

# ChemSep Tutorial: Absorber Case Study

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Here we consider the modeling of an absorption column using **ChemSep**. The following tutorials are included below:

1. Setting up a simple absorption column (this is Example 8.2 in *Multistage Separation Processes*, by F.M. Khoury (Prentice-Hall, 1999))
2. Using the Parametric Study option in *ChemSep* to investigate the influence of the solvent flow rate (this is a continuation of Example 8.2 from the book by Khoury)
3. Using the Parametric Study option in *ChemSep* to investigate the influence of the number of stages (this is Example 8.3 in the book by Khoury)

## Tutorial 1: Absorption of Propane by n-Dodecane

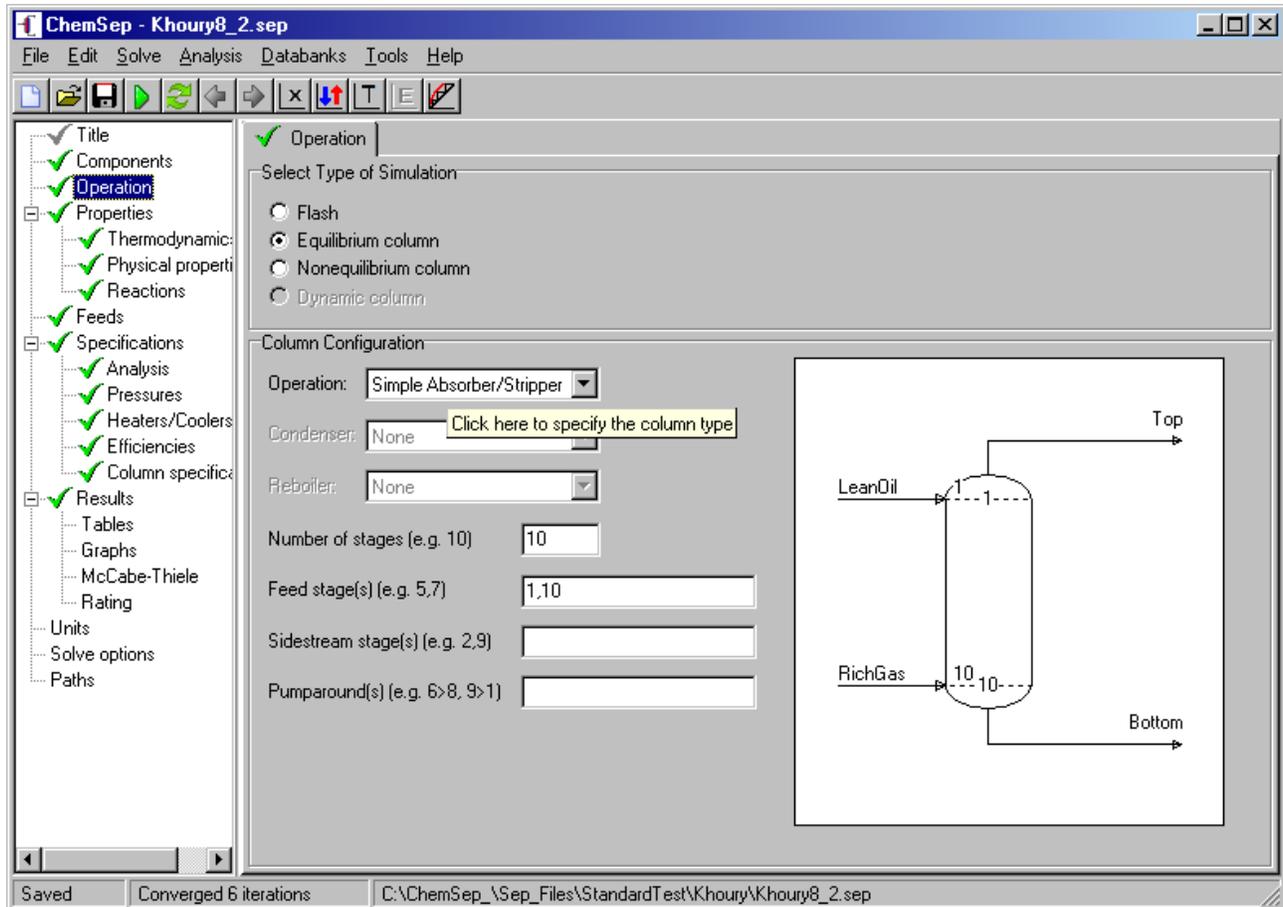
Dodecane is to be used as the solvent in an absorption process to recover propane (and any heavier components present) from a gas mixture. Both feed streams and the column (which has 10 stages) are at a pressure of 400 psia; in addition, the feeds are at a temperature of 100 °F. The components and their respective feed rates are summarized in Table 1 (which also includes the results obtained by Khoury).

