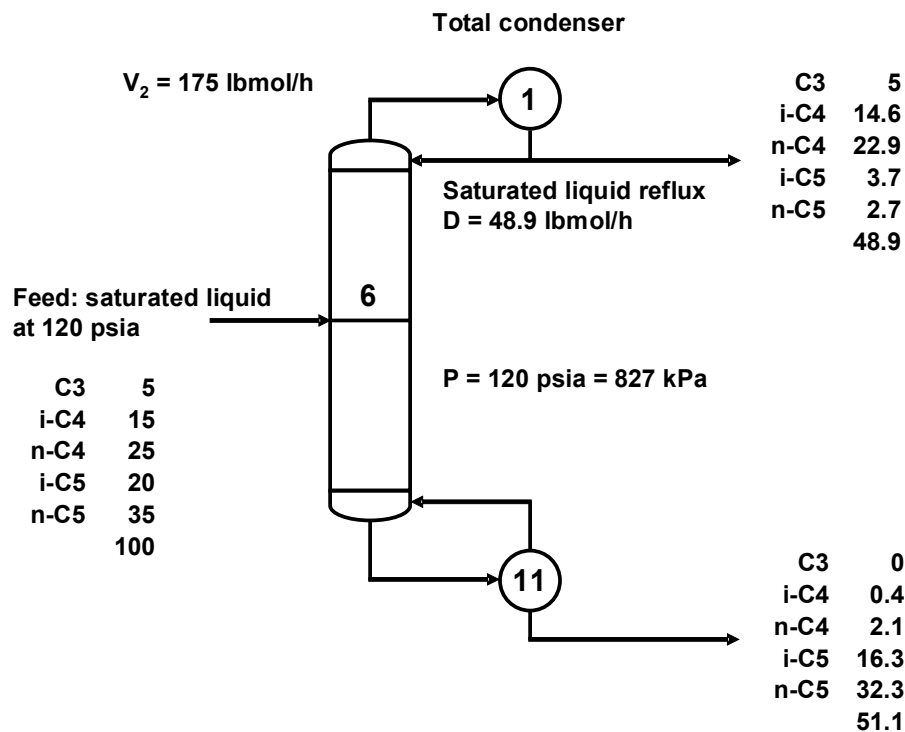


ChemSep Tutorial: Simple (Multicomponent) Distillation

Harry Kooijman and Ross Taylor

In the material below we illustrate the use of *ChemSep* to solve a multicomponent distillation problem posed by J.D. Seader [Perry's Chemical Engineers Handbook, 7th Edition (1986)]. The results here differ only very slightly from those obtained by Seader (almost certainly due to differences in physical property models).

The specifications for this problem are summarized in the figure below.



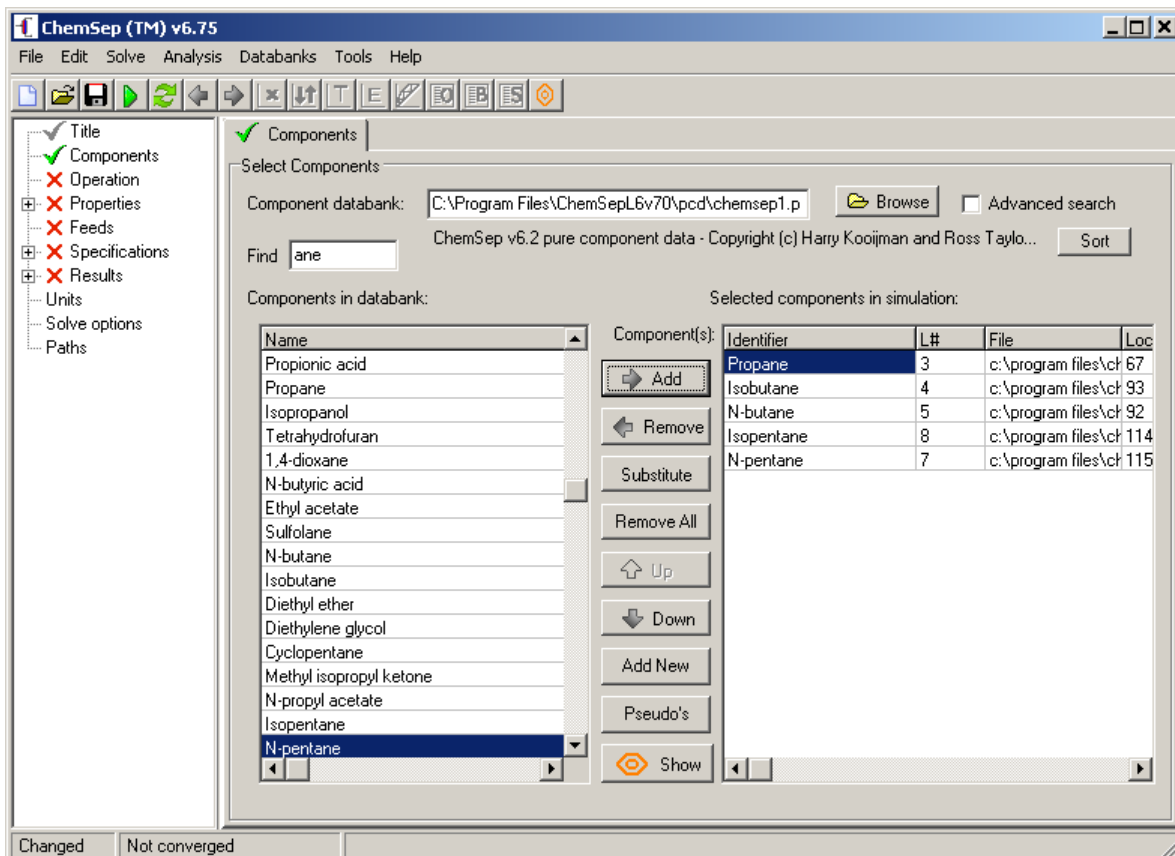
The specifications made in this case are summarized in the table below:

