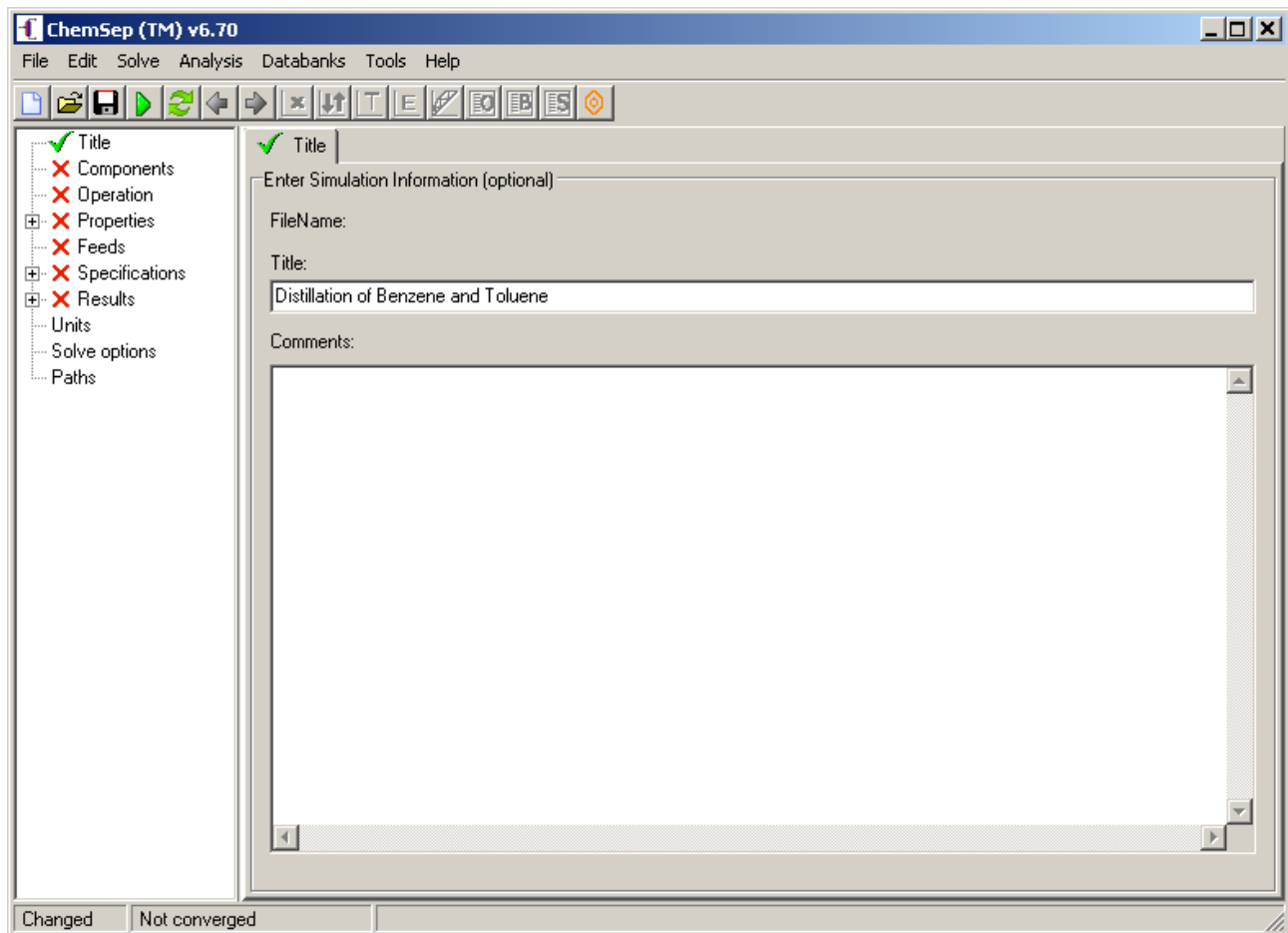


## ChemSep Tutorial: Simple Distillation

Harry Kooijman and Ross Taylor

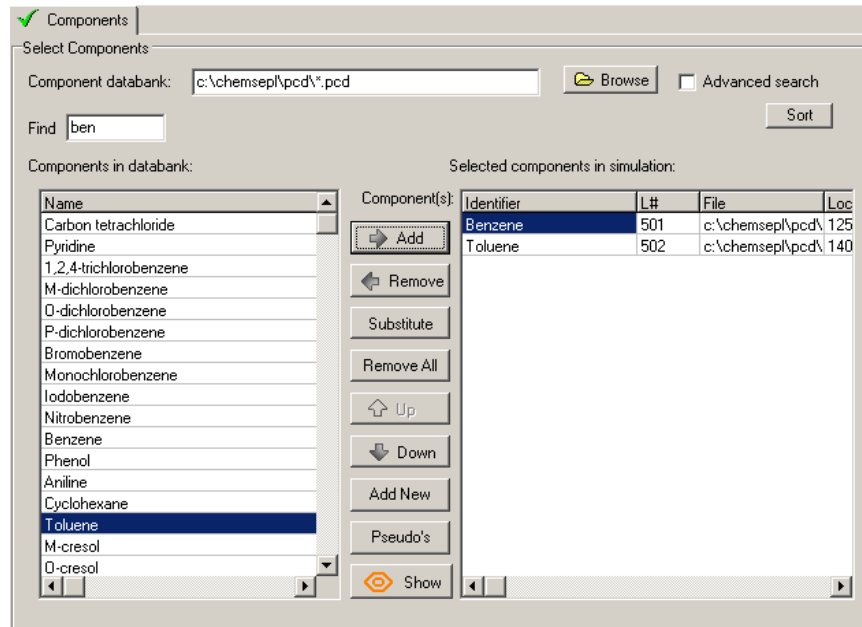
In this tutorial we take you on a quick tour of *ChemSep* by showing you how to input the specifications for the simulation of a simple distillation column for a simple binary separation.

We begin by entering a name for this simulation on the title panel:



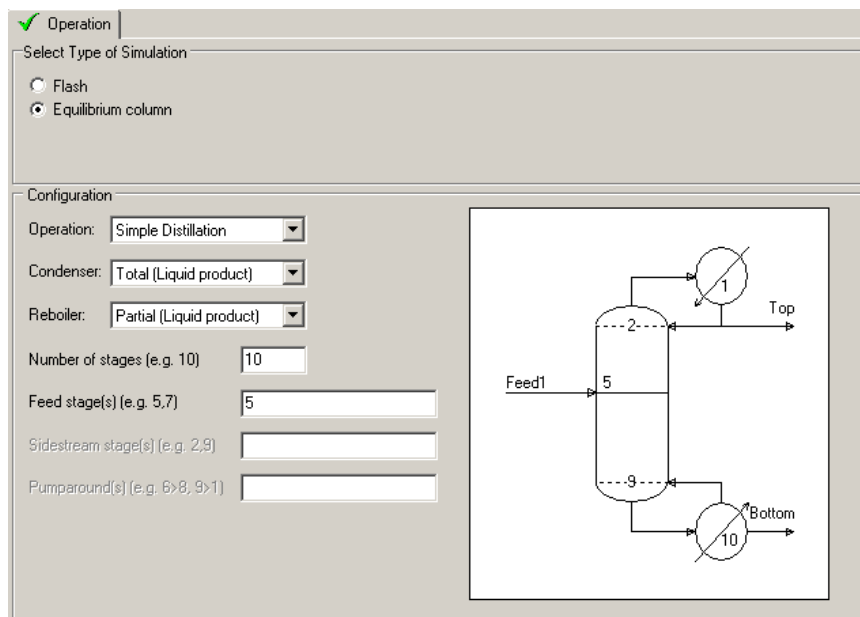
Notice the title panel now is complete (as denoted by the green check in the tree to the left). This does not mean that you need refrain from adding any information that you wish to record in the comments box seen in the screen shot, only that you are not required to record anything here.

Use the next button to move to the component selection panel. A longer discussion of the many ways to select compounds is given in a separate tutorial, Here we assume that you have either read that tutorial or otherwise know how to select compounds. The screen shot below shows that for this exercise we have selected benzene and toluene.



Note that as soon as the first compound was selected, the interface marked the component selection panel as complete (and displayed a green check mark). Of course, for a distillation column model we need to select at least two components.

The next step is to select the type of simulation: in this case we are selecting an *Equilibrium column*. Once we make this selection we need to specify the configuration of our column. Here the interface supplies us with all kinds of defaults and for this exercise we will accept most of the defaults as shown below:



We continue by selecting the *thermodynamic models* used to simulate the vapor-liquid equilibria on the stages in the column. **Process simulation makes extensive use of thermodynamic properties, and they can have a profound influence on the simulation results. Selecting the right models sometimes requires insight and experience from the user. It is your responsibility to assess whether or not the thermodynamic model you have selected is adequate for your needs.** The main specification here is the selection of the K-value model. Other model selections depend on the type of K-value model selected. A more complete guide to model selection is provided in a separate tutorial. The image below shows the models selected for this particular exercise.

Thermodynamics    Physical properties    Reactions

Select Thermodynamic Models

K-value:     Show enthalpy/exergy settings:

Equation of state:

Activity coefficient:

Vapour pressure:

Enthalpy:

We have selected the *DECHEMA* K-model, *UNIFAC* for the activity coefficients, and *Antoine* for the vapor pressures. These are reasonably good model selections for the nearly ideal Benzene - Toluene system of our example. The enthalpy model *None* means that the enthalpies for the liquid and vapor are assumed constant and equal for all the components. This assumption is often referred to as *Equimolar Overflow* or *Constant Molar Overflow (CMO)*. It implies that the vapor and liquid flows up and down the column are constant from stage to stage (except around stages that involve feed or product streams). We shall investigate the consequences of changing the enthalpy model later in this tutorial.