Table 1: Absorber Stream Flows: Feed Specifications and Predicted Products

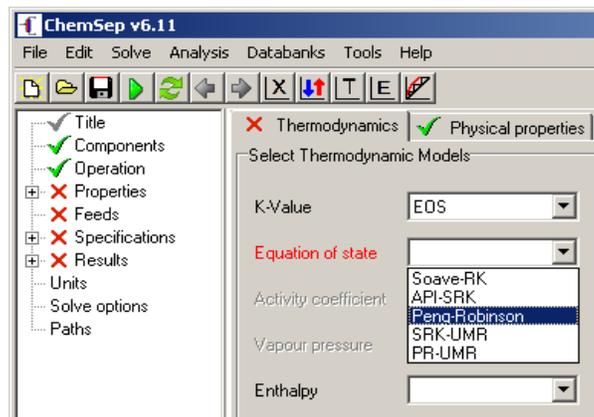
Stream	LeanOil	RichGas	Top	Bottom
Stage	1	10	10	10
Pressure (psia)	400	400	400	400
Vapour fraction (-)	0	1	1	0
Temperature (oF)	100	100	106.1	117.8
<b>Mole flows (mol/h)</b>				
Nitrogen	0	20	19.4	0.6
Methane	0	800	722.8	77.2
Ethane	0	80	48.5	31.5
Propane	0	70	3.3	66.7
N-butane	0	20	0	20
N-pentane	0	20	0	10
N-dodecane	500	0	0	499.9
Total molar flow	500	1000	794.1	706.9

We begin by clicking on the Components Panel and selecting the components that are listed in Table 1.

Next, select the **Operation** tab and choose **Equilibrium Column**. Complete the specification of the column configuration as shown in the screen shot below:



The next step is to select the appropriate thermodynamic models. Khoury does not tell us what model he used in his example calculations; we use the Peng-Robinson Equation of State for the estimation of both the K-values and the enthalpy.



The next step is to provide the details of the two feeds. Click on the **Feeds** line and complete the feeds panel so that it appears as it does in the screen shot below:

Insert Remove Molar flows ▼

Feed:	1	2
Name	LeanOil	RichGas
Stage	1	10
Two-phase feed	Split	Split-below
State	T & p	T & p
Pressure (psia)	400.000	400.000
Vapour fraction (-)		
Temperature (oF)	100.000	100.000
Flowrates (mol/h):		
Nitrogen	0.000000	20.0000
Methane	0.000000	800.000
Ethane	0.000000	80.0000
Propane	0.000000	70.0000
N-butane	0.000000	20.0000
N-pentane	0.000000	10.0000
N-dodecane	500.000	0.000000
Total flowrate	500.000	1000.00

Enter the details of each feed stream

The column pressures are specified as shown below:

Column Pressure Specifications

Condenser pressure  (psia)

Column pressure  ▼

Top pressure  (psia)