Variable	Number	Value
Number of stages	1	11
Feed stage location	1	6
Component flows in feed	$c = 5$	5, 15, 25, 20, 35 lbmol/h
Feed pressure	1	120 psia
Feed vapor fraction	1	0
Pressure on each stage including condenser and reboiler	$N = 11$	$P_j = 120$ psia
Heat duty on each stage except reboilers and condensers	$N - 2 = 9$	$Q_j = 0$
Vapor flow to condenser (replaces heat duty of reboiler)	1	$V_2 = 175$ lbmol/h
Distillate flow rate (replaces heat duty of condenser)	1	$D = 48.9$ lbmol/h
Total	31	

In addition, we have assumed that the pressure of the reflux divider is the same as the pressure of the condenser, the heat loss from the reflux divider is zero, and the reflux temperature is the boiling point of the condensed overhead vapor.

The entry of these specifications into *ChemSep* is shown in the screen images that follow.

Component Selection



Operation

We select an *Equilibrium Column* and create a column configuration to match that above where we summarized the specifications.

Configuration

Operation:

Condenser:

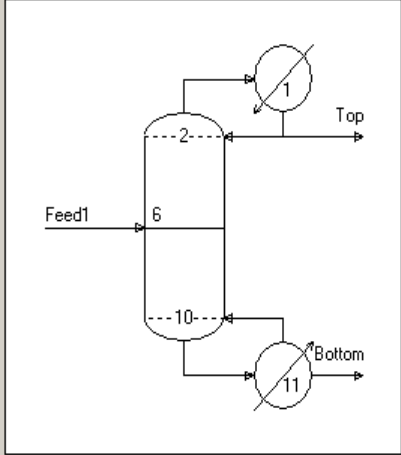
Reboiler:

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)



Properties

Thermodynamics Physical properties Reactions

Select Thermodynamic Models

K-value Show enthalpy/exergy settings:

Equation of state

Activity coefficient

Vapour pressure

Enthalpy

Enter Thermodynamic Model Parameters (when required)

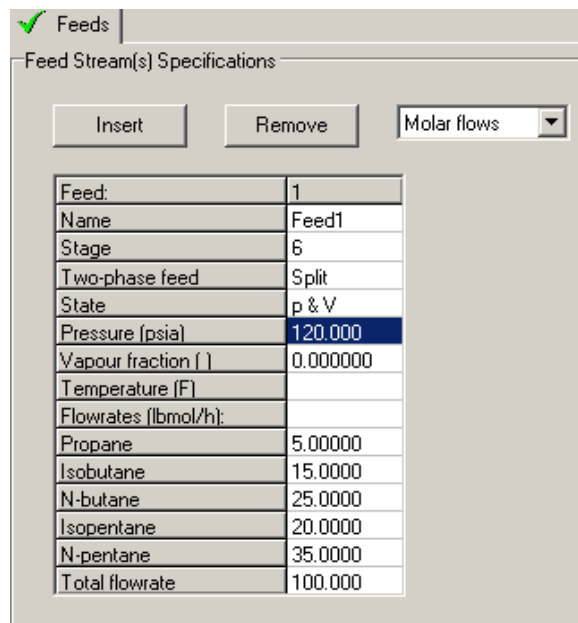
Peng-Robinson T dependence

i - j	k-ij
Propane - Isobutane	-7.800E-03
Propane - N-butane	0.00330000
Propane - Isopentane	0.0111000
Propane - N-pentane	0.0267000
Isobutane - N-butane	-4.000E-04
Isobutane - Isopentane	*
Isobutane - N-pentane	*
N-butane - Isopentane	*
N-butane - N-pentane	0.0174000
Isopentane - N-pentane	0.0600000

The Peng-Robinson equation of state was selected to estimate K-values and enthalpy departures (as opposed to the De Priester charts by Seader who solved this problem using the Thiele-Geddes method).

It can be seen that we have loaded the binary interaction parameters from the library that comes with *ChemSep*. Missing parameters will be assumed to be zero. (This is probably a safe assumption in this example, but it will not always be wise to make this assumption and every effort should be made to find binary interaction parameters if they are not available in the library).

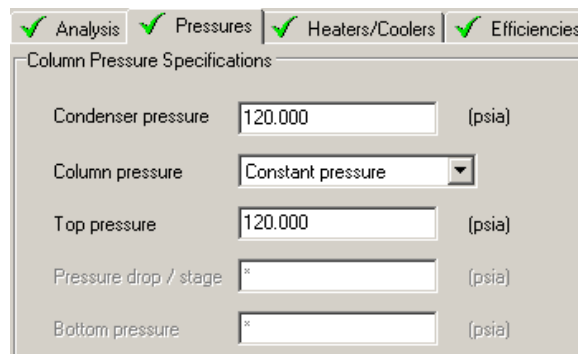
Feeds



Property	Value
Feed:	1
Name	Feed1
Stage	6
Two-phase feed	Split
State	p & V
Pressure (psia)	120.000
Vapour fraction ()	0.000000
Temperature (F)	
Flowrates (lbmol/h):	
Propane	5.00000
Isobutane	15.00000
N-butane	25.00000
Isopentane	20.00000
N-pentane	35.00000
Total flowrate	100.000

Pressures

The pressure is assumed constant throughout the column.



