KM 331 PROSES BENZETİM PROGRAMLARI DERS NOTLARI [1-4]

Kaynaklar

1. Chemcad User Guide and Tutorial, Chemstations, Inc. Version 6.1.
2. Aspen Technology, Inc., Apsen HYSYS ® Version 7.
3. ChemCad Eğitim Notları , Chemstations, Inc- Houston,TX,USA.
4. A Guide for Getting Started in Aspen HYSYS
   Dinu Ajikutira, Sr. Director, Engineering Product Marketing, Aspen Technology, Inc.

Plug Flow Reactor with Multiple Reactions

THE PROBLEM STATEMENT

Allyl chloride is to be produced in a 12-ft. long 2-in ID tube operating at isothermal PFR. The feed is a 4:1 molar ratio of propylene to chlorine and enters at a feed rate of 0.85 lbmole/hr and 2 atm of pressure and temperature of 1000 Rankine. The reactor pressure is assumed to be constant.

$$Cl_2 + C_3H_6 \xrightarrow{k_1} C_3H_5Cl + HCl \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \textit{Reaction1}$$

$$Cl_2 + C_3H_6 \xrightarrow{k_2} C_3H_6Cl_2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \textit{Reaction2}$$

The rate constants have units of lbmoles/(hr-ft^3-atm^2) and are:

$$k_1 = 206000 * \exp(\frac{-27200}{RT})$$

$$k_2 = 11.7 * \exp(\frac{-6860}{RT})$$

where *T* is in degrees Rankine and R is in Btu/(lbmole ºR). The rate expressions are

$$r_1 = k_1 \times P_{C_3H_6} P_{Cl_2}$$

$$r_2 = k_2 \times P_{C_3H_6} P_{Cl_2}$$

Calculate

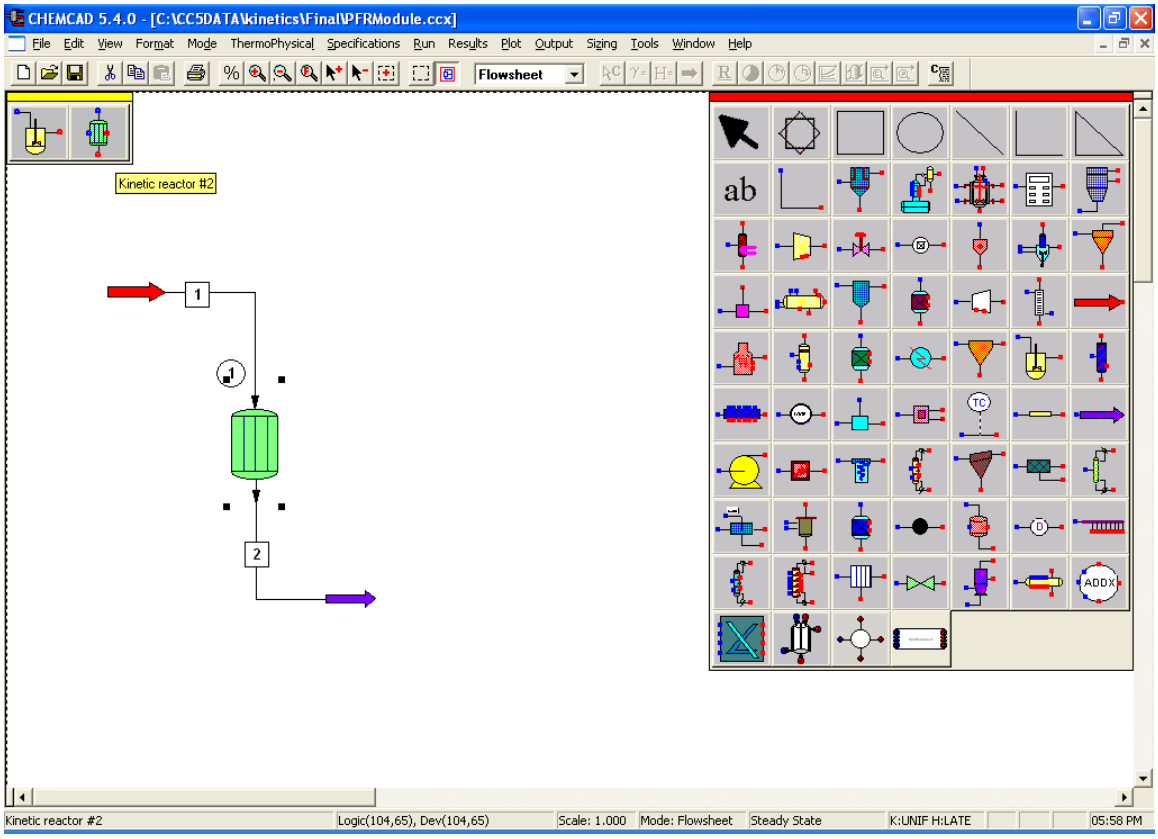
1) The exiting stream concentrations from the reactor.
2) Plot the change in concentration of the reactants and products along the volume of the reactor.

Procedure:

Step 1: Creating the flow sheet
Step 2: Entering the components and formatting engineering units
Step 3: Entering the feed stream composition
Step 4: Entering the reactor specs
Step 5: Running the simulation and retrieving the results

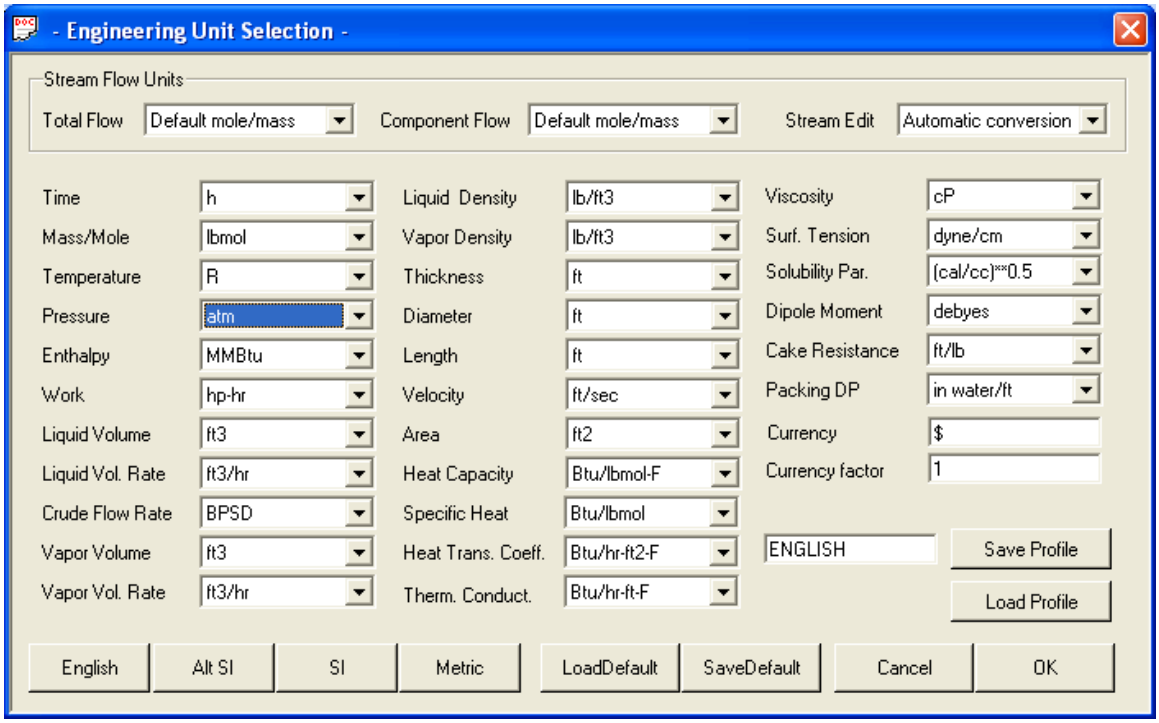
Step 1: Creating the flow sheet

Select and right click on the *kinetic reactor* and choose the *kinetic reactor #2 (plug flow reactor), feed* and *product* icons on the workspace. Connect the three using the *stream.* Click on the drop down menu that currently says *Flowsheet* and change it to *Simulation.*

