Table of Contents

Introduction to UniSim

In our first lab we will seek to get acquainted with our process simulator, UniSim R440 from Honeywell. The various steps to using this simulator are summarised as follows:

- Setting up the Basis Environment
  - Creating the component list
  - Choosing the fluid package
  - Adding reactions
- Creating the Process Flowsheet
  - Adding and configuring process streams
  - Adding and configuring process equipment
- Presenting output from the process

In today's work we will create a feed stream of a 50/50 mixture of water and acetone, we will pass it into a separator, we will look at the composition and flow rates of the ensuing vapour and liquid streams, and we will ensure that material balance conditions are met by our simulator.

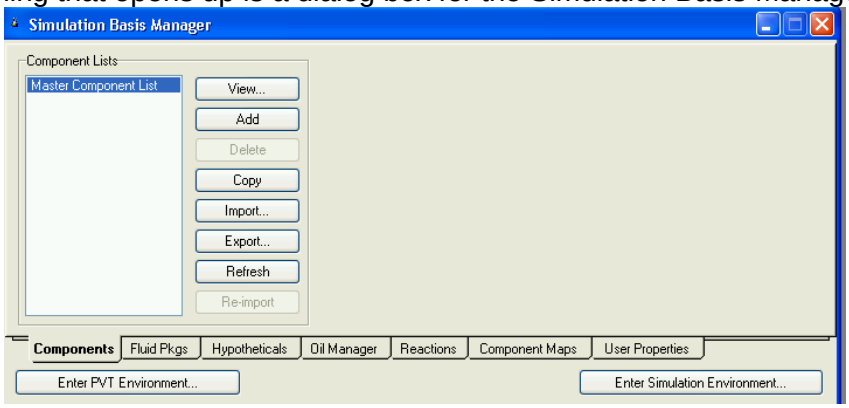
1. Getting Started

To log on to the PC's in room 116 you should use our regular login and password. The programme we use should have a shortcut on the desktop that looks a little like this:

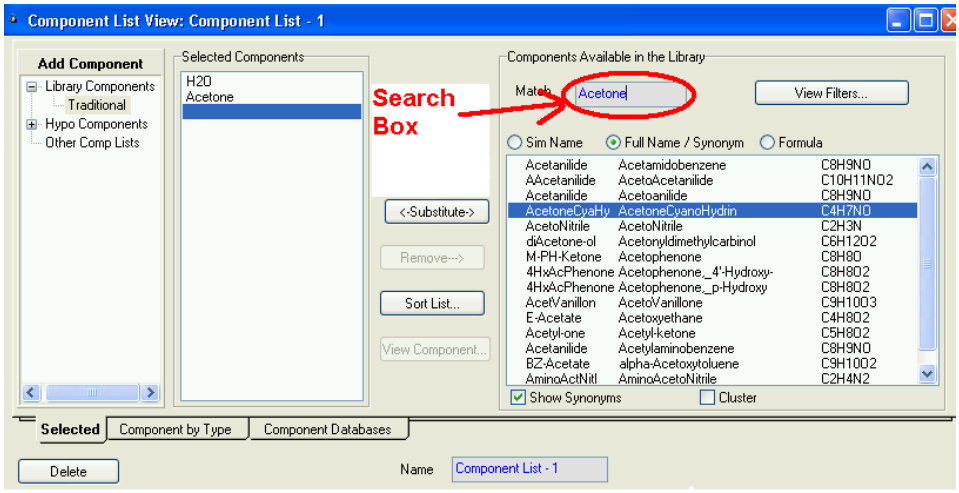
You can also find it under *Start, All Programs, Honeywell, Unisim Design R440.* Once the programme opens, click on *File, New, Case*

2. Basis Environment

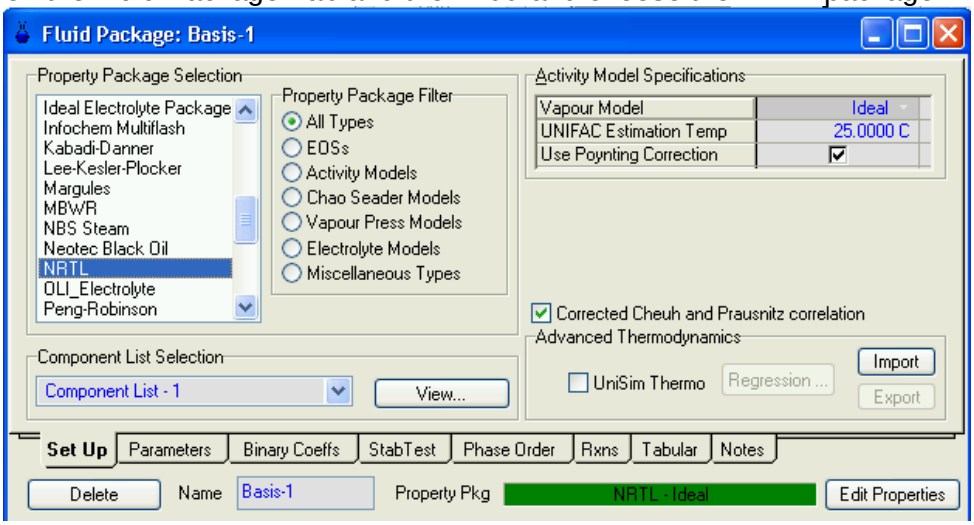
The first thing that opens up is a dialog box for the Simulation Basis Manager



Click *Add* and then add water and acetone to the components list. Using the *Match* search box helps a lot here.



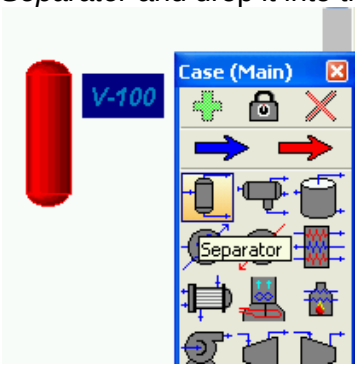
Close the *Component List View.*
Click on the Fluid Package Tab and then *Add* and choose the NRTL package.



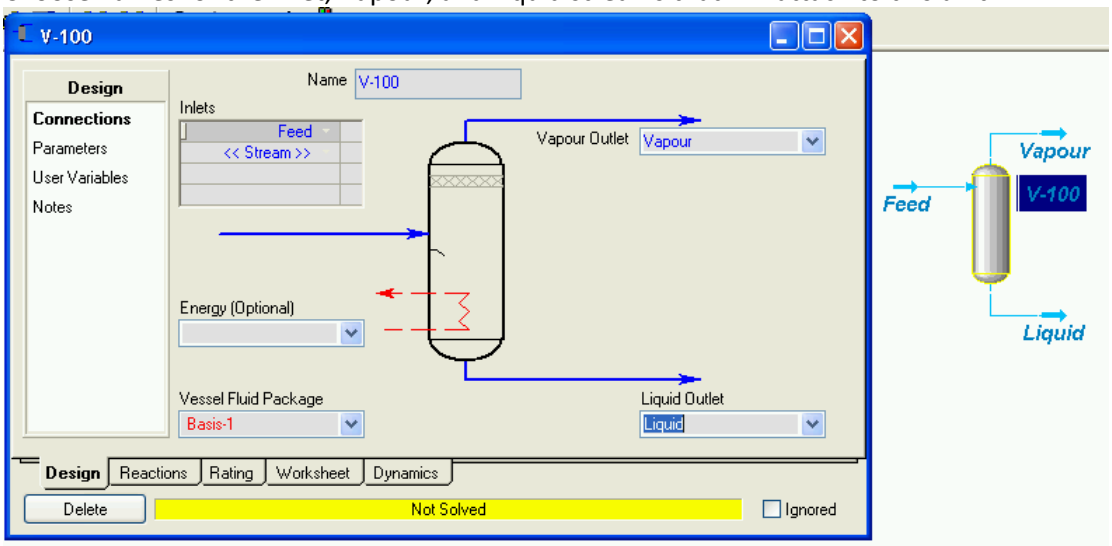
Check on the Binary Coefficients tab that the two interaction parameters have been successfully calculated (they should be in red type).
In this simulation we won't deal with any reactions, but normally we would also be visiting the Rxns tab to add reactions to our fluid package.
Close the Fluid Package dialog box.

3. Creating the Process Flowsheet

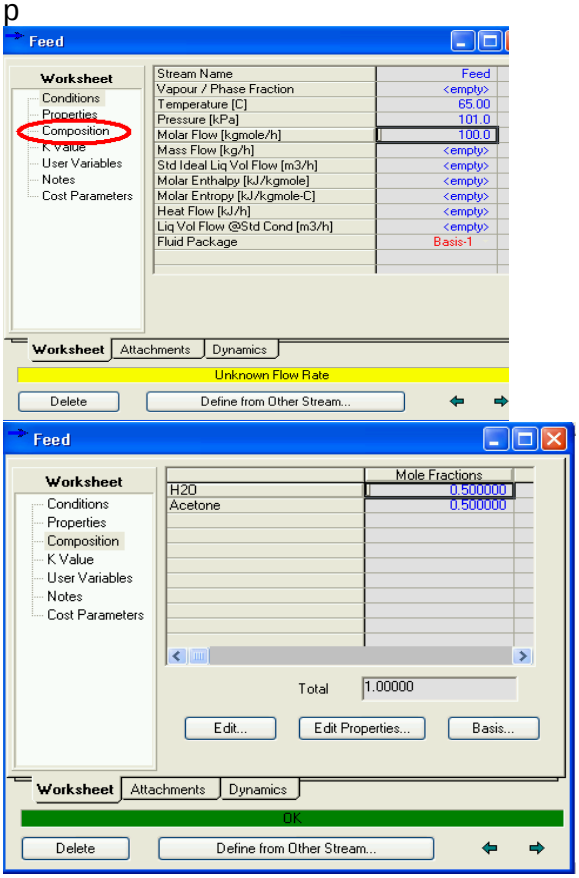
From the Simulation Basis Manager dialog box, click on the *Enter Simulation Environment…* button in the lower right corner. This opens up a new screen called *PFD Case (Main)* and also a menu dialog box with units and streams.
From this menu, click on the *Separator* and drop it into the main window.



Double click on the new separator vessel, V-100, to enter its dialog box
Choose names for the Inlet, Vapour, and Liquid streams that will attach to this unit.



Because they don't already exist, these streams will be automatically generated by the programme, you might even see them pop up on the main PFD screen. Note that we could have created them separately by clicking on the blue arrow in the Case (Main) menu list.
Now close the V-100 dialog box.
Configure the conditions of the Feed stream by double clicking on it. Choose its temperature to be 65°C, its pressure to be 101kPa, and its molar flow rate to be 100kgmol/hr. Click on the *Composition* option from the *Worksheet* list and enter 0.5 for the mole fractions of both water and acetone.
p

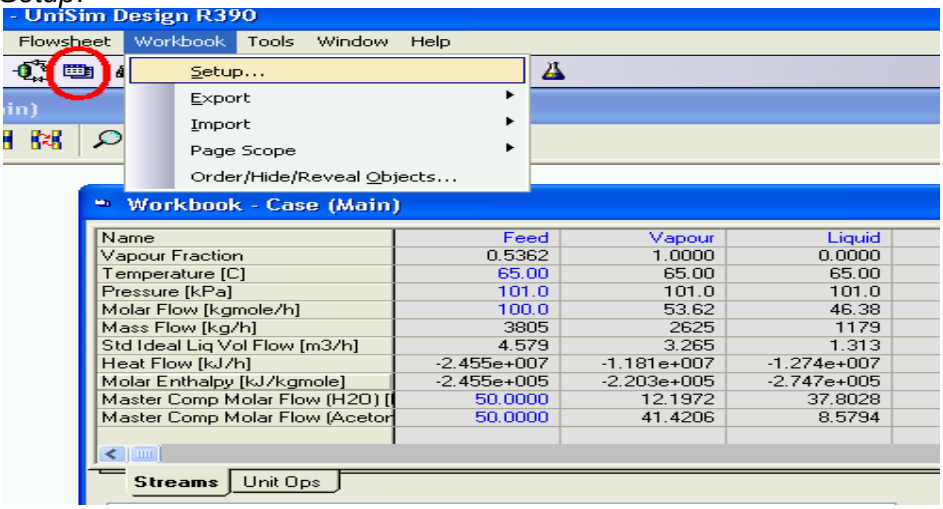


Close the Feed stream dialog box. Notice that the icons for all three streams have now turned from light to dark blue. This is because they have been solved.