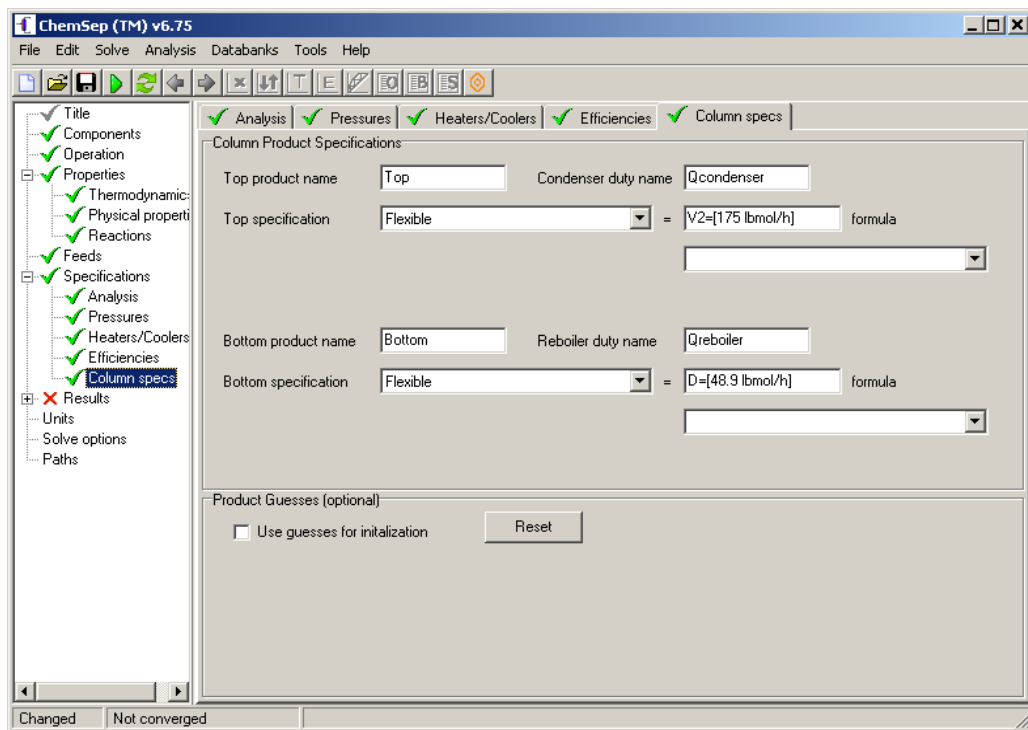
Condenser pressure	120.000	(psia)
Column pressure	Constant pressure	
Top pressure	120.000	(psia)
Pressure drop / stage	*	(psia)
Bottom pressure	*	(psia)

There are no heaters or coolers in this example so this panel is quickly completed (and, therefore, not shown). The stage efficiencies are assumed equal to their default value of 1.

Column Specifications

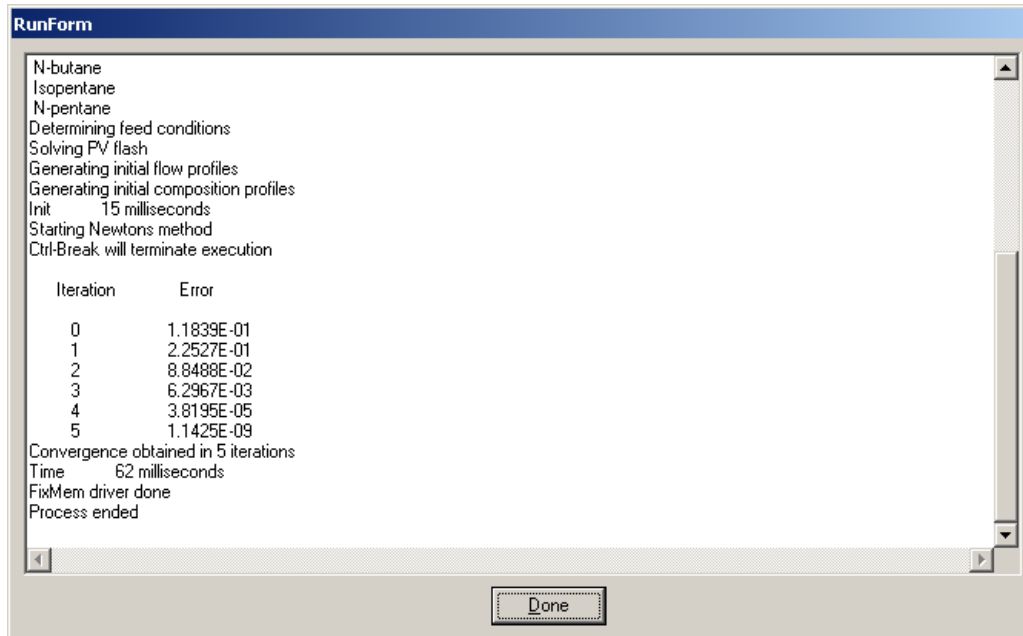
Seader specified the flow rate entering the condenser and the distillate flow rate. This combination is a little unusual in that both specifications involve flows around the top of the column. *ChemSep* normally expects one specification for the top and another specification for the bottom of the column. The specifications chosen by Seader allow us to easily calculate the bottoms product rate, and the reflux rate, and hence the reflux ratio. Thus, we could, in principle choose any combination of these five variables (as long as we don't choose two mutually exclusive specifications at the same time such as the distillate rate and the bottoms product rate). However, *ChemSep* can accept the specifications made by Seader and this is how we have chosen to complete the input for this example.

From the pull down specification menu we select the last option: *Flexible*. We may then choose to specify any variable in the column model (although we would be unwise to pick most of the possible choices). Here, following Seader, we pick the flow rate of vapor leaving stage 2 and the distillate flow rate. Note that when using the flexible specification option we may need to enter units as part of the specification equation.