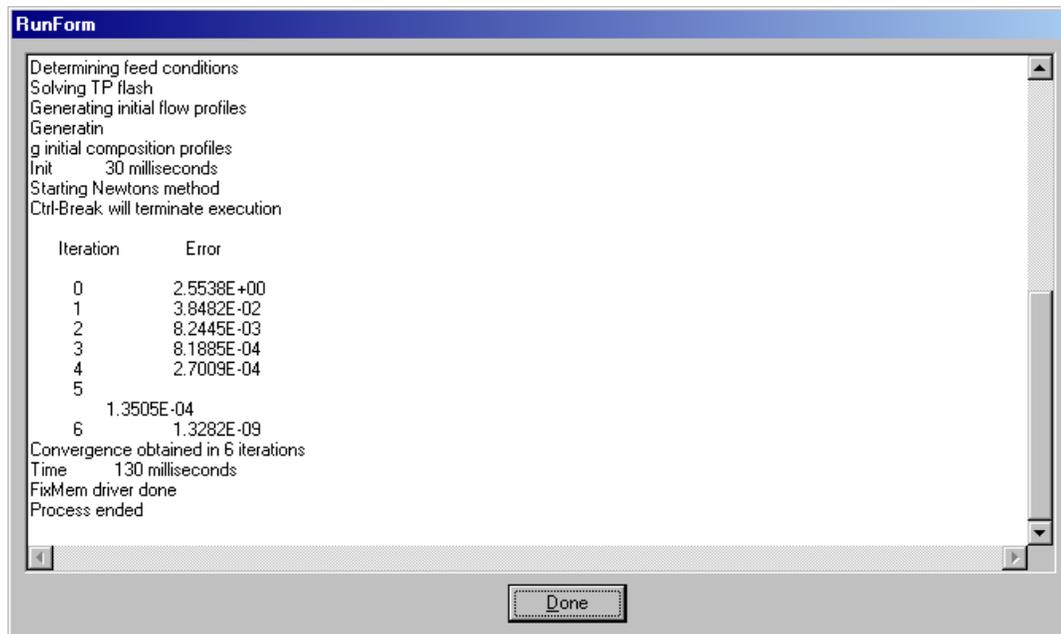
Pressure drop per stage  (psia)

Bottom pressure  (psia)

The column specifications are completed by setting the heat losses to zero and the default efficiency to one.

The next step is to save the file (using the **File** menu – note that the file name appears on the blue bar at the top of the ChemSep window) and then click on the green arrow head icon to start the calculations.

This will bring up the solve window – which looks like this:



Click on **Done** to close the window and bring up the results panel.

ChemSep - Khoury8\_2.sep

File Edit Solve Analysis Databanks Tools Help

Tables | Graphs | McCabe-Thiele | Rating

Select table: Streams

Stream	LeanOil	RichGas	Top	Bottom
Stage	1	10	1	10
Pressure (psia)	400.000	400.000	400.000	400.000
Vapour fraction (-)	0.000000	1.00000	1.00000	0.000000
Temperature (oF)	100.000	100.000	106.394	118.459
Enthalpy (J/kmol)	-5.312E+07	-194645	100933	-3.796E+07
Entropy (J/kmol/K)	-111459	-20944.6	-23532.4	-80209.9
Mole flows (mol/h)				
Nitrogen	0.000000	20.0000	19.1536	0.846408
Methane	0.000000	799.999	721.518	78.4813
Ethane	0.000000	79.9999	48.6892	31.3107
Propane	0.000000	69.9998	3.62909	66.3708
N-butane	0.000000	20.0000	1.3618E-04	19.9999
N-pentane	0.000000	10.0000	4.0866E-09	10.0000
N-dodecane	500.000	0.000000	0.0722171	499.928
Total molar flow	500.000	999.999	793.062	706.937
Mole fractions (-)				
Nitrogen	0.000000	0.0200000	0.0241514	0.00119729
Methane	0.000000	0.800000	0.909787	0.111016
Ethane	0.000000	0.0800000	0.0613940	0.0442906
Propane	0.000000	0.0699999	0.00457604	0.0938849
N-butane	0.000000	0.0200000	1.7172E-07	0.0282909

