

ChemSep Tutorial: Efficiencies

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In actual operation the trays of a distillation column rarely, if ever, operate at equilibrium despite attempts to approach this condition by proper design and choice of operating conditions. The usual way of dealing with departures from equilibrium in multistage towers is through the use of stage efficiencies and/or overall efficiencies. Efficiencies often are used in conjunction with the equilibrium stage model to fit actual column operating data, along with the number of equilibrium stages in each section of the column (between feed and product take-off points). There are many parts to this tutorial:

1. **Efficiencies in Tray Columns – a review of some basic concepts**
2. **Efficiencies in Packed Columns – more basic concepts**
3. **The Baur Efficiency**
4. **Estimating Efficiencies – The O'Connell Method**
5. **Specifying Efficiencies in *ChemSep* – Method 1**
6. **Specifying Efficiencies in *ChemSep* – Method 2**
7. **Equilibrium Stage Mass Transfer Model with Internals Design**
8. **Efficiency Derating**
9. **Case Study: Modeling an Industrial C4 Splitter**

1. Efficiencies for a Tray Column – A Review of Some Basic Concepts

The **overall column efficiency** for a tray column may be defined by:

$$E_o = N_{EQ} / N_{actual}$$

where N_{EQ} is the number of equilibrium stages and N_{actual} is the number of actual trays in the column.

There are many different definitions of stage (or tray) efficiency, that of Murphree [*Ind. Eng. Chem.*, **17**, 747–750, 960–964 (1925)] being by far the most widely used in separation process calculations:

$$E_{i,j}^{MV} = \frac{y_{i,j} - y_{i,j+1}}{y_{i,j}^* - y_{i,j+1}}$$

where $E_{i,j}^{MV}$ is the **Murphree vapor efficiency** for component i on stage j and $y_{i,j}^*$ is the composition of the vapor in equilibrium with the liquid leaving the tray. Other types of efficiency include that of Hausen [*Chemie Ingr. Tech.*, **25**, 595 (1953)], vaporization and the generalized Hausen efficiencies of Standart [*Chem. Eng. Sci.*, **20**, 611 (1965)]. Arguments for and against various types are presented by, among others, Standart, Holland & McMahon [*Chem. Eng. Sci.*, **25**, 431 (1972)] and by Medina et al. [*Chem. Eng. Sci.*, **33**, 331 (1978), **34**, 1105 (1979)]. Possibly the most soundly based definition, the generalized Hausen efficiency of Standart are never used in industrial practice. Seader [*Chem. Eng. Progress*, **85**(10), 41 (1989)] summarizes some of the shortcomings of efficiencies.

The fact that mole fractions must sum to unity means that for binary systems the Murphree (and Hausen) efficiencies of both components in a binary mixture are equal.

$$E_1^{MV} = \frac{\Delta y_{1,L}}{\Delta y_1^*}, \quad E_2^{MV} = \frac{\Delta y_{2,L}}{\Delta y_2^*} = \frac{-\Delta y_{1,L}}{-\Delta y_1^*} = E_1^{MV}$$

In addition, binary Murphree efficiencies cannot be negative (although they can be greater than one).

For multicomponent systems, the restriction on the sum of the mole fractions means that there are $c - 1$ independent component efficiencies (c being the number of compounds), and there is no requirement that they be equal. For a three-component system, for example, we have:

$$E_1^{MV} = \frac{\Delta y_{1,L}}{\Delta y_1^*}, \quad E_2^{MV} = \frac{\Delta y_{2,L}}{\Delta y_2^*}, \quad E_3^{MV} = \frac{\Delta y_{3,L}}{\Delta y_3^*} = \frac{\Delta y_1^* E_1^{MV} + \Delta y_2^* E_2^{MV}}{\Delta y_1^* + \Delta y_2^*}$$

where $\Delta y_{i,L} = y_{i,L} - y_{i,E} = y_{i,L} - x_i$ and $\Delta y_i^* = y_i^* - y_{i,E} = y_i^* - x_i$.

It has been known for a long time that the Murphree component efficiencies are not the same for all components on a stage (tray). In fact, they are also not required to take values between zero and one as they are for a binary system and may indeed be found anywhere in the range

$-\infty < E_i^{MV} < \infty$. There is abundant experimental evidence that demonstrates that Murphree component efficiencies vary from component to component and from stage to stage (readers are referred to the compilation of data in Chapter 13 of Taylor & Krishna, *Multicomponent Mass Transfer*, Wiley, New York 1993). Component efficiencies are more likely to differ for strongly nonideal mixtures. While models exist for estimating efficiencies in multicomponent systems (see, again, Chapter 13 in Taylor and Krishna), they are not widely used and have not (as far as we know) been included in any of the most widely used commercial simulation programs.

Murphree efficiencies are easily incorporated into *some* of the methods used for solving the equilibrium stage model equations (this includes the method used in *ChemSep*). Some column simulation programs based on the equilibrium stage model allow users to specify Murphree efficiencies for each component on each stage. We do not, however, advocate taking advantage of such a feature (even if available) for the reasons discussed below.

The maximum number of Murphree component efficiencies is the number of independent efficiencies per stage ($c - 1$) times the number of stages; potentially a very large number indeed. This many adjustable parameters may lead to a model that fits one set of operating data very well, but has no predictive ability (i.e. cannot describe how the column will behave when something changes). At the other extreme, the overall efficiency is just a single parameter that can improve robustness of the model and speed of convergence, but it may be difficult to match actual temperature and/or composition profiles since there is unlikely to be a one-to-one correspondence between the model stages and actual trays. A compromise often used in practice is to use just one value for all components on any single stage (and sometimes for all stages in a single section of a column).

The fact that component efficiencies in multicomponent systems are unbounded also means that a simple arithmetic average of the component Murphree efficiencies is useless as a measure of the performance of a multicomponent distillation process.

For these reasons *ChemSep* does not allow you to specify different component efficiencies; the program permits only the specification of just one efficiency per stage. (Note that the efficiency is allowed to vary from stage to stage if so desired and there are no ambiguities that result from doing so.) Efficiencies should not be used to model condensers and reboilers; it is safer to assume that they are equilibrium stage devices (*ChemSep* does not use efficiencies for condensers and reboilers). It is also unwise to employ Murphree efficiencies for trays with a vapor product since any Murphree efficiency less than one will necessarily lead to the prediction of a sub-cooled vapor.

2. Efficiencies in Packed Columns – More Basic Concepts

The performance of a packed column often is expressed in terms of the HETP (Height Equivalent to a Theoretical Plate) for packed columns. The HETP is related to the height of packing (H) by:

$$HETP = H / N_{EQ}$$

In this case N_{EQ} is the number of equilibrium stages (theoretical plates) needed to accomplish the separation that is possible in a real packed column of height H .

The concept of HETP for multicomponent systems suffers from many of problems that plague component efficiencies. In particular, the HETP for one compound is not often the same as the HETP for another compound. Thus, although they are widely used as a measure of column performance, they can also become a source of confusion.