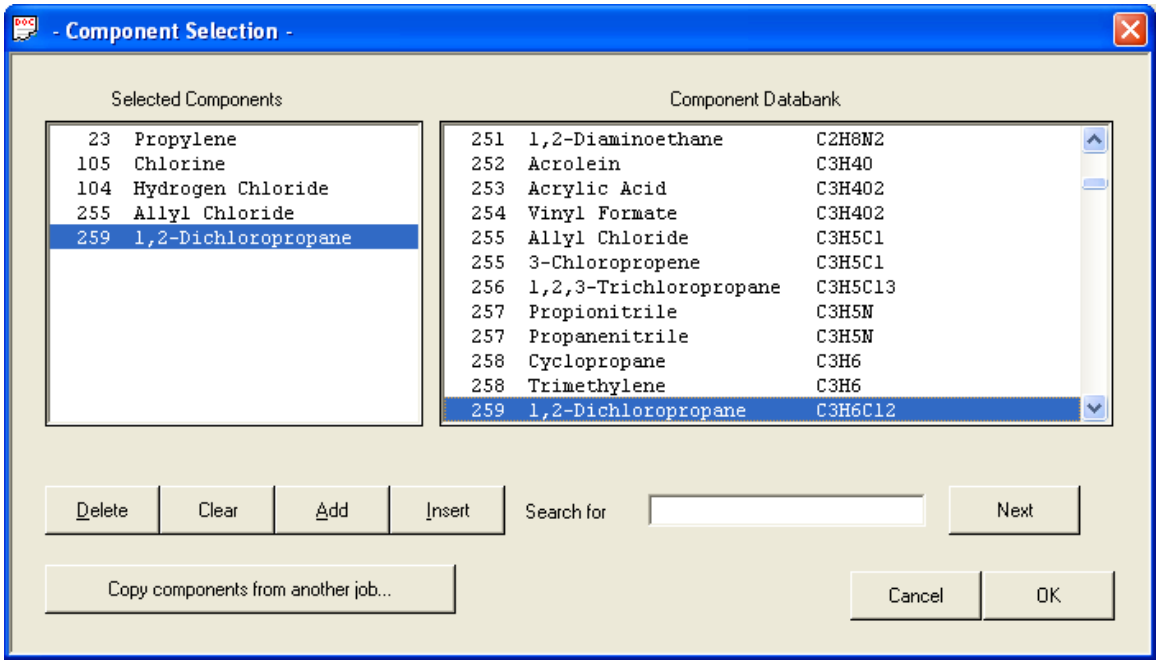


Step 2: Entering the components and formatting engineering units

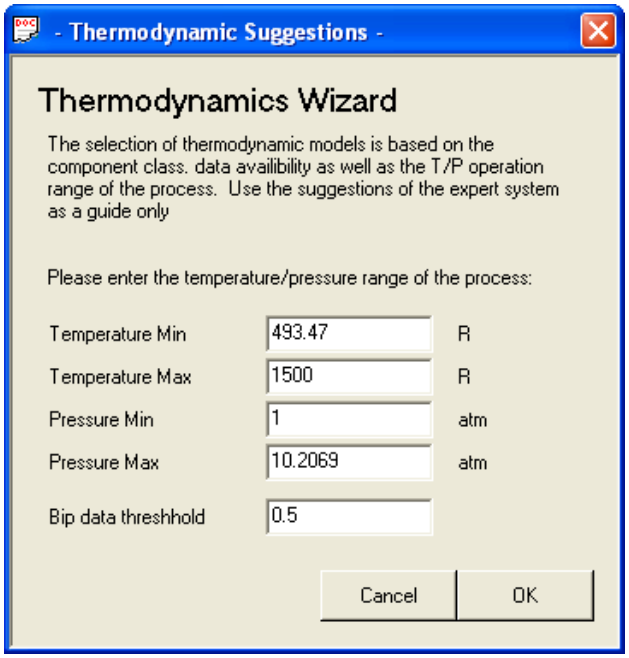
Go to the *Format* menu and click on *Engineering Units* and select the desired units for such properties as R for temperature, and atm for pressure etc. Use *English* units option to convert all units at the same time. Click OK to continue.



Go to the *Thermophysical* on the menu bar and click on *Components List*. Find propylene, chlorine, hydrogen chloride, allylchloride and 1,2-DiCl-Propane from the CHEMCAD component databank and click *Add*.

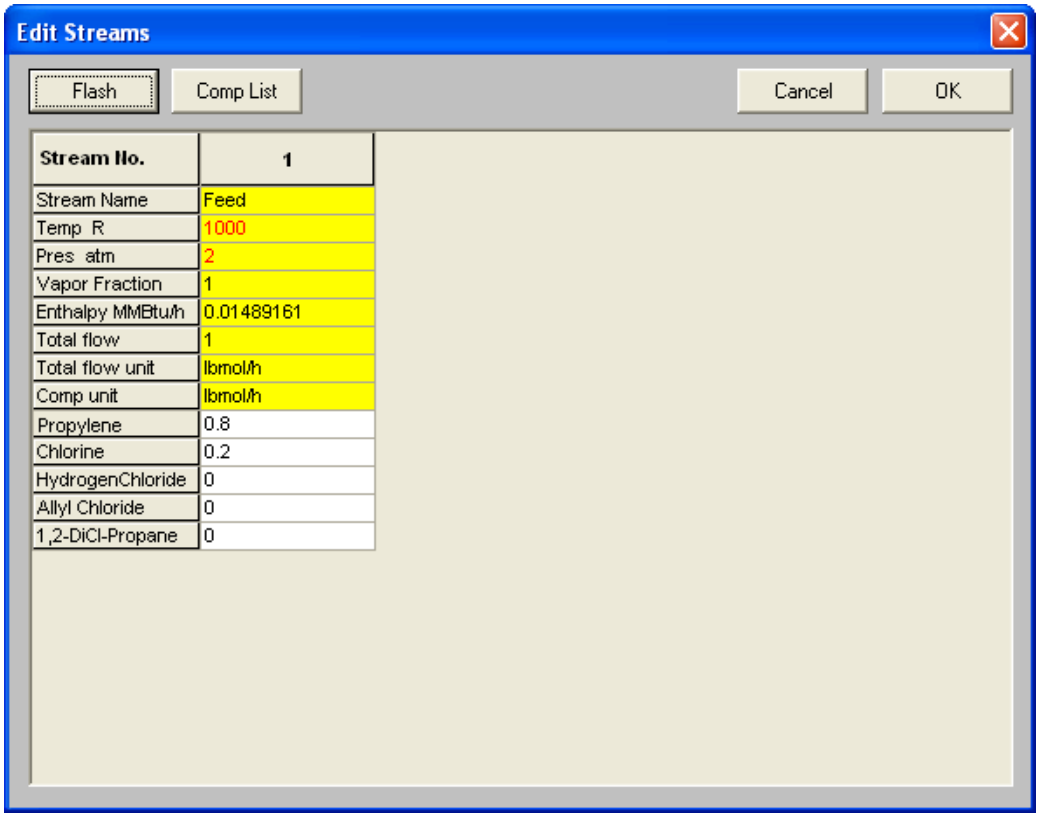


When the *Thermodynamic Suggestions* window appears, input the desired ranges of temperatures and pressures, then click OK. (Also click OK through the next 3 windows that pop up.)



Step 3: Entering the feed stream composition

Double click on the feed stream and enter the feed information (temperature, pressure, total flow rate and component mole fractions) given in the problem statement. Click once on *Flash* to get the feed stream enthalpy and vapor fraction in feed at the feed conditions.



Step 4: Entering the reactor specs
Double click on the reactor.

General Specifications Page:

a. *Number of reactions:* Since there are two reactions in the given problem, enter '2'

b. *Reactor Pressure:* Enter the reactor pressure as given in the problem statement (2 atm)

c. *Pressure Drop:* There is no pressure drop in the reactor given in the problem statement.

d. *Kinetic Rate Expression:* There are two options for this. The default option *(Standard)* is used when the rate equation is in standard form. The other option *(User Specified)* is used when the rate law is not in its standard form and the user needs to enter this manually. For more information on this, the user can always click on the *help* button that appears at the bottom left corner on this page. For this problem, the kinetic rate expression is given, so select the *(User Specified)* option.

e. *Reaction Phase:* Since the reactants and products are in vapor phase, click on the *vapor only* option.

f. *Specify Reactor Type:* As the reactor described in the problem statement is a plug flow reactor, *PFR* should be selected form the drop box.

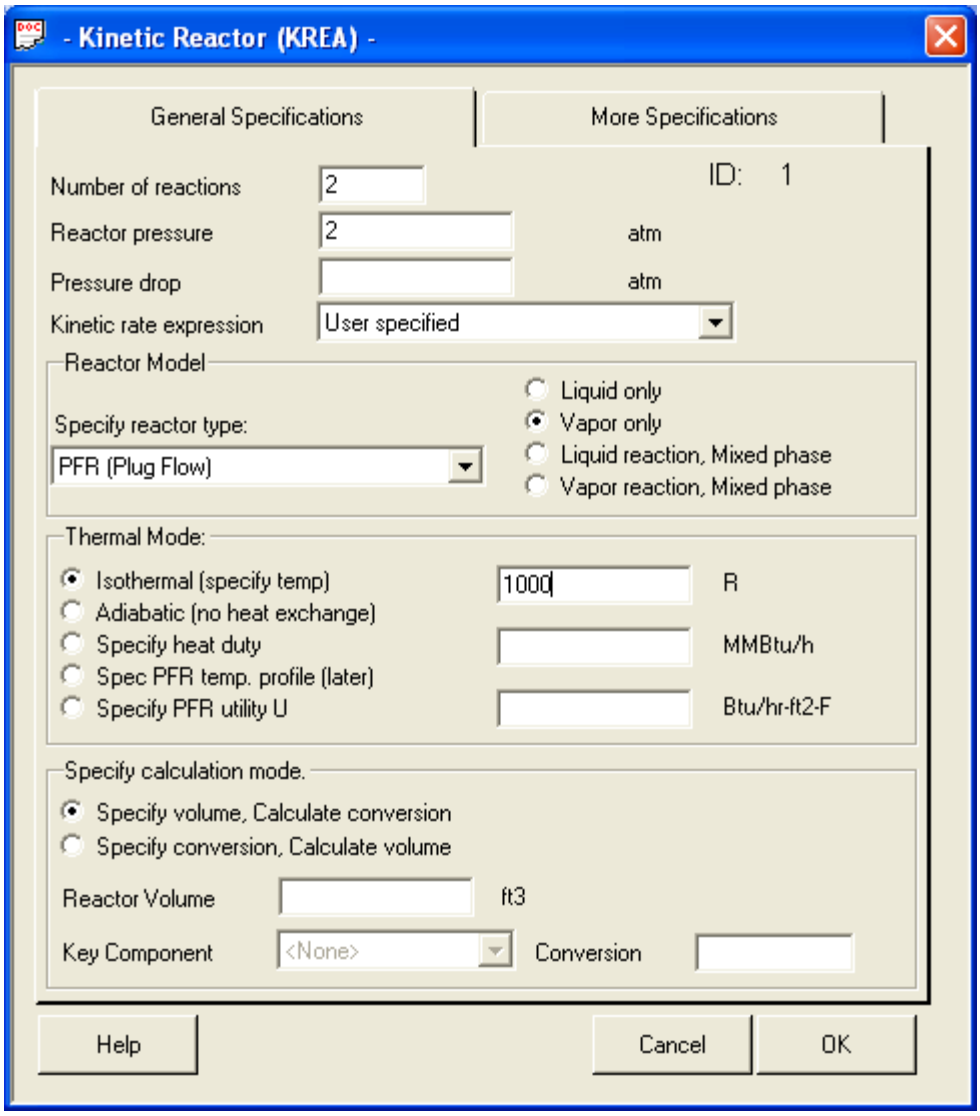
g. *Thermal Mode:* As the temperature of the reaction is given at 1000 Rankine, select *isothermal* and imput 1000 in the box next to it.