4. Process Simulator Output

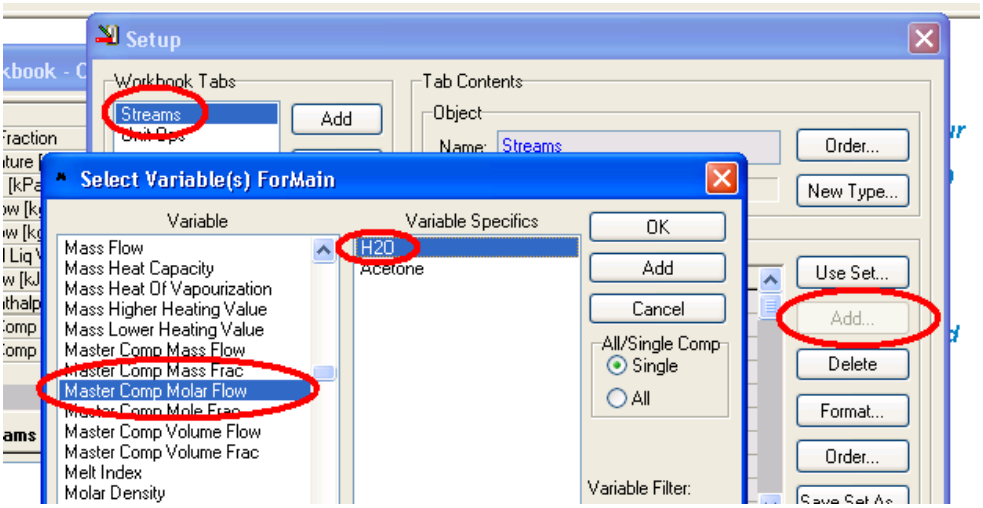
Output from the simulator can consist of tables, graphs, calculations, etc. For today's work we will content ourselves with the flow rates and compositions of the three process streams so that we can verify that material balance has been observed by our simulation.

From the main window, click on the *Workbook* icon on the toolbar (circled in red in the screenshot below). Then click on the *Workbook* text on the upped toolbar, then *Setup*.



Name	Feed	Vapour	Liquid
Vapour Fraction	0.5362	1.0000	0.0000
Temperature [C]	65.00	65.00	65.00
Pressure [kPa]	101.0	101.0	101.0
Molar Flow [kgmole/h]	100.0	53.62	46.38
Mass Flow [kg/h]	3805	2625	1179
Std Ideal Liq Vol Flow [m3/h]	4.579	3.265	1.313
Heat Flow [kJ/h]	-2.455e+007	-1.181e+007	-1.274e+007
Molar Enthalpy [kJ/kgmole]	-2.455e+005	-2.203e+005	-2.747e+005
Master Comp Molar Flow (H2O) [	50.0000	12.1972	37.8028
Master Comp Molar Flow (Acetor	50.0000	41.4206	8.5794

From the *Setup* dialog box, make sure the workbook tab *Stream* is clicked, then from the *variables* area click *Add* then choose *Master Comp Molar Flow* as the variable and then H2O and acetone in turn. Click *OK*, then close the *Setup* dialog box. Note the two new rows in the workbook.



Examine the output from the workbook and verify that material balance is good for total molar flow, and for each component molar flow fraction.

5. Report

Your report will consist of:

- A screenshot of your PFD **(2 marks)**
- A screenshot of the workbook **(2 marks)**
- The material balance calculations **(2x3 marks)**

Submit your report over moodle at:
https://elearning.it-tallaght.ie/mod/turnitintool/view.php?id=288820

Reactions and Case Studies

In our second lab we will further explore the capabilities of process simulators. We will set up a reaction in a reactor and we will then investigate the influence of process parameters such as temperature and pressure on the conversion ratio of the reaction.

The reaction we will use is the production of methanol from carbon dioxide and hydrogen. The reaction is:

$$CO_2 + 3H_2 \Leftrightarrow CH_3OH + H_2O$$

This is a reversible reaction with different reaction kinetics in the forward and reverse directions.

A similar same set of procedures will be followed as in last week's lab. They are:

- Setting up the Basis Environment
  - Creating the component list
  - Choosing the fluid package
  - Adding reactions
- Creating the Process Flowsheet
  - Adding and configuring process streams
  - Adding and configuring process equipment
- Presenting output from the process

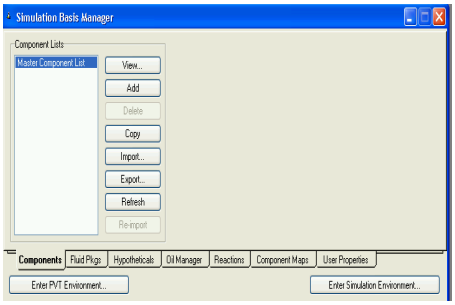
6. Getting Started

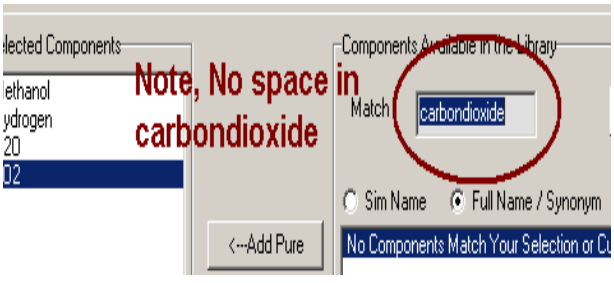
To log on to the PC's in room 116 you should use our regular login and password. The programme we use should have a shortcut on the desktop that looks a little like this:

You can also find it under *Start, All Programs, Honeywell, Unisim Design R440.* Once the programme opens, click on *File, New, Case*

7. Basis Environment

The first thing that opens up is a dialog box for the Simulation Basis Manager





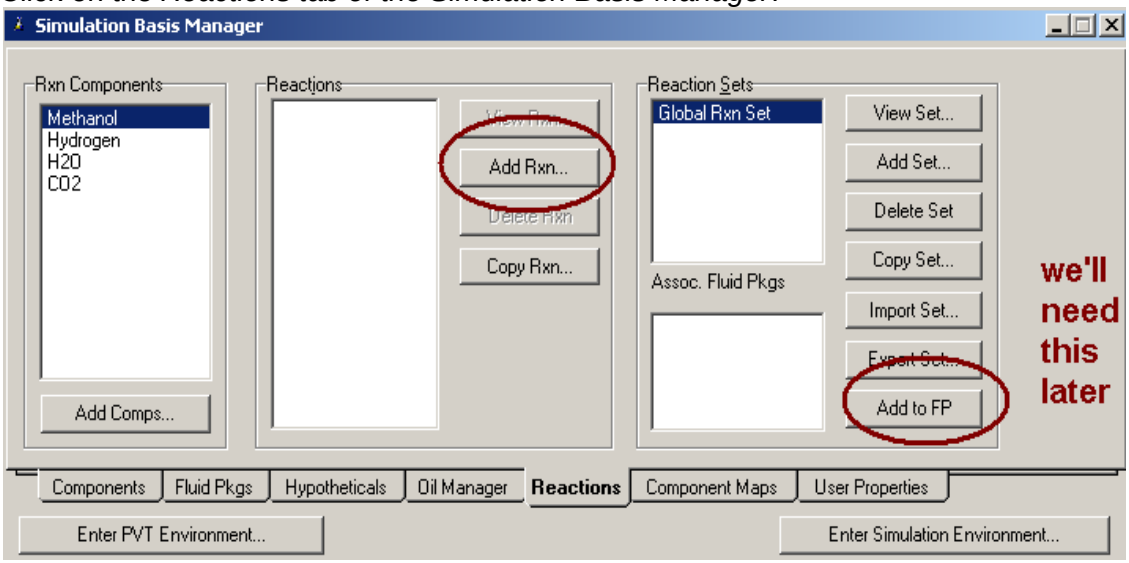
Click *Add* and then add methanol, water, hydrogen, and carbon dioxide to the components list. Using the *Match* search box helps a lot here.

Close the *Component List View.*
Click on the Fluid Package Tab and then *Add* and choose the SRK package.

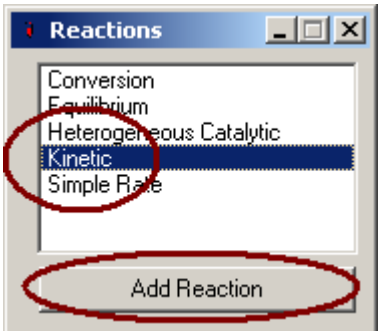
Check on the Binary Coefficients tab that all the interaction parameters have been successfully calculated (they should be in red type).

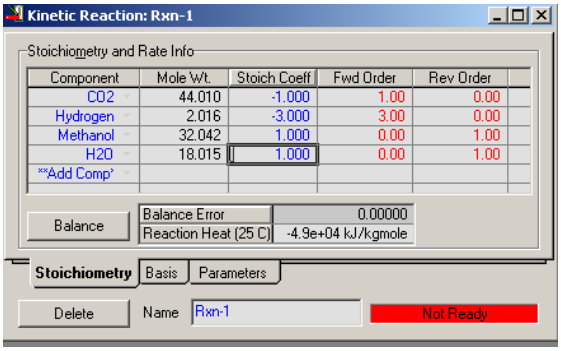
8. *Setting up the Reaction:*

Click on the *Reactions tab of the Simulation Basis Manager*.

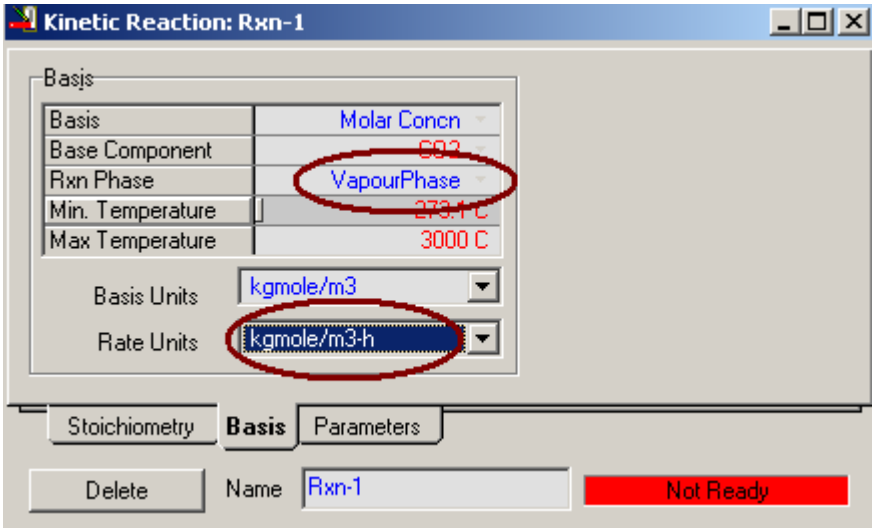


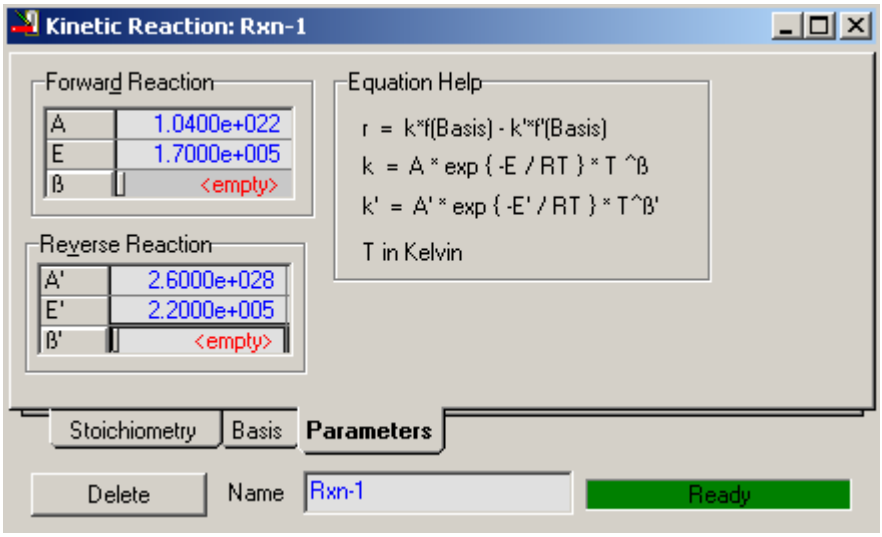
Click on *Add Rxn*. Choose a Kinetic Reaction and then press the *Add Reaction* button





Fill out the *Stoichiometry* tab as shown above. Note that the stoichiometry coefficients mirror the reaction equation shown above. Note that minus values (e.g. -3 for H_2) indicate that the agent is consumed in the forward order of the reaction. Also note that the balance error should be 0.000. Depending on the version of UniSim, you may have to input the Fwd Order and Rev Order columns above by hand, in which case they will be in blue rather than red. Fill out the *Basis* and *Parameters* tabs as shown below.