3. The Baur Efficiency

The **Baur efficiency** [see Taylor, Baur & Krishna, *AIChE J.*, **50**, 3134 (2004)] is defined as follows:

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

The Baur efficiency as defined above has a simple and appealing physical significance: it is the ratio of the length of the actual composition profile (in mole fraction space) to the length of the composition profile. For this reason, and in contrast to other measures of efficiency, the Baur efficiency applies both to tray and to packed columns. For a binary mixture in a tray column, for example, the Baur efficiency is equal to the Murphree efficiency.

$$\varepsilon = \frac{\sqrt{(\Delta y_{1,L})^2 + (\Delta y_{2,L})^2}}{\sqrt{(\Delta y_1^*)^2 + (\Delta y_2^*)^2}} = \frac{\Delta y_{1,L}}{\Delta y_1^*} = E_1^{MV} = E_2^{MV}$$

In fact, it is possible to show that for a multicomponent system in which the component Murphree efficiencies are the same for all components (that is, if) the Baur efficiency can be shown to be equal to the Murphree efficiency. In other words,

$$\text{if } E_1^{MV} = E_2^{MV} = \dots = E_i^{MV} = \dots = E_{c-1}^{MV} = E_c^{MV} = E^{MV} \text{ then } \varepsilon = E^{MV}$$

What this means is that if you specify a value for the Murphree efficiency that is the same for all compounds on a given stage (again, it may vary from stage to stage) you are, in effect, also specifying the Baur efficiency (but the fact that the Baur efficiency has but one value per stage does not imply that the individual component efficiencies are, in fact, equal).

For binary systems in packed columns the HETP may be approximated by

$$HETP = H_{OG} \frac{\ln(\Lambda)}{\Lambda - 1}$$

where Λ is the stripping factor. Strictly speaking this relationship is valid for cases where the operating lines and stripping lines are straight (but not parallel). It is, however, often used to estimate the HETP in circumstances where one or both of these lines is curved.

For binary systems in packed columns the overall height of a transfer unit is related to the Baur efficiency by

$$H_{OG} = \frac{H}{\varepsilon}$$

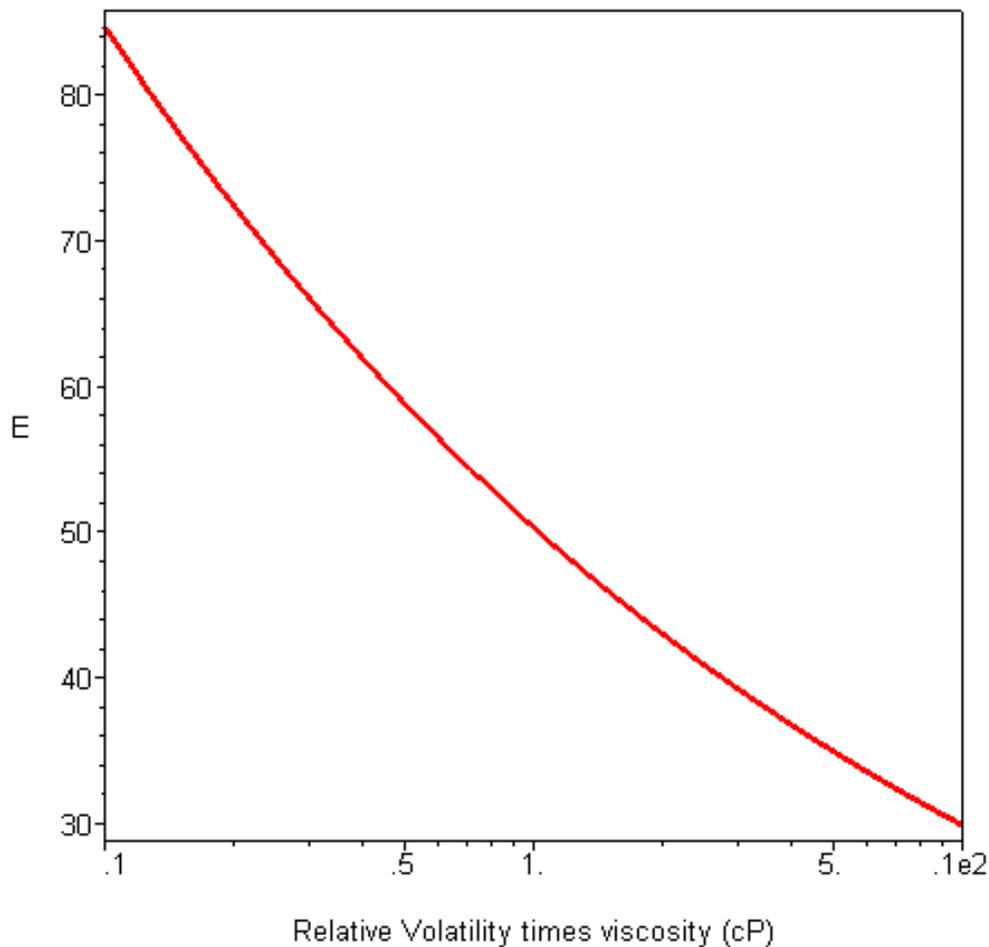
Unlike the component Murphree efficiencies and HETPs, there is just one Baur efficiency per tray or section of packed column regardless of the number of compounds; the Baur efficiency is “well-behaved” in that it cannot be negative, or tend to infinity (although it can be greater than one). For all of the reasons put forth here, we suggest that the Baur efficiency is the most convenient single quantity for column performance assessment.

4. Estimating Efficiencies – The O'Connell Method

There are many methods that have been developed to estimate distillation efficiencies. Readers are referred to sources such as *Distillation Design* by H.Z. Kister (McGraw-Hill, 1992) and *Separation Process Principles* by J.D. Seader and E.J. Henley (2nd Ed., Wiley, 2006) for considerable further discussion of this topic. Here we consider just one method; that of H.E. O'Connell (*Trans. AIChE*, **42**, 741, 1946). O'Connell obtained his correlation for the efficiency of distillation processes from an analysis of data on several operating columns. The original correlation was graphical, but equations have been proposed to represent the correlation. One such equation is:

$$E_{oc} = 50.3(\alpha\mu)^{-0.226}$$

Where α is the relative volatility between the key components and μ is the viscosity in cP. The correlation is shown below.



5. Specifying Efficiencies in *ChemSep* – Method 1

ChemSep permits efficiencies to be specified (with two versions of the standard equilibrium stage model), estimated using the O'Connell method (in combination with the third version of the equilibrium stage model), or back-calculated from the results of a nonequilibrium simulation. In this tutorial we demonstrate the first of these approaches with an example of a valve tray column based studied by Biddulph and Ashton (*Chem. Eng. J.*, 1977).

Choose the equilibrium stage model is on the *Operation* panel and complete the column configuration as shown below.