Using F6 we switch to the next input screen. This brings us to the *physical properties* where we can define models for densities, viscosities, thermal conductivities, surface tension, and diffusivities. *ChemSep* provides a default set of model selections so no user input is required. If you want to make your own selection, uncheck the checkbox "Use default methods" and all the selections will become visible. This is not needed now and we use F6 again for the next input screen, which is *Reactions*. As benzene and toluene do not react with each other, we can skip this item and move to the next item in the input: *Feeds*.

Feeds

Feed Stream(s) Specifications

      Molar flows

Feed:	1
Name:	Feed1
Stage:	5
Two-phase feed:	*
State:	Temperature & pressure
Pressure [bar]:	Temperature & pressure
Vapour fraction [ ]:	Pressure & vapour fraction
Temperature [C]:	*
Flowrates [mol/s]:	*
Benzene:	*
Toluene:	*
Total flowrate:	*

Note that *ChemSep* has already filled in a name for the feed we entered during the specification of the column operation. You may, of course, change the feed stream name (and any changes will be reflected in the diagram on the operation panel).

*ChemSep* numbers the feeds in the sequence of the feed stage numbers we supplied but that can be changed here if necessary.

Two different types of specifications can be given to fix the feed state: the temperature and pressure or the vapor fraction and the pressure (of the feed). This specification is necessary to determine how much of the feed is vapor or liquid. This allows the program to determine the internal flow rates.

We must also select the feed stage model, a choice of *Split*, *Not split*, or *Split below*. The last of these options is for feed to the bottom stage of columns that do not have a reboiler. Either of the other options will suffice for this exercise but it should be noted that *Split* should normally be selected for feeds to stages other than the bottom stage. For more on the feed stage model we refer readers to a separate discussion.

In this example we want to specify a 'saturated feed' and we do this by selecting the vapor fraction specification. When a vapor fraction of zero is specified, the feed is taken to be at its boiling point (in the simulation a flash calculation is performed to calculate the boiling point of the feed mixture). Of course, we must specify a pressure to determine the feed temperature. Here our column operates just above atmospheric pressure in order to prevent ingress of any air in case any leak might develop.

We enter "1.1 atm" and we are asked to confirm the conversion to the default units for the pressure, namely in bar. If you enter the wrong type of units *ChemSep* will warn you and let you try again. Next we need to set the feed composition and total flow rate. Here we want a equimolar feed with a total *mass* flow rate of 1 kg/s. To do this we first enter equimolar feedrates of Benzene (B) and Toluene (T). Any amount will do as long as we enter the same rates for the two components. Then we enter "1 kg/s" in the total flowrate field.

Flowrates (mol/s):	
Benzene	1.00000
Toluene	1.00000
Total flowrate	1kg/s

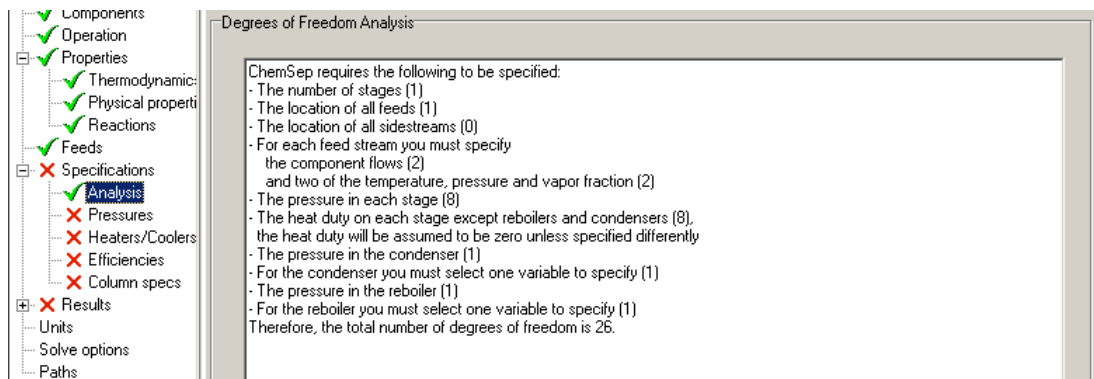
Press *Enter* and you will now see this:

Flowrates (mol/s):	
Benzene	5.87354
Toluene	5.87354
Total flowrate	11.7471

*ChemSep* knows the molecular weights of the components it automatically carried out the conversion of the mass flowrate to the molar flowrate. The 1 kg/s corresponds to 11.7471 mol/s as total feed flow as shown above.

Note that we can also switch from displaying the feed flows in mass or molar units using the pull down list that appears just above the feed table.

As our simple distillation column only has one feed, we are done and can move to the next input screen: expand the tree for the 'specifications'. There are five tab screens listed for this input: *Analysis*, *Pressures*, *Heaters/Coolers*, *Efficiencies*, and *Column* specifications. The analysis screen shows us the degrees of freedom for the equilibrium staged column and therefore what needs to be specified.



We see that we need to specify the pressures on each stage and we do this by selecting the *Pressures* tab after we opened the *Specifications*. Since the column has a condenser *ChemSep* asks us to specify pressure in the condenser first.

Column Pressure Specifications	
Condenser pressure	1.11458 (bar)
Column pressure	Constant pressure
Top pressure	1.11458 (bar)
Pressure drop / stage	* (bar)
Bottom pressure	* (bar)

There you will notice that each item that needs to be specified is shown as an asterisk (\*) in *ChemSep*. Upon selecting such a field, the asterisk usually is replaced by a default value or else a value that is consistent with the other specifications that already have been made. In this example we already have entered a feed pressure and thus *ChemSep* assumes that the condenser pressure equals this pressure. Normally, the condenser is not located on top of the column but at some lower elevation. There is, therefore, a considerable length of pipe between the column and the condenser over which a certain pressure drop exists. Thus, it is likely that the condenser has a lower pressure than the top of the column but to keep this problem simple we assume that the pressure is the same throughout the column as well as in the condenser. Thus, we accept the

defaults *ChemSep* provides for the condenser and column top pressures and select the constant pressure specification.

The degrees of freedom also tells us that on each stage we need to specify a *heat duty*, representing either a heater when positive or a cooler when negative.



Define Column Heat Exchangers

Column heat loss: 0 (MW)

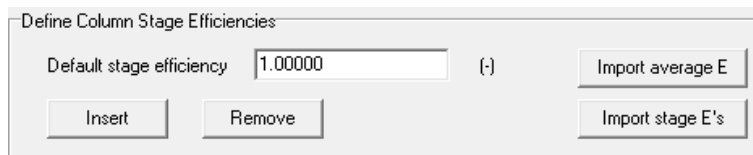
Name column duty: Qcolumn

Stage heat exchangers:

Insert Remove

These heat duties are optional, and you, therefore, need to "insert" such a cooler or heater if required. When doing so the program asks you to specify the stage number, name of the heat exchanger, and its duty. As columns typically operate at temperatures above ambient, there is typically also a heat loss over the column. This is modeled as a separate duty that gets subtracted from each stage, except for the condenser and reboiler. The default name for this the heat loss is set to 'Qcolumn' and you only need to specify a value for it. In this example we will assume the column is insulated well enough that the heat loss is negligible and therefore we assume the default value of zero.

After the specifications of the heaters and coolers the next sheet brings us to the *Stage Efficiencies*. A default stage efficiency for all the stages is to be specified. This value is used for all stages in the column except the condenser and reboiler, which are assumed to operate at equilibrium. We can specify stage specification for specific stages by inserting and deleting stage efficiencies. These are Murphree vapour efficiencies and we use the default efficiency value of one.



Define Column Stage Efficiencies

Default stage efficiency: 1.00000 (-)

Import average E

Import stage E's

Insert Remove

Further discussion of the options available in *ChemSep* for specifying efficiencies is available elsewhere.

The next and also the last specification tab sheet is that for the *column product specifications*. As we have equipped our column with both a condenser and a reboiler, we have to make two additional specifications that are going to fix the heat duties of these heat exchangers and that will determine the internal flow rates as well as the overall mass balance by means of the distillate and bottoms flows. Again, we see that *ChemSep* has provided default names for the product flow names (here *Top* and *Bottom*) and heat duties of the condenser and reboiler (indicated with a Q). For the top specification there is a long list of possible specifications that we are allowed to make.

The first is the reflux ratio, RR, a very common specification that determines the ratio between the distillate top product and the flow that is refluxed back to the column. *ChemSep* provides a default value for the reflux ratio of two, however, this value will depend very much on the application and system at hand. This means that the ratio of refluxed liquid flow rate to the product distillate flow is two (twice as much liquid is returned to the top of the column as reflux compared to the liquid drawn as distillate product).

Column Product Specifications

Top product name: Top      Condenser duty name: Qcondenser

Top specification: Reflux ratio = 2.00000 (-)

Bottom product name: Bottom      Reboiler duty name: Qreboiler

Bottom specification: Bottom product flow rate = 5.87400 (mol/s)

For the reboiler select the total bottoms flow rate. As we fed an equimolar mixture to the column, we want to draw equal bottoms as distillate flows, so we specify a bottoms flow of 5.874 mol/s. The operation specifications spreadsheet shows both these specifications. The combination of reflux ratio and bottoms flow rate is one that gives the most rapid convergence in our experience. You can make other combinations but not all will converge very quickly, and some combinations might even give rise to impossible specifications. That's why we advocate the reflux ratio – bottoms flow combination for each (distillation) problem. After you have solved the problem with this specification you can see what the column does and when necessary switch to a different set of specifications.