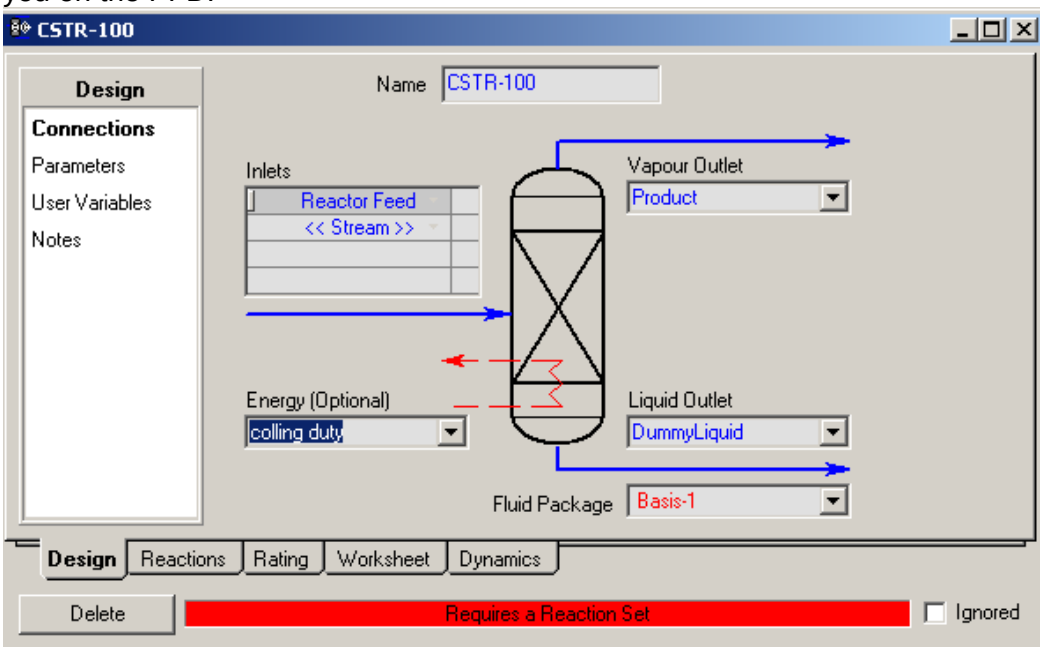
Once this is done you can close the Kinetic Reactions window. Then you must press *Add to FP* on the *Reactions tab of the Simulation Basis Manager* (this is shown in an image above).

9. Creating the Process Flowsheet

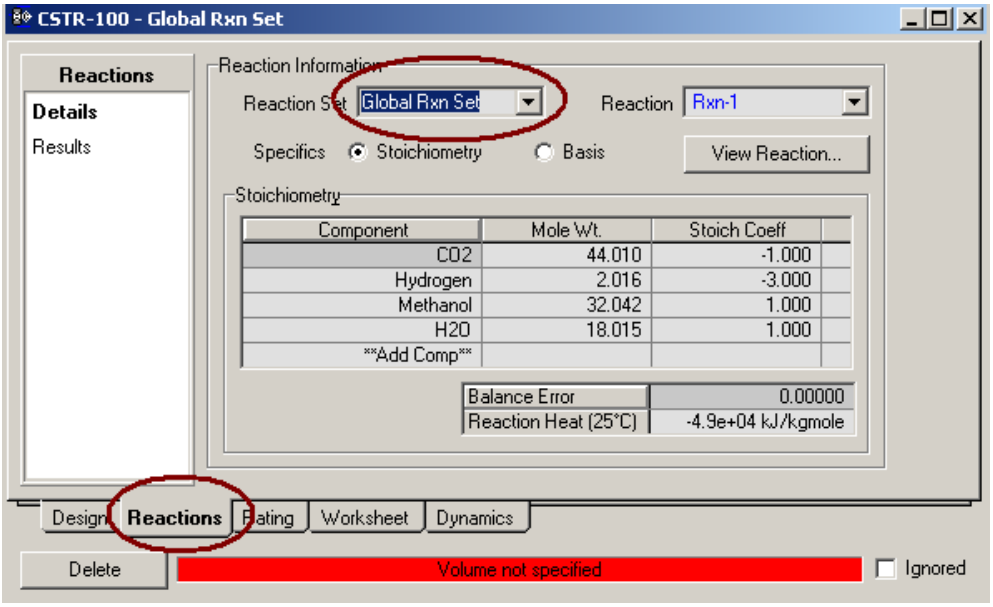
From the Simulation Basis Manager dialog box, click on the *Enter Simulation Environment…* button in the lower right corner. This opens up a new screen called *PFD Case (Main)* and also a menu dialog box with units and streams.

From this menu, click on the *CSTR (* ) and drop it into the main window.

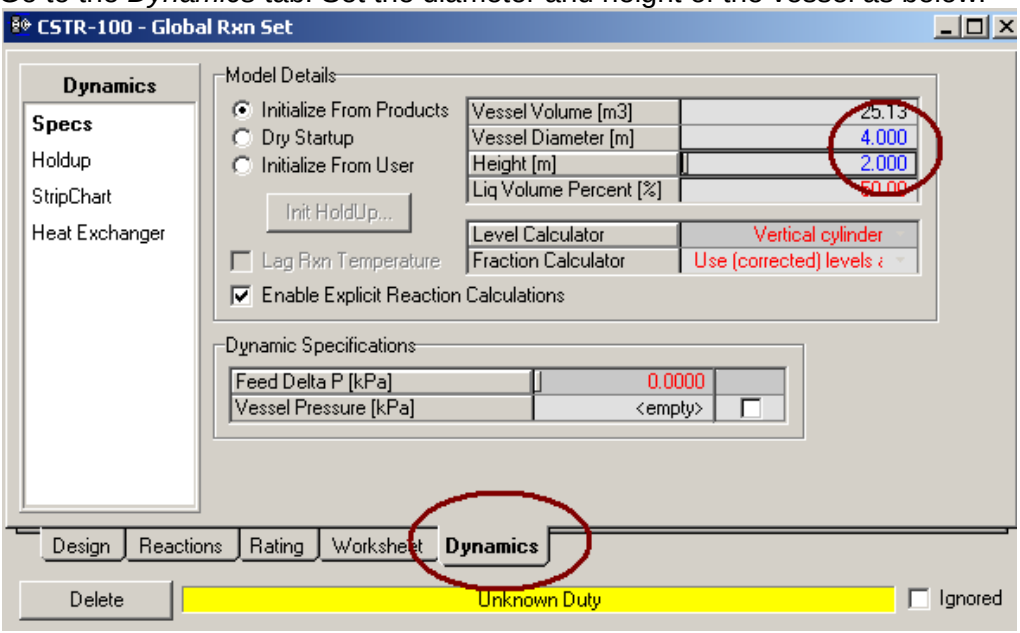
Double click on the new CSTR, *CSTR*-100, to enter its dialog box. Configure it as shown below. Note that material and energy streams will be made automatically for you on the PFD.



On the *Reactions* tab, configure as shown below:

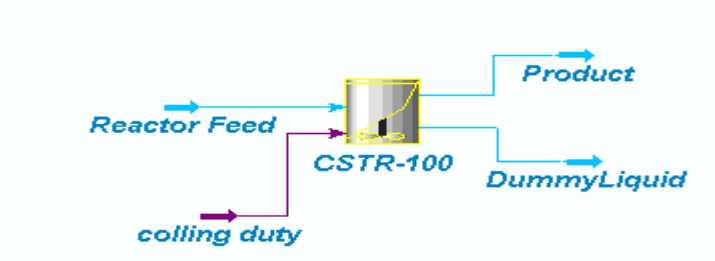


Go to the *Dynamics* tab. Set the diameter and height of the vessel as below.

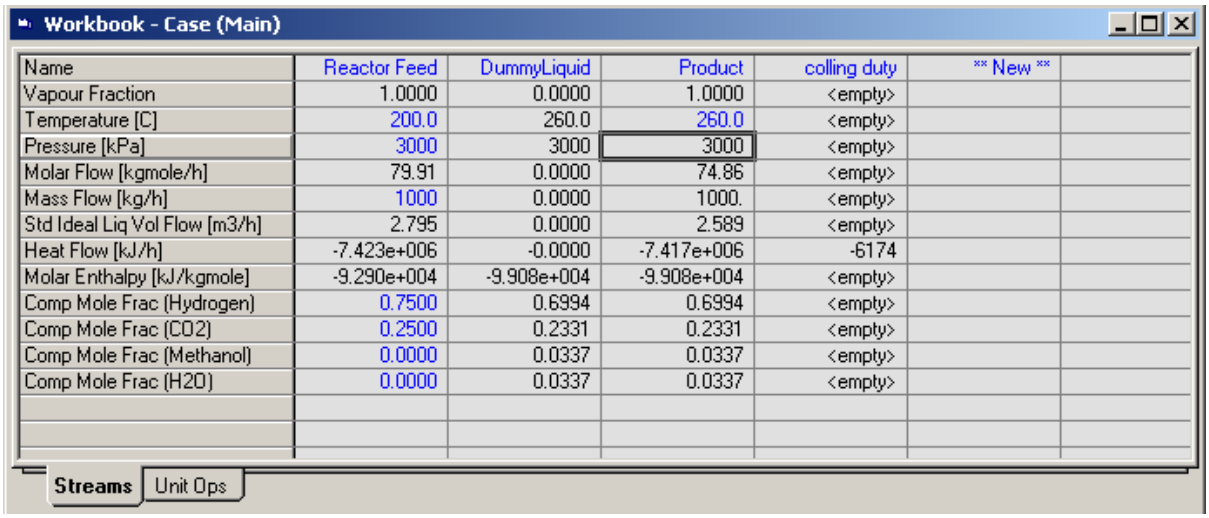


You can now close the *CSTR-100 – Global Rxn Set* window.

The PFD should now look something like this:

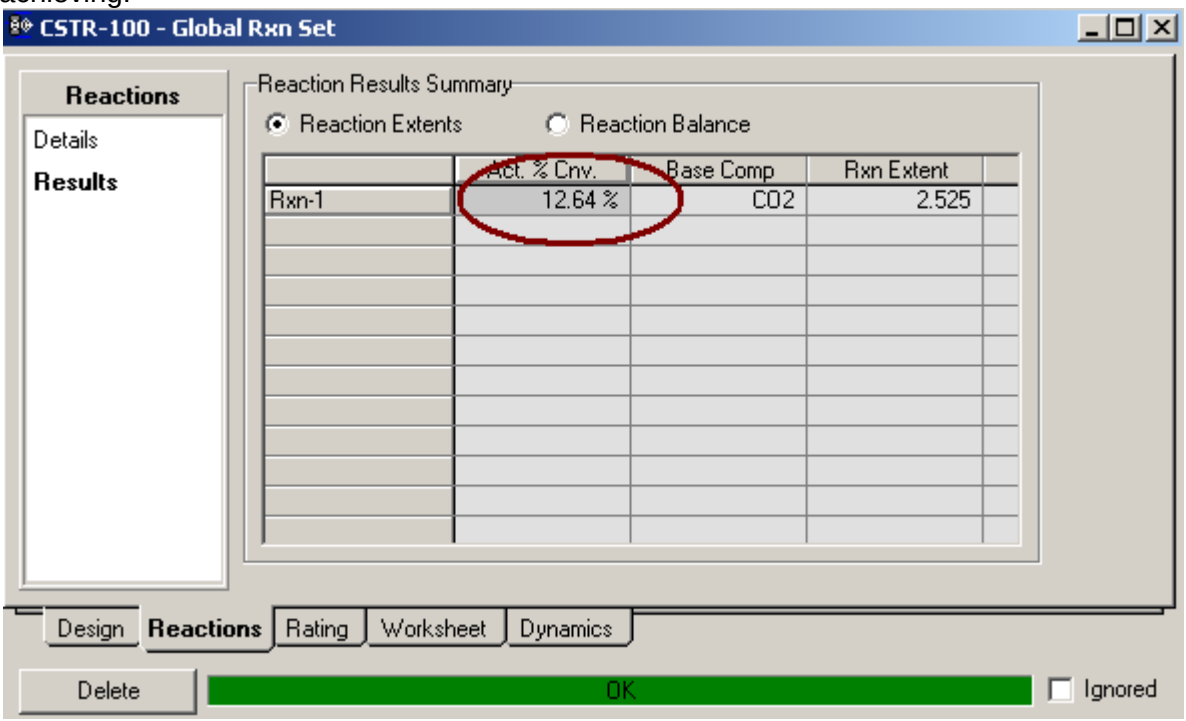


Open the *Workbook* ( ) from the toolbar. Use *Set Up* like we did last week to add the *Comp Mole Frac* for the four components. Configure the workbook as shown below, remember you just add the parameters in blue, those in black are calculated.