The screenshot displays the *ChemSep (TM) - Biddulph_eq.sep* window. The left sidebar shows a tree view with the following items checked: Title, Components, Operation, Properties, Thermodynamic, Physical property, Reactions, Feeds, Specifications, Analysis, Pressures, Heaters/Coolers, Efficiencies, Sidestreams, Column specific, Results, Tables, Graphs, McCabe-Thiele, Rating, Units, Solve options, and Paths. The main panel is titled "Operation" and contains the following settings:

- Select Type of Simulation:
 - Flash
 - Equilibrium column
 - Nonequilibrium column
 - Dynamic column
- Column Configuration:
 - Operation: Complex Column
 - Condenser: Total (Liquid product)
 - Reboiler: Partial (Liquid product)
 - Number of stages (e.g. 10): 56
 - Feed stage(s) (e.g. 5,7): 27
 - Sidestream stage(s) (e.g. 2,9): 7
 - Pumparound(s) (e.g. 6>8, 9>1):

To the right of the configuration panel is a schematic diagram of a distillation column. It shows a vertical column with a feed stream labeled "Feed1" entering at stage 27. A condenser is at the top, labeled "1", with a "Top Side1" outlet. A reboiler is at the bottom, labeled "56", with a "Bottom" outlet. A sidestream is drawn from stage 7, labeled "7". A pumparound is shown between stages 2 and 55, labeled "2-7" and "55".

The thermodynamic properties are selected as shown below:

Thermodynamics Physical properties

Select Thermodynamic Models

K-Value:

Equation of state:

Activity coefficient:

Vapour pressure:

Enthalpy:

The feed and side streams are as shown below

Feeds

Feed Stream(s) Specifications

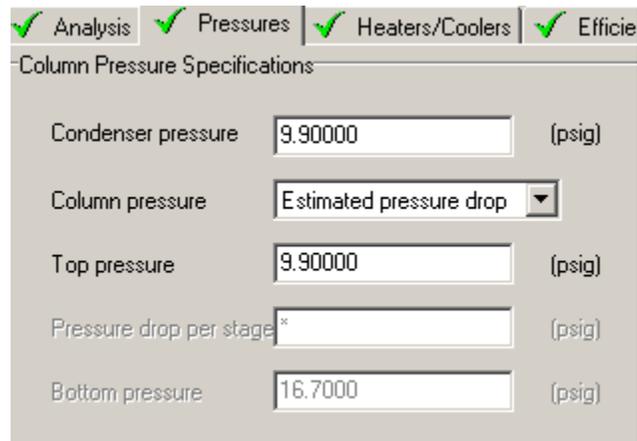
Feed:	1
Name	Feed1
Stage	30
Two-phase feed	Split
State	T & p
Pressure [psig]	10.0000
Vapour fraction (-)	
Temperature [oF]	164.000
Flowrates [kmol/s]:	
Benzene	0.0285112
Toluene	0.0439202
M-xylene	0.00425786
Total flowrate	0.0766893

Analysis Pressures Heaters/Coolers Efficiencies Sidestreams

Sidestreams

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

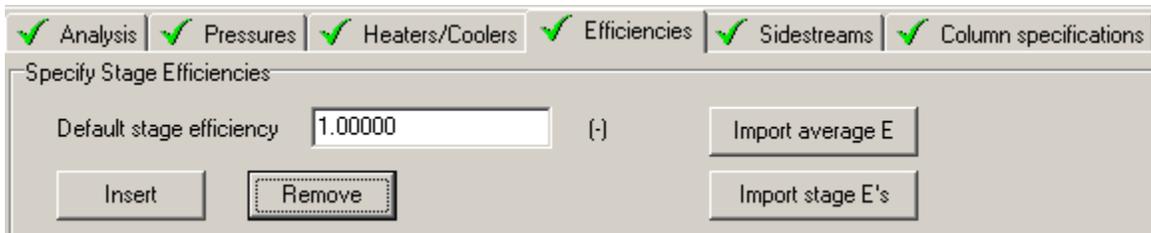
The column pressure profile is specified as:



Condenser pressure	9.90000	(psig)
Column pressure	Estimated pressure drop	
Top pressure	9.90000	(psig)
Pressure drop per stage*		(psig)
Bottom pressure	16.7000	(psig)

Finally, we specify the stage efficiencies. These are Murphree efficiencies, but they are assumed to be same for all components on a stage. Thus, as shown above, they are the same as Baur efficiencies.

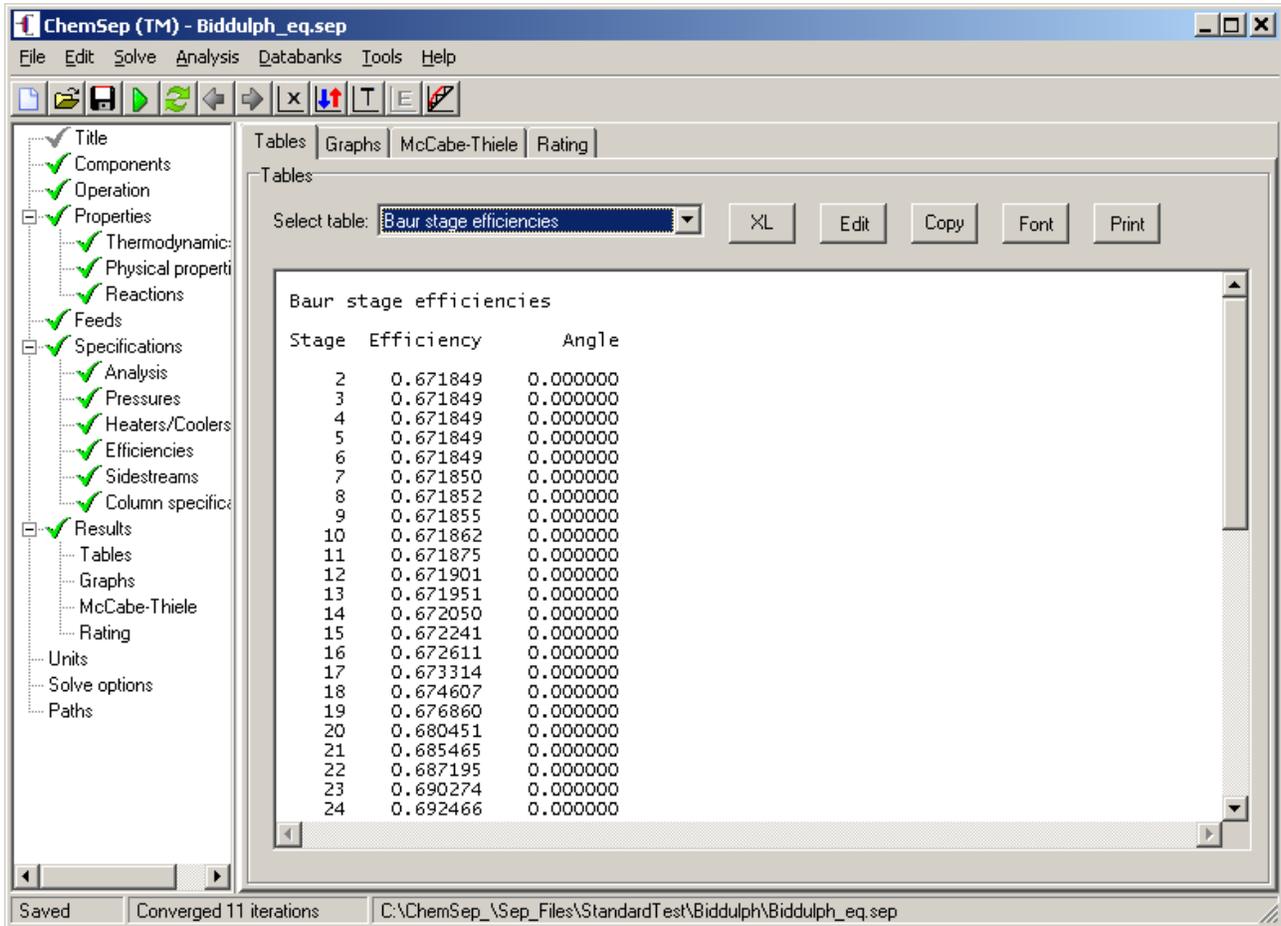
For a new problem the efficiencies panel looks like this