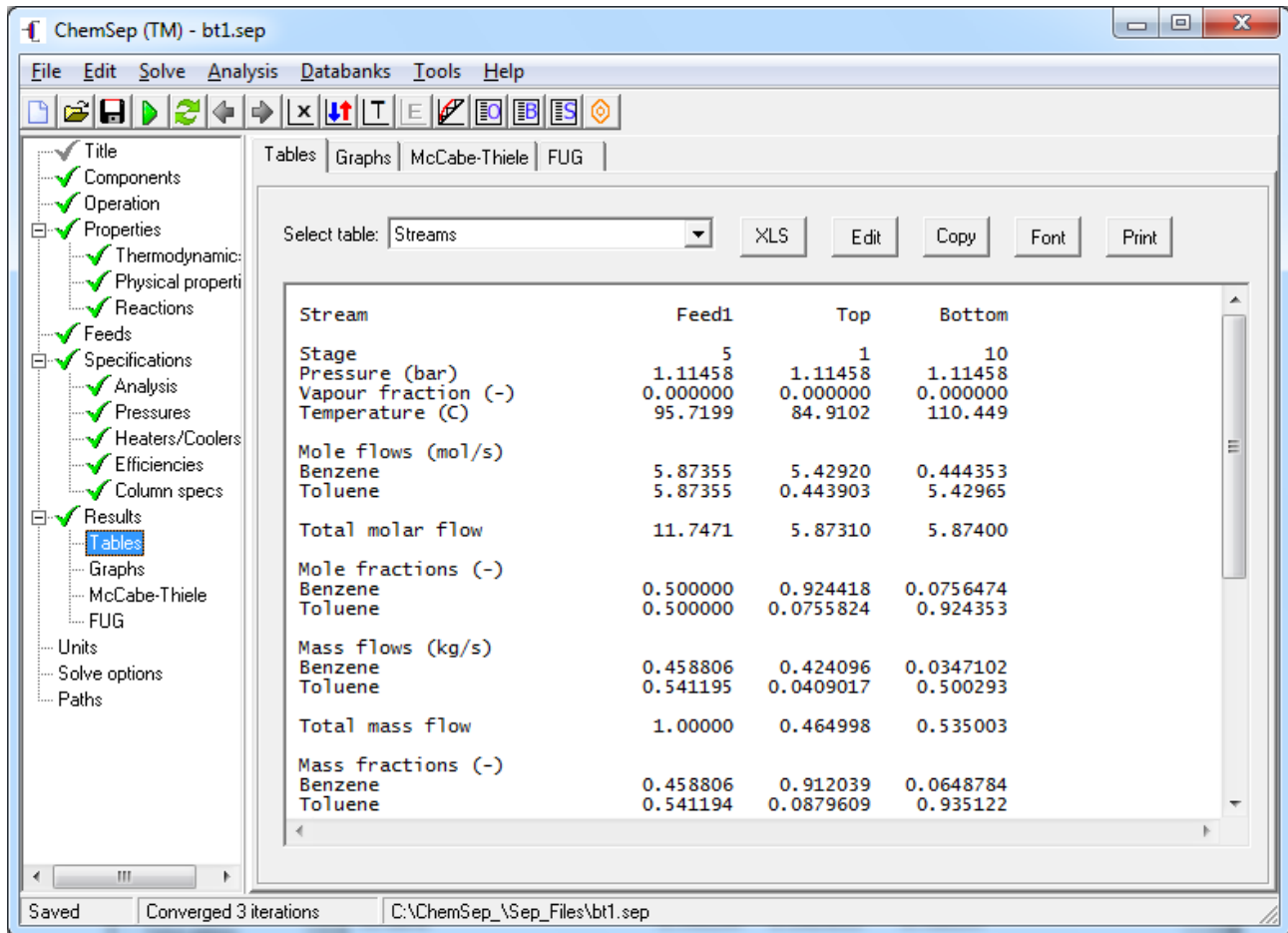
After the column specifications have been set all the red crosses in the input tree list have become green check marks, meaning we have successfully completed the input specification for our binary distillation example and can go ahead with solving the column. We can do so by pressing `{\it Alt-S}` or clicking the little calculator on the toolbar. This will also check our input and if we forgot something bring us to the window where more input is required or where there is a problem with the specifications. To solve the problem we must also save it into a simulation file in order to pass the problem on to the simulator programs. They are separate programs that read the problem from the simulation file and append the results to the same file. Thus, we are prompted for a valid file name and path. The default extension (.sep) is automatically appended by *ChemSep*. After the simulation file name is specified, say "bt1", the input is saved and the column simulation starts.

During the *solve* process a window shows the progress of the calculations in the form of messages of reading the problem and while solving a sum of errors for each iteration. This error sum is a norm for the convergence obtained and needs to become less than the accuracy set under the Solve options. When the error sum is small enough the process ends.



## Results: Tables

Following a successful simulation *ChemSep* will reload the sep-file and enable the results tab sheets: *Tables*, *Graphs*, *McCabe-Thiele*, and *FUG*. The latter is an acronym for Fenske-Underwood-Gilliand and is a collection of short-cut models. **Note that the *FUG* panel is not available in all versions of *ChemSep*.** The interface will automatically display the stream table.



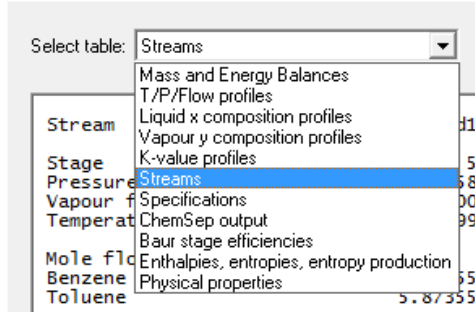
The screenshot shows the ChemSep (TM) - bt1.sep application window. The 'Tables' tab is active, and the 'Streams' table is selected. The table displays the following data:

Stream	Feed1	Top	Bottom
Stage	5	1	10
Pressure (bar)	1.11458	1.11458	1.11458
Vapour fraction (-)	0.000000	0.000000	0.000000
Temperature (C)	95.7199	84.9102	110.449
Mole flows (mol/s)			
Benzene	5.87355	5.42920	0.444353
Toluene	5.87355	0.443903	5.42965
Total molar flow	11.7471	5.87310	5.87400
Mole fractions (-)			
Benzene	0.500000	0.924418	0.0756474
Toluene	0.500000	0.0755824	0.924353
Mass flows (kg/s)			
Benzene	0.458806	0.424096	0.0347102
Toluene	0.541195	0.0409017	0.500293
Total mass flow	1.00000	0.464998	0.535003
Mass fractions (-)			
Benzene	0.458806	0.912039	0.0648784
Toluene	0.541194	0.0879609	0.935122

The stream table shows a complete overview of the feed(s) and products of the distillation column. It shows pressure, vapor fraction, temperature, enthalpy, molar and mass flows for the (component) flows of each stream.

In this table we see that the feed is equimolar; both component mole fractions are 0.5. The distillate top product and the bottoms product compositions are almost exactly mirrors of each other in respect to the mole fractions. As there is a modest difference in molecular weights between the components, the weight fractions are somewhat different. To edit the table just click in the table and start typing.

Other tables can be selected from the pull down list of tables:



Below we display the *material and energy balances*.

Select table: **Mass and Energy Balances** [XLS] [Edit]

Mass and Energy Balances	
Stream / Apparatus	Mass (mol/s)
Feed1	11.7471
Top	-5.87310
Bottom	-5.87400
Balance	----- + 4.6566E-07
Component discrepancies (mol/s)	
Benzene	2.6970E-07
Toluene	2.8327E-07

Here we can see in whether the overall and component mass balance have been met. The overall balances should be equal to zero or close to 0 (within the criterion used to converge the simulation). Also, the component balances must be (approximately) zero. When this is not the case, the solution found is not a physically meaningful solution. It is important to *always* check this.

To see a different table, select it from pull down list of the table selector. For example the *T/P/Flow profiles*.

Select table: **T/P/Flow profiles** [XLS] [Edit] [Copy] [Font] [Print]

Stage	Temperatur (C)	Pressure (bar)	Flow rates (mol/s)		Feed	Product
			Liquid	Vapour		
1	84.9102	1.11458	11.7462	RR=2	11.7471	5.87310 L
2	87.1615	1.11458	11.7462	17.6193		
3	90.1049	1.11458	11.7462	17.6193		
4	93.2790	1.11458	11.7462	17.6193		
5	96.1035	1.11458	23.4933	17.6193		
6	98.5078	1.11458	23.4933	17.6193		
7	101.601	1.11458	23.4933	17.6193		
8	104.963	1.11458	23.4933	17.6193		
9	108.036	1.11458	23.4933	17.6193		
10	110.449	1.11458	BR=2.99954	17.6193		
Stage	Temperatur (C)	Pressure (bar)	Flow rates (kg/s)		Feed	Product
			Liquid	Vapour		
1	84.9102	1.11458	0.929996	RR=2	1.00000	0.464998 L
2	87.1615	1.11458	0.946338	1.39499		
3	90.1049	1.11458	0.966162	1.41134		
4	93.2790	1.11458	0.985842	1.43116		
5	96.1035	1.11458	2.00420	1.45084		
6	98.5078	1.11458	2.03010	1.46919		
7	101.601	1.11458	2.06134	1.49510		
8	104.963	1.11458	2.09291	1.52634		
9	108.036	1.11458	2.11982	1.55791		

In this table we see that the reflux ratio we specified was indeed also obtained and that together with the bottoms flow rate specification this implied a boilup ratio of three (within the tolerance we supplied at the solve options). We see that the pressures are all the same throughout the whole column – also as specified -- and the temperatures vary from 85°C in the condenser to 111°C in the reboiler. This is typical of the temperature profile one would expect for a simple distillation column.

Note, also, the T/P/flow profile table shows the flows in both molar (top) *and* mass units (bottom).

Note that we can use one of the buttons above the table to export the table into an Microsoft Excel table or an ASCII table we can edit in a text editor. Alternatively, we can copy the table to the clipboard. The table can also be edited from hand in the interface before we do that. Of course, as soon as we select a new table with the table selector we lose any changes we make.

The next table shows the liquid mole fractions.

Select table:

Liquid x composition profiles		
Stage	Benzene	Toluene
1	0.924418	0.0755824
2	0.825234	0.174766
3	0.704915	0.295085
4	0.585472	0.414528
5	0.487041	0.512959
6	0.408441	0.591559
7	0.313627	0.686373
8	0.217832	0.782168
9	0.136170	0.863830
10	0.0756474	0.924353

There is a similar table for the vapor mole fractions. In either table we see that the benzene concentrates in the top of the column.