h. *Specify Calculation Mode:* As the conversion is to be calculated, *Specify Volume, Calculate Conversion* option should be selected.

i. *Reactor Volume:* This can be left blank or can be calculated. The volume can be specified as a combination of the reactor diameter and length in *more specifications*.

j. *Key Component:* The key component is to be specified when we choose the *Specify conversion, Calculate volume* option. So this can be left blank

k. *Conversion:* This needs to be left blank, as this is the value that is calculated in the simulation.



Don't Click *OK* yet! There is more to complete in the *More Specifications* page!

More Specifications:

Length of tubes: Enter the Length of the reactor specified in the problem statement (12 ft)

Diameter of tubes: Enter the Length of the reactor (note: convert 2 inches to feet = 0.1667 ft)

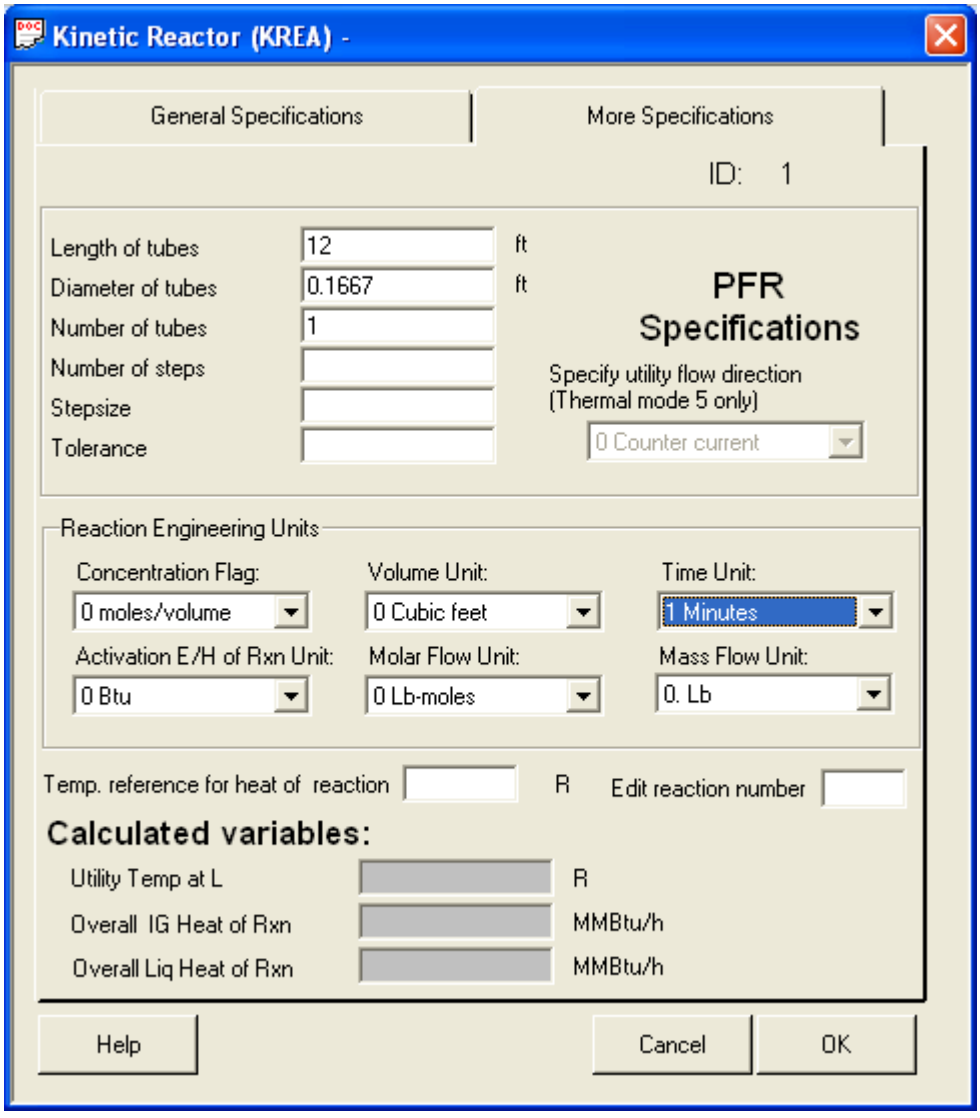
Number of tubes: Enter '1'

# of steps, *Stepsize* and *Tolerance* can be left blank as these are optional fields.

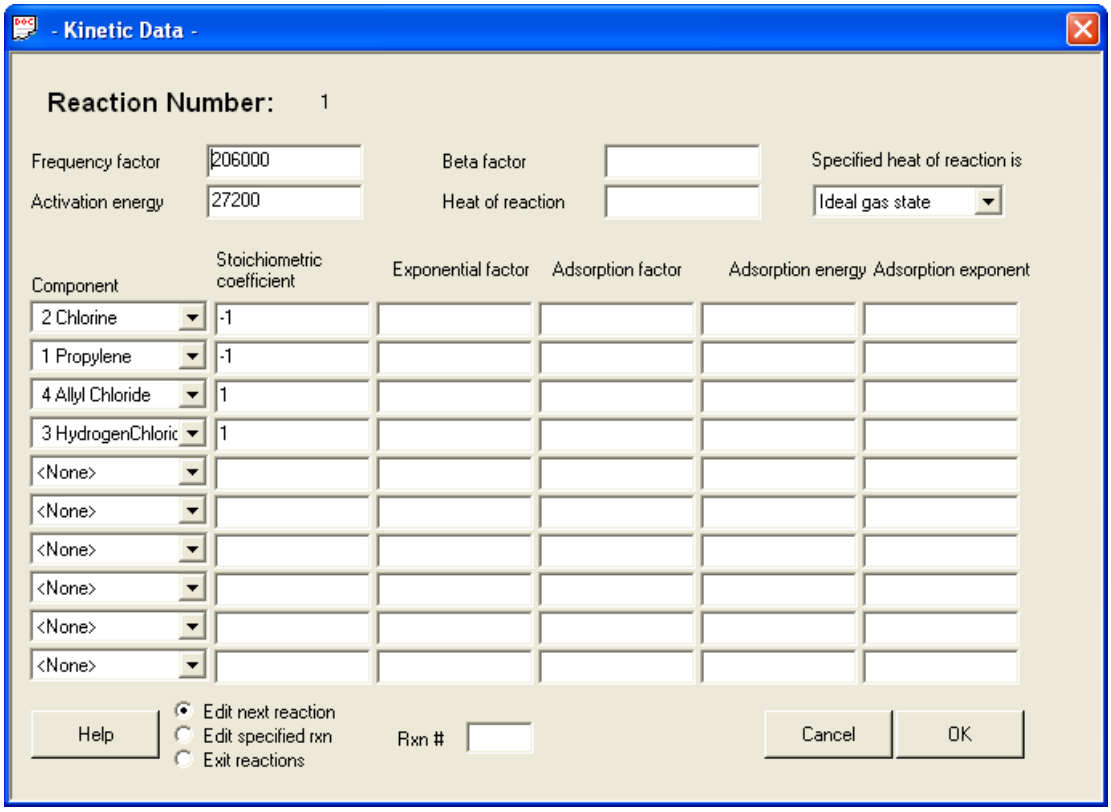
Reaction Engineering Units: Change the units so that the units are consistent with the rate law (Change *time* units to *minutes*

Temperature reference for heat of reaction: Can be left blank. Chemcad chooses the default reference temperature.