Name	Reactor Feed	DummyLiquid	Product	colling duty	** New **
Vapour Fraction	1.0000	0.0000	1.0000	<empty>	
Temperature [C]	200.0	260.0	260.0	<empty>	
Pressure [kPa]	3000	3000	3000	<empty>	
Molar Flow [kgmole/h]	79.91	0.0000	74.86	<empty>	
Mass Flow [kg/h]	1000	0.0000	1000.	<empty>	
Std Ideal Liq Vol Flow [m3/h]	2.795	0.0000	2.589	<empty>	
Heat Flow [kJ/h]	-7.423e+006	-0.0000	-7.417e+006	-6174	
Molar Enthalpy [kJ/kgmole]	-9.290e+004	-9.908e+004	-9.908e+004	<empty>	
Comp Mole Frac (Hydrogen)	0.7500	0.6994	0.6994	<empty>	
Comp Mole Frac (CO2)	0.2500	0.2331	0.2331	<empty>	
Comp Mole Frac (Methanol)	0.0000	0.0337	0.0337	<empty>	
Comp Mole Frac (H2O)	0.0000	0.0337	0.0337	<empty>	

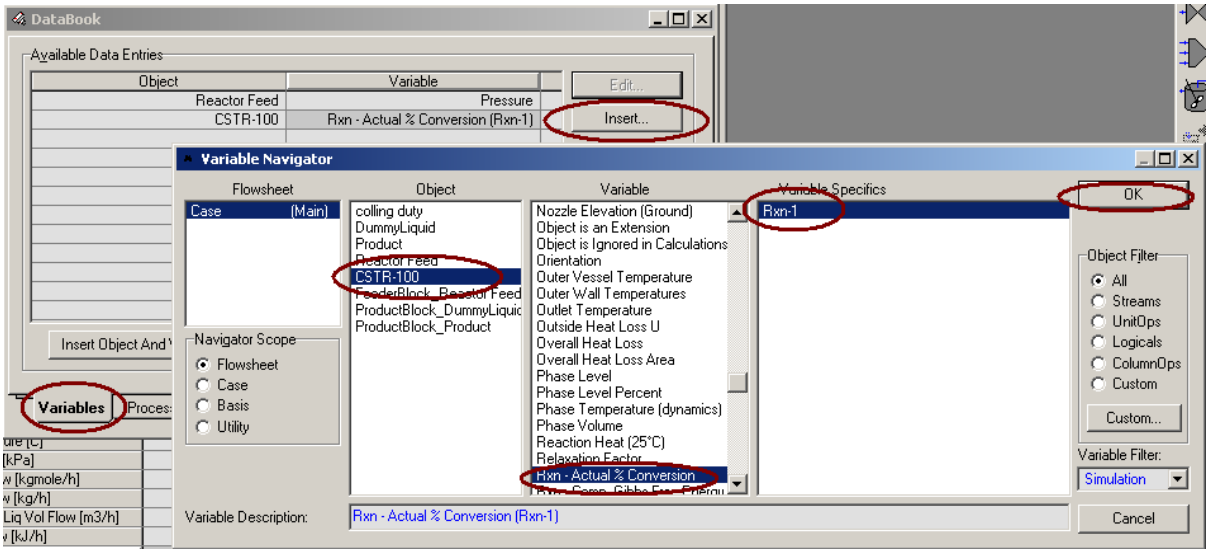
Now are process is solved, note that there is a certain amount of methanol in the product stream so the reaction is working. If you double click on the CSTR again and look at its *Reactions, Results* tab you'll see the amount of conversion we are achieving.



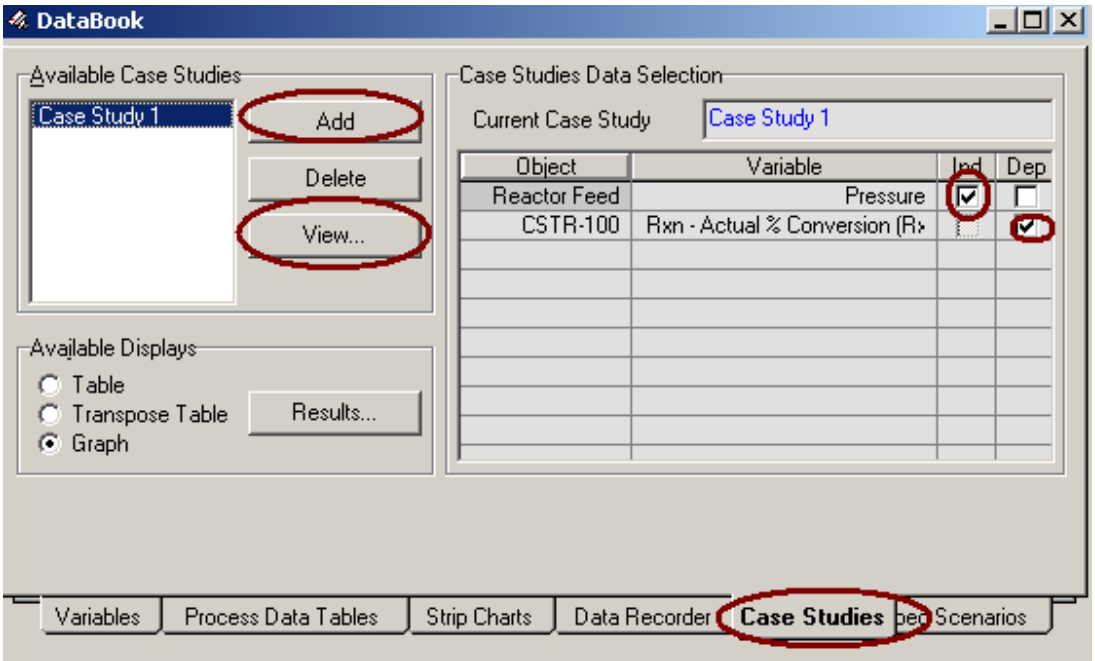
5. Case Studies

UniSim lets examine how the process will change as we alter some parameters of the system. As a first instance we'll see how the conversion rate in the reactor (the *Act % Cnv*.) above changes as the reactor volume changes. This kind of examination is called a *Case Study*.

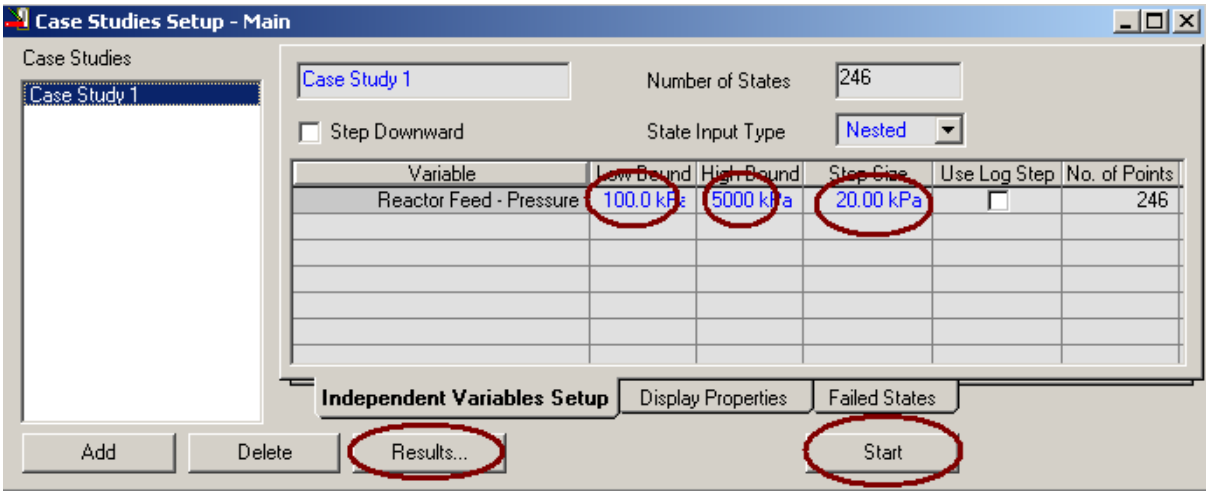
1. Click on *Tools, Databook*
2. Insert the variables *Reactor Feed Pressure and CSTR Actual % Conversion.*



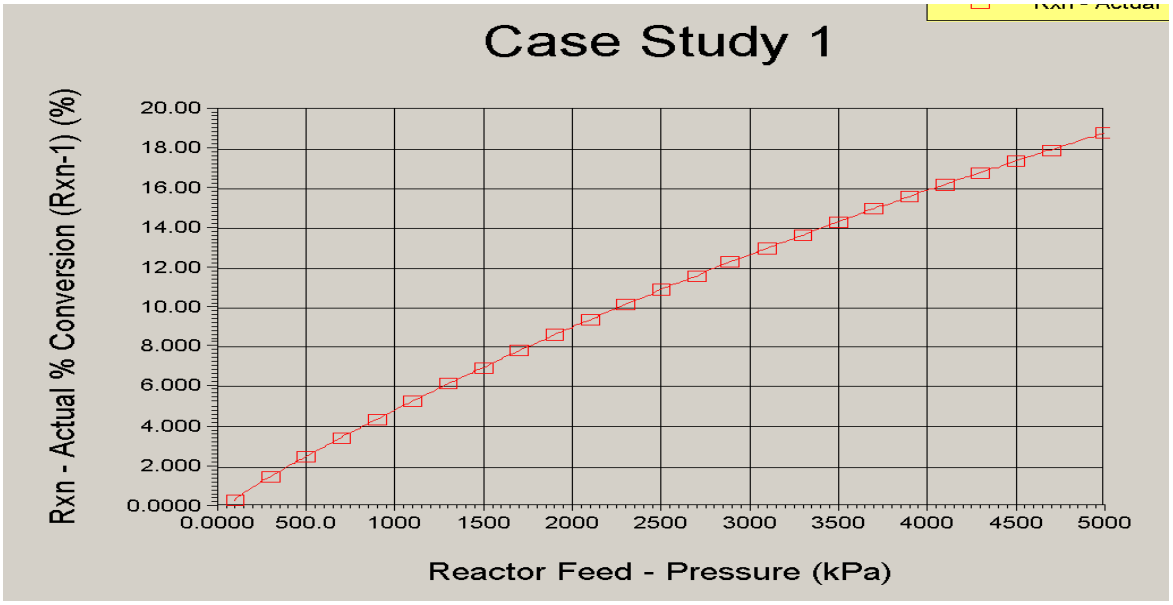
On the Case Studies tab Add a new case study and choose the Reactor Feed Pressure as the independent variable and the CSTR Rxn – Actual % Cnv as the dependent variables as shown below



Click on View to see the Case Study and fill it out as below



Now click *Start* and when it finishes running click *Results.* You should see a graph akin to the one below. Note how these results are consistent with Le Chatelier's Principle.



You are also asked to examine two other parameters that influence Actual % Conversion and produce Case Studies for them.

6. Report

Your report will consist of:

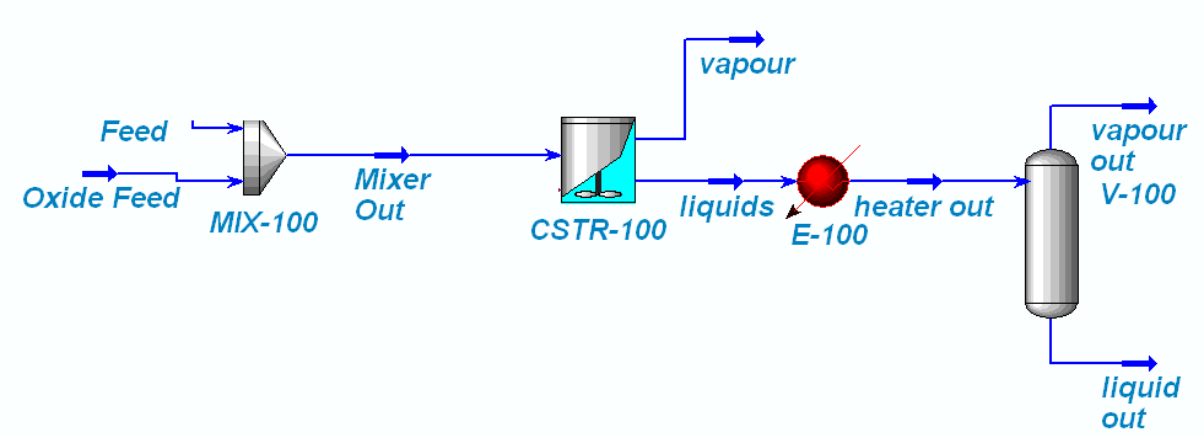
- A screenshot of your PFD **(1 marks)**
- A screenshot of the workbook **(1 marks)**
- Screenshots of your Case Studies **(2x3 marks)**
- Explanation of the principle behind your case studies (e.g. for the first one it is Le Chatelier's Principle **(2 marks)**

Reaction and Separation

This lab won't present too much new material, it will mostly serve to reinforce the learning outcomes from the first two labs and also give less hand-holding. To remind you, the skills we've developed so far are:

- Constructing the component database
- Configuring a reaction
- Setting up a PFD
- Inputting the required parameters into the workbook
- Displaying the results of the simulation

In today's work we will have two feed streams, water and propylene oxide. We will mix them together and feed to a reactor. Here the reaction: $H_2O + C_3H_6O \rightarrow C_3H_8O_2$ takes place, producing propylene glycol. We'll be setting up a PFD something like this:

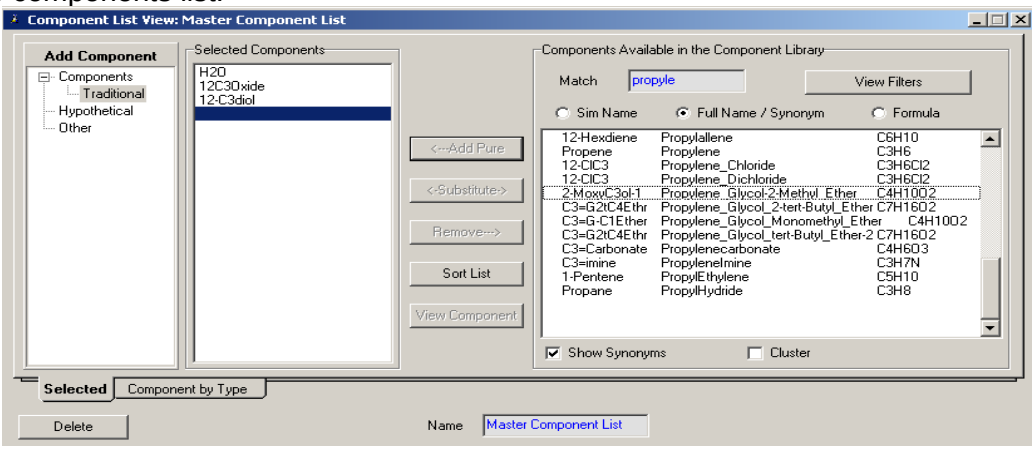


10. Getting Started

As before, to log on to the PC's and launch a new case of UniSim Design R400.