The K-values can also be listed:

Select table:

K-value profiles		
Stage	Benzene	Toluene
1	1.04922	0.397983
2	1.12019	0.432478
3	1.21759	0.480217
4	1.32898	0.535350
5	1.43408	0.587856
6	1.52823	0.635281
7	1.65607	0.700218
8	1.80398	0.776092
9	1.94783	0.850590
10	2.06678	0.912696

Here we see that the the K-values for benzene are greater than one – and those for toluene are lower than one. The K value was defined as the ratio of the vapor mole fraction to the liquid mole fraction, this means that the relative amounts of benzene are higher in the vapor than in the

liquid. This is why the fraction of benzene increases as the vapor rises up the column, condensing at 92 mole% whereas the feed was only 50%.

Two more tables are available that are not shown here: a summary of the specifications and a table showing the output from the column simulator which was written to the run window. The specification summary is a very useful table for it contains the complete problem specification of the simulation, with this table anyone can reproduce the simulation. It also includes the little schematic drawing of the column flowsheet to show the column configuration.

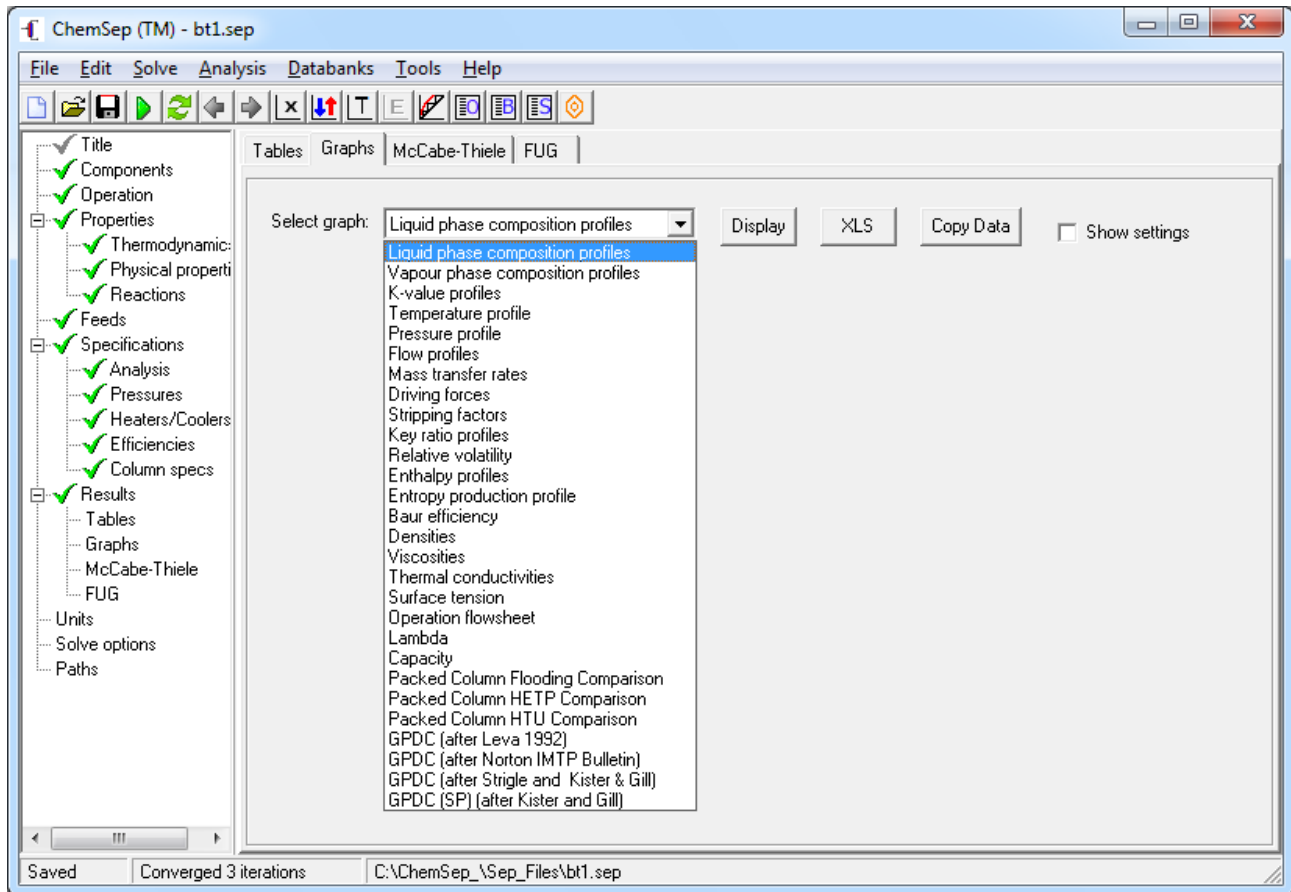
Finally, we show the table of physical properties. To display the whole table we need to increase the width of the *ChemSep* window.

The screenshot shows the ChemSep (TM) - bt1.sep software interface. The 'Tables' tab is active, and the 'Physical properties' table is displayed. The table contains 10 rows of data corresponding to the stages of the distillation column. The columns are: Stage, Vapour Density (kg/m<sup>3</sup>), Liquid Density (kg/m<sup>3</sup>), Vapour Viscosity (Pa.s), Liquid Viscosity (Pa.s), Vapour Molecular weight (kg/kmol), Liquid Molecular weight (kg/kmol), Vapour Heat capacity (J/kmol/K), Liquid Heat capacity (J/kmol/K), Vapour Thermal conductivity (J/s/m/K), Liquid Thermal conductivity (J/s/m/K), and Surface tension (dyn/cm).

Stage	Vapour Density kg/m <sup>3</sup>	Liquid Density kg/m <sup>3</sup>	Vapour Viscosity Pa.s	Liquid Viscosity Pa.s	Vapour Molecular weight kg/kmol	Liquid Molecular weight kg/kmol	Vapour Heat capacity J/kmol/K	Liquid Heat capacity J/kmol/K	Vapour Thermal conductivity J/s/m/K	Liquid Thermal conductivity J/s/m/K	Surface tension dyn/cm
1	2.94045	807.419	9.0539E-06	3.0199E-04	78.5359	79.1742	100687	152478	0.0155356	0.121840	20.5499
2	2.94582	805.070	9.0765E-06	2.9562E-04	79.1742	80.5654	102553	155464	0.0156438	0.120529	20.3138
3	2.95618	801.991	9.1008E-06	2.8756E-04	80.1017	82.2532	105186	159207	0.0157727	0.118921	20.0112
4	2.97174	798.666	9.1199E-06	2.7915E-04	81.2268	83.9286	108286	163071	0.0158946	0.117302	19.6922
5	2.98956	795.708	9.1303E-06	2.7185E-04	82.3438	85.3093	111289	166382	0.0159874	0.115950	19.4141
6	3.00780	793.192	9.1342E-06	2.6575E-04	83.3854	86.4118	114038	169118	0.0160541	0.114856	19.1813
7	3.03556	789.959	9.1320E-06	2.5800E-04	84.8555	87.7418	117852	172542	0.0161226	0.113517	18.8869
8	3.07144	786.453	9.1202E-06	2.4969E-04	86.6289	89.0855	122374	176155	0.0161739	0.112140	18.5728
9	3.10969	783.254	9.1003E-06	2.4216E-04	88.4205	90.2309	126877	179373	0.0161992	0.110942	18.2905
10	3.14351	780.746	9.0786E-06	2.3628E-04	89.9479	91.0799	130675	181849	0.0162041	0.110038	18.0719

## Results: Graphs

*ChemSep* has a rich set of plotting options for the column simulation results. It is much easier to analyze the results in graphical than in table format (as is true for most other problems). The graph menu shows the different plots that are available.



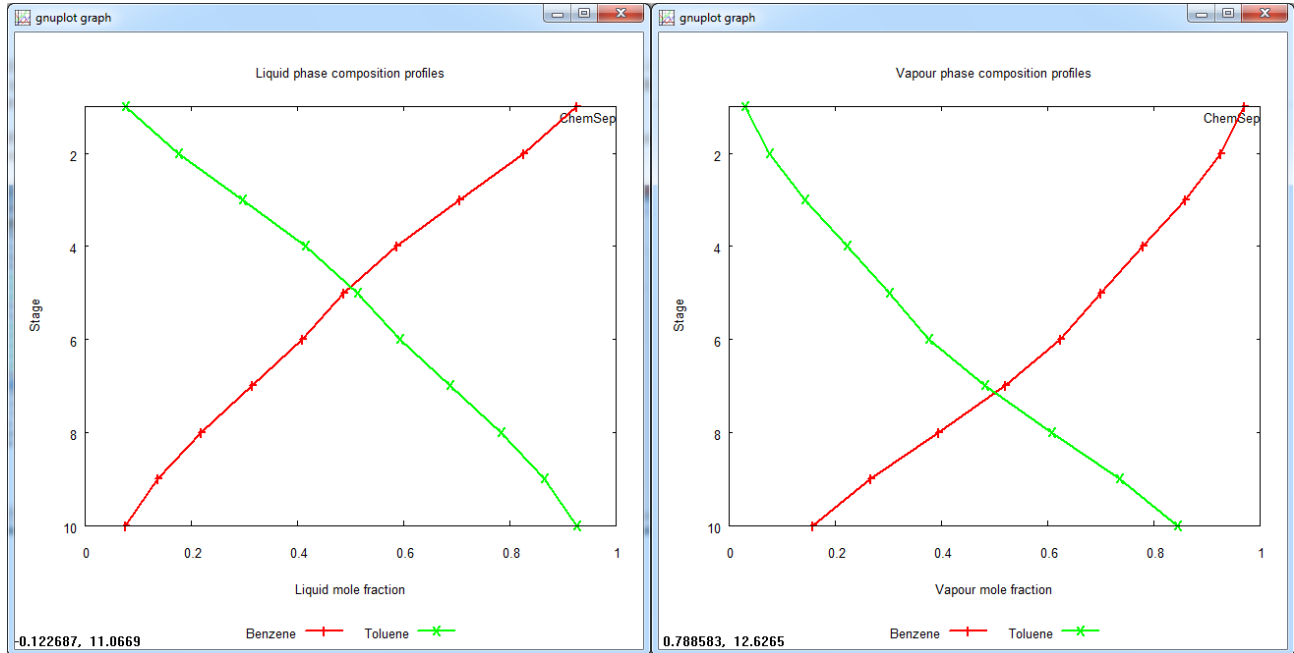
Not all of these plots are available in every case. For example, the last eight in the list above are available only for rate-based model simulations (which this particular example is not).