Units  
Solve options  
Paths

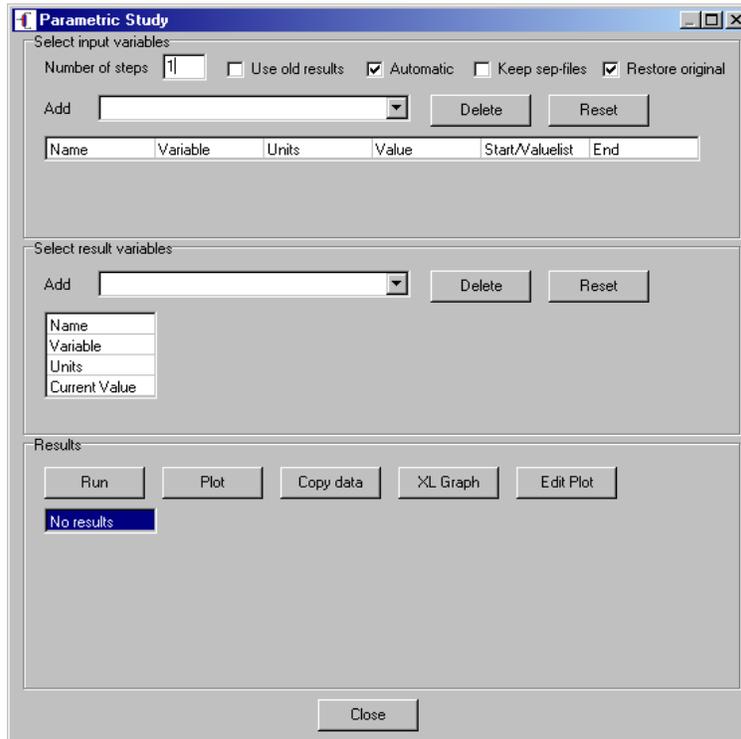
Saved | Converged 6 iterations | C:\ChemSep\_Sep\_Files\StandardTest\Khoury\Khoury8\_2.sep

The results shown above are close to those reported by Khoury (see Table 1). Remember that Khoury does not tell us what thermodynamic model he used so the close agreement can be considered to be quite satisfactory.

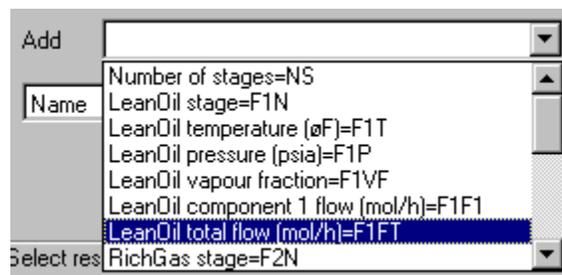
## Tutorial 2: Effect of Solvent Flow Rate on Component Recovery

This tutorial continues with Example 8.2 from Khoury in which he investigates the effect of the solvent flow rate on the propane recovery. This is a question that can best be answered using the Parametric Study option of *ChemSep*.

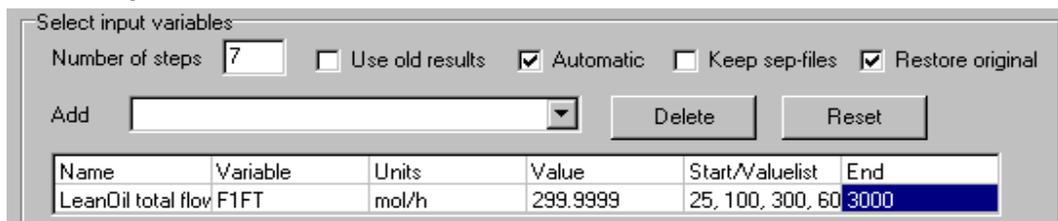
Click on the **Analysis** menu and select **Parametric Study**. This will bring up a window that looks like this:



Click on the drop down list next to **Add** near the top of this window. Scroll down and select the LeanOil flow:

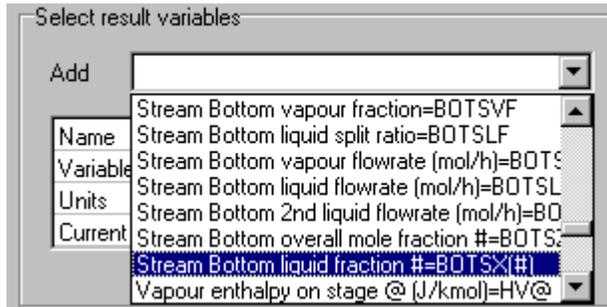


Fill in the values of the solvent flows that will be investigated (they are 25, 100, 300, 600, 750, 1000, and 5000 mol/h). Type in the number of simulations that will cover this range in the box next to **Number of steps**.



The next task is to select the output variables of interest. If we click on the drop down list under **Select result variables** (central section of the parametric study panel) we see a very long list of the possible result variables. We are interested in the recovery of each compound (C1 to C5), but compound recovery is not one of the listed variables. Nevertheless, we can obtain the species recoveries by making use of *ChemSep*'s ability to combine result variables as we now show.

Start by selecting the mole fraction of methane in the rich oil (Bottoms).



This puts the string BOTSX(#) in the result variable list:

Name	LeanOil total flow	Stream Bottom li
Variable	F1FT	BOTSX(#)
Units	mol/h	
Current Value	299.9999	0

The # sign must be replaced by the number of the component in the component list. Methane is the second component so we can replace the # by 2. This, of course, just means that the mole fraction of methane in the bottoms is recorded, how may we obtain the recovery? The component recovery is defined as the component flow (in the bottoms here) divided by the component flow in the feeds (in this case we need be concerned only with the gas feed). The component flow rate is the component mole fraction multiplied by the total stream flow rate. Thus, the component flow in the bottoms is the mole fraction in the bottoms (already selected as shown above) multiplied by the bottoms flow rate. If we scroll down the list of result variables we see that the bottoms flow rate is named **BOTSL**. Thus, we can record the component flow of methane in the bottoms by multiplying the bottoms mole fraction by the bottoms flow rate. To obtain this click in the field that shows BOTSX(#) in the above illustration (it should now be BOTSX(2) and add BOTSL so that the entire string reads BOTSX(2)\*BOTSL.

Now we have the component flow rate of methane. To obtain the recovery we need to divide by the component flow rate of methane in the gas feed. Scroll down the list of result variables to find that the component flow of species 1 in the gas feed is F2F1 (where the last digit refers to the component number). We return to the cell of interest and add /F2F2 so that we divide the component flow of methane in the bottoms by the component flow of methane in the gas feed. This string now reads: BOTSX(2)\*BOTSL/F2F2\*100 (the \*100 is to convert the recovery to a percentage).

To add the recoveries of the other hydrocarbon compounds we repeat the above steps starting with the selection of the Bottoms mole fraction.

When we have completed this step the central portion of the Parametric Study panel appears as shown below (note that we have also typed in meaningful names in the first cell in each of columns 3 to 7).