Solving the Simulation

With 11 stages and 5 components the equilibrium stage model has 143 equations to be solved for 143 variables (the unknown flow rates, temperatures, mole fractions). Convergence of the computer algorithm was obtained in just 5 iterations.



Results

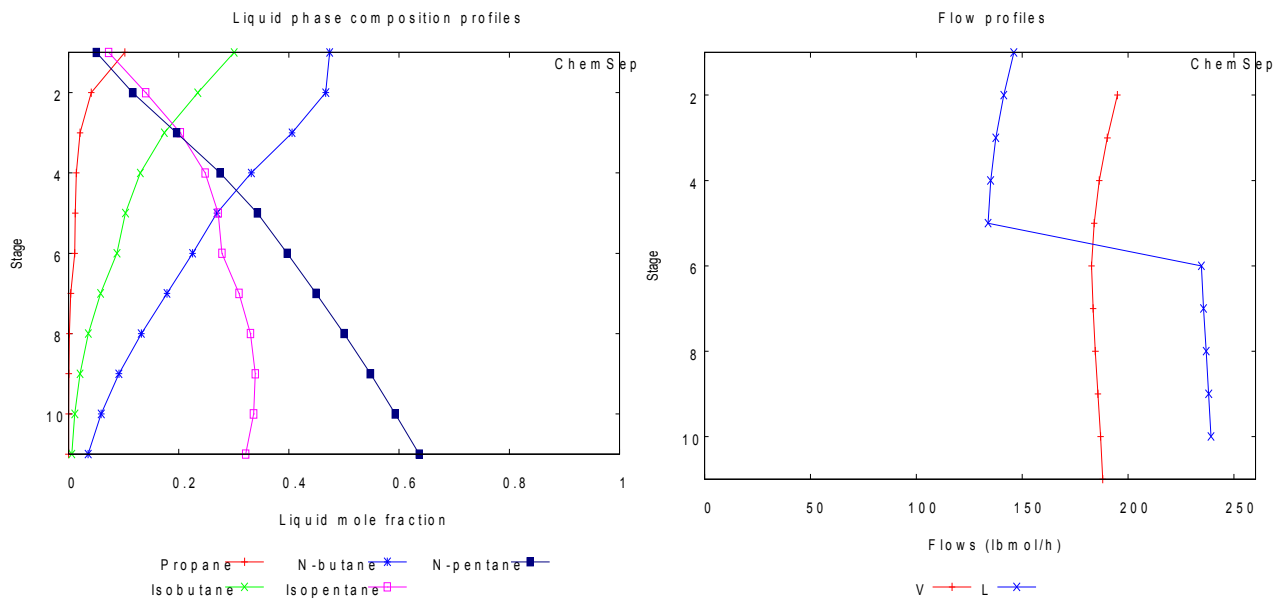
ChemSep can display an enormous amount of information. We refer readers to the sections on *Tables* and *Graphs* for more information; here we show some of the more useful results.

The stream table is shown below:

The Tables window shows the following stream table:

Stream	Feed1	Top	Bottom
Stage	6	1	11
Pressure (psia)	120.000	120.000	120.000
Vapour fraction (-)	0.000000	0.000000	0.000000
Temperature (F)	180.553	144.332	229.761
Enthalpy (Btu/lbmol)	-6055.58	-6637.92	-4503.01
Entropy (Btu/lbmol/R)	-9.69188	-11.9235	-7.85208
Mole flows (lbmol/h)			
Propane	5.00000	4.99726	0.00273815
Isobutane	15.0000	14.6999	0.300158
N-butane	25.0000	23.1726	1.82739
Isopentane	20.0000	3.56452	16.4355
N-pentane	35.0000	2.46576	32.5343
Total molar flow	100.000	48.9000	51.1001

The composition and flow profiles is obtained by clicking on the appropriate icons on the button bar.



A McCabe-Thiele diagram can be obtained by clicking on the McCabe-Thiele icon on the button bar. We may also elect to select the McCabe-Thiele panel:

Tables | Graphs | **McCabe-Thiele** | Rating | FUG

Auto-select key components

Criterion: Largest mass transfer rate [Display]

User selected key components [Copy data]

Light key: N-butane [Lumped]

Heavy key: Isopentane [Show settings]