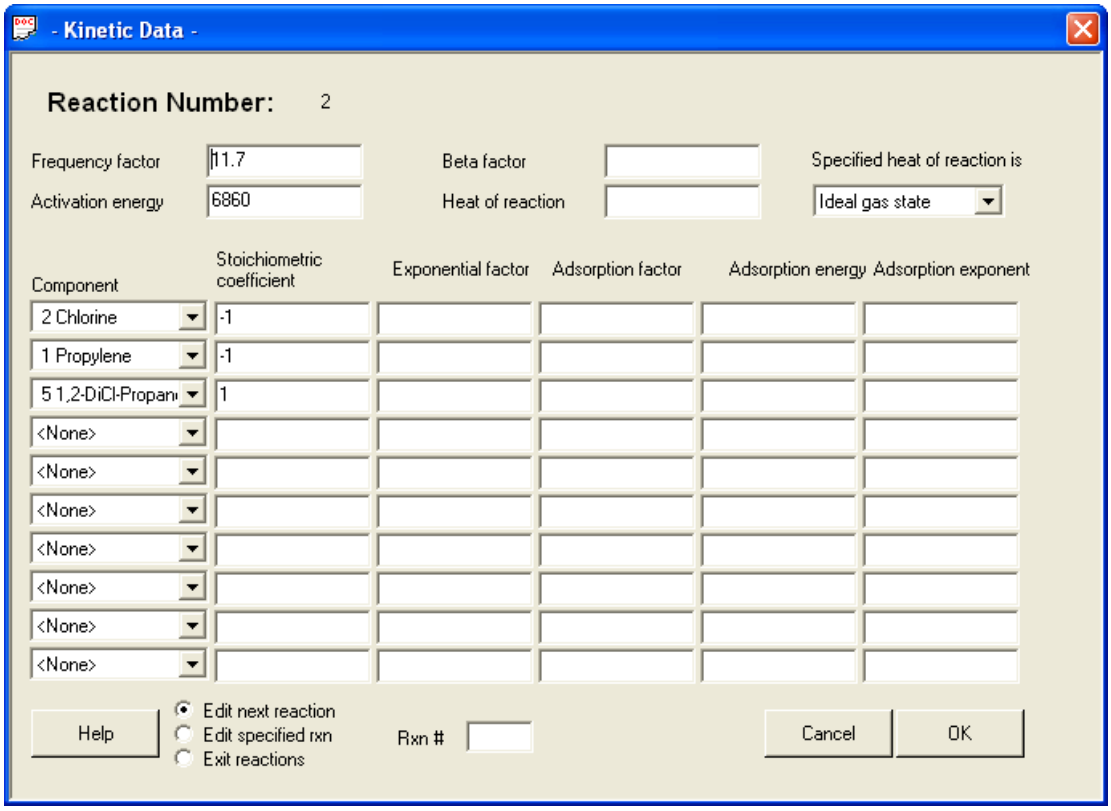
Edit reaction number: Can be left blank.



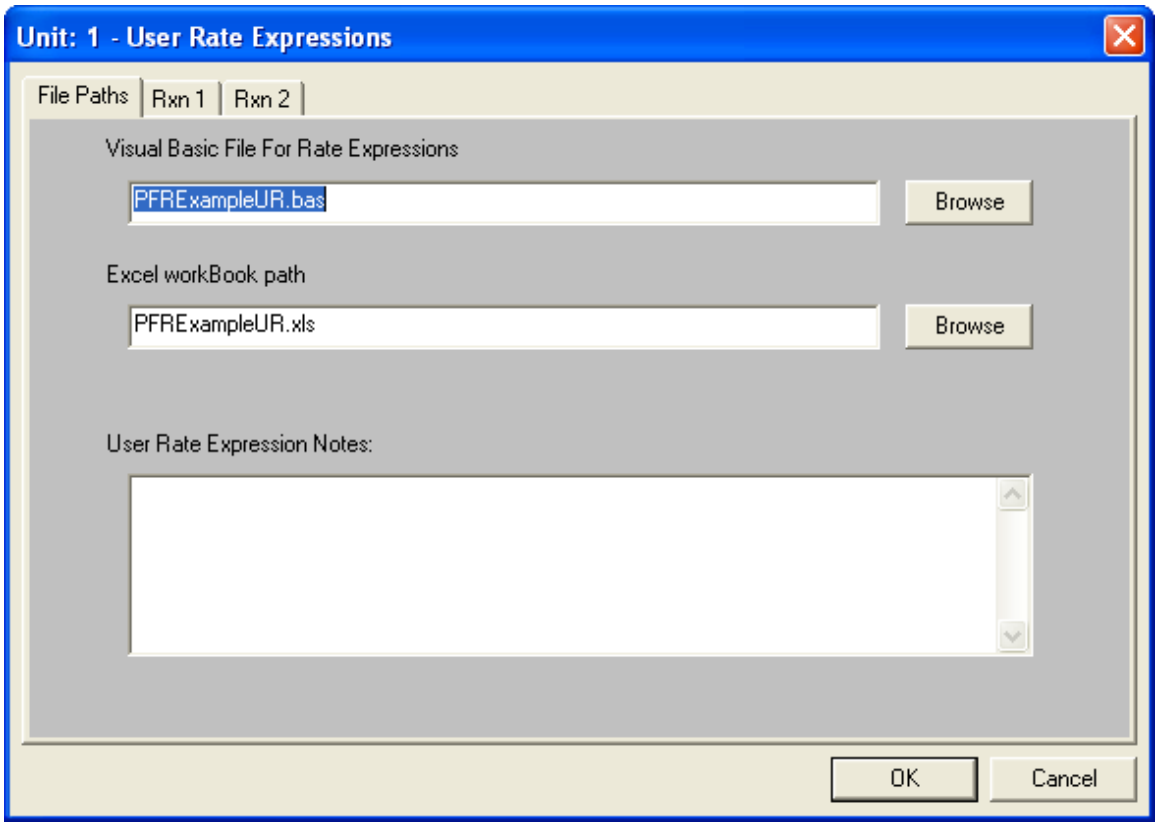
Click *OK* after completing the specifications page. A new window appears and the stoichiometric coefficients for *Reaction 1* (The reaction number is displayed on the top left hand corner of this window) of all the components are entered in this window as shown in the following figures. Also, enter the values in for the activation energy and the frequency factor as shown below. Click *OK* after entering these coefficients.



Similarly, enter the stoichiometric constants for *reaction 2* and click OK.



As the *User Specified* option is selected for kinetic rate expression, another window with the title *User Rate Expressions* appears. If a separate Visual Basic code is available, the user can browse those files using options available on *File path* tab. For most practical purposes, the user can go directly to the *Rxn1* tab or the *Rxn2* tab:

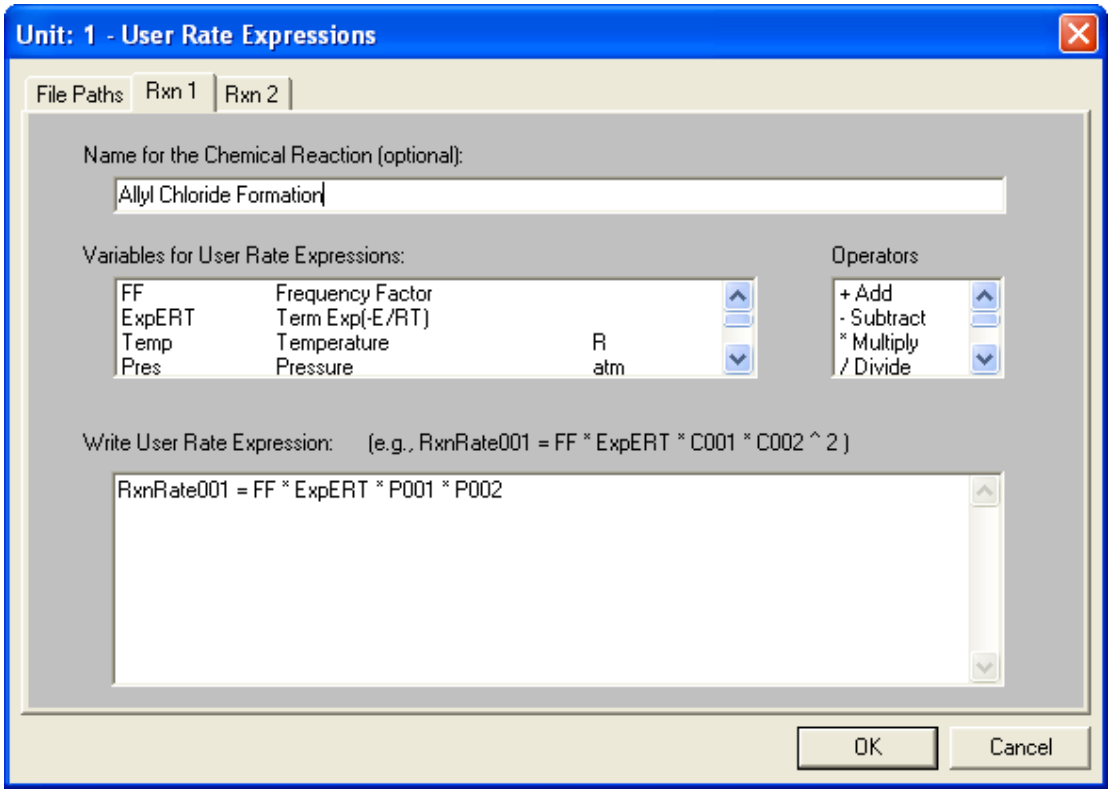


Select the *Rxn1* Tab and enter the rate expression for the reaction1.

Name for the Chemical Reaction: Allyl Chloride formation

Variables for User Rate Expressions: CHEMCAD supplies the user with the variables described in this section to be used for user rate expressions.