Name	LeanOil total flow	C1 Recovery	C2 Recovery	C3 Recovery	n-C4 Recovery	n-C5 Recovery
Variable	F1FT	BOTSX(2)*BOTS	BOTSX(3)*BOTS	BOTSX(4)*BOTS	BOTSX(5)*BOTS	BOTSX(6)*BOTS
Units	mol/h					
Current Value	299.9999	6.050972	23.49231	53.96777	85.01016	96.96105

We now click on the **Run** button in order to fill in the table of results. This will appear in the bottom panel (we have stretched this window in both lateral and vertical directions in order to accommodate the entire table):

Results

Run Plot Copy data XL Graph Edit Plot

Step	LeanOil total flow	C1 Recovery	C2 Recovery	C3 Recovery	n-C4 Recovery	n-C5 Recovery
Units	mol/h					
1	25	0.73965	3.136484	9.040213	25.64757	66.91493
2	100.0001	2.309105	9.305969	25.42666	64.11004	99.43123
3	299.9999	6.059105	23.85364	64.04287	99.85631	99.99999
4	600.0012	11.67389	47.09121	98.73702	99.99991	100
5	749.9988	14.46077	59.07566	99.82853	99.99998	99.99999
6	1000.001	19.11014	78.02914	99.9897	99.99999	99.99999
7	5000.004	96.85551	99.99999	100	100	100

Readers of Khoury's book will be able to confirm that the results shown here are in good agreement with his Table 8.4 (and again we note that Khoury does not tell us what thermodynamic model he used).

To display these results graphically we may click on the **Plot** button, but we prefer **Edit Plot** because that choice allows us to customize the plot as shown below:

Plot

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

Axes

	Title	Start	End	Tic interval	Small tics	Grid	Logarithmic	Scientific not
x1	Lean Oil total	0	5100	500	0	Off	Off	Off
y1	Recovery	0	110	20	0	Off	Off	Off
x2					0	Off	Off	Off
y2					0	Off	Off	Off

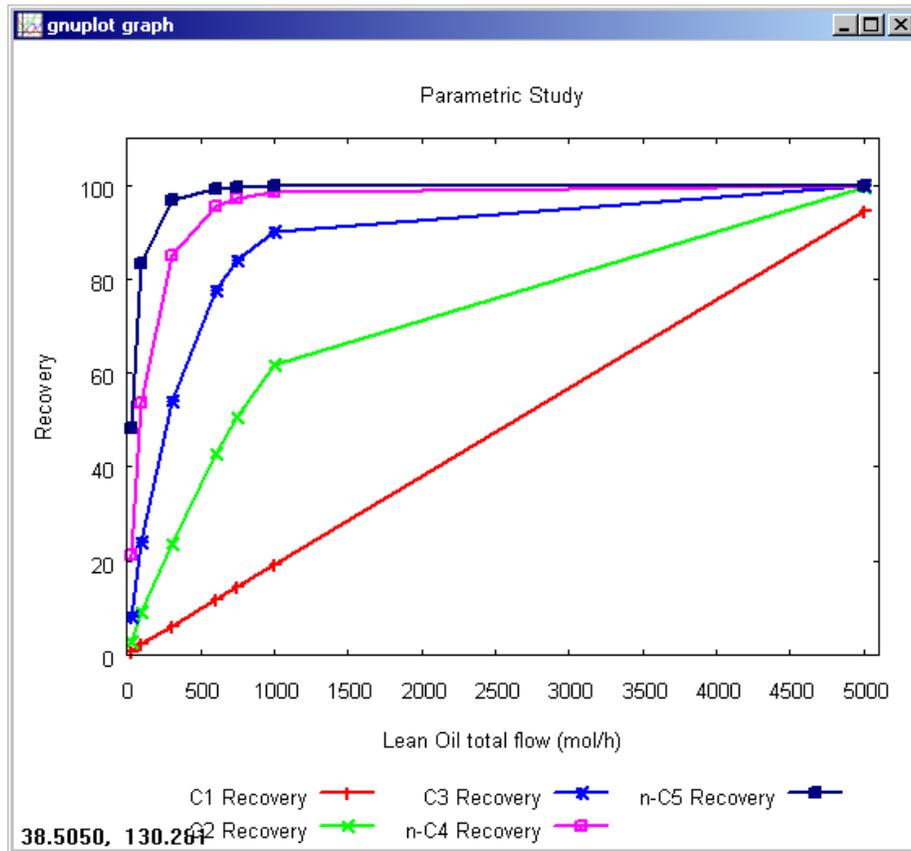
Add set Reset sets Calc.Dev's Save graph Auto Axis  Auto colors Black