Default stage efficiency	1.00000	(-)	Import average E
Insert	Remove		Import stage E's

The default value of the stage efficiency is shown in the white cell above. If you don't specify a value then it will be taken to be 1. *ChemSep* allows you to specify different values of the efficiency for each stage if desired. Click on the *Insert* button shown above to add stages on which to specify an efficiency. We will not, however, avail ourselves of that opportunity here.

This completes the specifications for this example and we may proceed to run the simulation. One table in particular is of interest to us here in the context of this tutorial: the table of Stage Efficiencies shown below.



These efficiencies were estimated from the O'Connell correlation using the results of the simulation. These efficiencies were *not* used during the calculations. However, we may now do so. Return to the efficiencies panel (see image above) and click on *Import Average E*. The screen should now look like this:



where the default value of 1 has been replaced by the average of the estimated efficiencies.

Now click on *Import stage E's*:

ChemSep (TM) - Biddulph_eq.sep

File Edit Solve Analysis Databanks Tools Help

Analysis
 Pressures
 Heaters/Coolers
 Efficiencies
 Sidestreams
 Column specifications

Specify Stage Efficiencies

Default stage efficiency (-)

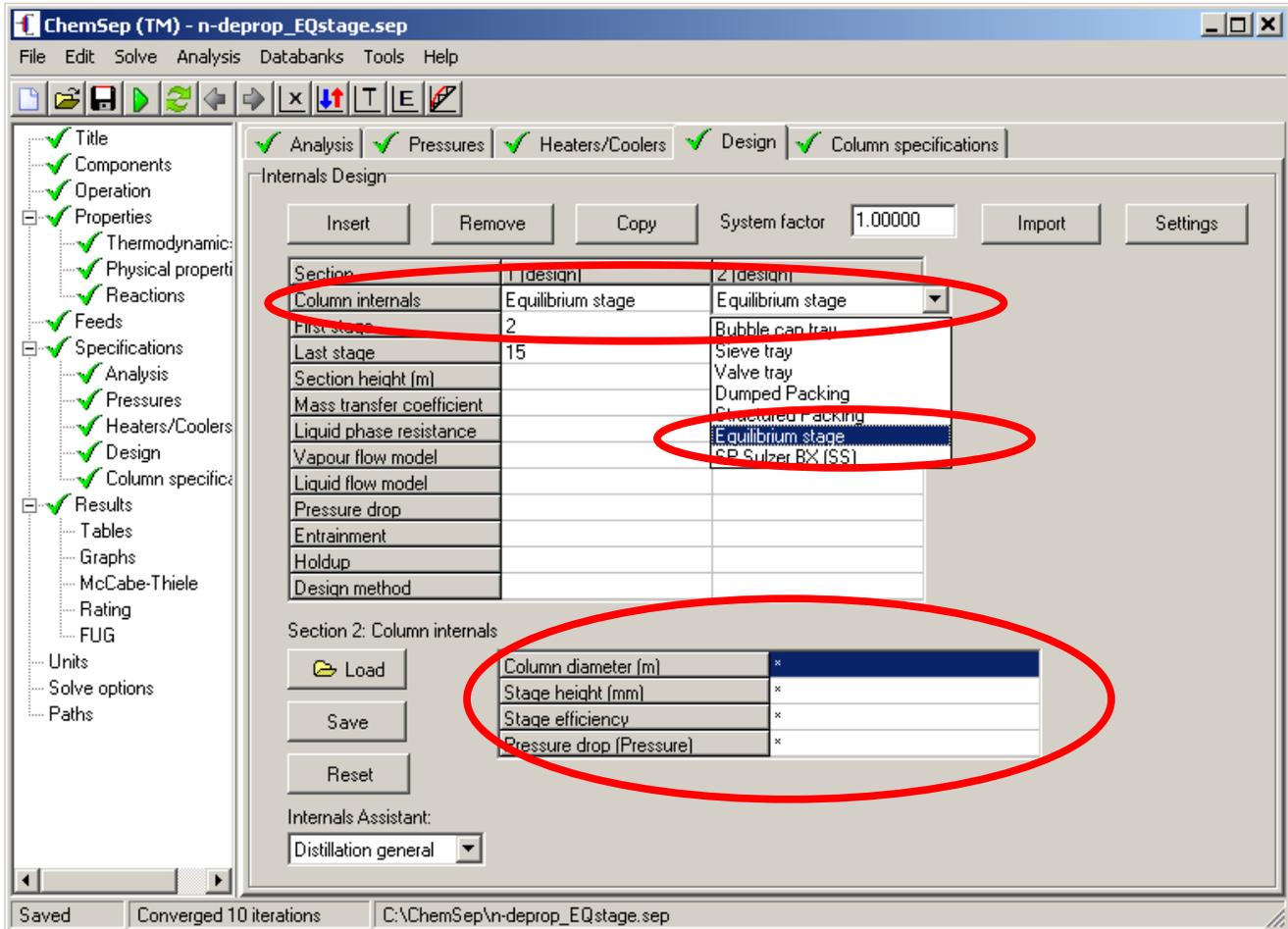
Stage	Efficiency (-)
2	0.671849
3	0.671849
4	0.671849
5	0.671849
6	0.671849
7	0.671850
8	0.671852
9	0.671855
10	0.671862
11	0.671875
12	0.671901
13	0.671951
14	0.672050
15	0.672241
16	0.672611
17	0.673314
18	0.674607
19	0.676860
20	0.680451
21	0.685465

Changed Converged 11 iterations C:\ChemSep_\Sep_Files\StandardTest\Biddulph\Biddulph_eq.sep

We see that all of the individual stage efficiencies have been loaded. We can now rerun the simulation using these efficiencies if we wish to do so. The results, will of course, differ from those obtained before, possibly very different. We advise caution when interpreting the results of such an exercise.