The default orientation in *ChemSep* profiles is to plot the stages vertically, with the condenser at the top and the reboiler on the bottom. Imagine the profile projected over the column standing straight up on the left axis. This orientation can be changed as can almost all other details of the plots by clicking in the *Show settings* check box. Configuration of plots is covered in more detail elsewhere.

In what follows we look at some of the standard plots available following equilibrium (and rate-based) simulations.

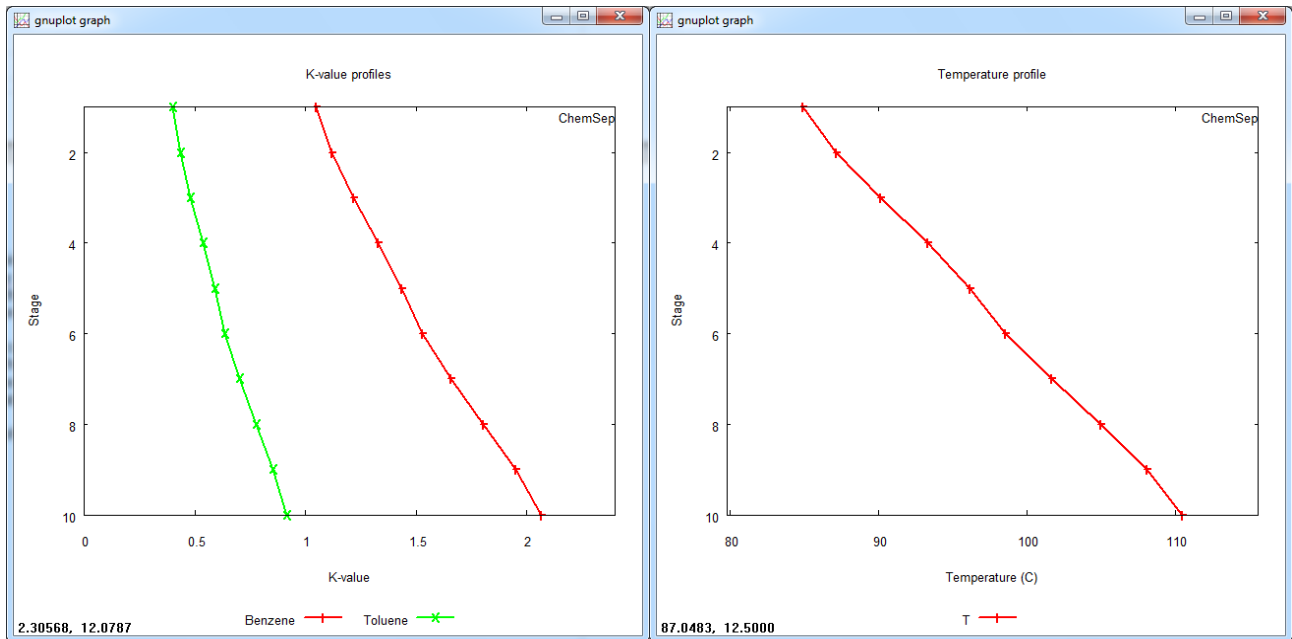
## Composition profiles

The first two plots listed in the graph menu are the liquid and vapor mole fraction profiles that show how the components are distributed over the column. The first of these is shown below.



Looking at the composition profiles we observe that benzene concentrates in the top of the column and toluene in the bottom. This is to be expected as benzene boils at 80 and toluene at 110.6°C at atmospheric pressure. Note that the composition profiles show an almost symmetric behavior. This is an indication that benzene and toluene form a relatively ideal mixture.

## The K-value and temperature profiles

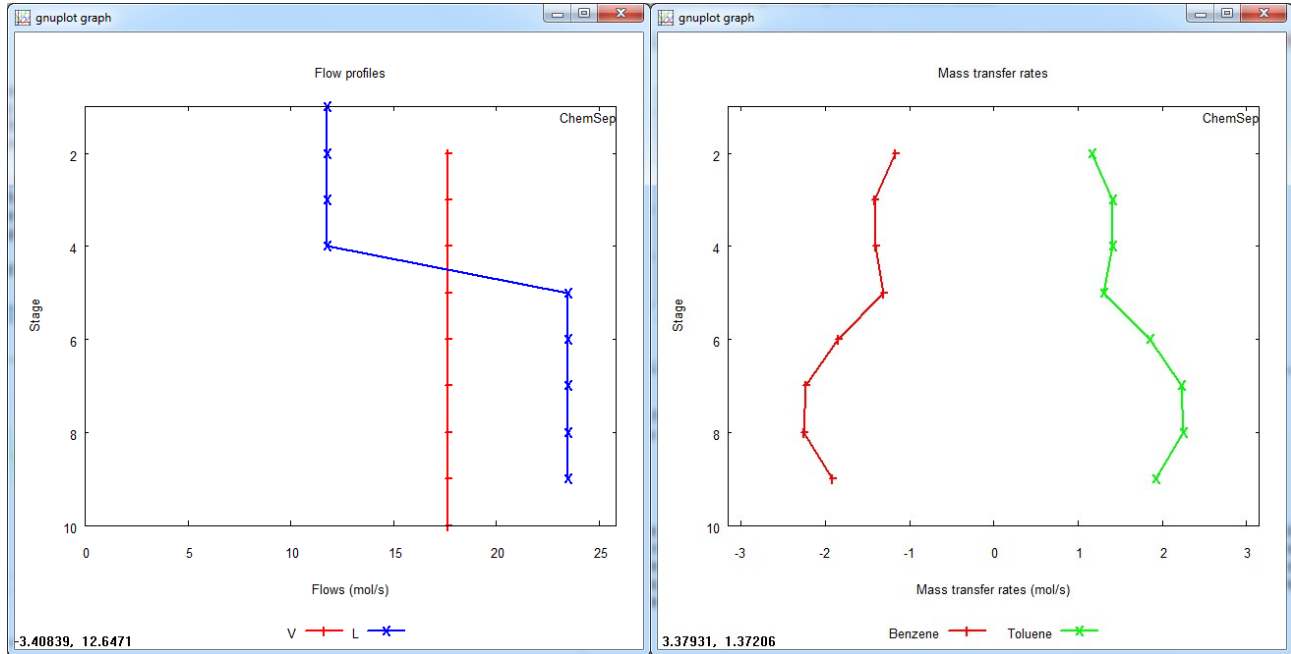


Both the K-values and temperatures increase from top to bottom. In this case the behavior of the K-values can be explained from the temperatures. We used the DECHEMA K-model:

$$K_i = \frac{y_1 P_{i, sat}}{P}$$

where the pressure is constant over the whole column. As benzene and toluene form an relatively ideal mixture, the activity coefficients are close to unity and do not vary much over the height of the column. Therefore, the K values are dictated mostly by the behavior of the component vapor pressures, which increase with increasing temperatures. The temperature profile shows that the temperatures increase from top to bottom, which explains why the K-values do the same.

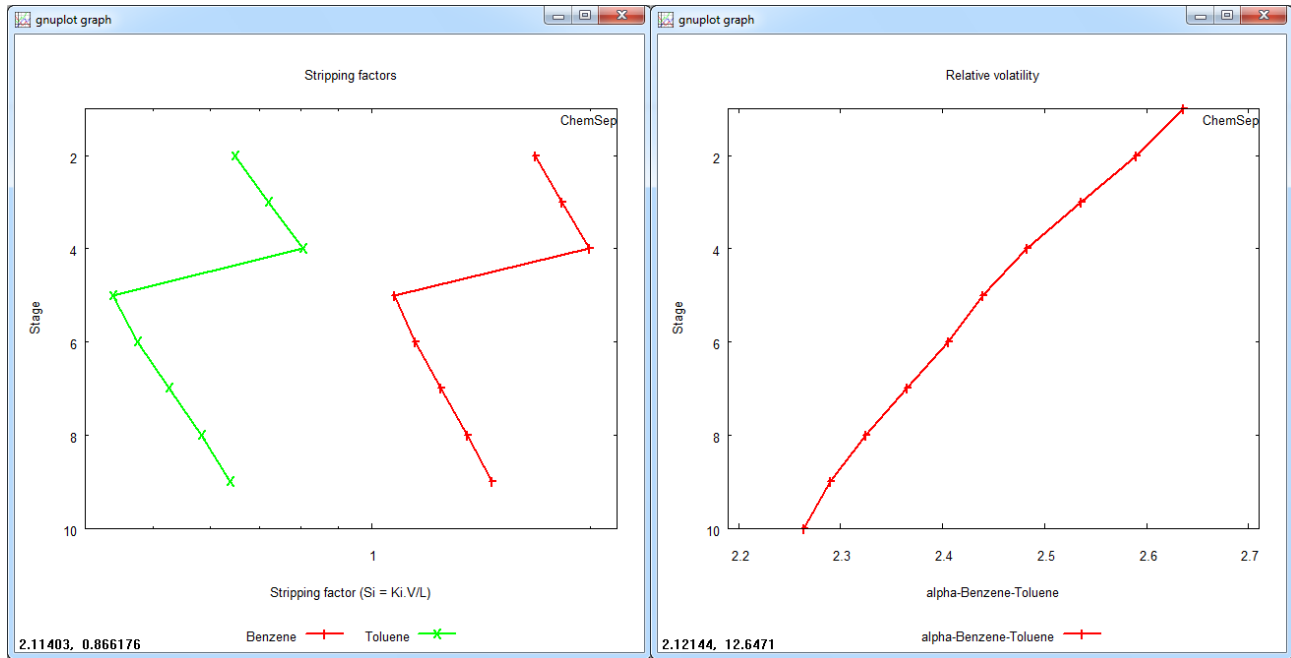
## Vapor and liquid flows and mass transfer rate profiles



Here we see that the vapor flow rates are constant through the whole column. This can be explained by the fact that the feed enters as a saturated liquid on stage 5. At this stage we also see an increase in the liquid internal flowrate. As the feed is at its boiling point, no vapor is condensed, nor is any vapor added at the feedstage. The only vapor generation is done in the reboiler. The difference in the liquid from stage 1 (the condenser) and the vapor from stage 2 (which enters the condenser) equals the distillate flowrate. We see that this difference is half the size of the reflux flow from the condenser (the liquid flow stage 1); thus, the reflux ratio is equal to 2.

