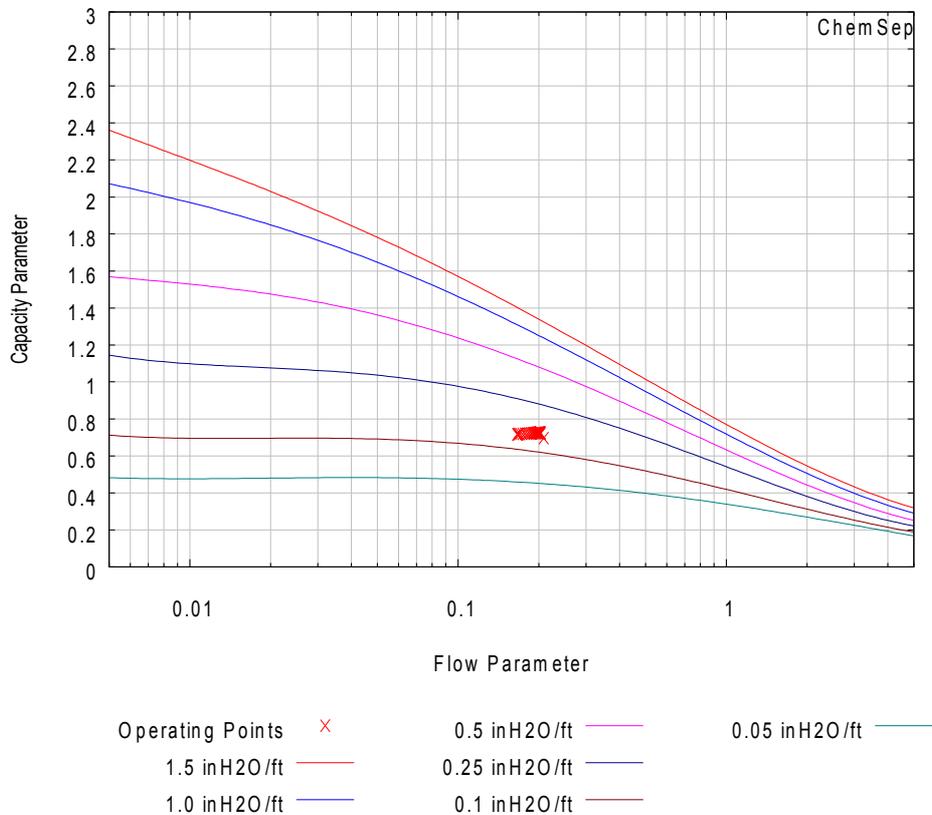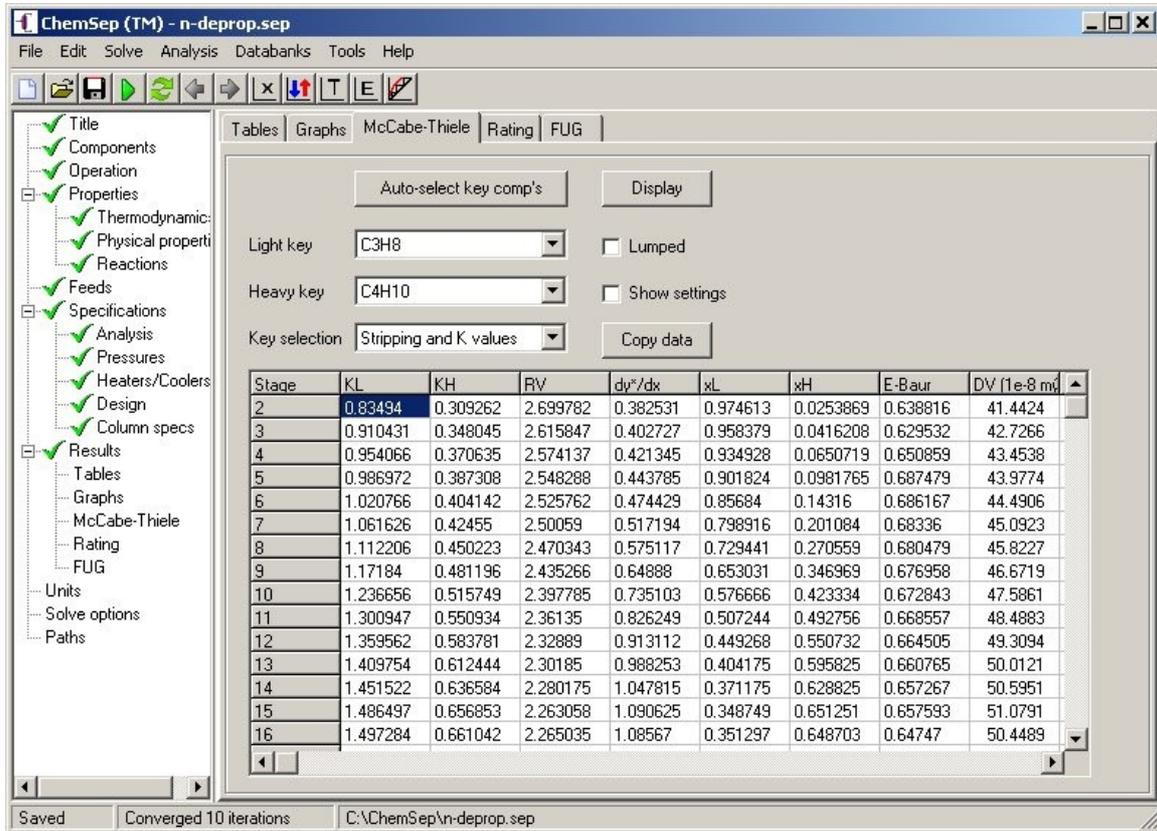
# New: Getting more from the McCabe-Thiele Diagram