6. Specifying Efficiencies in ChemSep – Method 2

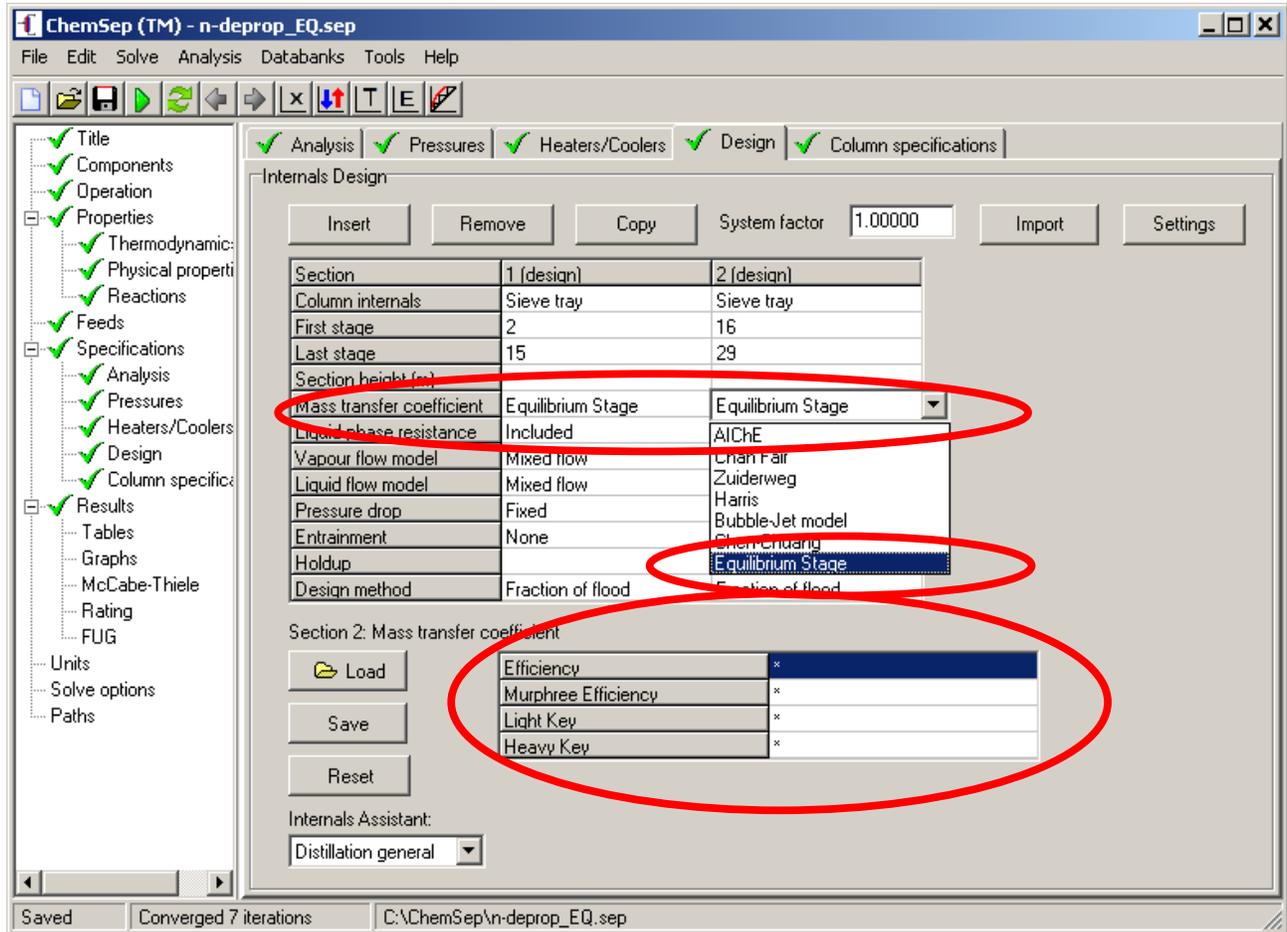
It may come as something of a surprise to many *ChemSep* users that the equilibrium stage model also is available after selecting the *Nonequilibrium model* on the above panel. In fact, the second method of selecting the equilibrium stage model, via the *Design* panel as shown below has always been part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

7. Equilibrium Stage Mass Transfer Model with Internals Design!

The third 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:

Section 2: Mass transfer coefficient

Efficiency	Specified
Murphree Efficiency	Specified
Light Key	O'Connell Absorption
Heavy Key	*

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:

Section 2: Mass transfer coefficient

Efficiency	O'Connell Distillation
Murphree Efficiency	C2H6
Light Key	C2H6
Heavy Key	C3H8
	C4H10
	C5H12

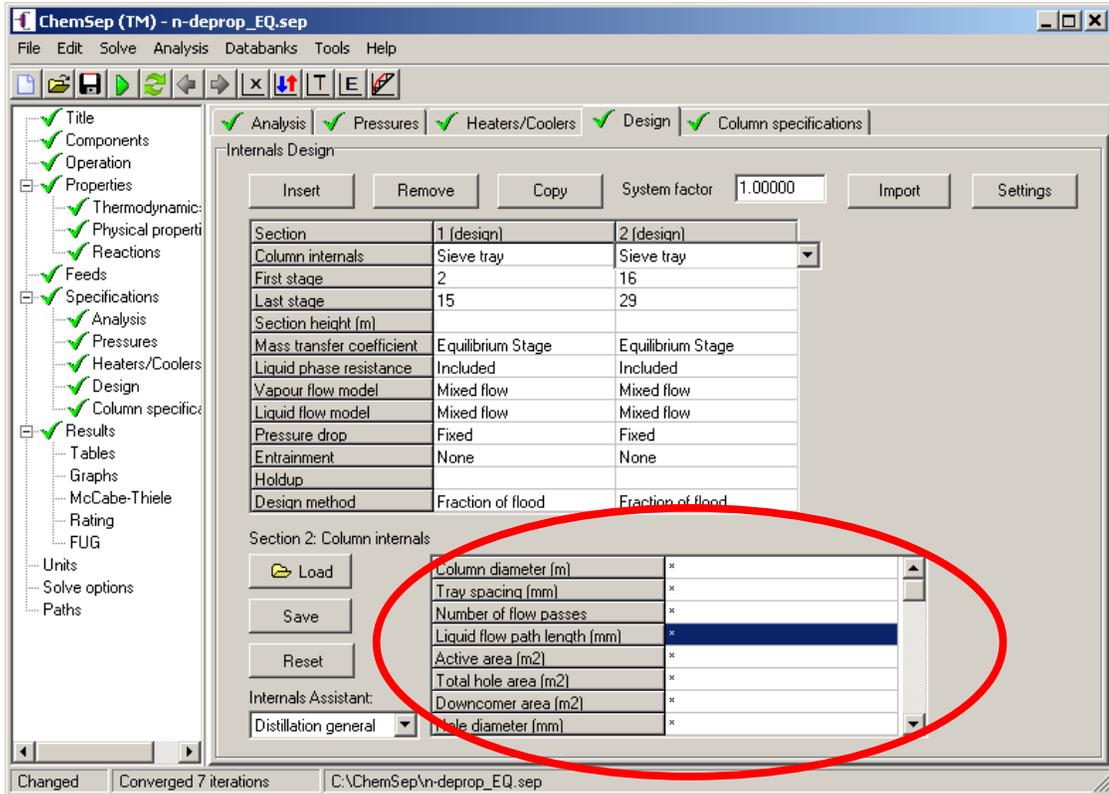
Select the light key from the list that appears. Repeat this action to select the heavy key in the white cell below. For the example shown here this part of the design panel now looks like this:

Section 2: Mass transfer coefficient

Efficiency	O'Connell Distillation
Murphree Efficiency	*
Light Key	C3H8
Heavy Key	C4H10

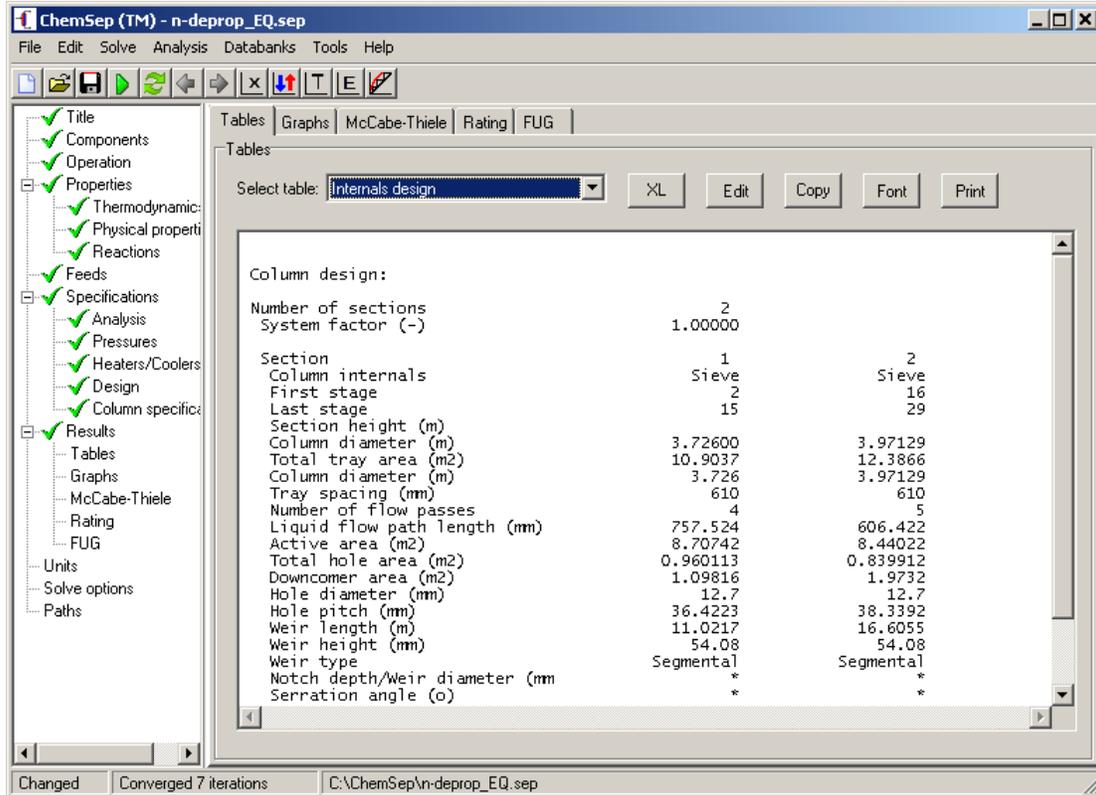
If the key compounds are not specified then *ChemSep* will estimate the O'Connell efficiency for all possible binary pairs in the mixture and then compute the average value of all of these efficiencies to use in the simulation!

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

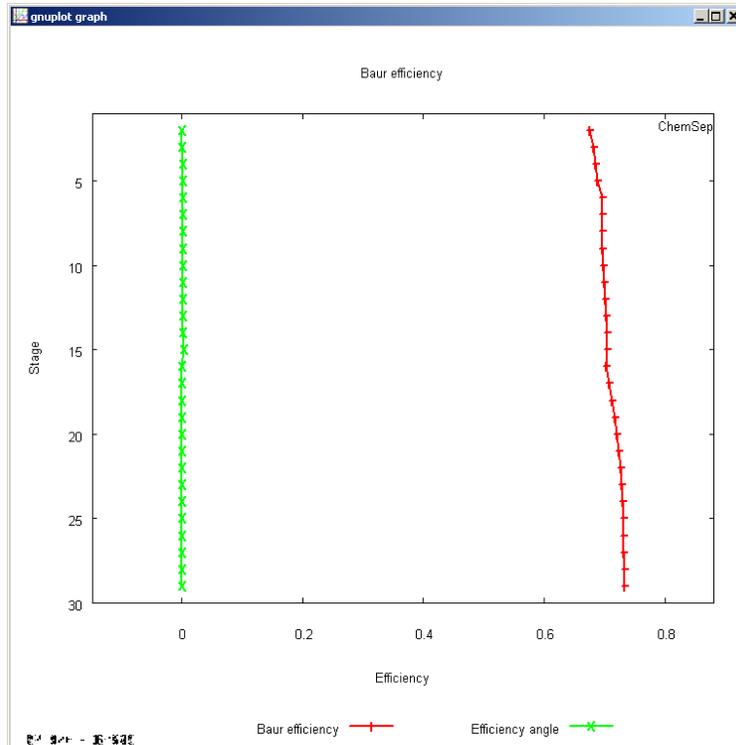


If we leave this section empty (as is the case here) then *ChemSep* will carry out tray (or packed column) sizing calculations. These equipment sizing calculations are not done for the equilibrium stage internal (because *ChemSep* does not then know what kind of column section – tray or packing – to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

8. Efficiency Derating

ChemSep 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.

The first screenshot shows the 'Design method' dropdown set to 'Fraction of flood'. Below it, the 'Section 1: Design method' panel contains a table with the following rows:

Fraction of flooding	*
Fraction of weeping	*
System factor model	*
System factor	*
Efficiency derating factor	*

The second screenshot shows the 'Design method' dropdown set to 'Fraction of flood (Leva)'. Below it, the 'Section 1: Design method' panel contains a table with the following rows:

Fraction of flooding	*
System factor	*
Efficiency derating factor	*

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).

9. Case Study: An Industrial *i*-Butane/*n*-Butane Fractionator

Klemola and Ilme [*Ind. Eng. Chem.*, **35**, 4579 (1996)] and Ilme [Ph.D. Thesis, University of Lappeenranta, Finland (1997)] report data from an industrial *i*-butane/*n*-butane fractionator that is used here as the basis for this tutorial.

The column has 74 valve trays, the feed was introduced onto tray 37. The initial column configuration in *ChemSep* is, therefore: as shown below:

Select Type of Simulation

Flash
 Equilibrium column
 Nonequilibrium column
 Dynamic column

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)

Note that the condenser is counted as stage 1 and the reboiler is the highest numbered stage: thus, the total number of stages here is set to 76 with the feed to stage 38 (one higher than the known feed tray location). The condenser is initially specified to be a total condenser, but we will revisit this selection shortly.