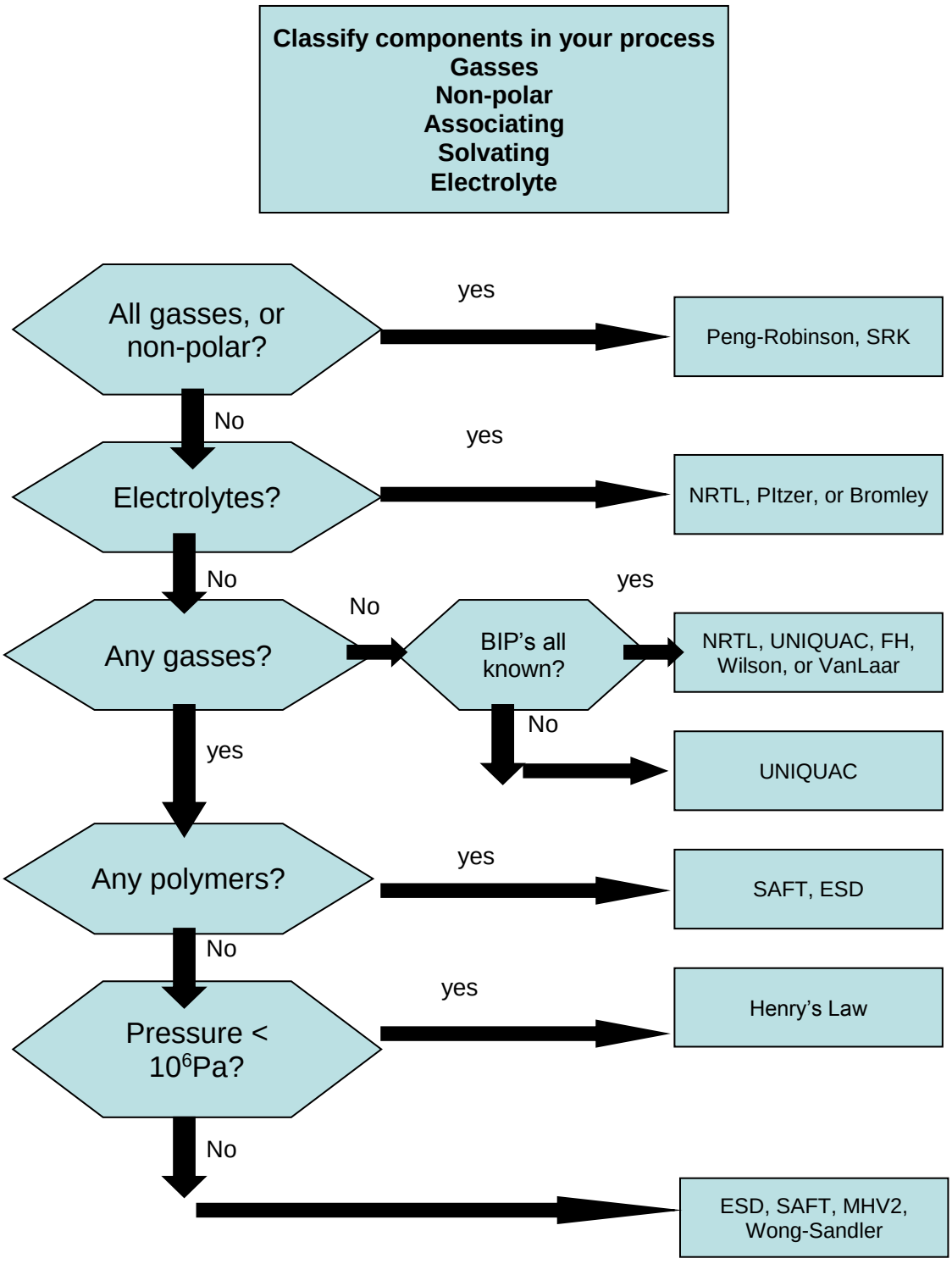
11. Component Database

In the Simulation Basis Manager add water, propylene oxide and propylene glycol to the components list.

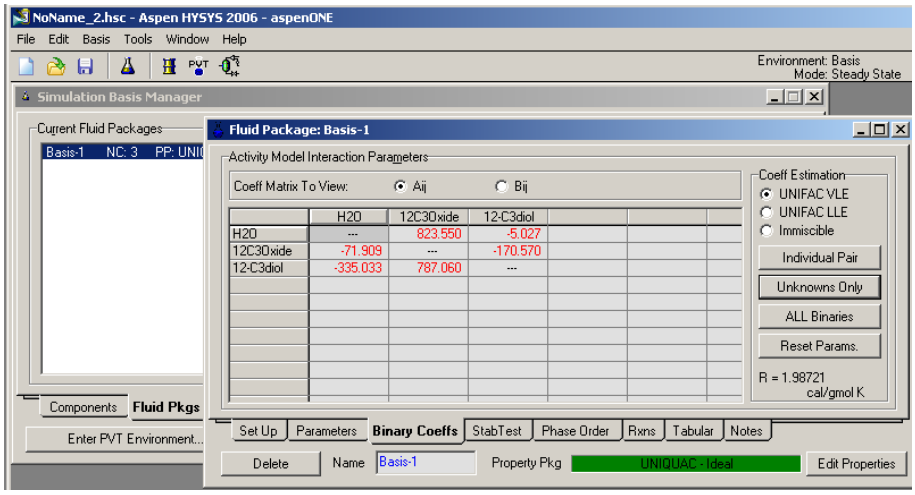


Close the *Component List View.*

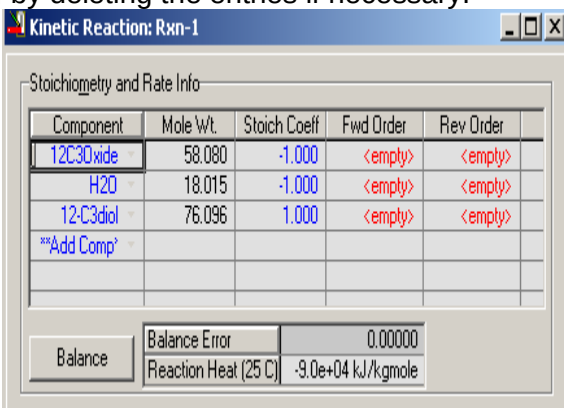
Click on the Fluid Package Tab and then *Add* and choose the relevant fluid package. The flowchart below should help you choose the correct one, bearing in mind that we don't have gasses, electrolytes, and that the Binary Interaction Parameters are not all known.



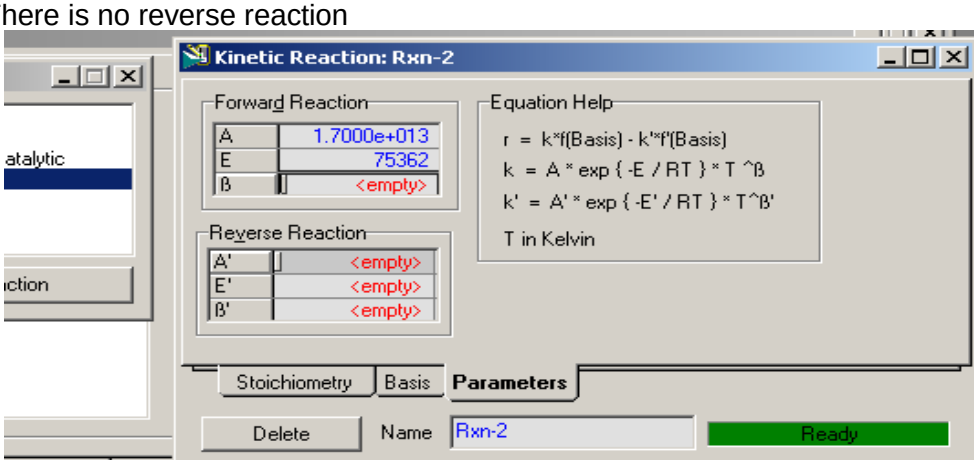
The connection between temperature and pressure will depend not only on what chemicals are present but also on how they mix together. For this we need the binary reaction coefficients.
Click Binary Coeffs. To complete the table click on Unknowns Only, making sure the radio button UNIFAC VLE is selected



Next we define the reaction between our components.
Return to the Simulation Basis Manager and click on the Reactions tab.
Click the ADD RXN button, the Reactions pop-up will appear. Choose Kinetic by double clicking and the Kinetic Reactions pop-up will appear.
Choose the three components using the drop down lists from the Components column of the table. Input their stoichoimetries as -1 for water and propOxide (-1 because they are consumed in the reaction) and +1 for propGlycol. Note the balance error should be 0 (reaction is materially balanced) and the reaction heat should be negative, indicating an exothermic reaction. Make sure the Fwd Order and Rev Order boxes are empty, by deleting the entries if necessary.



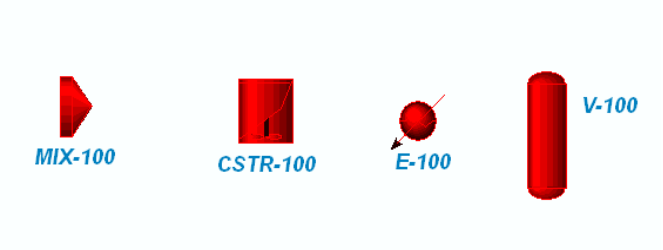
Next, select the Basis tab of the Kinetic Reactions pop-up and change the Base Component from H_2O to PropOxide and also change the Rxn Phase to Combined Liquid. Change the Basis Units to lbmol/ft3 and the rate units to lbmol/ft3-hr.
Then click on the Parameters tab to input the Arrhenius parameters for the reaction. Type in 1.7e13 for the forward A parameter and 75362 for forward parameter E. There is no reverse reaction



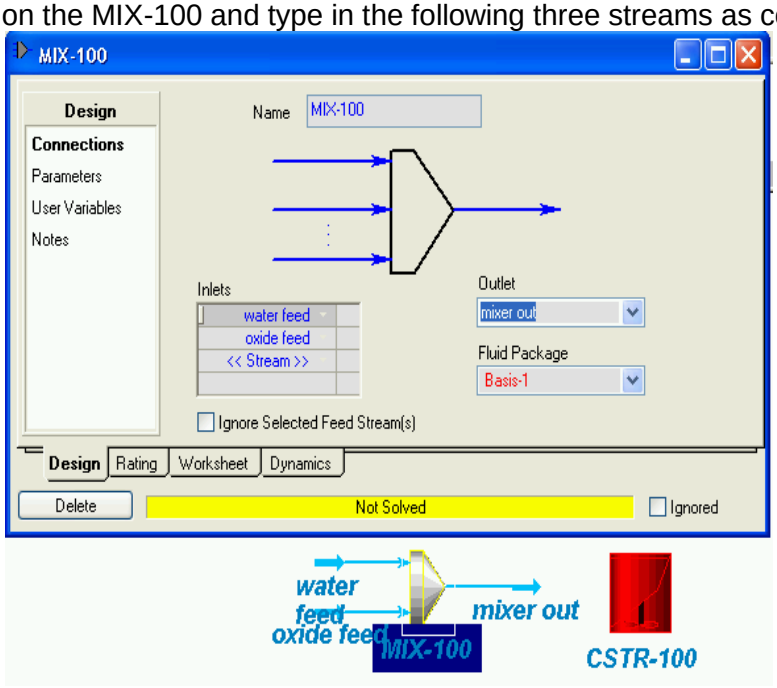
The status indicator at the bottom of the pop-up changes from Not Ready to Ready.
Close the two reactions windows
On the Simulation Basis Manager, click Add to FP then Add Set to Fluid Package

12. Creating the Process Flowsheet

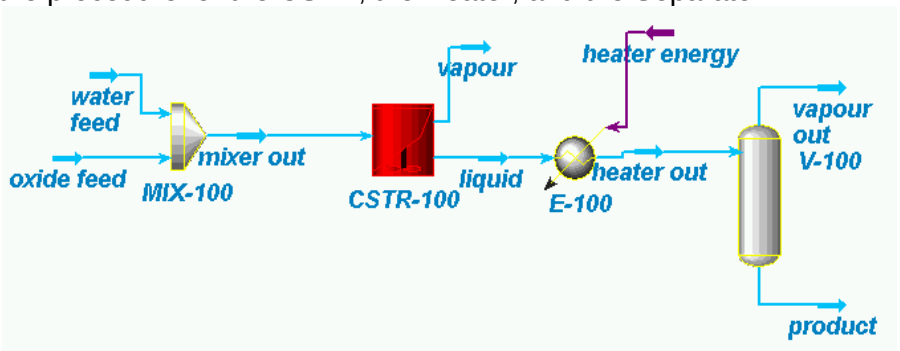
From the Simulation Basis Manager dialog box, click on the *Enter Simulation Environment…* button in the lower right corner. This opens up a new screen called *PFD Case (Main)* and also a menu dialog box with units and streams.
From this menu, click on a *Mixer, CSTR, Heater,* and a *Separator*.