*ChemSep* 6.5 adds a new ways to display McCabe-Thiele diagrams and more information that can be obtained from these informative illustrations.

The McCabe-Thiele panel now looks like this:



The most obvious change is the appearance of the spreadsheet that provides information pertaining to the McCabe-Thiele diagram. This spreadsheet displays the following quantities:

| Variable | Description |
|----------|-------------|
| KL | K-value of light key component |
| KH | K-value of heavy key component |
| RV | Relative volatility RV = KL / KH |
| dy*/dx | Slope of the equilibrium line |
| xL | Mole fraction of the heavy key |
| xH | Mole fraction in the liquid of the light key |
| E-Baur | Baur efficiency |
| DV | Diffusion coefficient in the gas/vapor phase for the light-heavy key pair |
| DL | Diffusion coefficient in the liquid phase for the light-heavy key pair |

Less obvious is the check box to the settings for this illustration and the *Key selection* line. Click on the drop down list and we will see three different methods for picking the pair of key components:

| Key selection | Stripping and K values ▼ |
|---|---|
| | Stripping and K values |
| Stage | K Largest mass transfer rates |
| 2 | 0 Net flux |

The default method is the first one, but it does not always pick the right pair of key components (but then, neither do the others). It remains possible to choose the key compounds using the drop down lists above the *Key selection* line.

An example of the McCabe-Thiele diagram appears below:

McCabe-Thiele diagram - C4H10
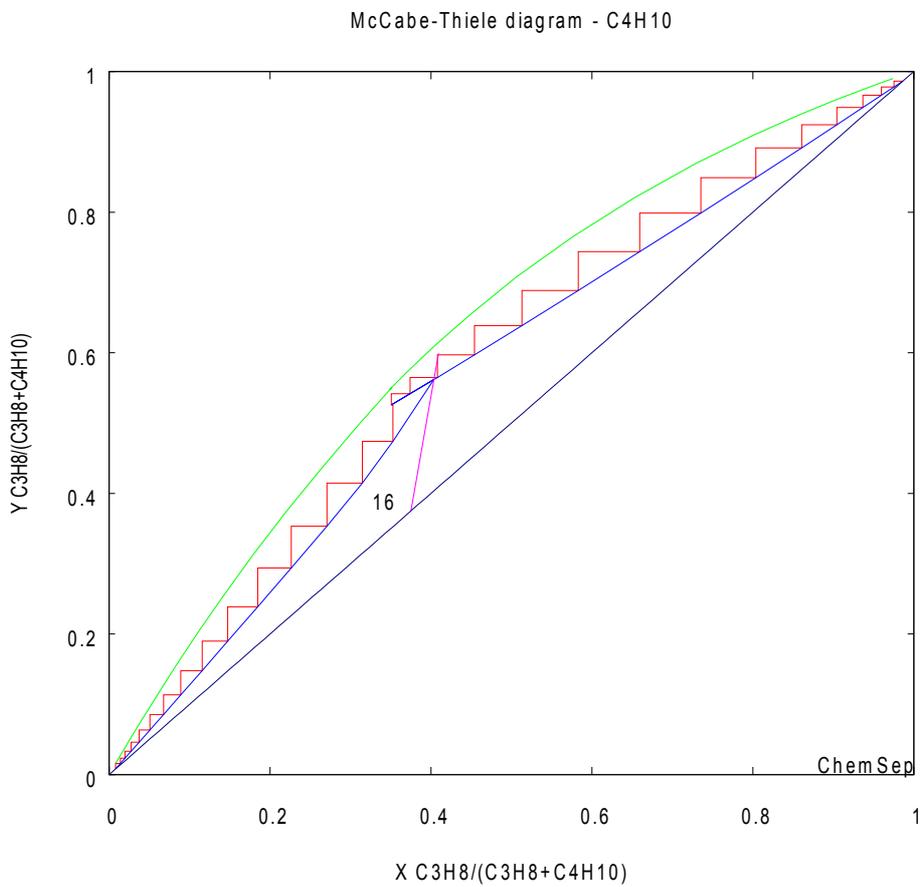
The other change is the inclusion of the *Lumped* check box. Click here and the quantities in the table are automatically recomputed (and the diagram redrawn) using the lumped mole fractions. If the lumped box is checked then the lumped light key component in the liquid phase is computed from the sum of the mole fractions of the designated light key and the mole fractions of all compounds that have a K-value higher than that of the designated light key. The mole fraction of the lumped heavy key is computed by summing the mole fractions of the designated heavy key with those of all compounds that have a K-value smaller than that of the designated heavy key. Similar calculations are made for the lumped gas/vapor keys. The lumped K-values follow from:

$$K_L = y_L / x_L \qquad K_H = y_H / x_H$$

The relative volatility is the ratio of these K-values

$$RV = K_L / K_H$$

and this is used to compute the vapor liquid equilibrium line and the slope (by differentiation). Note that no assumptions regarding constancy of the relative volatility need to be made since it can be calculated at each stage from the local composition.

The lumped version of the diagram shown above appears below.



Lumped McCabe-Thiele diagram
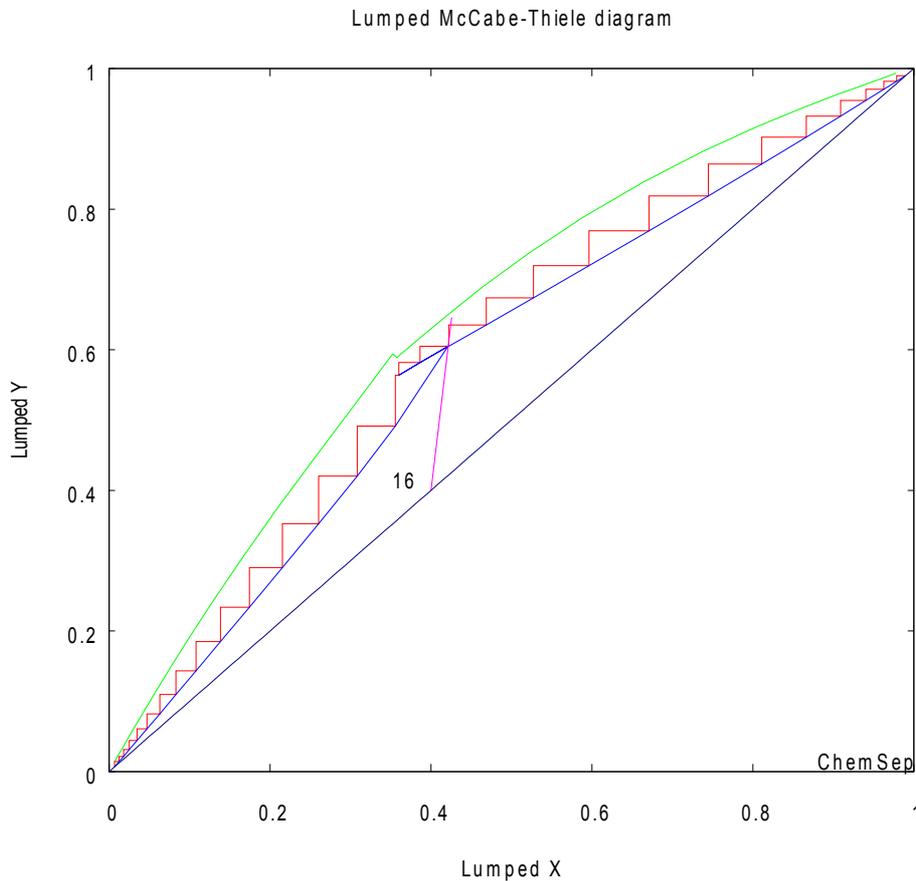
The lumped McCabe-Thiele diagram (sometimes callled a Hengstebeck diagram often is similar to our standard form, but not always. Both can be useful in the interpretation of a column simulation.