The key design parameters for the valve trays will be provided in Tutorial X. The measured compositions and flow rates of the feed and products for the C4 splitter as reported by Ilme are summarized in the table below.

Measured Feed and Product Flows and Compositions (mass %)
for *i*-Butane/*n*-Butane Fractionator (Ilme, 1997)

Species	Feed	Top	Bottom
Propane	1.50	5.30	0.00
Isobutane	29.4	93.5	0.30
<i>n</i> -Butane	67.7	0.20	98.1
C4 olefins	0.50	1.00	0.20
Neopentane	0.10	0.00	0.20
Isopentane	0.80	0.00	1.10
<i>n</i> -Pentane	0.10	0.00	0.10
Total flow (kg/h)	26234	8011	17887

Other measured parameters are as follows:

Other details of the *i*-Butane/*n*-Butane Fractionator

Reflux Flow Rate	kg/h	92838
Reflux Temperature	°C	18.5
Column Top Pressure	kPa	658.6
Pressure drop per tray	kPa	0.47
Feed Pressure	kPa	892.67
Boiler Duty	MW	10.24

Rarely, and this is a case in point, are plant data in exact material balance and it will be necessary to reconcile errors in such measurements before continuing. The feed and product compositions as adjusted by Ilme so that they satisfy material balance constraints, are provided below. Note how the C4 olefins were assigned by Ilme to isobutene and 1-butene.

Adjusted feed and product compositions (mass %) and flows
for *i*-Butane/*n*-Butane Fractionator (Ilme, 1997)

Species	Feed	Top	Bottom
Propane	1.54	4.94	0.00
Isobutane	29.5	94.2	0.3
<i>n</i> -Butane	67.7	0.20	98.1
Isobutene	0.13	0.23	0.08
1-butene	0.20	0.41	0.10
Neopentane	0.11	0.00	0.17
Isopentane	0.77	0.00	1.12
<i>n</i> -Pentane	0.08	0.00	0.11
Total flow (kg/h)	26122	8123	17999

The feed is assumed to be saturated liquid (the feed temperature is not specified) to stage 38.

To proceed with building a model of this column we specify the number of stages equal to the number of trays plus condenser and reboiler ($N = 76$).

If we computing the bubble point of the overhead product we will find that the measured reflux temperature is well below the estimated boiling point. Thus, we choose the subcooled condenser model. We assume a partial reboiler.

The specifications made to model this column are summarized below:

Variable	Number	Value
Number of stages	1	$N = 76$
Feed stage location	1	39
Component flows in feed	$c = 8$	See other table
Feed pressure	1	120 psia
Feed vapor fraction	1	0
Pressure at the top of the column	1	658.6 kPa
Pressure drop per stage	$N - 1 = 75$	0.47 kPa
Heat duty on each stage except reboilers and condensers	$N - 2 = 74$	$Q_j = 0$
Reflux ratio (replaces heat duty of condenser)	1	$R = 11.588$
Bottoms flow rate (replaces heat duty of reboiler)	1	$B = 17999 \text{ kg/h}$
Temperature of reflux	1	291.65 K
Total	165	

Finally, we must select appropriate methods of estimating thermodynamic properties. Ilme (1997) used the SRK equation of state to model this column, whereas Klemola and Ilme (1996) had earlier used the UNIFAC model for liquid phase activity coefficients, the Antoine equation for vapor pressures and the SRK equation for vapor phase fugacities only. For this exercise we used the Peng-Robinson equation of state. Computed product compositions and flow rates are shown in the table below.

Specified feed (Ilme, 1997) and computed product compositions (mass %) and flows for *i*-Butane/*n*-Butane Fractionator

Compound	Feed	Top	Bottom
Propane	1.54	4.95	0.00
Isobutane	29.49	93.67	0.53
<i>n</i> -Butane	67.68	0.73	97.89
Isobutene	0.13	0.29	0.06
1-butene	0.20	0.36	0.13
Neopentane	0.11	0.00	0.16
Isopentane	0.77	0.00	1.12
<i>n</i> -Pentane	0.08	0.00	0.12
Total flow (kg/h)	26122	8123.01	17999

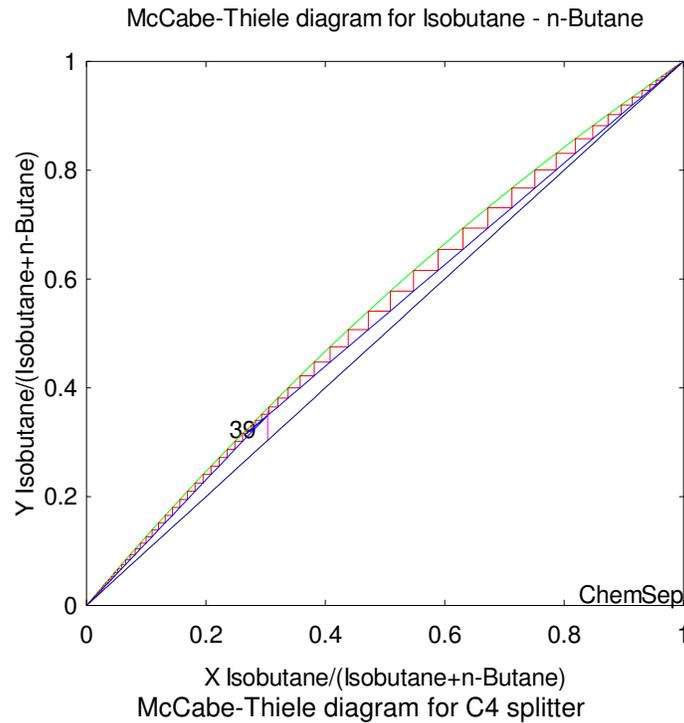
The agreement with the adjusted material balance (tabulated above) appears to be quite good and to a first approximation it seems that we have a good model of the column.

It must be noted that although this column is distilling a mixture containing at least 8 identifiable compounds, only two are present in significant amounts and, therefore, this is essentially a binary separation. It is usually relatively straightforward to match product compositions in processes involving only two different species simply by adjusting the number of equilibrium stages. We shall return to this point later.