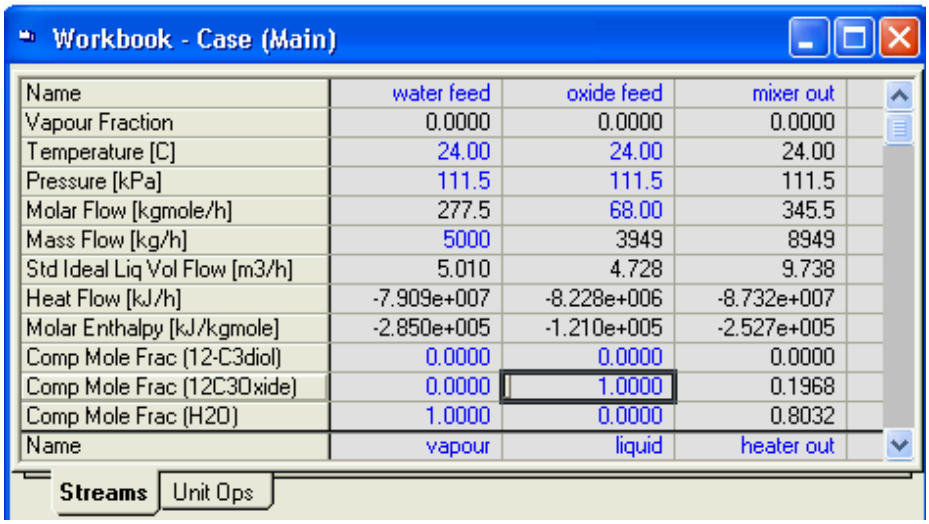
Double click on the MIX-100 and type in the following three streams as connections.



Note that these streams pop into the PFD as they are created on the MIXER dialogue box.
Repeat the procedure for the CSTR, the Heater, and the Separator.



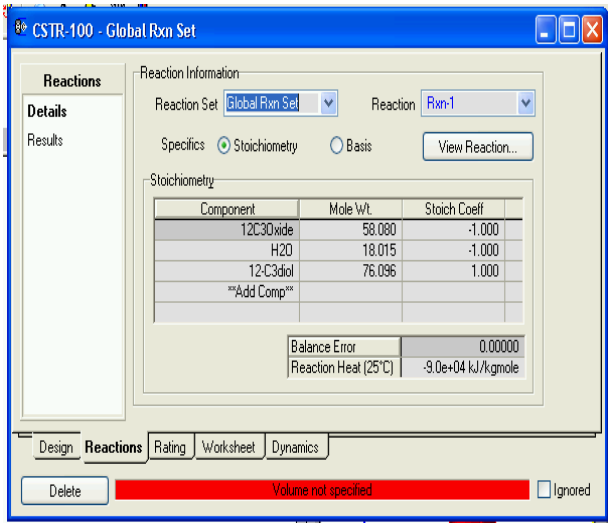
We need to specify the parameters of the two feed streams, their temperatures, pressures, flow rates, and compositions.

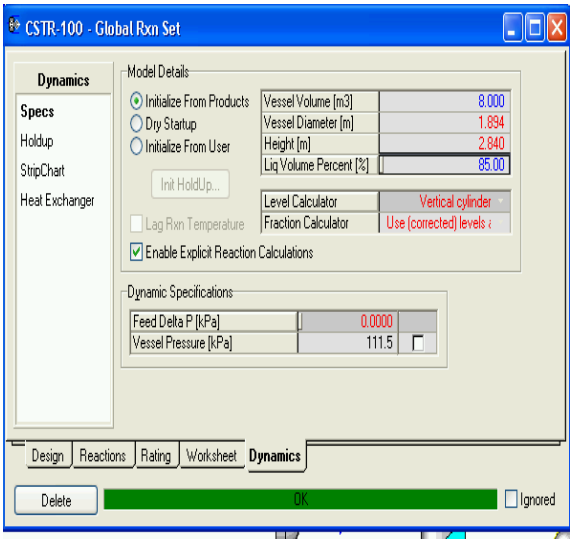


Name	water feed	oxide feed	mixer out
Vapour Fraction	0.0000	0.0000	0.0000
Temperature [C]	24.00	24.00	24.00
Pressure [kPa]	111.5	111.5	111.5
Molar Flow [kgmole/h]	277.5	68.00	345.5
Mass Flow [kg/h]	5000	3949	8949
Std Ideal Liq Vol Flow [m3/h]	5.010	4.728	9.738
Heat Flow [kJ/h]	-7.909e+007	-8.228e+006	-8.732e+007
Molar Enthalpy [kJ/kgmole]	-2.850e+005	-1.210e+005	-2.527e+005
Comp Mole Frac (12-C3diol)	0.0000	0.0000	0.0000
Comp Mole Frac (12C3Oxide)	0.0000	1.0000	0.1968
Comp Mole Frac (H2O)	1.0000	0.0000	0.8032
Name	vapour	liquid	heater out

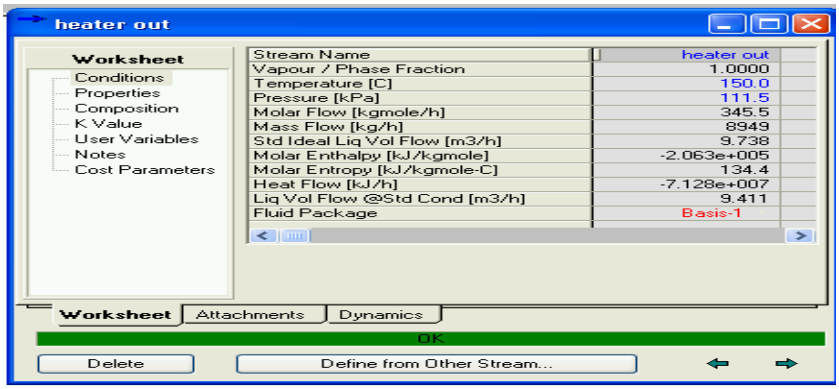
The parameters in blue type are entered by the user, those in black are calculated. The Comp Mole Fractions are added to the work book using the workbook, setup options from the toolbar as we have done before.

Next we need to configure the reactor. It needs to be told the reaction that we are using in it. Double click on it, go to the reactions tab, and add the reaction we created earlier. Also, on the dynamics tab specify the reactor volume to be 8m^3 and the liquid fill to be 85%. The reactor needs this to be able to calculate the residence time in the reactor and thus the reaction extent.





Lastly we need to configure the heater. We'll do this by specifying the heater out stream by stipulating its temperature and pressure. We'll make it isobaric but let it warm the output stream to 150^{o}C.



At this point the entire PFD should be solved.

13. Process Simulator Output

Like last week, we will verify the material balance of the simulation. This is complicated because of the reaction.

From the main window, click on the *Workbook* icon on the toolbar.

Workbook - Case (Main)

Name	water feed	oxide feed	mixer out	vapour	liquid	heater out	vapour out	product	heater energy
Vapour Fraction	0.0000	0.0000	0.0000	1.0000	0.0000	0.7419	1.0000	0.0000	<empty>
Temperature [C]	24.00	24.00	24.00	113.5	113.5	150.0	150.0	150.0	<empty>
Pressure [kPa]	111.5	111.5	111.5	111.5	111.5	111.5	111.5	111.5	<empty>
Molar Flow [kgmole/h]	277.5	68.00	345.5	84.13	193.4	193.4	143.5	49.93	<empty>
Mass Flow [kg/h]	5000	3949	8949	1592	7357	7357	4175	3182	<empty>
Std Ideal Liq Vol Flow [m3/h]	5.010	4.728	9.738	1.591	7.166	7.166	4.099	3.067	<empty>
Heat Flow [kJ/h]	-7.909e+007	-8.228e+006	-8.732e+007	-2.026e+007	-6.706e+007	-6.002e+007	-3.869e+007	-2.132e+007	7.042e+006
Molar Enthalpy [kJ/kgmole]	-2.850e+005	-1.210e+005	-2.527e+005	-2.408e+005	-3.467e+005	-3.103e+005	-2.697e+005	-4.271e+005	<empty>
Master Comp Mole Frac [12-C3di	0.0000	0.0000	0.0000	0.0157	0.3448	0.3448	0.1908	0.7873	<empty>
Master Comp Mole Frac [12C3Ox	0.0000	1.0000	0.1968	0.0000	0.0000	0.0000	0.0000	0.0000	<empty>
Master Comp Mole Frac [H2O]	1.0000	0.0000	0.8032	0.9843	0.6552	0.6552	0.8092	0.2127	<empty>

Examine the output from the workbook and verify that material balance is good for total molar flow, and for each component molar flow fraction. Also, do a material balance for the mixer, the reactor, and the separator. Calculate the conversion and the yield for the reactor.

14. Report

Your report will consist of:

- A screenshot of your PFD **(1 marks)**
- A screenshot of the workbook **(1 marks)**
- The material balance calculations **(0.75x8 marks)**
  There are eight of these:
  i) Total molar balance around the mixer
  ii) Component balance on water around the mixer
  iii) Component balance on oxide around the mixer
  iv) Total mass balance around the CSTR
  v) Component balance on glycol around the separator
  vi) Component balance on water around the separator
  vii) Total molar balance around the separator
  viii) Total mass balance around the entire process
- Conversion and yield calculations **(2 marks)**
  Calculate the conversion rate on water in the reactor. Because there are no competing reactions, this will also equal the yield.

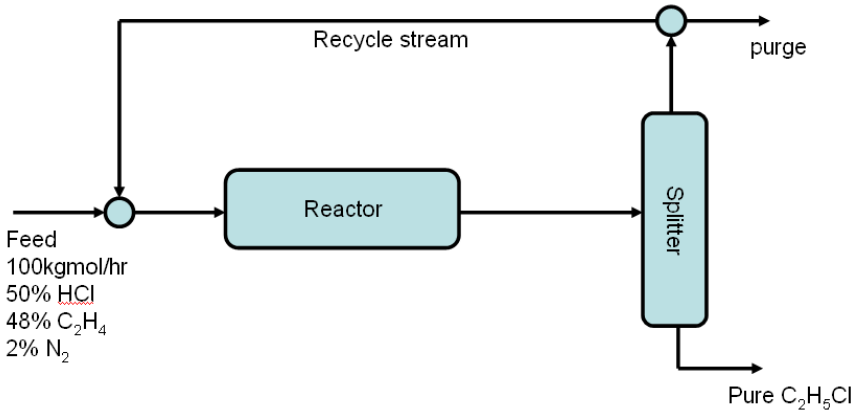
Production of Ethyl Chloride

Introduction:

One of the routes to produce ethyl chloride is by the gas phase reaction of HCl with ethylene:

$$C_2H_4 + HCl \rightarrow C_2H_5Cl$$

The PFD for the process is shown below:



Since the reaction only achieves 90% conversion the unreacted components are separated from the ethyl chloride and recycled.

The process is operated at 25°C, atmospheric pressure (100kPa) and pressure drops are ignored.

To prevent the accumulation of interts (N_2) in the system 10kgmol/hr is purged from the system. We want to investigate the effect of the flow rate of the purge stream on the recycle rate and the feed to the reactor.