# New: Convergence methods in ChemSep

*ChemSep* includes several different approaches to solving the model equations, all based on Newton's method, but now automatically incorporating various "tricks" that we have found helpful in our own use of the program. The options are shown in the partial screen shot (from **Solve Option**) shown below. In the drop down list next to **Method** (look in the top left corner) we can see a list of methods:
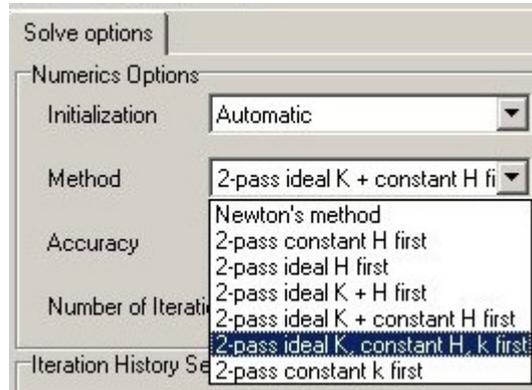


Part of Solve Options tab sheet showing new algorithms

## *Method 1: Newton's method*
Newton's method is the default setting and will be the method used unless you select something else from the drop-down list shown above. Newton's method will be successful 90% of the time; however, it is those cases that Newton's method fails to solve that demand 90% of the users time.

## *Method 2: 2-pass constant H first*
Distillation is a process in which one often assumes that the molar flows are constant from stage    to stage. The practical consequence of this assumption is that the energy balances for each stage can be ignored. The calculations are much simpler and convergence often is very rapid.

Thus, in this option *ChemSep* first attempts to solve a problem with constant enthalpies (for each    phase). This is done by resetting the enthalpy model to **None**; once that problem has converged the  program automatically resets the enthalpy model to be whatever was initially selected and the simulation re-run using the solution to the constant H-model as the starting point.

## *Method 3: 2-pass ideal-H first*
The approach taken here is very similar to that of method 2. Rather than select **None** as the enthalpy model, in this version of our algorithm, the enthalpy model used in the first pass is **Ideal**.

## *Method 4: 2-pass ideal K+H first*
In this third version of the 2-pass Newton method, the first problem is solved using ideal enthalpies *and* ideal K-values (in practice this means the Raoult's law-like **Wilson K-value model**).

## *Method 5: 2-pass ideal K+ constant H first*
This version of the 2-pass Newton method combines the key aspect of method 2 (constant enthalpies) with the use of ideal (Wilson model)  K-values in the first pass.

## *Method 6: 2-pass ideal K+ constant H + constant k first*
This is another two pass method that builds on Method 6; in this version the mass transfer coefficients are maintained constant in the first pass as well as the enthalpies and the use of ideal K-values.

### *Method 7: 2-pass constant k first*

This method keeps constant only the mass transfer coefficients in the first pass. K-values and enthalpies are evaluated using the selected models in both passes.

**Methods 6 and 7 are only for use with rate-based or nonequilibrium models.**

### *Recommendations*

Newton's method should be the first choice (it is the default setting) until it has been shown not to work. In the event of failure then one of the alternative options can be tried (but not all of these methods will allow every problem to be solved). Method 2 can be useful for hard-to-converge distillation-type models. It is less useful for hard-to-converge reboiled absorbers and strippers. One of the alternatives might work better for those applications.

Our experience is that **Method 6 (*2-pass ideal K+ constant H + constant k first*) is very successful when applied to solving rate-based separations at high pressure**. Many problems that were extremely difficult to converge with earlier versions of *ChemSep* and that often required a great deal of help from the user, can be solved immediately using this new option.

# Improved: Parametric Study Feature

The Parametric Study feature in *ChemSep* has been enhanced to include some new features:

1. Can calculate (and display) several new variables:

| Name | Description |
|------|-------------|
| FFAC# | F-Factor of stage # |
| AFFAC# | Average F-Factor of section # |
| CFAC# | C-Factor of stage # |
| ACFAC# | Average C-Factor of section # |
| HETP# | HETP of stage # |
| AHETP# | Average HETP of section # |
| DP# | Pressure drop of stage # |
| ADP# | Average pressure drop of section # |
| DDP# | Dynamic pressure drop of section # |
| ADDP# | Average dynamic pressure drop of section # |
| Lam# | Stripping factor of stage # |
| HTU# | Height of a Transfer Unit on stage # |