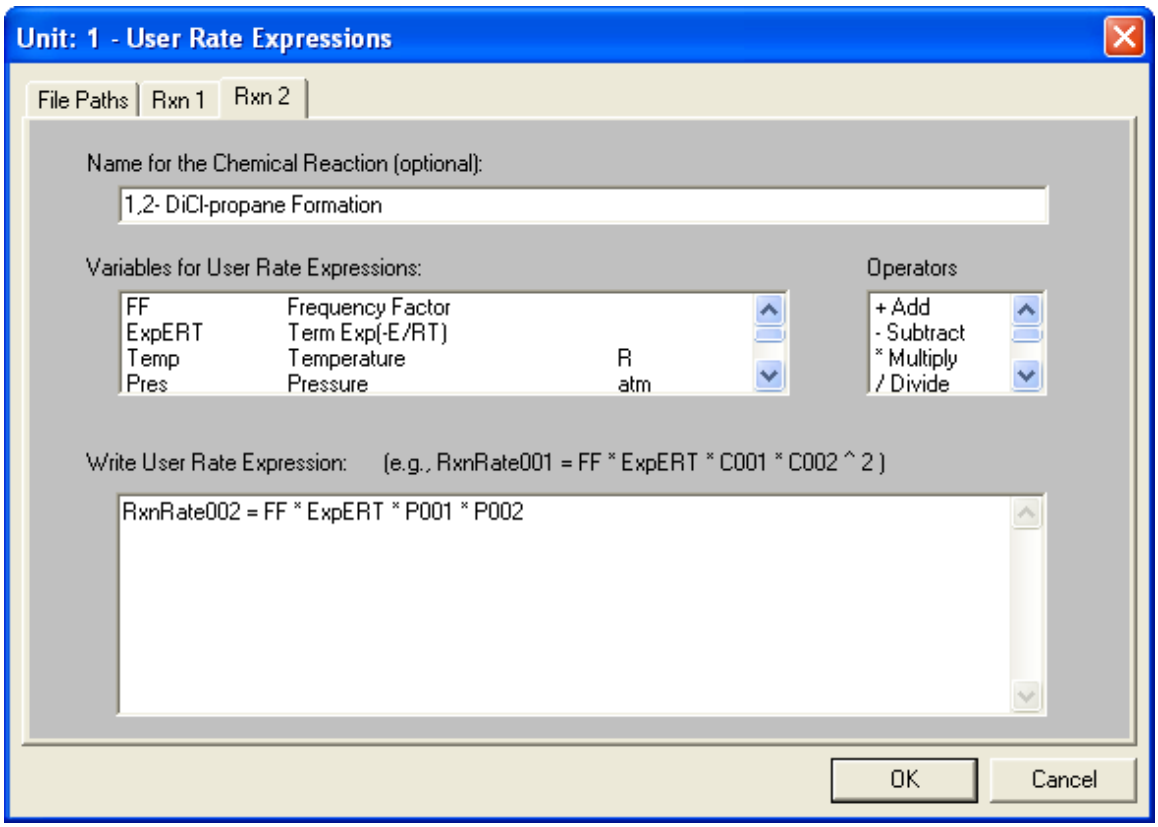
*Write User Rate Expression: RxnRate001 = FF * ExpERT * P001 * P002*



Select the *Rxn2* Tab and enter the rate expression for the reaction2.

Name for the Chemical Reaction: 1,2- DiCl-propane formation

*Write User Rate Expression: RxnRate001 = FF * ExpERT * P001 * P002*

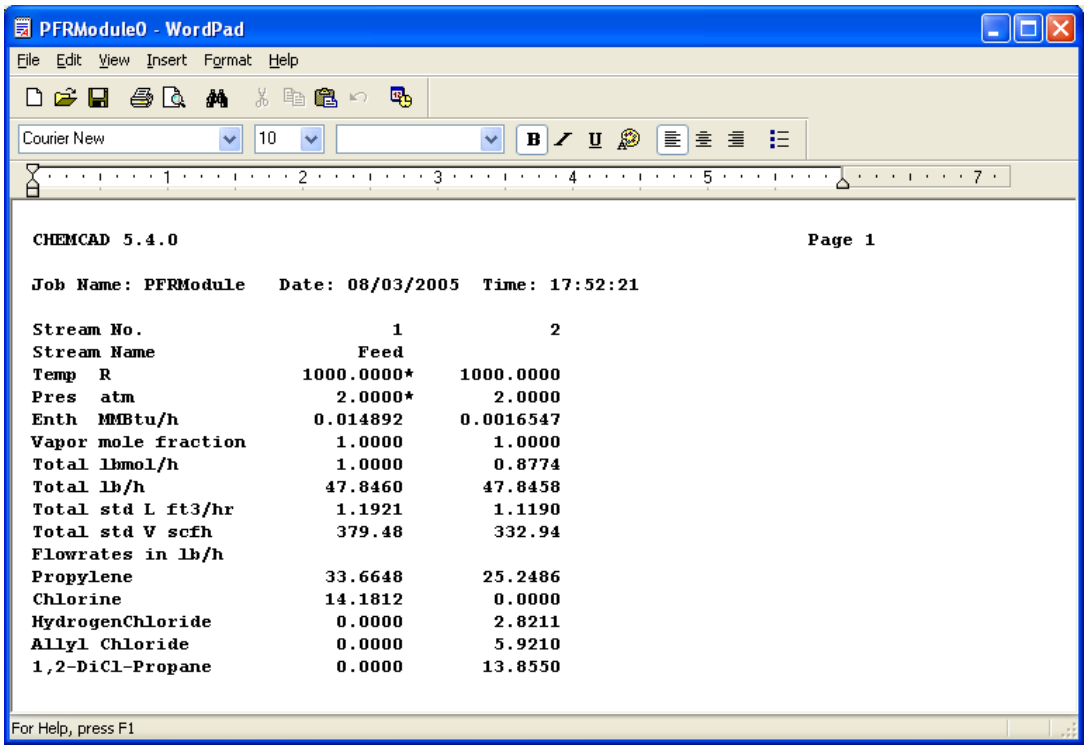


Click *OK* when finished. A window appears to confirm that we allow the cookies from an existing excel file so that the Visual Basic program accesses the rate expression specified by us. Click on *Yes* to continue.

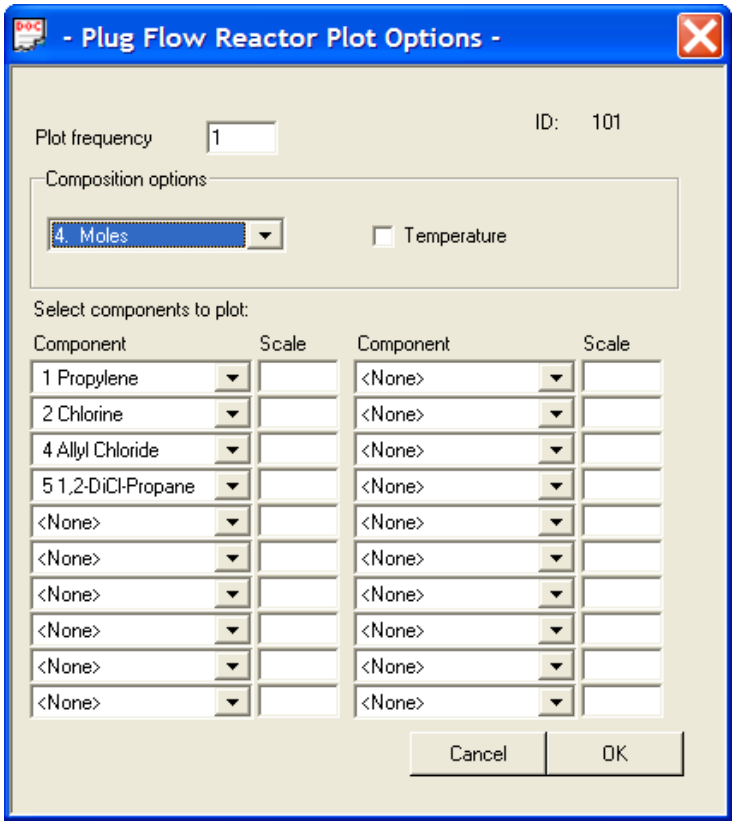
Step 5: Running the simulation and retrieving the results:

Now the simulation is ready to be run. Click once on *R* to run the simulation. Alternatively, one can run the simulation by clicking on *Run* on the menu bar and selecting *Run all.* The status of the simulation can be found at the bottom left hand corner of the screen. The message, *Run Finished* appears in this place if the run is successfully completed.

The product stream properties can be found either by double clicking on the product stream or by clicking once on *Results* on the menu, selecting *Stream Composition* and then clicking on *All Streams.* The results will be available in a WordPad file.



To plot the concentrations along the volume of the reactor, Select *plot* from the toolbar and then choose *plug flow reactor profile*. The following screen will appear.