The mass transfer rate profiles for the two components are symmetric either side of the line denoting zero. Mass transfer rates are defined to be positive for condensing components. That is why the mass transfer rates for benzene are negative as it evaporates at each stage in the column (note the condenser and reboiler are not shown!). The fact that the profiles for benzene and toluene are symmetric is obvious when we realize that we are separating a binary mixture under equimolar overflow conditions: if one component evaporates the same amount of the other component needs to condense.

## Stripping factor and relative volatility profiles



The stripping factor is defined as the ratio of the vapor and liquid component molar flows:

$$S_i \equiv \frac{V y_i}{L x_i} = \frac{V}{L} K_i$$

Stripping factors indicate the direction a component is moving at the specific stage. If it is larger than one, this means the component flow upwards in the column is larger than the component flow downwards at this stage. As we can see in \figure{FEXstrippingfactors}, the stripping factor for benzene is larger than unity at all points in the column. The stripping factor for toluene is less than 1 at all points in the column.

The ratio of the K-values is the relative volatility:

$$\alpha_{ij} = \frac{K_i}{K_j}$$

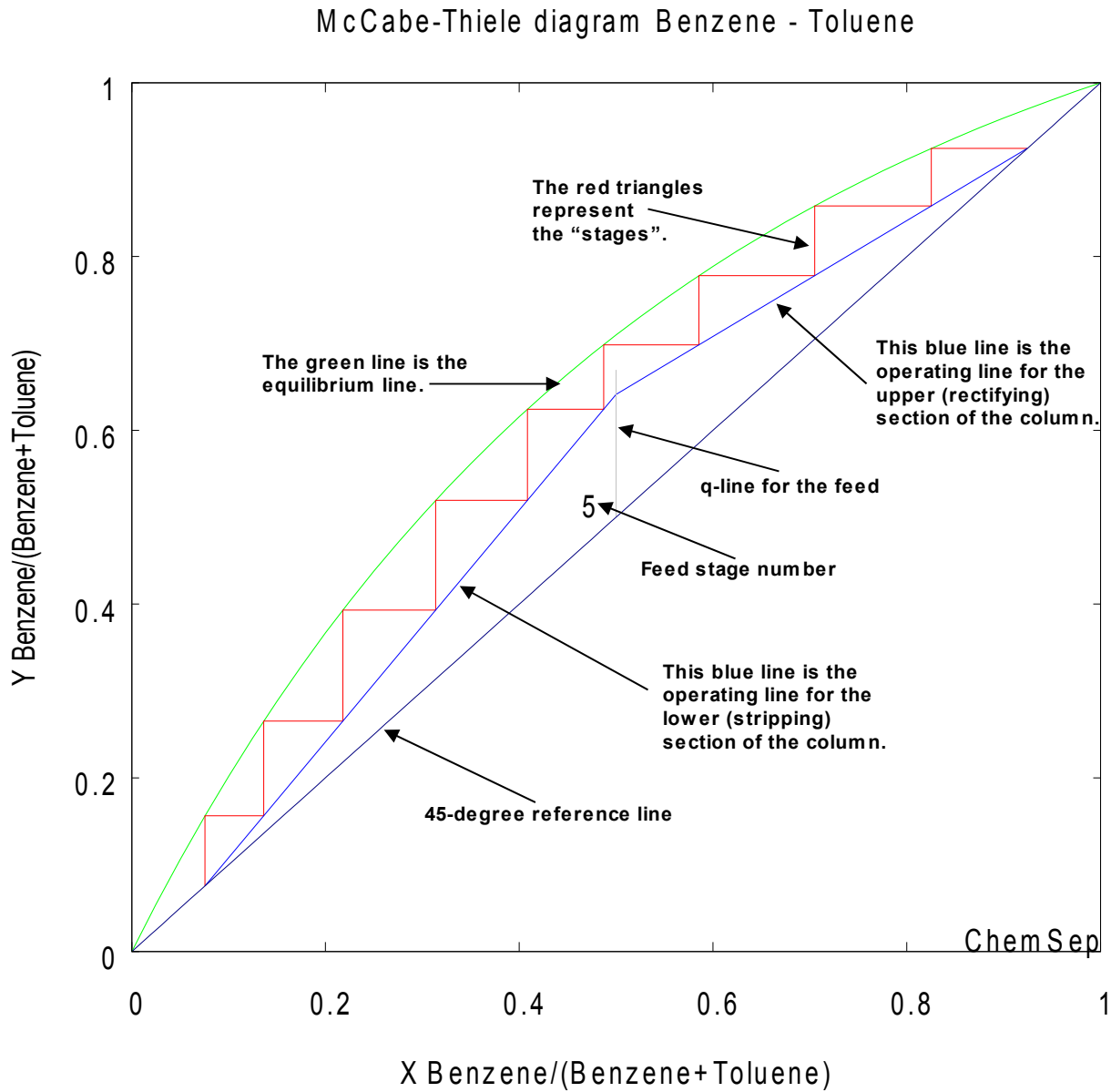
This ratio is a measure of how easy it is to separate two components from each other. In our example – using the DECHEMA model – this ratio becomes:

$$\alpha_{ij} = \frac{\gamma_i P_{i,sat}}{\gamma_j P_{j,sat}}$$

When the activity coefficients are close to unity (true for ideal mixtures) the relative volatility is just the ratio of the component vapor pressures. As the latter increase with temperature, the relative volatility is often only a weak function of temperature. This is especially so when the boiling points of the two components are close. In our case the relative volatility varies from 2.25 in the reboiler to 2.6 in the condenser

## The McCabe-Thiele Diagram

The McCabe-Thiele diagram for this example is shown below with explanatory labels superimposed on the diagram created by *ChemSep*.



In the x-y diagram we add the *45-degree line* or  $x=y$  line as a useful reference line.

For binary mixtures the vapor mole fraction can be calculated from:

$$y_1 = \frac{\alpha_{12} x_1}{1 + x_1(\alpha_{12} - 1)}$$

where  $\alpha_{12} = K_1/K_2$  is the relative volatility between benzene and toluene. We saw from the plot shown above that the relative volatility is not constant (although it does not vary all that much over the height of the column). *ChemSep* uses the actual relative volatility calculated on each stage from the ratio of K-values as defined above.

The larger the relative volatility, the further away the equilibrium line is from the  $x=y$  line and the easier it is to separate the two components.

At  $x=0.5$  another small line is drawn that represents the feed or 'q' line. A number indicates the feed stage (5). Here 'q' stand for the 'quality' or liquid fraction in the feed. Using the component balance for the feed divided by the feed we find:

$$z_i = \frac{L^F}{F} x_i + \frac{V^F}{F} y_i$$

substituting the total molar balance  $F = V^F + L^F$  and  $q = L^F/F$  gives

$$z_i = q x_i + (1 - q) y_i$$

Thus, the slope of the so-called *q-line* is  $q/(1 - q)$

When  $q=1$  the q-line is vertical line as is shown in this example.

The blue lines in the diagram are the operating lines. These lines define the molar balances for the two column sections in our column. The material balance for the top section of the column or rectifying section is:

$$V_j y_{i,j} = L_j x_{i,j} + D x_{i,D}$$

If the molar flow rates in the column section are constant this becomes:

$$y_i = \frac{r}{r+1} x_i + \frac{1}{r+1} x_{i,D}$$

where  $r$  is the reflux ratio defined by  $r = L/D$ .

This is a straight line with slope  $L/V = r/(r+1)$

which crosses the  $x=y$  line at  $x_D$ .

For the lower part of the column (the stripping section) the material balance is:

$$V'_j y_{i,j} = L'_j x_{i,j} - B x_{i,B}$$

which can be written as

$$y_i = \frac{s+1}{s} x_i - \frac{1}{s} x_{i,B}$$

where  $s$  is the reflux ratio defined by  $s = V/B$ .

This also is a straight line with slope  $L'/V'$  which crosses the  $x=y$  line at  $x_B$ . Now it becomes clear why we used the  $x=y$  line as our reference line: the two operating lines and the  $q$ -line cross this line at the feed and top/bottom compositions, respectively.

The red lines drawn in between the equilibrium line and the operating lines represent the stages. We start drawing at the reboiler composition  $x_B$  on the  $x=y$  line. The reboiler generates a vapor with a vapor composition of  $y_B$ , which is the  $y$  value on the equilibrium line at  $x=x_B$ . In other words, we draw a dotted line straight up to the equilibrium line. The liquid composition from the stage above can be obtained by moving horizontally to the operating line, as the operating line determined the mass balance for the internal flows. Then, for the stage above we draw again a vertical line to the equilibrium line and repeat this process. When we pass the feed stage we switch from using the stripping operating line to using the rectification operating line. A total condenser does not generate another triangle for as all the vapor is condensed into a liquid and no further separation is achieved.