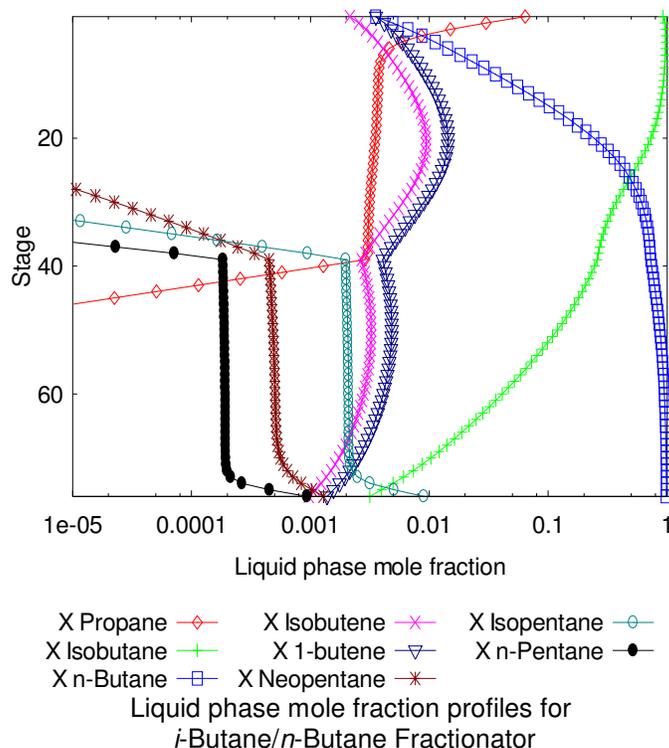
It is possible to estimate the overall efficiency for a column such as this one simply by adjusting the number of equilibrium stages in each section of the column that are needed to match the mass fractions of *i*-butane in the distillate and *n*-butane in the bottoms. Using the SRK equation of state for estimating thermodynamic properties Ilme (1997) found that 82 equilibrium stages (plus condenser and reboiler) and the feed to stage 38 were required. This corresponds to an overall column efficiency of $82/74 = 111\%$. Klemola & Ilme (1996) used the UNIFAC model for liquid phase activity coefficients, the Antoine equation for vapor pressures and

the SRK equation for vapor phase fugacities only and found that 88 ideal stages were needed; this corresponding to an overall efficiency of 119%. With the Peng-Robinson equation of state for the estimation of thermodynamic properties we find (using *ChemSep*) that 84 stages are needed (while maintaining the feed to the center stage as is the case here); the overall column efficiency for this model being 114%. The differences between these efficiencies are not large in this case, but the important point here is that efficiencies – all kinds – depend on the choice of model used to estimate thermodynamic properties. Caution must, therefore, be exercised when using efficiencies determined in this way to predict column performance.

As an alternative to varying the number of stages we may prefer to maintain a one-to-one correspondence between the number of stages and the number of actual trays, 74 in this case (plus condenser and reboiler), with the feed to tray 38. Using the Peng-Robinson equation of state and a Murphree stage efficiency of 116% we find the product mass fractions that are in excellent agreement with the plant data. The McCabe-Thiele diagram for this case, assembled from the results of the simulation, is shown below



Composition profiles computed from this model are shown below. Note that the mole fractions are shown on a logarithmic axis so that all of the composition profiles can easily be seen.



It must be remembered that this is essentially a binary separation and that it is usually relatively straightforward to match product compositions in processes involving only two different species. In other cases involving a greater number of species with significant concentrations it will likely be necessary to vary both the number of stages and the component efficiencies to match plant data. We do not recommend adjusting thermodynamic model parameters in order to fit plant data since this can have unfortunate consequences on the prediction of product distributions, process temperatures and/or pressures.

When we create a nonequilibrium model of this – or any – column we do not need to guess how many stages to use in each section of the column. The real column had 74 valve trays; the model column includes 74 model trays with the feed to tray 38 (plus a (subcooled) condenser and a reboiler, both of which are modeled as equilibrium stages as described above). All operating specifications are the same as for the corresponding equilibrium stage model. It is necessary to choose models that allow for the estimation of the rates of interphase mass transfer; that means selecting vapor and liquid flow models and correlations to estimate the mass transfer coefficients in each phase as discussed above. In this case the AIChE correlations were used. It is known that this method is more conservative than others (i.e. the predicted efficiencies are lower). The importance of the flow model is clear from the simulation results tabulated below. The predicted component Murphree efficiencies vary more widely from stage to stage and from component to component than might be expected for a system like this. The Baur efficiency, on the other hand, does not change by more than a few percentage points over the height of the column; the value in the table below is an average of that computed for each tray from the simulation.

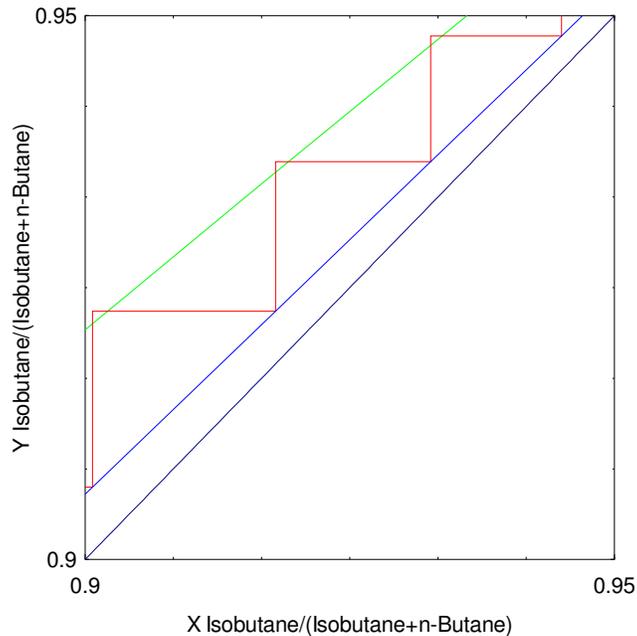
Vapor flow model	Liquid flow model	iC4 in Distillate (%)	nC4 in Bottoms(%)	Efficiency(%)
Mixed	Mixed	90.2	96.3	63
Plug	Mixed	92.2	97.2	78
Plug	Dispersion	93.9	98.0	106

Internal vapor and/or liquid composition data rarely is available, but such data is the best possible for model discrimination and validation. It is often relatively easy to match even a simple model only to product

compositions. In the absence of composition profiles, the internal temperature profile can often be as useful provided that it is known to which phase a measured temperature pertains. The table below compares the few available measured tray temperatures with those computed during the simulation. The agreement is quite good.

Tray	Temperature (°C)	
	Measured	Predicted
9	47.5	48.6
65	62.2	62.5
74	63.2	63.1

A portion of the McCabe-Thiele diagram for the simulation involving plug flow of vapor and dispersion flow of the liquid is shown below. For a nonequilibrium column these diagrams can only be constructed from the results of a computer simulation. Note that the triangles that represent the stages extend beyond the curve that represents the equilibrium line; this is because the efficiencies are greater than 100%.



Expanded view of upper right corner of McCabe-Thiele diagram for C4 splitter.

In this particular case the converged composition and temperature profiles have the same shape as those obtained with the equilibrium stage model (with specified efficiency) and, therefore, are not shown. The reason for the similarity is that, as noted above, this is basically a binary separation of very similar compounds. The important point here is that, unlike the equilibrium stage model simulations, the nonequilibrium model predicted how the column would perform; *no parameters were adjusted to provide a better fit to the plant data*. That is not to say, of course, that NEQ models cannot be used to fit plant data. In principle, the mass transfer coefficients and interfacial area (or parameters in the equations used to estimate them) can be tuned to help the model better fit plant data.