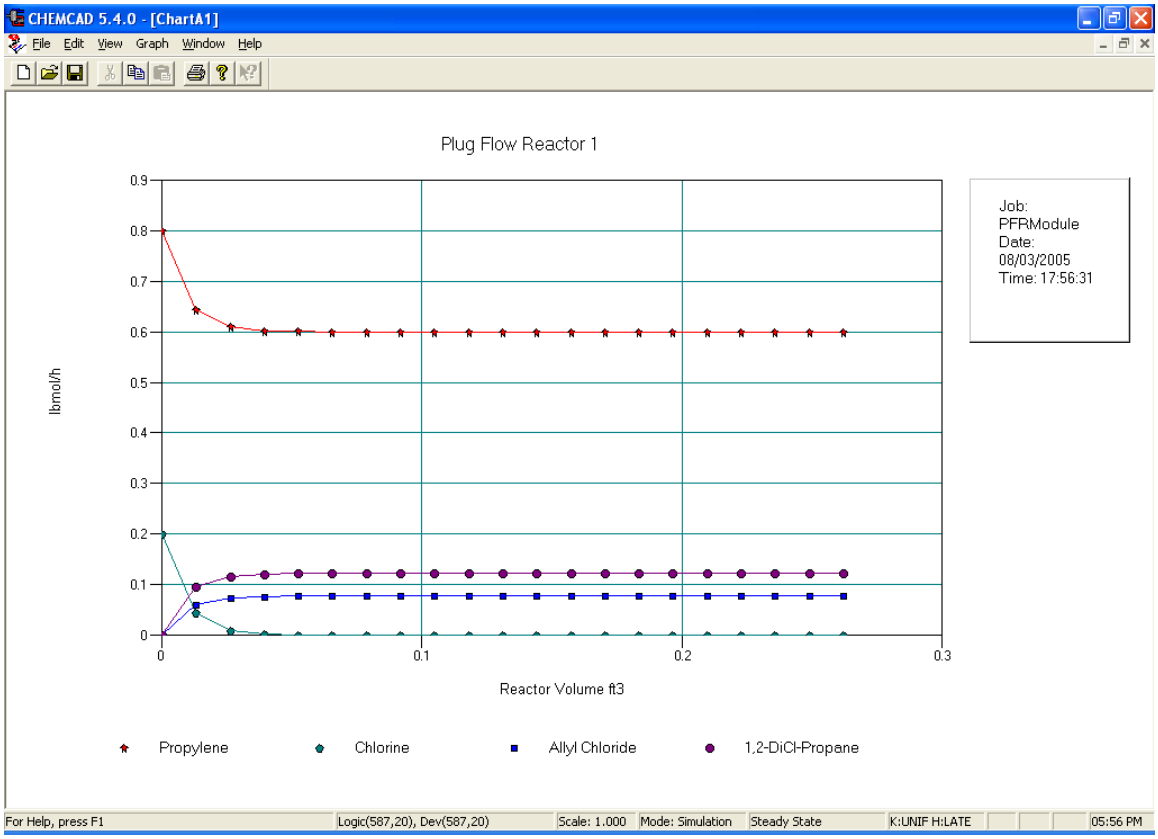


Plot Frequency: select a value of '1'.

Composition Option: Since we want the compositions in moles choose moles. The temperature change along the reactor can also be plotted. Since ours is an isothermal case we need not select it.

Select Component to Plot: Select all the components of which we want to see the change in concentration. Click *OK*.

The following graph plots the change in concentration along the reactor volume.



SHORTCUT COLUMN

Problem Statement:

A 100 kmol/hr stream of ethanol (50 mol%) and n-propanol (50 mol%) is fed to a continuous distillation column at room temperature (298 K) and atmospheric pressure. The pressure drop across the column is negligible and a reflux ratio of 1.5 is used. About 93 mol% of ethanol in feed and 5 mol% of n-propanol in feed is desired to be present in the distillate stream.

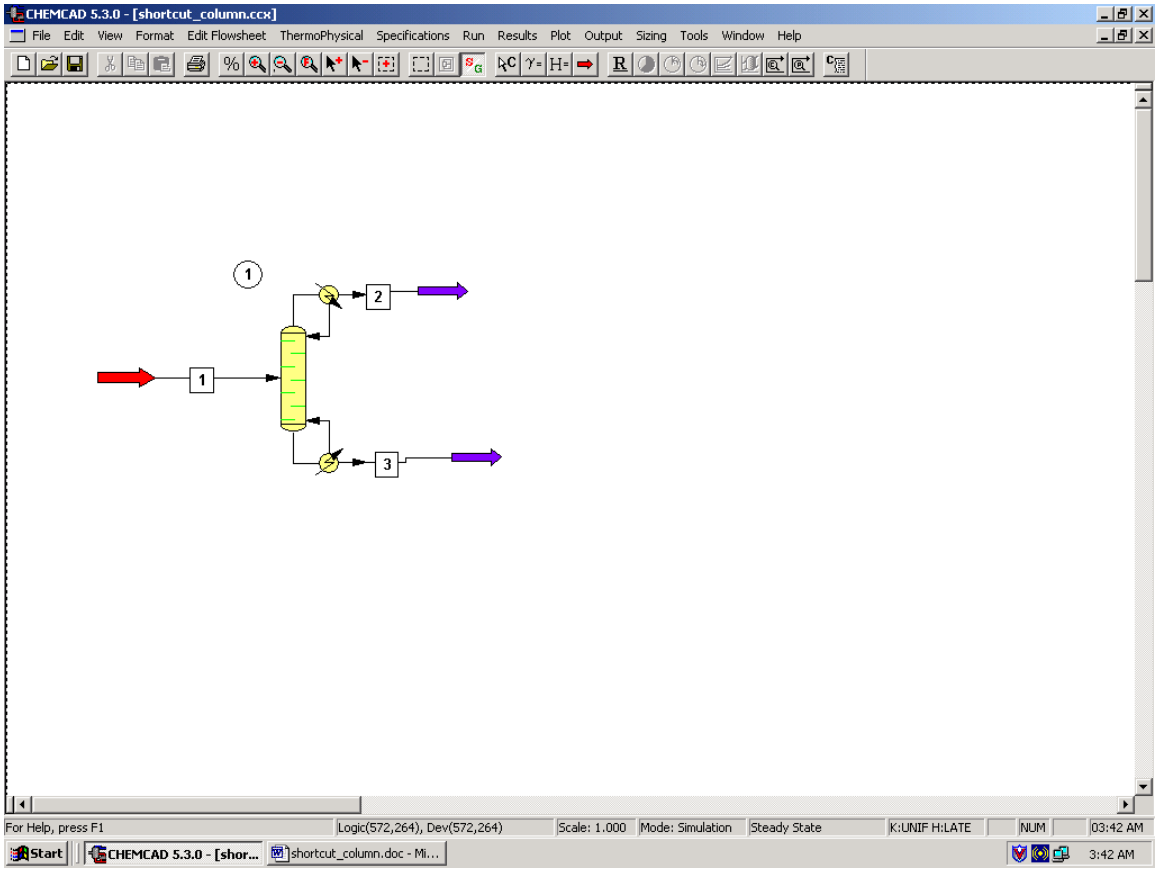
Design a continuous distillation column to meet the desired specifications using *Shortcut column* in CHEMCAD and report the total number of stages, minimum number of stages, feed stage location, minimum and calculated reflux ratios, final distillate and bottom stream concentrations and the reboiler and condenser heat duties.

Procedure:

Step 1: Creating the flow sheet
Step 2: Entering the components and engineering units
Step 3: Entering the composition of feed stream
Step 4: Entering the shortcut column specs
Step 5: Running the simulation and retrieving the results

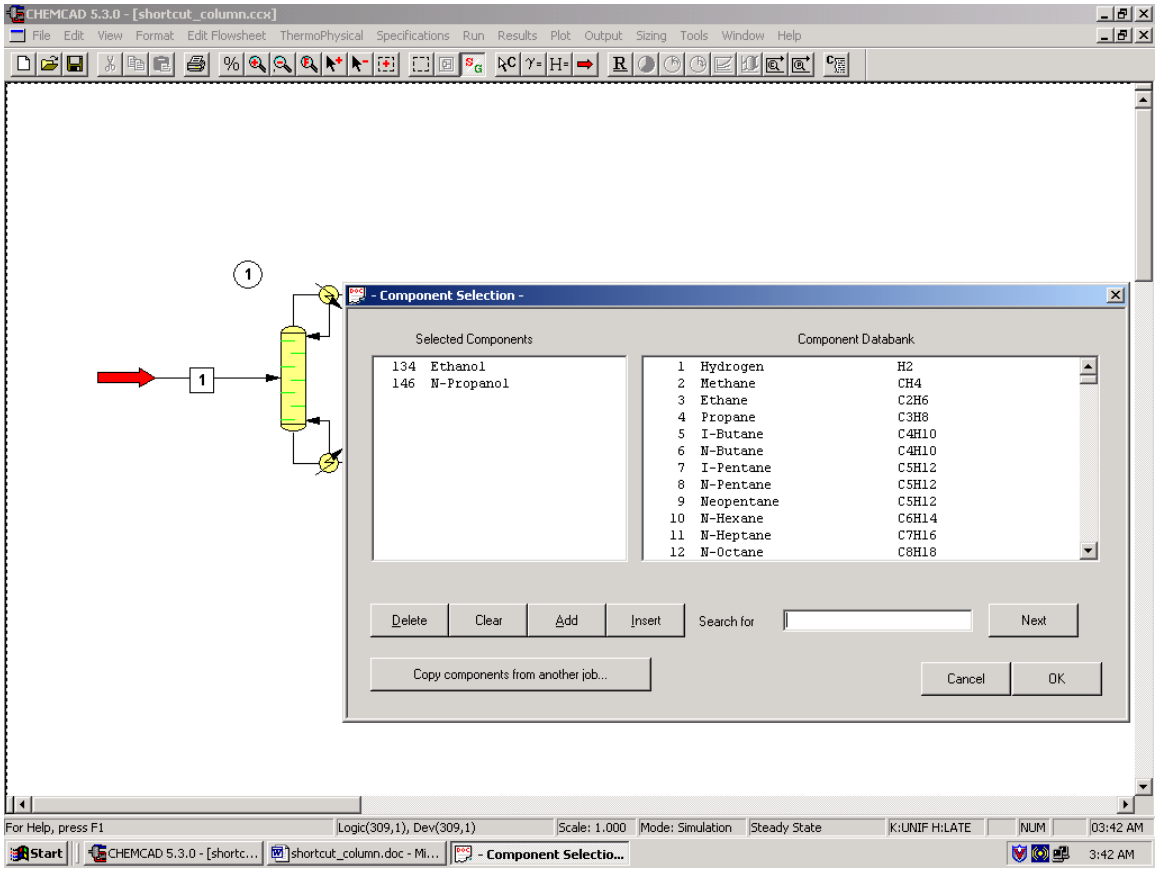
Step 1: Creating the flow sheet

Go to *new* on the *File* menu and save the blank simulation. Click on *Shortcut column* on the CHEMCAD palette and click once on simulation window to paste it. Click on the feed icon on the palette and paste it on the workspace. Similarly, click on the product icon and place it on the workspace (do the product twice as there are two product streams). After making sure that all the necessary icons are placed on the workspace, they can be connected by using *stream.* CHEMCAD automatically assigns numbers to streams and unit operations the order in which they are placed on the workspace. After completing the flow sheet, click once in the **S/G** icon found on the menu bar so that the simulation is changed from *edit* mode to *run* mode. The same icon can be used to toggle between these two simulation modes. Alternatively, one can toggle between *Edit Flowsheet* and *Run Simulation* on the menu bar to achieve the same.