Initial Setup:

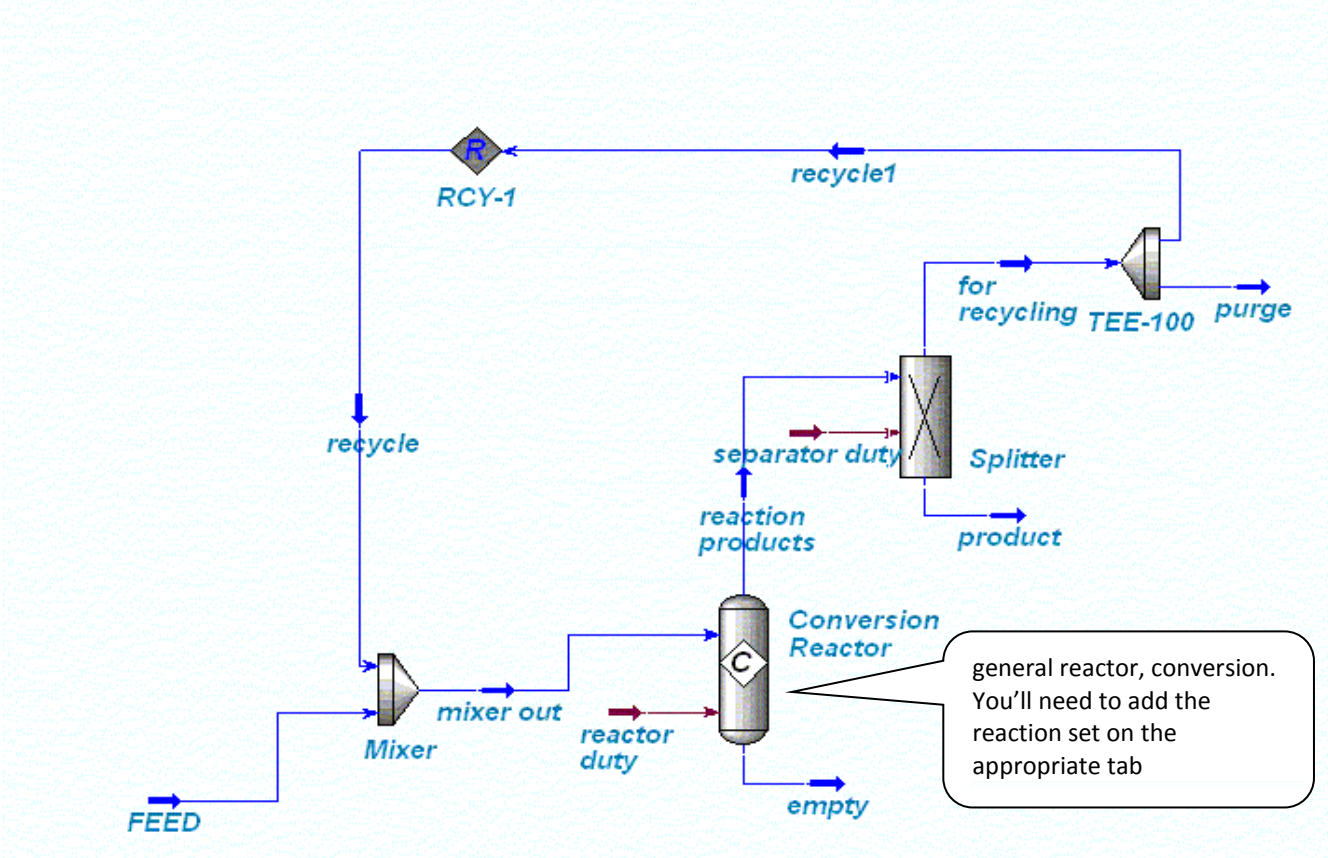
1. Start a new case in UniSim
2. Select ethylene, HCl, ethyl chloride, and nitrogen as components.
3. Choose the correct fluid package bearing in mind that everything here is gas phase.
4. Check the binary coefficients, (should be mostly 0).

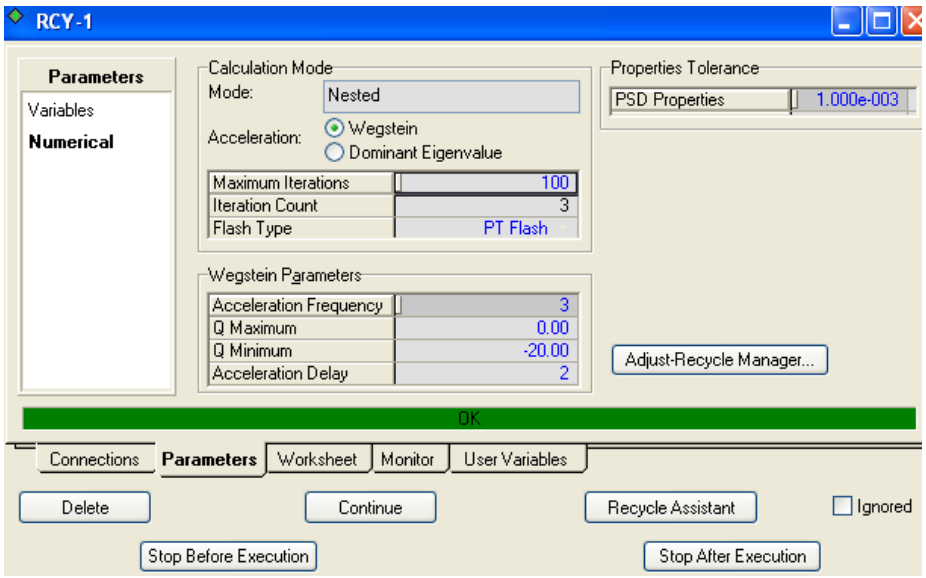
Setting up the Reaction:

In the simulation basis manager, click the reactions tab, click Add Reaction, then choose conversion reaction. Enter the stoichiometry for the reaction (remember, -1 for consumed in reaction, +1 for produced). On the Basis tab enter Ethylene for the base component, Overall for the Rxn Phase, and 90 for C_0. Leave C_1 and C_2 blank, we are not considering any temperature dependence for this reaction. Don't forget to add the reaction to the fluid package.

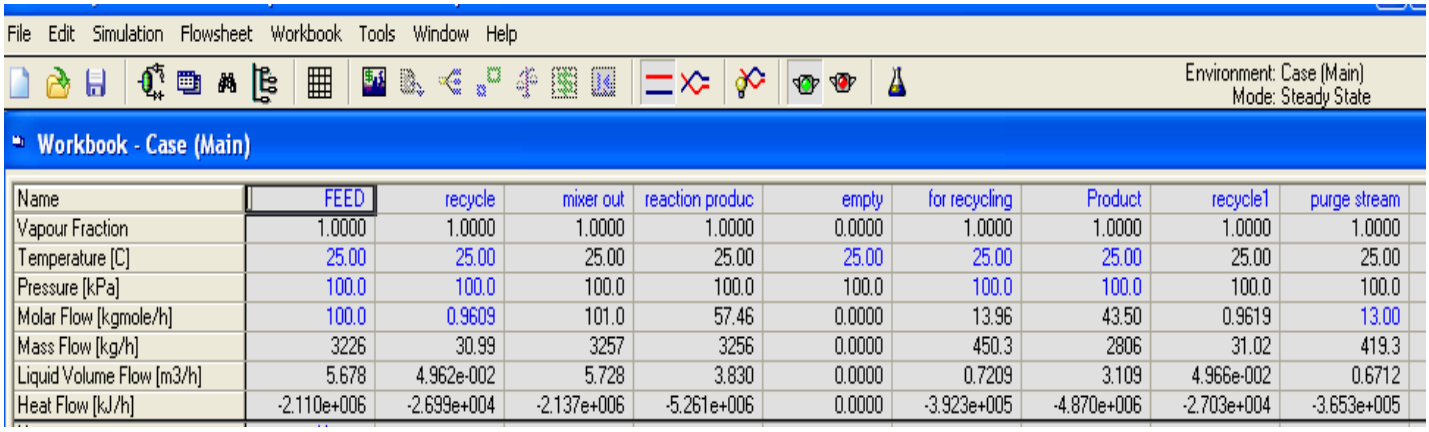
Setting up the PFD:

Set up the PFD as shown below. For the Splitter, click on *Design* then *Splits* and make sure all the Ethyl Chloride goes to *product* and everything else goes to *For Recycling*. **Make sure the very last thing you do to complete the PFD is to connect the *Recycle* stream into the Mixer.** Set the flow rate in the purge stream to be 13kgmol/hr.





1. As a check, the worksheet should look as follows:

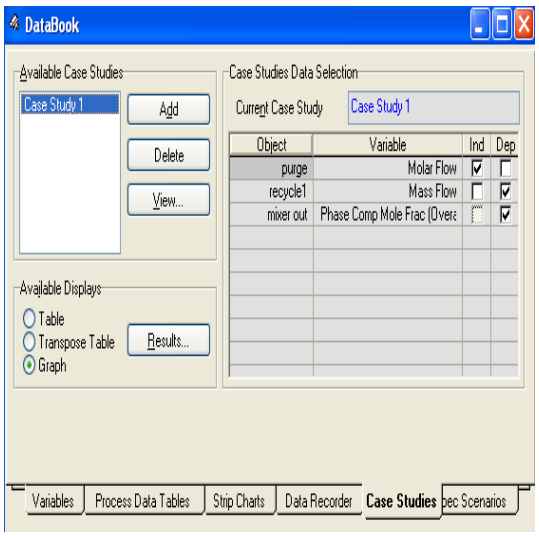


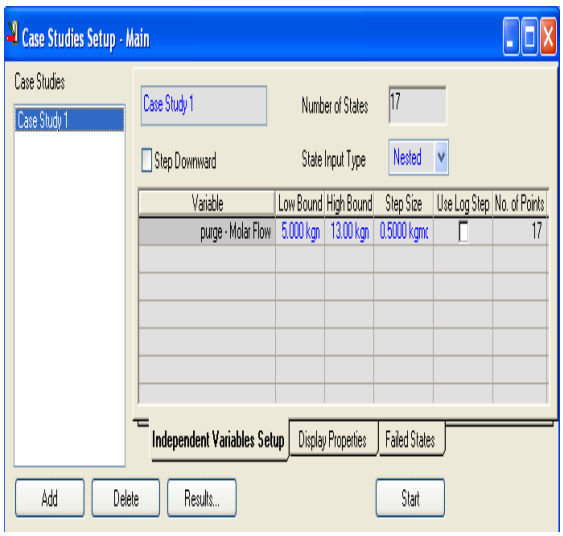
Name	FEED	recycle	mixer out	reaction produc	empty	for recycling	Product	recycle1	purge stream
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	1.0000	1.0000
Temperature [C]	25.00	25.00	25.00	25.00	25.00	25.00	25.00	25.00	25.00
Pressure [kPa]	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Molar Flow [kgmole/h]	100.0	0.9609	101.0	57.46	0.0000	13.96	43.50	0.9619	13.00
Mass Flow [kg/h]	3226	30.99	3257	3256	0.0000	450.3	2806	31.02	419.3
Liquid Volume Flow [m3/h]	5.678	4.962e-002	5.728	3.830	0.0000	0.7209	3.109	4.966e-002	0.6712
Heat Flow [kJ/h]	-2.110e+006	-2.699e+004	-2.137e+006	-5.261e+006	0.0000	-3.923e+005	-4.870e+006	-2.703e+004	-3.653e+005

Case Studies, Effect of Flow Rate of Purge on Process:

|UniSim has a handy way of examining dependencies. We're going to look at the effect of the flow rate of the purge stream.

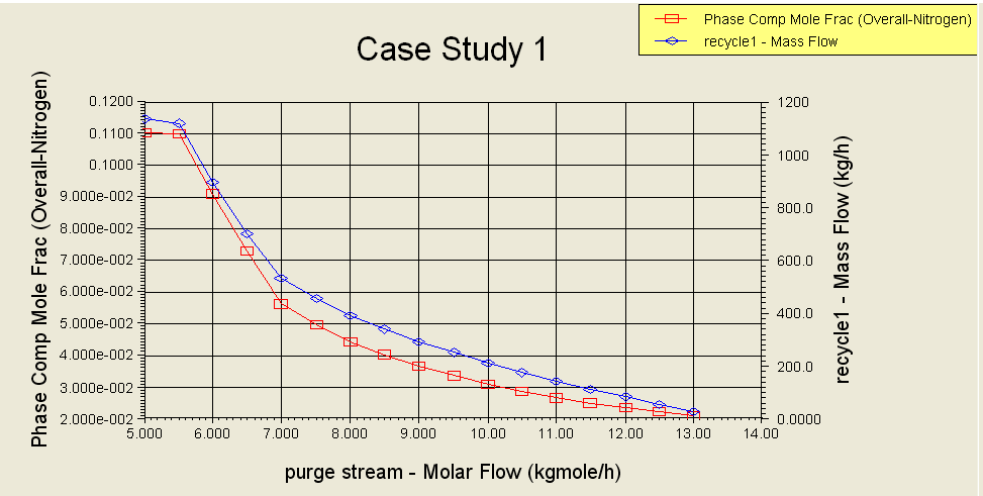
1. Click on Tools, Databook.
2. In the Variables tab choose the following variables:
    a. purge – Molar Flow
    b. recycle1 – mass flow
    c. mixer out – Phase Component Mole Fraction (Overall-Nitrogen)
3. On the Case Studies tab Add a new case study and choose the purge stream as the independent variable and the mixer out and recycle1 as the dependent variables as shown below





4. Click View to enter the Case Studies Set-Up screen and fill it out as above:

5. Now click Start and the Results to get the required graph, something like below. Interpret your results in terms of the efficiency of using the input ingredients versus the problem of build-up of inerts in the process.