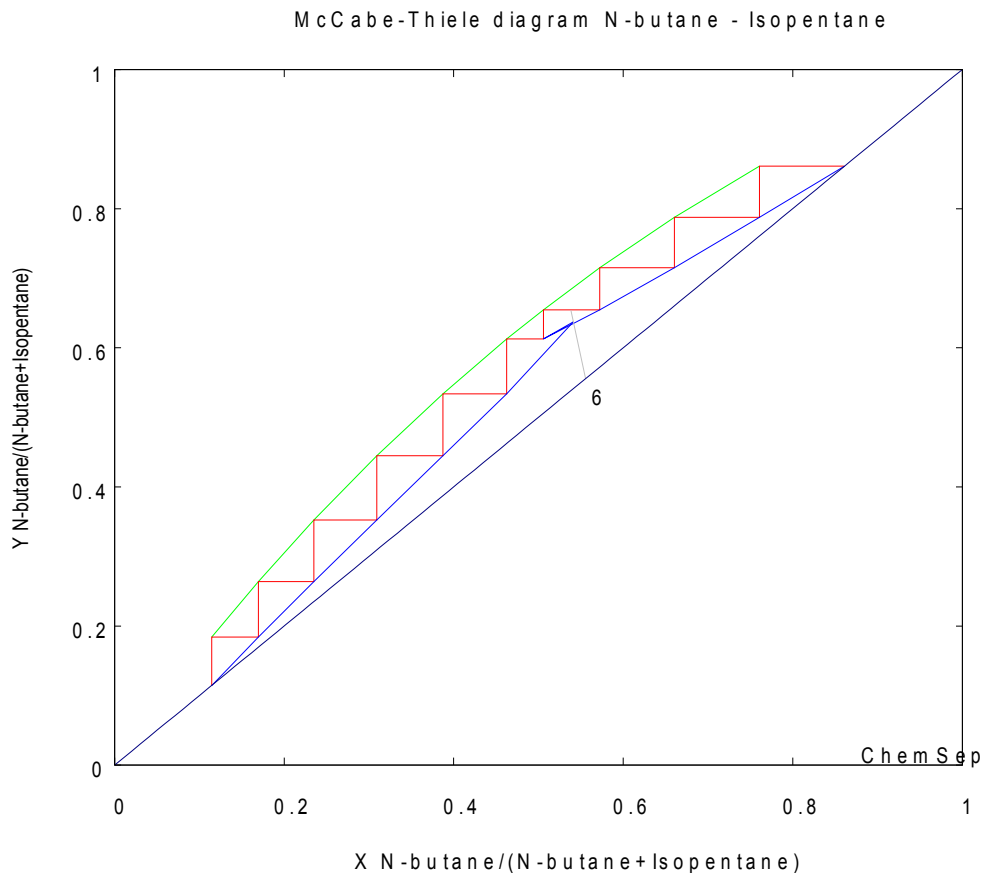
Stage	KL	KH	RV	dy*/dx	xL	xH	E-O'Connell	DV (m ² /s)
2	1.014777	0.519797	1.952257	0.65054	0.76905	0.23095	0.718316	7.0719E-07
3	1.155319	0.605433	1.908252	0.740473	0.666473	0.333527	0.72224	7.3377E-07
4	1.276435	0.680929	1.874551	0.83261	0.572262	0.427738	0.725294	7.5558E-07
5	1.371622	0.741396	1.850053	0.913396	0.497839	0.502161	0.727814	7.7217E-07
6	1.439241	0.784949	1.833547	0.973058	0.44713	0.55287	0.730447	7.8370E-07
7	1.554591	0.860866	1.805846	1.076733	0.366136	0.633864	0.735248	8.0308E-07
8	1.653115	0.92682	1.783641	1.190833	0.285654	0.714346	0.738052	8.1934E-07
9	1.733213	0.981208	1.766407	1.306294	0.212489	0.787511	0.740774	8.3239E-07
10	1.795396	1.023889	1.753507	1.414736	0.150377	0.849623	0.743102	8.4244E-07

ChemSep has automatically selected the two key components to be used as the basis for this diagram. It has made the correct determination of the two keys in this case; there are, however, situations where it is unable correctly to pick the right key components. For those cases it is possible for you to make your own selections as can be seen in the screen image above. For more information about the options available for McCabe-Thiele diagrams please consult the section on *Graphs*.

For systems with more than two components these diagrams can only be computed from the results of a computer simulation. The axes are defined by the relative mole fractions:

$$X = \frac{x_{LK}}{x_{LK} + x_{HK}} \quad Y = \frac{y_{LK}}{y_{LK} + y_{HK}}$$

where the subscripts *LK* and *HK* refer to **light key** and **heavy key** respectively. The lines in the diagram have the same significance as would be expected from our knowledge of McCabe-Thiele diagrams for binary systems; the triangles corresponding to equilibrium stages.



The fact that the staircase of triangles fails to come close to the corners of the diagram where $X = Y = 1$ and $X = Y = 0$ shows that the separation is not especially sharp. In addition, we can see that the feed is not in the best possible location.

Parametric Studies

It is worth asking what can be done to improve the separation obtained with this column. The parameters that have a significant effect on the separation are the numbers of stages in the sections above and below the feed, the reflux ratio, and a product flow rate (or reflux flow).

In order to see how changes in these variables affect the simulation we will use the Parametric Study feature of *ChemSep*.

Click on *Analysis* and then *Parametric Study* to bring up the appropriate window.

1. Set the number of steps (problems to solve) in covering the range of variable values.
2. Select variable(s) to vary. Here it is the reflux ratio. Set the start and end values.
3. Select output variables to monitor. Note that the index numbers of the light and heavy key components must be typed in (to replace the # sign that appears on selection of these mole fractions).
4. Click *Run* to generate results. *ChemSep* will then carry out the specified number of column simulations and the results tabulated in the lower section of the window as shown.

Parametric Study

Select input variables:

Number of steps: 11 Use old results Automatic Keep sep-files Restore original

Add: [Dropdown] Remove Reset

Name	variable	Units	Value	Start/Value list	End
Reflux ratio	RR		2.578725	1.5	6

Select result variables:

Add: [Dropdown] Remove Reset

Name	Reflux ratio	Stream Top liquid	Stream Bottom liquid	Reboiler duty (Btu/h)
Variable	RR	TOPSX(4)	BOT SX(3)	QR
Units				Btu/h
Current Value	2.578725	0.0734773	0.0412710	1477742

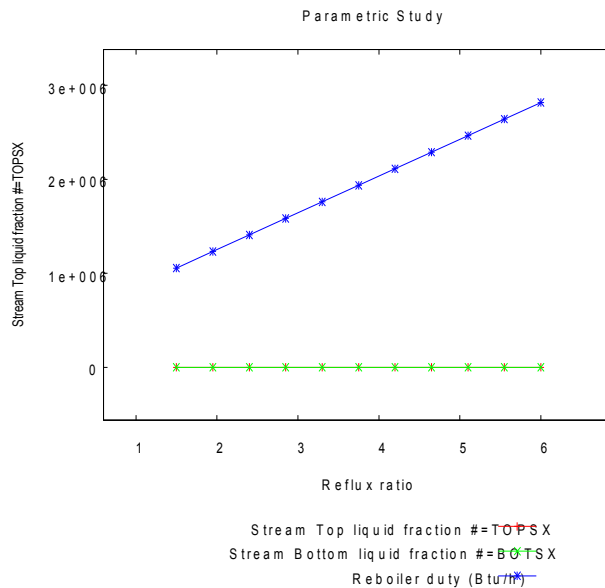
Results:

Run Graph Copy data XL Graph Edit Graph

Step	Reflux ratio	Stream Top liquid	Stream Bottom liquid	Reboiler duty (Btu/h)
Units				
1	1.5	0.0882194	0.068795	1055217
2	1.95	0.0814942	0.0541311	1231756
3	2.4	0.076888	0.0442761	1407849
4	2.85	0.0736772	0.0374347	1583809
5	3.3	0.0713811	0.0325111	1759751
6	3.75	0.0696953	0.0288468	1935715
7	4.2	0.0684267	0.0260384	2111711
8	4.65	0.067451	0.023831	2287742
9	5.1	0.0666861	0.0220587	2463805
10	5.55	0.066076	0.0206086	2639895
11	6	0.0655821	0.0194034	2816008

Close

5. Click *Graph* to display results.



Unfortunately this plot is not as clear as we would like; the reason being the rather different magnitudes of the heat duty and the product mole fractions that were selected as output variables.

Click on the *Edit Graph* button to bring up the plot configuration panel.

Tables | Graphs | McCabe-Thiele | Rating | FUG

Select graph: Parametric Study Display XLS Copy Data Show settings

Title	Labels	Stages	Axis color	Commands	Box	Labels box	Import data
Parametric Study	On	Vertical	Black		On	Off	

	Title	Start	End	Tic interval	Small tics	Grid	Logarithmic	Scientific not
x1	Reflux ratio	0.6	6.9	1	0	Off	Off	Off
y1	Stream Top li	-563201.6	3379210	1000000	0	Off	Off	Off
x2					0	Off	Off	Off
y2					0	Off	Off	Off

 Auto colors
Black

 Oversize 0.2
 Auto points
Diamond

	Label	Plot X	Plot Y	X axis	Y axis	Units X	Units Y	Color	Points	Thickne	Style	1st stag	Last sta
1	Stream	PS1	PS2	x1	y1			Red	Diamond	Normal	Solid	1	11
2	Stream	PS1	PS3	x1	y1			Green	+	Normal	Solid	1	11
3	Reboiler	PS1	PS4	x1	y1		Btu/h	Blue	Square	Normal	Solid	1	11

We can change the various plot settings here so that we can obtain something more useful.

The first change that we make is to assign the heat duty to the right hand vertical axis. If we then click on *Auto Axis* and then on *Display* we will obtain a plot that is more or less acceptable. However, we have made additional changes to the variable labels, the units of the heat duties and the axis limits as shown in this screen image. We have also removed the title that would otherwise appear over the top of the plot. The places where we have made changes are highlighted in the image below.

The screenshot shows a software interface with the following tables and controls:

Plot Table:

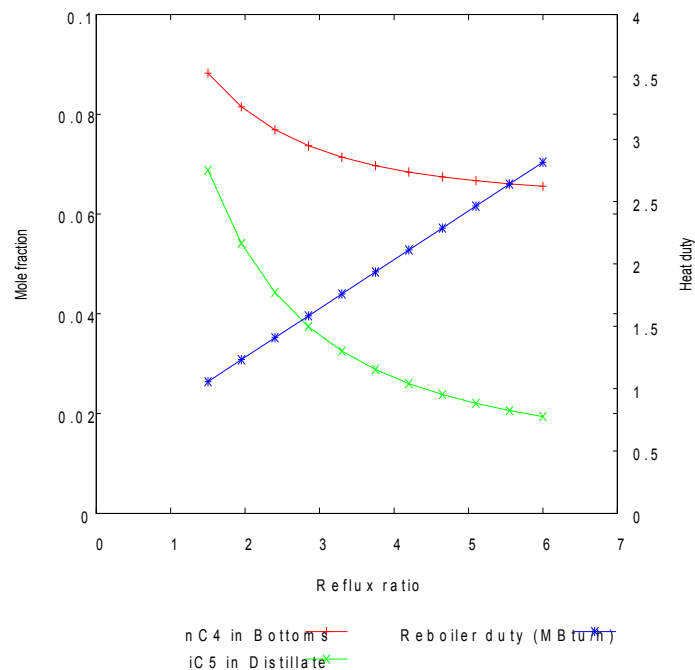
Name	Labels	Stages	Axis color	Commands	Box	Labels box	Import data
Di		Vertical	Black		On	Off	

Data sets Table:

Label	Plot X	Plot Y	X axis	Y axis	Units X	Units Y	Color	Points	Thickne	Style	1st stag	Last sta
nC4 in B PS1	PS2	x1	y1				Red	Diamond	Normal	Solid	1	11
iC5 in Di PS1	PS3	x1	y1				Green	+	Normal	Solid	1	11
Reboiler PS1	PS4	x1	y2			MBtu/h	Blue	Square	Normal	Solid	1	11

Buttons: Add set, Reset sets, Calc.Dev's, Store graph, Auto Axis, Auto colors (Black), Delete set, Save sets, Plot, Remove graph, Oversize (0.2), Auto points (Diamond), Show settings.

Now, when we click on *Display* we see the following.