Delete set Save sets Export Delete graph Oversize 0.2  Auto points Diamond

Data sets

	Label	Plot X	Plot Y	X axis	Y axis	Units	Units	Color	Points	Thickne	Style	1st st	Last st
1	C1 Recd	PS1	PS2	x1	y1	mol/h		Red	Diamond	Normal	Solid	1	7
2	C2 Recd	PS1	PS3	x1	y1	mol/h		Green	+	Normal	Solid	1	7
3	C3 Recd	PS1	PS4	x1	y1	mol/h		Blue	Square	Normal	Solid	1	7
4	n-C4 Re	PS1	PS5	x1	y1	mol/h		Magenta	x	Normal	Solid	1	7
5	n-C5 Re	PS1	PS6	x1	y1	mol/h		d-Blue	Inverse	Normal	Solid	1	7

In this example we have changed the default x and y axis titles, as well as the default axis ranges and incidence of tic-marks. The resulting plot is shown in a separate window and is reproduced below:



Khoury also tabulates the mole fraction of C1 to C5 in the overhead vapor. We leave the creation of this table (and appropriate plot) as an exercise for our readers.

### Tutorial 3: Effect of Number of Stages on Propane Absorption

We continue this tutorial with Example 8.3 from Khoury which concerns the effect of the number of stages in the propane absorption case considered above. Readers are advised to review Tutorial 2 before this one.

The determination of how the number of stages influences the separation involves another application of the Parametric Study in *ChemSep*. Following Khoury we will determine the separation accomplished by 2, 5, 10, 20, and 40 stages with a lean oil flow rate of 300 mol/h. The first step is to set the lean oil flow rate at 300 mol/h (instead of 500) and change the number of stages from 10 to 2 (strictly speaking this last step is not needed, but we think it wiser to start a parametric study from one end of the range of variables).

We then open the parametric study window and select the appropriate variables. Note that we *must* select both the number of stages *and* the stage number for the gas feed (since that is always to the bottom stage). Both of these variables must be varied in exactly the same way; note the cells containing the stage numbers to be used in this exercise as shown below.

Name	Variable	Units	Value	Start/Valuelist	End
Number of stage	NS		2	2,5,10,20,30,40	40
RichGas stage	F2N		2	2,5,10,20,30,40	40

For output variables we are interested only in the recovery of ethane, propane and butane; we determine these values in the way described in Tutorial 1.

Name	Number of stage	Ethane	Propane	n-Butane
Variable	NS	BOTSX(3)*BOTS	BOTSX(4)*BOTS	BOTSX(5)*BOTS
Units				
Current Value	2	23.49231	53.96777	85.01016

When ready we click on the Run button. On completion of the simulations the results section of the panel should have the following appearance:

Step	Number of stage	Ethane	Propane	n-Butane
Units				
1	2	23.49231	53.96777	85.01016
2	5	23.92548	62.47694	97.61867
3	10	23.85364	64.04287	99.85631
4	20	23.84811	64.15235	99.99946
5	30	23.84809	64.15285	100
6	40	23.84809	64.15285	100

Once again, readers of Khoury's book will be able to confirm the close agreement between the numbers in his Table 8.5 (page 207) and the results shown above. These results show that the component recoveries reach a constant value after some number of stages that varies from component to component. Note that these results are specific to a lean oil flow rate of 300 mol/hr. Khoury shows (in his Table 8.6) the same sort of behavior (but with different numerical results) for a lean oil flow rate of 600 mol/h. We leave this as an exercise for our readers.