2. Allows unit conversions for tabulating and plotting results

3. Can access physical properties of all feed and product streams

# New and Improved: Excel Export

*ChemSep* has long had the ability to export results to Microsoft Excel; that ability has been improved significantly in Version 6.5.
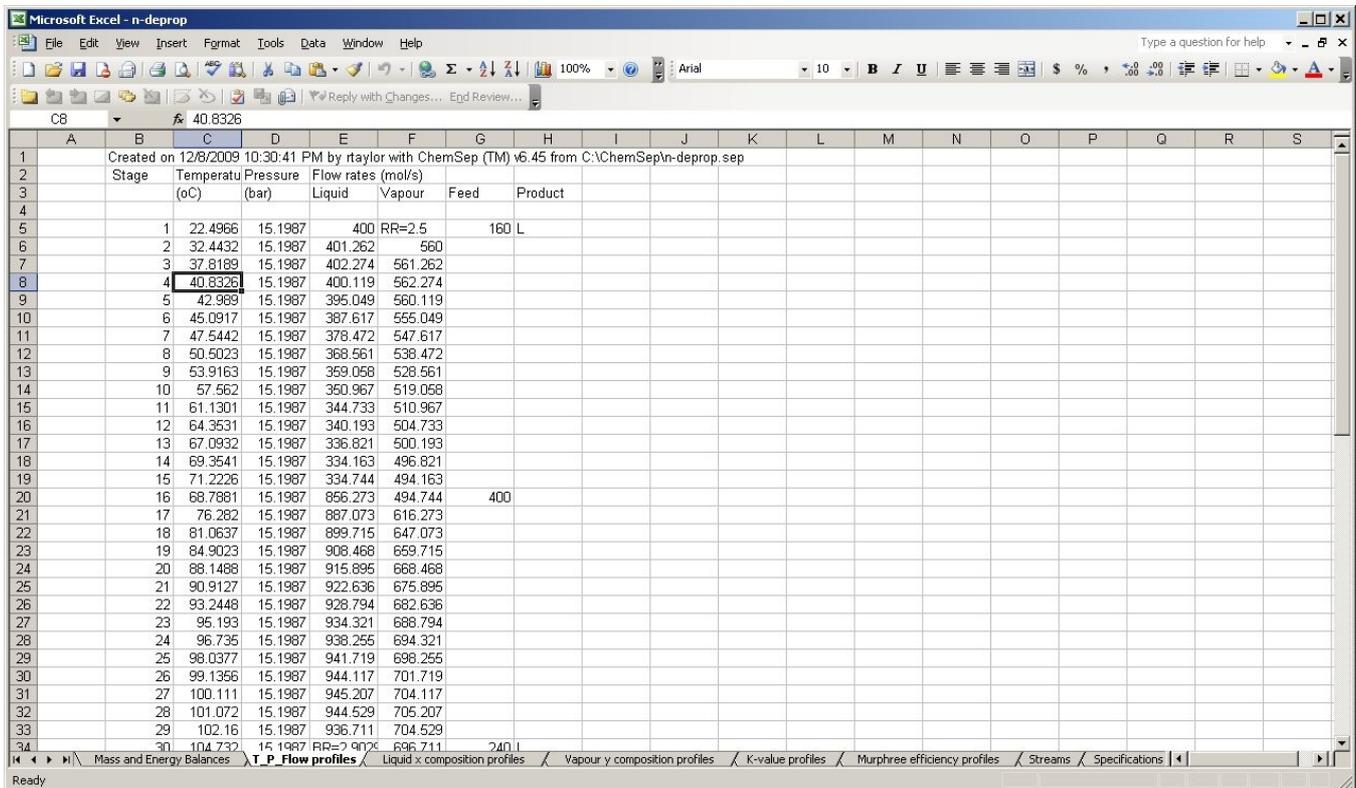
Click on the file menu and select *Export* and select *Save as type* to see the list of available export formats



Note that there are no less than 4 ways here to export results so that they can be imported directly into Microsoft Excel.

Select the first option to create a multi-tab Excel file. An example is shown below:



Each tab page corresponds to a table in the *Tables* section of *ChemSep*. An additional tab includes the spreadsheet from the McCabe-Thiele panel.

For simulations that involve many compounds the lists of compositions, K-values and efficiencies may be stacked one above the other. A file where all the mole fractions, K-values and efficiencies are listed side by side can be obtained by selecting the wide format option (see list above).

Finally, note the name *Export_Excel_Flexible* in the list above. This represents a completely new way of exporting ChemSep results to Excel. We have provided users with the ability to define just exactly what they want to see in an Excel file. Moreover, it is possible to create an unlimited number of different export formats (as long as the file that defines the output format begins with the word *Export*). This flexible export format is the subject of a separate tutorial.

# Other Important Improvements

1. Plots can now display up to 120 lines per plot (the old limit was 20 and that was sometimes a hindrance when plotting composition and efficiency profiles).

2. Several new methods for estimating the properties of pseudo-components and petroleum assays.

3. **Only one click needed to access pull-down lists in tables!**