Although it was devised for solving binary distillation problems graphically, the McCabe-Thiele diagram has value for simulation programs like *ChemSep*. The diagram can immediately show if the resulting design is optimum in some senses. It can also be used to interpret the results of a simulation of a multicomponent separation process (although, as we shall show elsewhere, there is more than one way to display a McCabe-Thiele diagram for such cases).

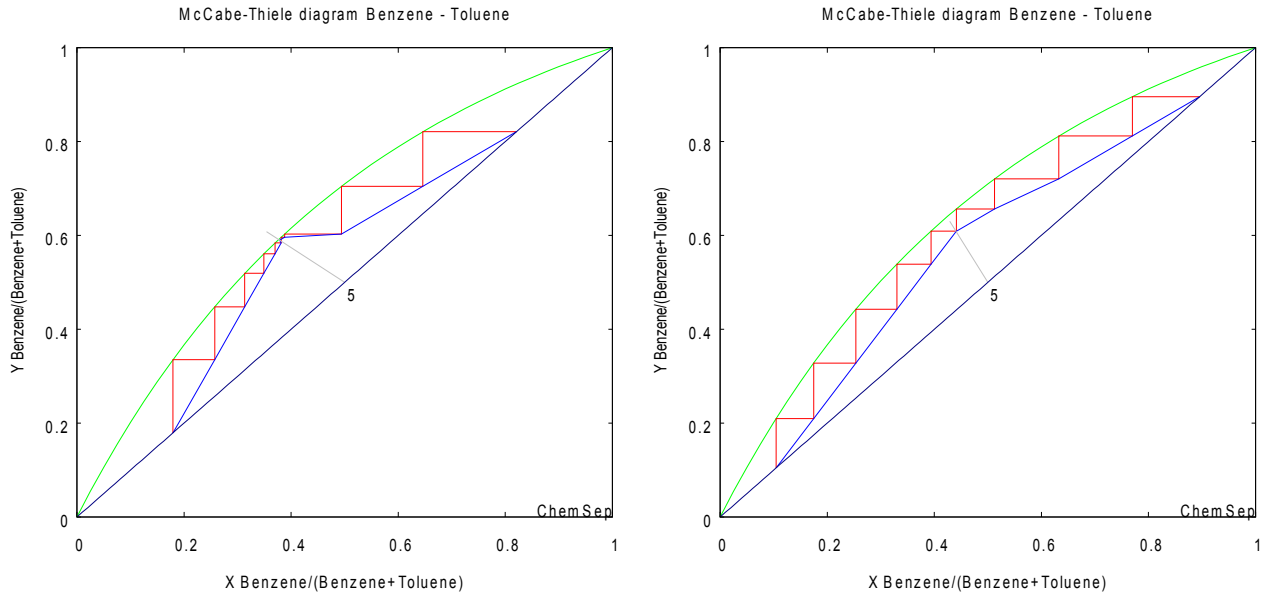
### **Influence of the Reflux Ratio**

We continue this tutorial by posing the question: What would happen if the feed were a saturated vapor (instead of a saturated liquid as was the case above)? To answer this question we need to go back to the *Feed specifications panel* and specify a vapor fraction of 1. When we use the solve option in the program we are asked whether we want to overwrite the simulation file. Don't; instead save the new problem under a different name. The McCabe-Thiele diagram (below left) that results from this simulation diagram looks quite different as we see below:

Observe that the distillate and bottoms compositions are closer to the feed composition. An enlargement of the area around the feed line shows what is going on. As the feed is now a vapor feed the  $q$ -line is a horizontal line. The slope of the  $q$ -line is given by  $q/(1-q)$  which is zero if

$q=0$ . This results in a misplaced feed and we have to keep stepping off stages on the stripping operating line when it would have been more advantageous to step off stages on the rectifying operating line. Two stages in the column are much less effective than they could be.

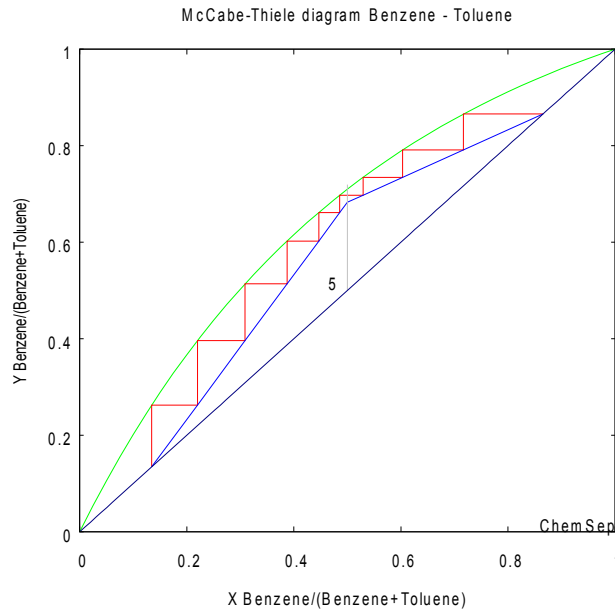
If the vapor fraction is specified as 0.5, we see (in the McCabe-Thiele diagram to the right below) that the feed line has a slope of -1 and that the feed is again much better placed (but still not optimally). In this case stage 6 is the optimal feed stage.



The feed quality  $q$  can also be larger than unity or smaller than zero. This occurs when subcooled liquid or superheated vapor feeds are introduced in the column. A subcooled liquid needs to be heated up to its boiling point, in which it will condense a certain amount of vapor generating a higher internal liquid flow. The opposite is true for a superheated vapor. For a subcooled liquid the slope of the feed line is even positive, the same for a superheated vapor.

Subcooled liquids are more common than superheated vapors for distillation columns for the simple fact that distillation feeds are often liquids (from storage) and a pre-heater represents an extra piece of equipment. The same task can be taken over by the reboiler, albeit at a higher temperature than the feed, requiring more energy (as well as shifting the operating line in the stripping section of the column).

When we change the reflux ratio of the column from 2 to 1, we see another change in the McCabe-Thiele diagram (the feed quality is set back to 0 for this case).



Now the operating lines have different slopes! The slopes of the operating lines are given by the ratios of the internal flows. For the rectification line we had a slope equal to  $L/V=r/(r+1)$ . For  $r=2$  this gives a slope of  $r/(r+1)=2/3$  and for  $r=1$  only a slope of  $r/(r+1)=1/2$ .

We also see that the operating lines intersect each other almost on the equilibrium line. When they intersect the equilibrium line we would need an *infinite* number of stages to switch from the stripping to the rectification operating lines. Therefore, this is called a *pinch-point*, as the equilibrium and the operating lines come together. The reflux ratio at which the operating lines intersect the point at which the feed line crosses the equilibrium line is called the *minimum reflux ratio*. At that point the column needs an infinite number of stages.

We can mimic this situation by changing the specifications so that the column has a large (but not infinite) number of stages (150 will suffice in this case). We must also change the top and bottom specifications (if we want to find the minimum reflux ratio it is wise NOT to specify it). Since we want to find the lowest reflux ratio that will give us the same separation as in our first simulation with this system we specify the mole fractions in the bottom and top equal to those we saw in the stream table shown above.

Column Product Specifications

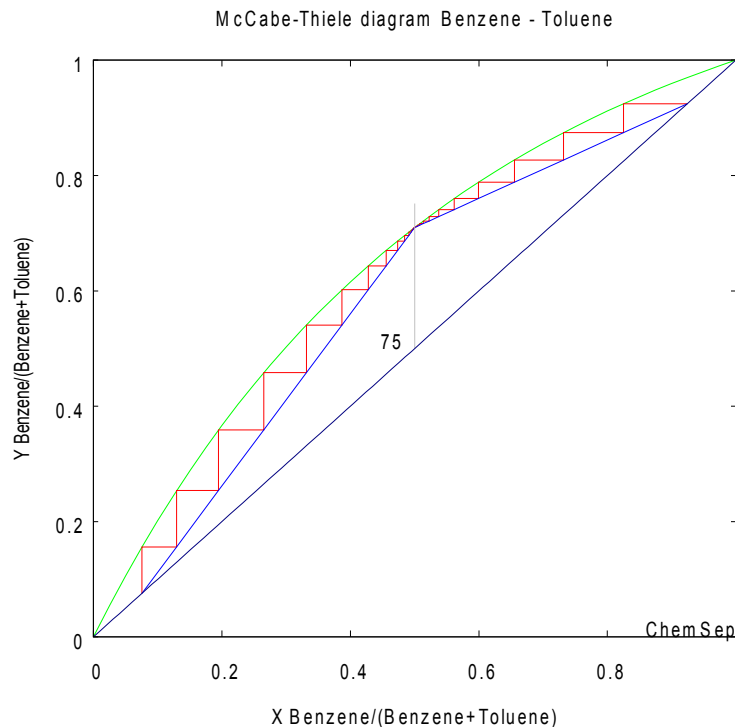
Top product name:  Condenser duty name:

Top specification: Mole fraction of a component =  (-)

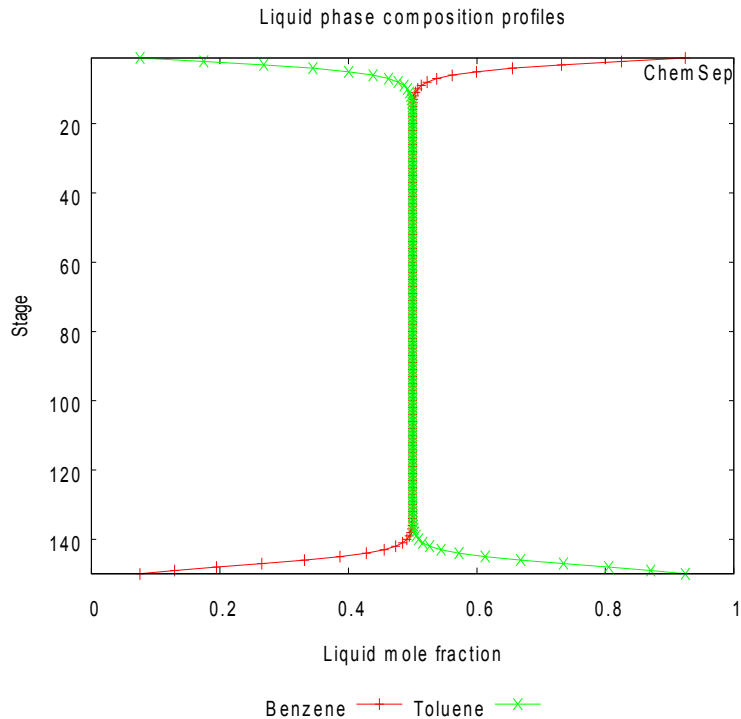
Bottom product name:  Reboiler duty name:

Bottom specification: Mole fraction of a component =  (-)

When we rerun the simulation we will obtain the McCabe-Thiele diagram shown below:



There are so many stages in this simulation that we cannot see all of them as distinct triangles (most of them are too small to show as more than isolated points). We can see that most of the stages perform essentially no separation by plotting the liquid phase composition profiles:

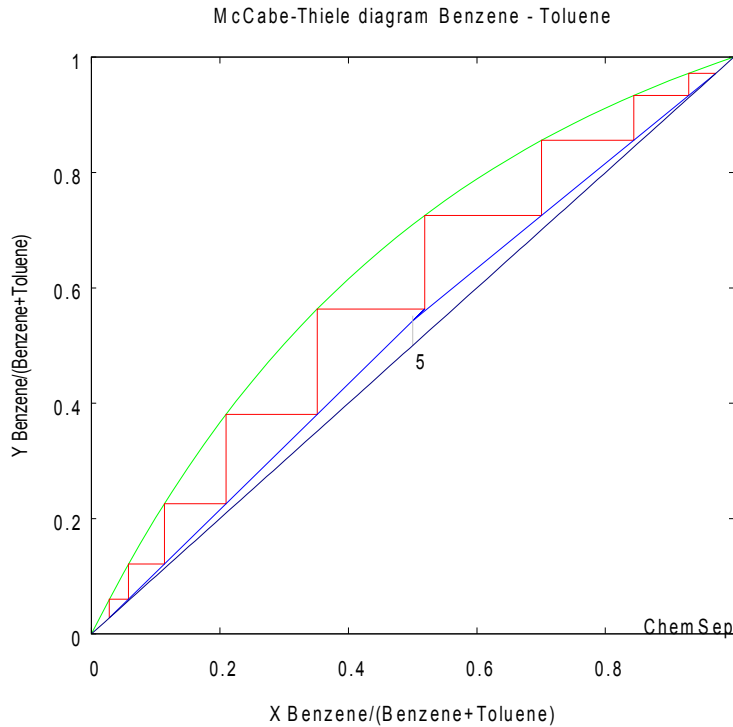


The value of the reflux ratio that gives this result can be seen in the flow table:

Stage	Temperatur (C)	Pressure (bar)	Flow rates (mol/s)		Feed	Product
			Liquid	Vapour		
1	84.9101	1.11458	6.01297	RR=1.02359		5.87436 L
2	87.1615	1.11458	6.01297	11.8873		

We see that a reflux ratio of slightly more than 1 is needed. Any reflux ratio lower than this will lead to top and bottom products with lower purities (try this as an exercise).

On the other hand, if we increase the reflux ratio to 10 (and set the number of stages back to 10) we obtain the McCabe-Thiele diagram shown below:

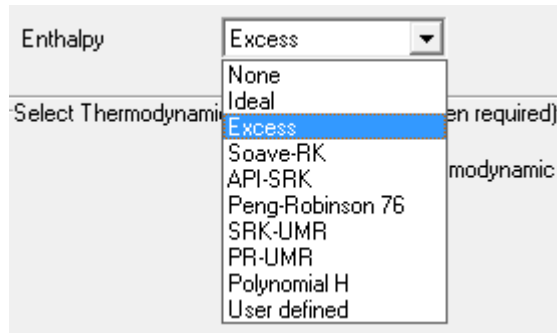


Observe here that the operating lines lie closer to the 45-degree reference line and that the stepping-off of stages leads to larger changes in mole fraction leading to a better separation. If we further increase the reflux the operating lines move closer to the  $x=y$  line until, at *total reflux*, they coincide with the  $x=y$  line. Of course, at total reflux  $r=\infty$ , all the vapor overhead is condensed and returned to the column so no product stream can be withdrawn (and hence, there is no production). At this point the separation uses the lowest number of stages to achieve a specific separation.

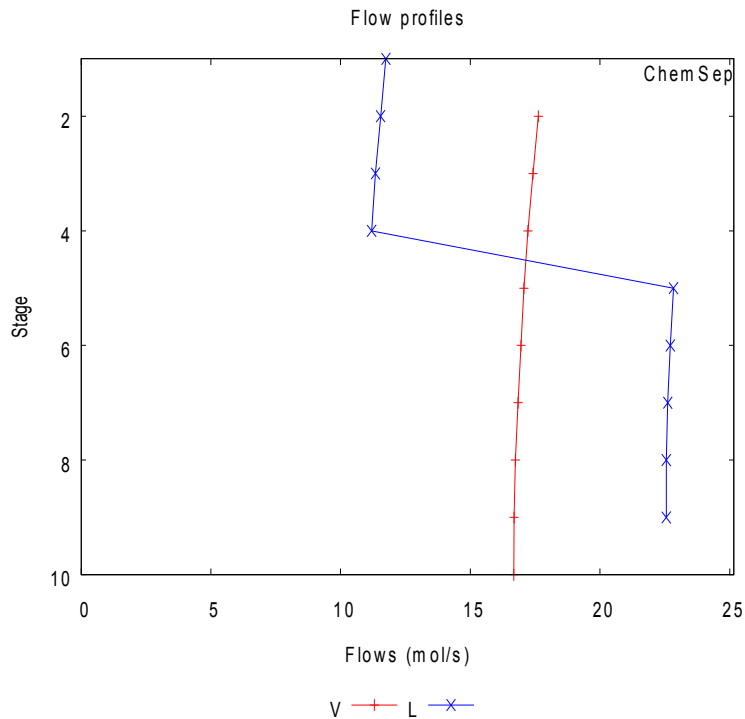
We see that there are two extremes for the separation for a given set of distillate and bottom compositions: the minimum reflux ratio at the pinch point and the minimum number of stages at total reflux. Real operation must lie somewhere between these two extremes. Typically, distillation columns operate at reflux ratios that are 1.1 to 1.5 times the minimum reflux ratio.

## The Influence of the Enthalpy Model

In all of the simulations carried so far out in this section we have set the enthalpy model to *None*. This leads to constant flowrates in each section of the column, a condition sometimes referred to as constant or equimolar overflow (CMO). We can relax this assumption by selecting a different enthalpy model: in the thermodynamic models under input. Here we select the *Excess* enthalpy model.

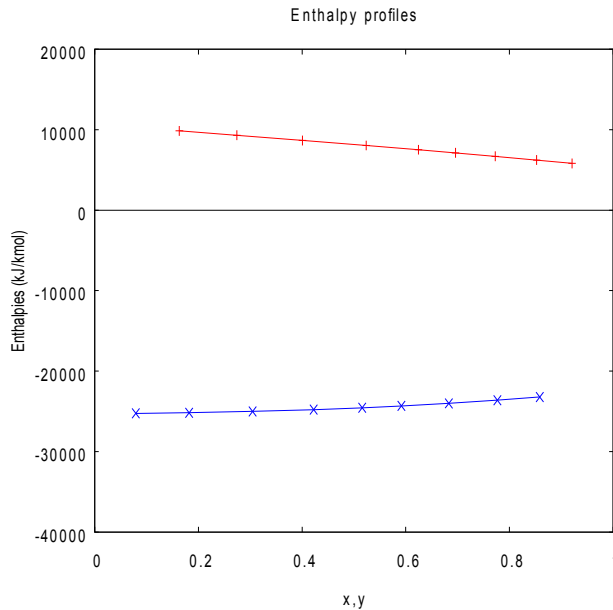


When we redo our column simulation and look at the flow profiles we see that the internal flows now change (albeit only slightly) from stage to stage.



As the internal flows change slightly, so do the slopes of the operating lines. The operating lines in the McCabe-Thiele plot now become also curved instead of straight lines (in this case the curvature is rather small so we have left out this plot).

When we select the Excess enthalpy model we are able to construct a Ponchon-Savarit diagram; in *ChemSep* it is actually just a H-xy plot as shown below.



Note that the vapor enthalpies are positive and liquid enthalpies are negative, the difference being the heat of vaporization. Vapor enthalpies are positive because the reference point for enthalpies is taken as gas at 298 K. As the column temperatures are higher than 298K, the vapor enthalpies are larger than 0. It is important to know what the reference point is when you are using enthalpies! Note that to display this plot as shown here some of the standard plot settings had to be changed as highlighted in the image below.

Select graph: Enthalpy profiles Display XLS Copy Data  Show settings

Plot

Title	Labels	Stages	Axis color	Commands	Box	Labels box	Import data
Enthalpy profiles	Off	Horizontal	Black	set label "Che On		Off	

Axes

	Title	Start	End	Tic interval	Small tics	Grid	Logarithmic	Scientific nota
x1	Enthalpies	-40000	20000	10000	0	Off	Off	Off
y1	x,y	0	1	0.2	0	Off	Off	Off
x2					0	Off	Off	Off
y2					0	Off	Off	Off

Add set Reset sets Calc.Dev's Store graph Auto Axis  Auto colors Black Delete set Save sets Plot Remove graph Enlarge 0.2  Auto points Diamond

Data sets

	Label	Plot X	Plot Y	X axis	Y axis	Units X	Units Y	Color	Points	Thickne	Style	1st stage	Last stage
1	y1	HV	y1	x1	y1	kJ/kmol		Red	Diamond	Normal	Solid	2	10
2	x2	HL	x2	x1	y1	kJ/kmol		Blue	+	Normal	Solid	1	9