This figure shows how the mole fraction of *i*-pentane in the overhead and *n*-butane in the bottom product change with reflux ratio. For the base case considered above the reflux ratio is 2.58 (calculated from the results of the simulation). It is clear that increasing the reflux ratio has the desired effect of improving product purity. This improvement in purity is, however, accompanied by an increase in both the operating cost, indicated by the increase in reboiler duty, and capital cost, because a larger column would be needed to accommodate the increased internal flow. Note, however, that the curves that represent the mole fractions of the keys in the overhead and bottoms appear to flatten showing that product purity will not increase indefinitely as the reflux ratio increases. Further improvement in product purity can only be made by changing a different specification.

Accordingly, we now run a second parametric study, this time varying the distillate flow. Note that since this was chosen as a flexible specification before we must first change the column specifications so that we don't end up specifying the distillate flow rate twice (which will mean the simulation will crash). We first rerun the original simulation by setting the distillate flow rate (to the value used before) and the reflux ratio (to 2.5, close to the value computed from the results of the last simulation). The specification panel now looks like this:

Analysis
 Pressures
 Heaters/Coolers
 Efficiencies
 Column specs

Column Product Specifications

Top product name: Condenser duty name:

Top specification: = (lbmol/h)

Bottom product name: Reboiler duty name:

Bottom specification: = formula

The parametric study panel will look like this (the top part is what we create, the lower part is where the results appear after clicking on *Run*).

Parametric Study

Select input variables

Number of steps: Use old results Automatic Keep sep-files Restore original

Add:

Name	Variable	Units	Value	Start/Valuelist	End
Distillate flowrate	D	lbmol/h	48.90003	40	50

Select result variables

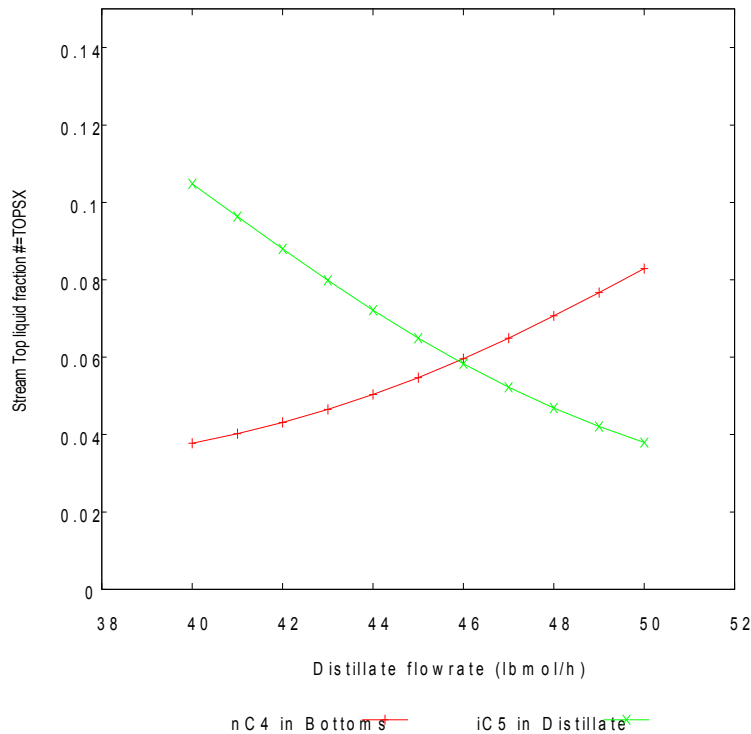
Add:

Name	Distillate flowrate	Stream Top liquid	Stream Bottom li
Variable	D	TOPSX(4)	BOT SX(3)
Units	lbmol/h		
Current Value	48.90003	0.0754773	0.0412718

Results

Step	Distillate flowrate	Stream Top liquid	Stream Bottom li
Units	lbmol/h		
1	40.00004	0.0377552	0.104791
2	40.99997	0.0402306	0.0963291
3	41.99999	0.0431211	0.0879858
4	43.00001	0.0464777	0.0798858
5	44.00002	0.0503385	0.0721567
6	44.99996	0.0547181	0.0649158
7	45.99998	0.0596022	0.0582534
8	46.99999	0.0649435	0.052225
9	48.00001	0.0706683	0.0468455
10	49.00003	0.0766866	0.042095
11	49.99997	0.0829029	0.0379289

Proceed as before (click on *Graph* and then on *Edit Graph* to tidy up the result).