CHEMCAD 5.3.0 - [shortcut_column.ccx]
File Edit View Format Edit Flowsheet ThermoPhysical Specifications Run Results Plot Output Sizing Tools Window Help
1
2
1
3
For Help, press F1
Logic(572,264), Dev(572,264)
Scale: 1.000
Mode: Simulation
Steady State
K:UNIF H:LATE
NUM
03:42 AM
Start
CHEMCAD 5.3.0 - [shor...
shortcut_column.doc - Mi...
3:42 AM

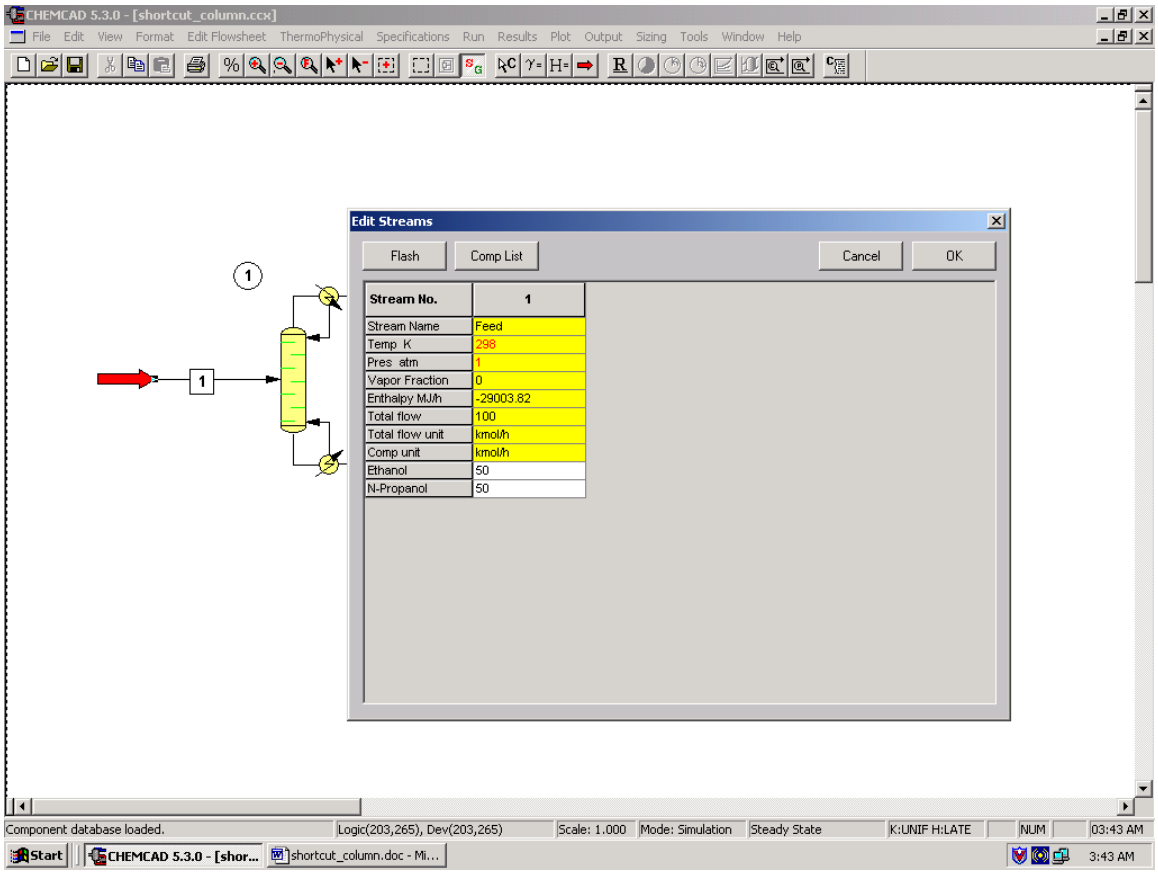
Step 2: Entering the components and engineering units

Go to the *Thermophysical* on the menu bar and click on *Components List*. Find ethanol and n-propanol from the CHEMCAD components list and add them to the component list. Go to the *Format* menu and click on *Engineering Units* and select the desired units for such properties as temperature, pressure etc. Click OK to continue.



Step 3: Entering the composition of feed stream

Double click on the feed stream and enter the feed information (temperature, pressure, total flow rate and component mole fractions) given in the problem statement. Click once on *Flash* to get the feed stream enthalpy and vapor fraction in feed at the feed conditions.



Step 4: Entering the Shortcut column specs

Double click on the *ShortCut Column.*

1. Select mode:
The *Shortcut column* can be used for both design and rating of a distillation column. As we need to design a column, option 2 or option 3 can be used for the design mode. Select one of these two and continue.

2. Select condenser type:
As this is not explicitly stated in the problem statement, the condenser can be assumed to be total and can be left to this default option.

3. Column pressure:
As there is negligible pressure drop across the column, one can enter the same pressure as that of the feed stream in this field (1 atm). This can also be left blank and CHEMCAD sets the pressure to default, which is the pressure of the feed stream.

4. Column pressure drop:
This can be left blank.

5. Number of stages:
CHEMCAD calculates the number of stages and stores the calculated number in this box. The user needs to leave this box blank.

6. Reflux ratio:
Enter the value '1.5' in this field.

7. R/Rmin:
One needs to enter only one of the two specs, reflux rato or R/Rmin. As the reflux ratio is specified, this field needs to be left blank.

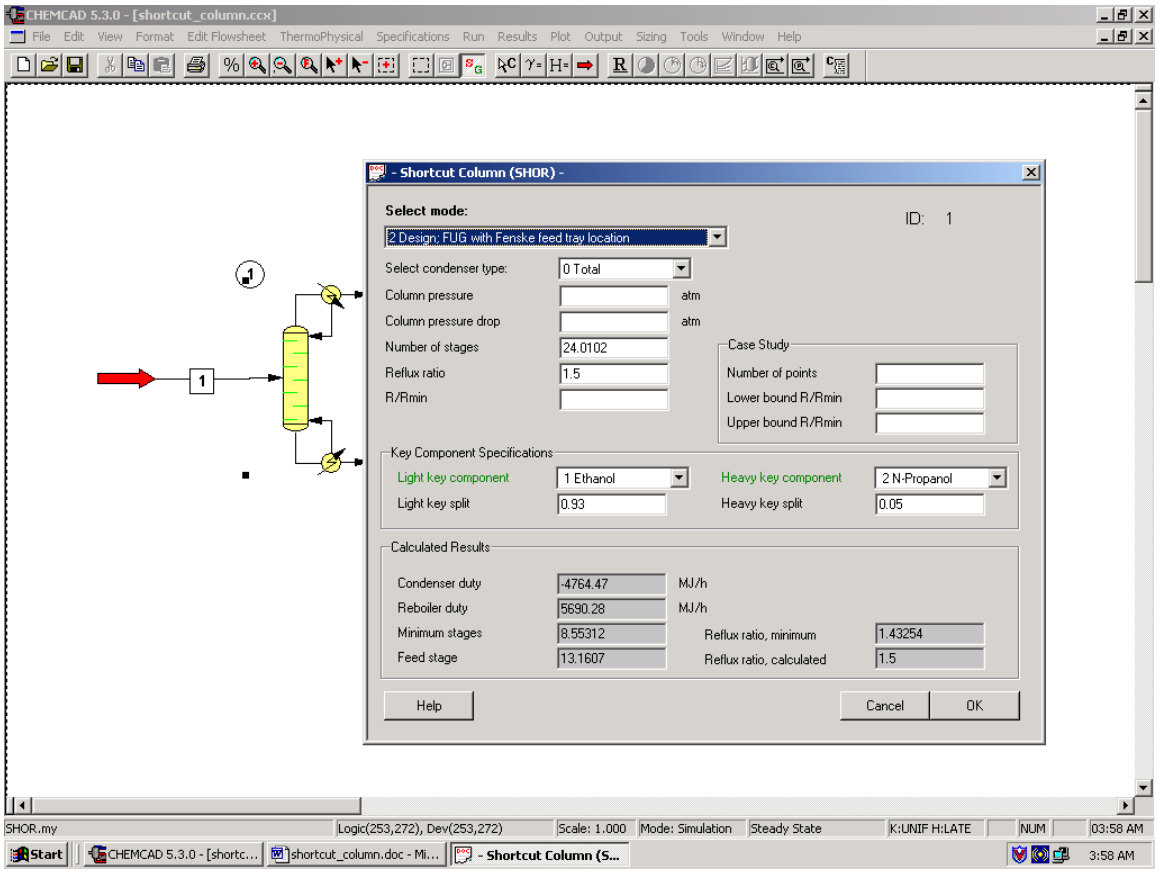
8. Case study:
This is optional and can be left blank for our purpose.