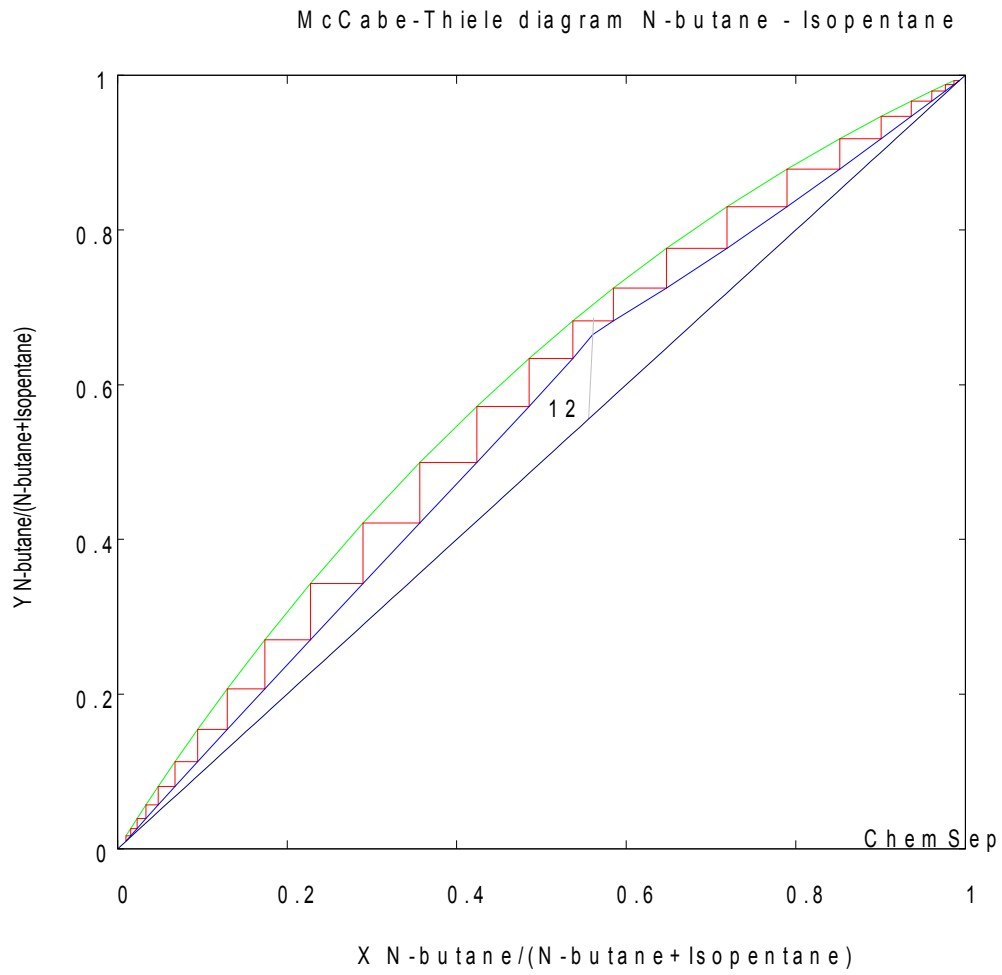


This figure shows what happens to product purity when we change the specified distillate flow rate. From this result we see that the best overall product purity is obtained when the distillate rate is 45 lbmol/h. On reflection this should not come as a surprise, the flow rate of the light key (*n*-butane) and all components with a higher volatility is 45 lbmol/h. However, even with the distillate flow rate set to 45 lbmol/h there remains room for improvement in the separation.

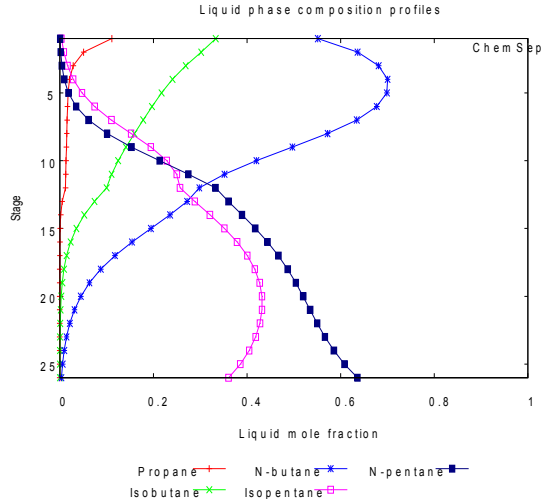
The other key design specifications here are the total number of stages and the location of the feed stage. In most cases, increasing the number of stages will improve the separation. On increasing the number of stages to 26, with the feed to stage 12, increasing the overhead vapor flow to 195 lbmol/h and decreasing the distillate rate to 45 lbmol/h we obtain the following products:

Mole flows lbmol/h)			
Propane	5	5	0
Isobutane	15	14.995	0.005
N-butan	25	24.8	0.196
Isopentane	20	0.168	19.83
N-pentane	35	0.033	34.97
Total molar flow	100	45	55

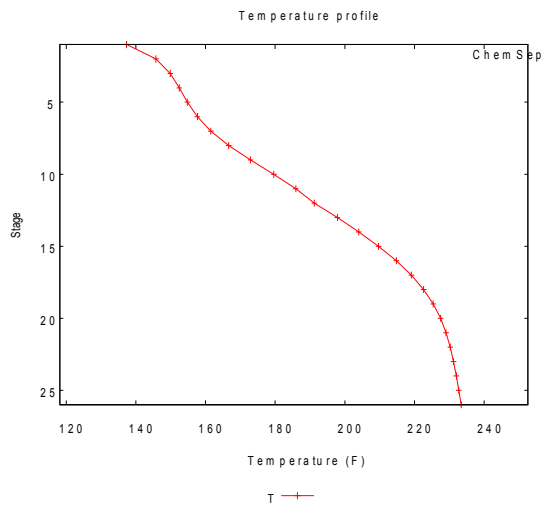
The McCabe-Thiele diagram for this configuration shown below appears to have the feed in the optimum location, and the product purities have improved.



The composition profiles are more or less as expected. The components more volatile than the light key (*n*-butane) are concentrated above the feed; those compounds less volatile than the heavy key (*i*-pentane) are concentrated below the feed. The mole fractions of the two keys exhibit maxima; the light key above the feed stage and the heavy key below the feed stage. The decrease in the mole fraction of light key over the top few stages is necessary to accommodate the increase in the composition of the lighter compounds. Similar arguments pertain to the decrease in the mole fraction of the heavy key over the stages towards the bottom of the column.



The temperature profile for this final case is shown here. It can be seen that the temperature increases from top to bottom of the column. This is normally the case in distillation columns (exceptions may occur with cold feeds or feeds with boiling points significantly lower than that of the mixture on stages above the feed stage).



Note the step change in the liquid flow rate around the feed stage. Had the feed been partially vaporized feed we would have observed changes in both vapor and liquid flows around the feed stage, and a saturated vapor feed would significantly change only the vapor flow profile. The slight (in this case) curvature in the flow profiles is due to enthalpy changes.