9. Key component specifications:

a. *Light key component:* Select 'Ethanol'
b. *Light key split:* Enter '0.93'
c. *Heavy key component:* Select 'n-propanol'
d. *Heavy key split:* Enter '0.05'

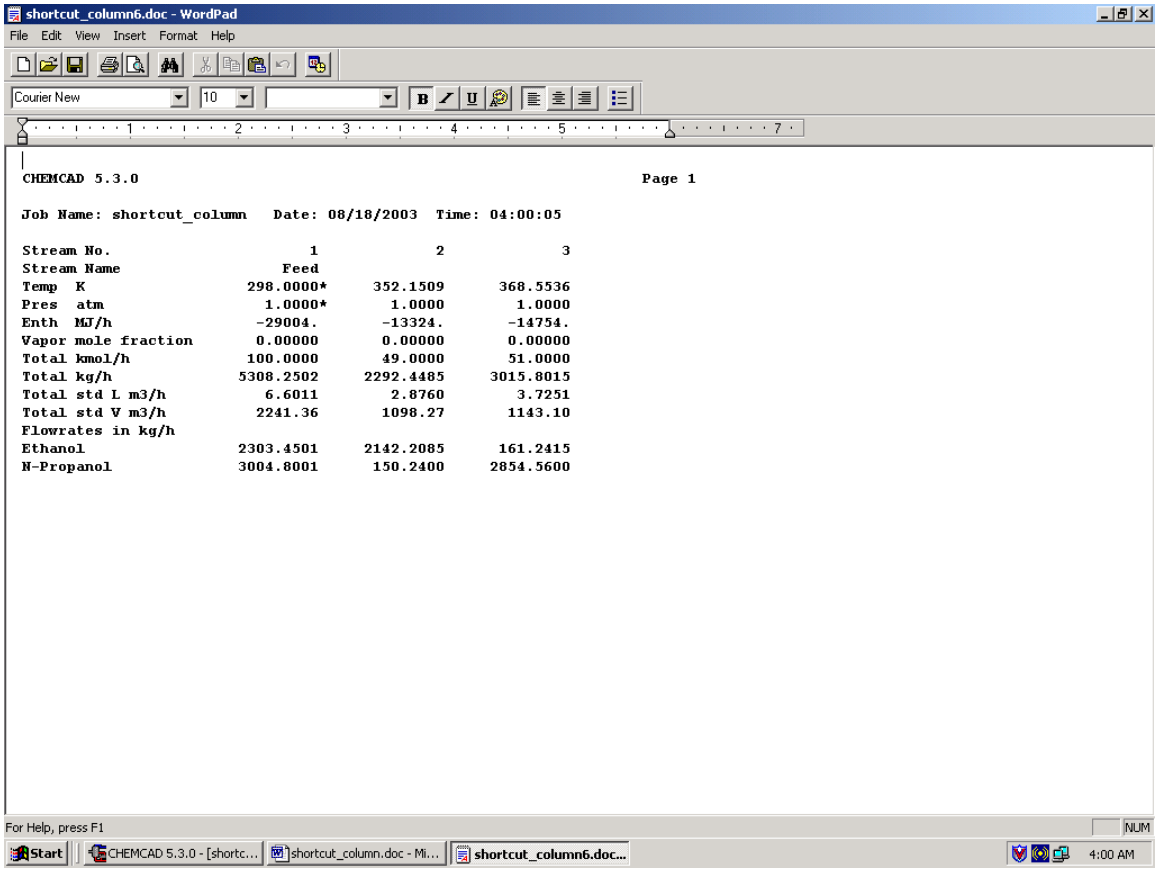
10. Calculated results:
These are the parameters that CHEMCAD calculates and stores the values of. All these fields need to be left blank.

Click *Ok* when finished.

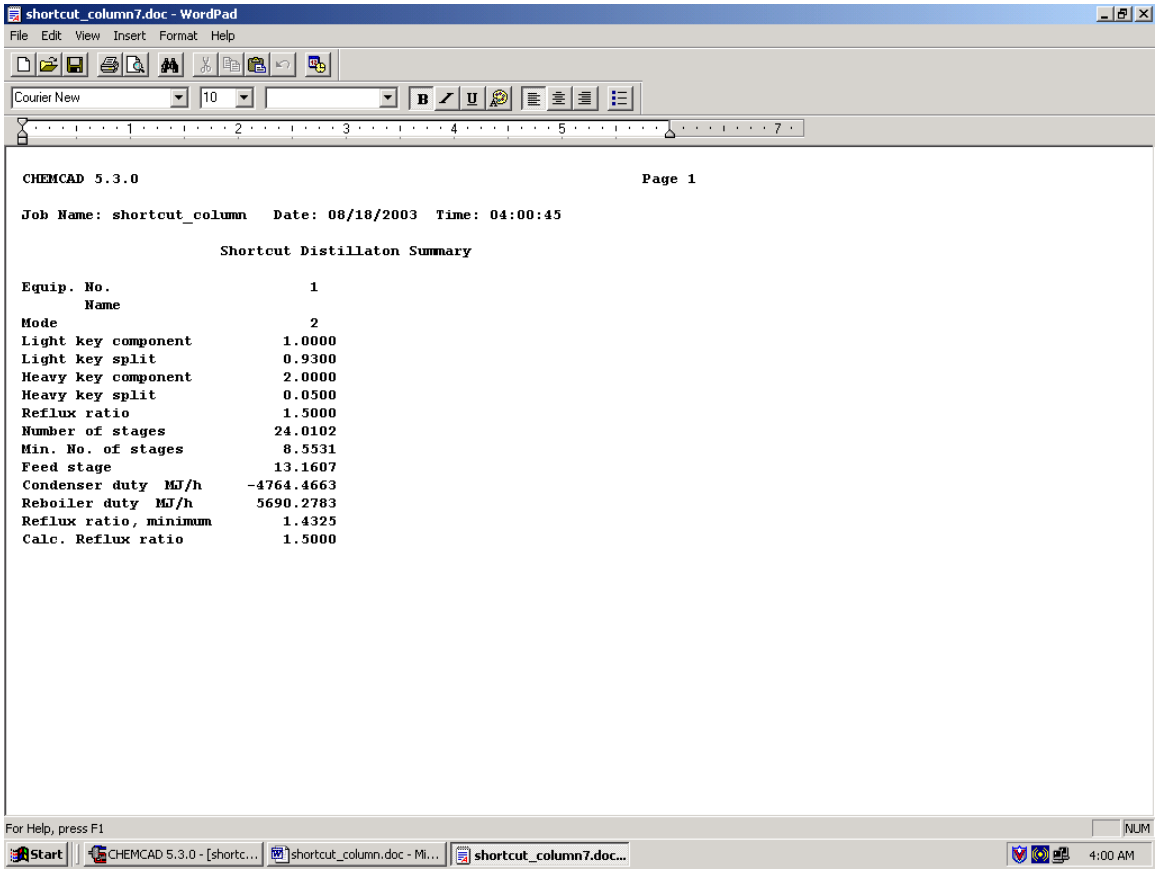

CHEMCAD 5.3.0 - [shortcut_column.ccx]
File Edit View Format Edit Flowsheet ThermoPhysical Specifications Run Results Plot Output Sizing Tools Window Help
- Shortcut Column (SHOR) -
Select mode:
ID: 1
2 Design; FUG with Fenske feed tray location
Select condenser type:
0 Total
Column pressure
atm
Column pressure drop
atm
Number of stages
24.0102
Reflux ratio
1.5
R/Rmin
Case Study
Number of points
Lower bound R/Rmin
Upper bound R/Rmin
Key Component Specifications
Light key component
1 Ethanol
Heavy key component
2 N-Propanol
Light key split
0.93
Heavy key split
0.05
Calculated Results
Condenser duty
-4764.47
MJ/h
Reboiler duty
5690.28
MJ/h
Minimum stages
8.55312
Reflux ratio, minimum
1.43254
Feed stage
13.1607
Reflux ratio, calculated
1.5
Help
Cancel
OK
1
SHOR.my
Logic(253,272), Dev(253,272)
Scale: 1.000
Mode: Simulation
Steady State
K:UNIF H:LATE
NUM
03:58 AM
Start
CHEMCAD 5.3.0 - [shortc...
shortcut_column.doc - Mi...
- Shortcut Column (S...
3:58 AM

Step 5: Running the simulation and retrieving the results

After entering the available information on the workspace as described in the previous steps, one can run the simulation by clicking on *R* on the menu bar. Alternatively, one can run the simulation by clicking on *Run* on the menu bar and selecting *Run all.* The simulator indicates the same warnings regarding the estimates as before and one can ignore them again and continue with the simulation by clicking on *Yes.* The status of the simulation can be found at the bottom left hand corner of the screen. The message, *Run Finished* appears in this place if the run is successfully completed. To view the product stream compositions, one can either double click on the individual product streams or by clicking *Results* on the menu bar and selecting *Stream Compositions* and further selecting *All Streams.* The results obtained from the latter method will be in a WordPad file.



All the results associated with the shortcut column can be found by clicking on *Results* menu and selecting *Unit Op's* and then the shortcut Column. The results will then be available in a WordPad file.


shortcut_column7.doc - WordPad
File Edit View Insert Format Help
Courier New
10
CHEMCAD 5.3.0 Page 1
Job Name: shortcut_column Date: 08/18/2003 Time: 04:00:45
Shortcut Distillaton Summary
Equip. No. 1
Name
Mode 2
Light key component 1.0000
Light key split 0.9300
Heavy key component 2.0000
Heavy key split 0.0500
Reflux ratio 1.5000
Number of stages 24.0102
Min. No. of stages 8.5531
Feed stage 13.1607
Condenser duty MJ/h -4764.4663
Reboiler duty MJ/h 5690.2783
Reflux ratio, minimum 1.4325
Calc. Reflux ratio 1.5000
For Help, press F1
NUM
Start
CHEMCAD 5.3.0 - [shortc...
shortcut_column.doc - Mi...
shortcut_column7.doc...
4:00 AM