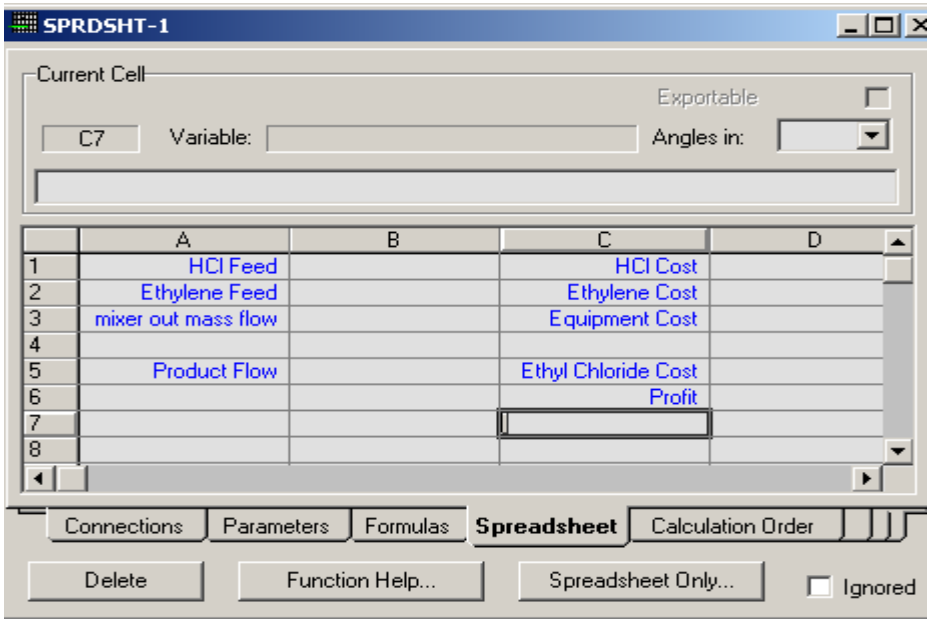
Profit Calculations

UniSim also lets us calculate the financial gain from this process. It contains an internal spreadsheet into which functions can be entered, featuring variables from the Workbook. In this way we can figure out the profit made from a given size of purge stream.

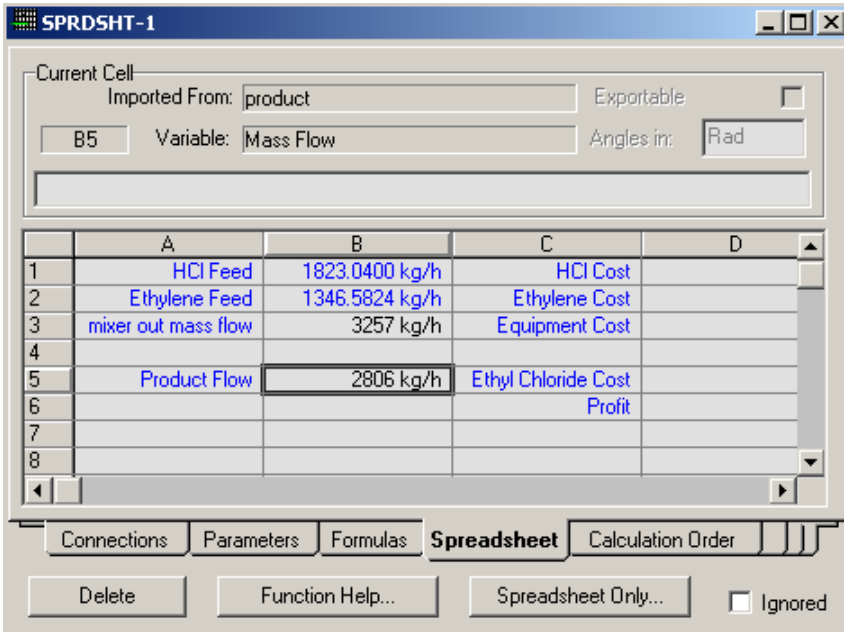
The purge stream wastes some of our reactants, so we want it to be small. However if the purge stream is too small the reactor will become unfeasibly large to accommodate all the N_2 drifting around the system.

To set up the Spreadsheet, drag a Spreadsheet from the Objects Palette anywhere onto the PFD (it doesn't connect to anything).

Type in the entries as shown below.



Right click in cell b1, chose Import Variables, FEED, Comp Mass Flow, HCl. Do the same for cells b2, b3, and b5 with the appropriate choice of variable. It should give you a spreadsheet as follows:



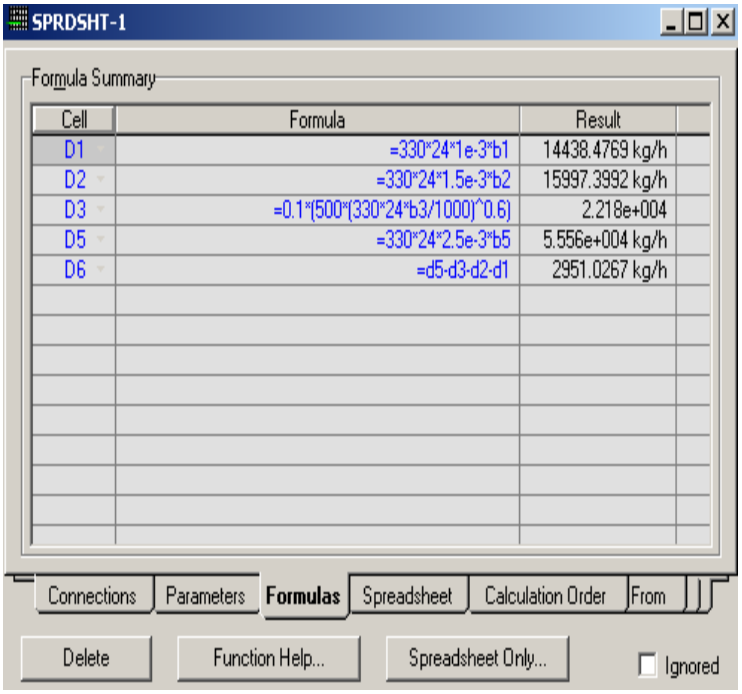
We want to calculate the profit based on the formula:

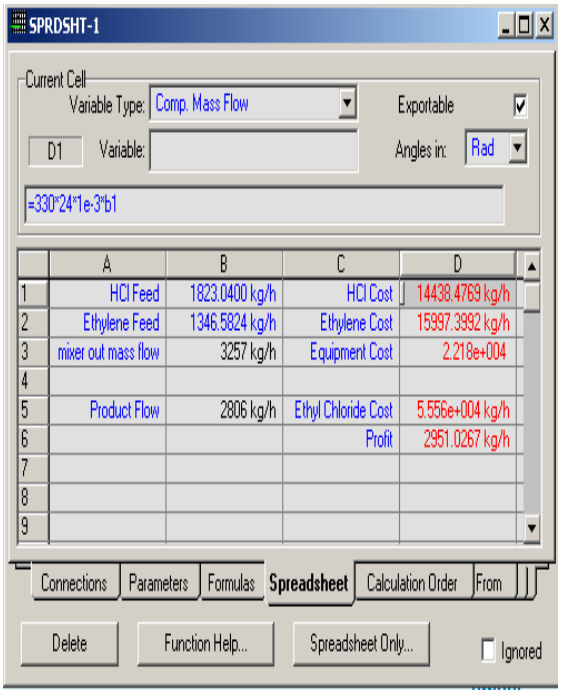
Profit = 330*24*[2.5*product-(1.5ethylene + HCl)*Feed]

$$- 0.1[500*(330*24*\text{ReactorIn}/1000)^{0.6}]$$

The raw cost of ethylene is 1.5x10-3 units per kg, that of HCl is 1.0x10-3 units per kg, and the sale price of Ethyl Chloride is 2.5x10-3 units per kg. The last term accounts for the price of the reactor.

To this end, in the spreadsheet tab enter the following data (note, the formulae are shown below in the formulas tab, but you must enter them in the spreadsheet tab):





Cell d5 gives us the profit.

Adjust the purge stream molar flow rate between 5kgmol/hr and 15 kgmol/hr and examine the profit recorded. Plot a graph of purge stream molar flow and profit. If you are clever you'll do this using the Case Studies Tool (you might have to knock off the two other dependent variables first).

Mass Balance

Do a mass balance on the Splitter by looking at the streams coming in and leaving this unit. Do the mass balance on the total mass flow and also on each component molar flow.

Write-Up

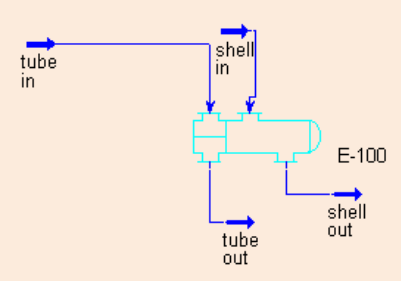
Include:

- copy of PFD (1 mark)
- copy of workbook (1 mark)
- case studies curves (2 marks)
- graph of profit versus purge flow (2 marks)
- purge flow rate value for optimal profit (1 marks)
- material balance around splitter (2 marks)
- conclusions (1 mark)

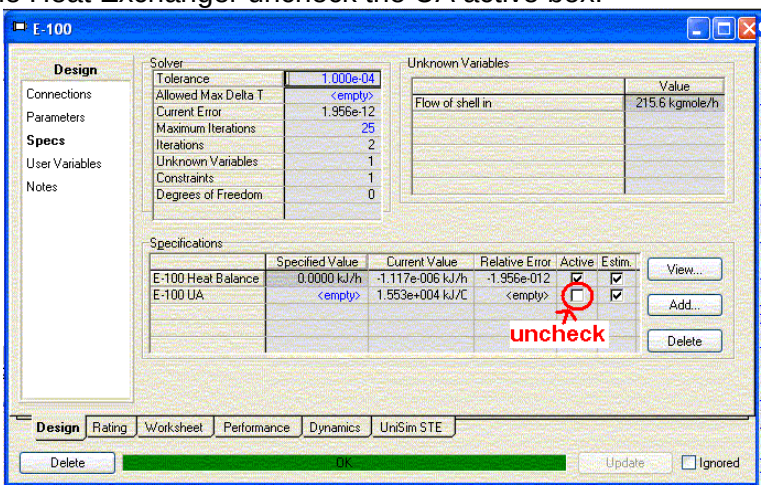
UniSim Heat Exchanger Calculations

Problem 1

- Set up a fluid package with H_2O and benzene. Use the UNIQUAC property package.
- Set up a heat exchanger with four material streams. Call them tube in/out and shell in/out.



- Set the compositions of both tube in and shell in to be 100% water. Set their temperatures to be tube in = 25°C and shell in = 90°C. Set the flow rate of tube in to be 9000kg/hr. Set their pressures to be 300kPa (tubes) and 200kPa (shell).
- Set the temperatures of tube out and shell out to be 40°C and 55°C respectively.
- Double click on the heat exchanger and connect the four streams to the appropriate inlets. On the Parameters page set the Delta P's (pressure drops) to 30kPa.
- To work correctly, we must let UniSim adjust the UA value. On the Design, Specs page of the Heat Exchanger uncheck the UA active box.



We have now specified seven of the nine parameters a heat exchanger needs, and this is enough to solve it uniquely. It's smart enough to figure out the composition of the outlet streams, and to calculate the flow rate through the shell and the UA value for the heat exchanger.

Do these calculations by hand and see if your results agree with UniSim.

i) calculate the shell side flow rate by conservation of energy ($m_s c_s \Delta T_s = m_t c_t \Delta T_t$).

ii) calculate the LMTD using the four temperatures

iii) divide the LMTD by the F_T factor on the performance details page (this takes account of the fact that the exchanger is a 2-1 pass and so is neither counter nor parallel flow.

iv) Calculate UA using $q = UA\ \Delta T$ where ΔT is the LMTD, assume counter flow.

You can check on the LMTD from UniSim from the Performance, Specs tab of the heat exchanger. Note that because this is a 1-2 heat exchanger we don't have a simple counter flow but this is corrected by an F_t factor; $LMTD_{actual} = F_t \times LMTD$.

For a 1-2 heat exchanger, Ft is calculated from the equation:

$$F_t = \frac{\sqrt{(R^2+1)}}{R-1} \frac{\ln\left[\frac{1-S}{1-RS}\right]}{\ln\left[\frac{2-S(R+1-\sqrt{R^2+1}}{2-S(R+1+\sqrt{R^2+1}}\right]}$$

$$\text{Where R} = \frac{T_{H_{in}} - T_{H_{out}}}{T_{C_{out}} - T_{C_{in}}}$$

and

$$\text{S} = \frac{T_{C_{out}} - T_{C_{in}}}{T_{H_{in}} - T_{C_{in}}}$$

In this case this gives F_t = 0.939. You should check this by doing the calculation by hand (or in Excel, as shown on the right).

UniSim won't let us use an uneven number of tube passes (see the Rating, Sizing tab of the heat exchanger) so the simplest heat exchanger we can configure is 1-2.

	tube	shell
In (°C)	25	90
Out (°C)	40	55
Flow (kg/hr)	9000	3857.143
Shc(Jkg^{-1} °C^{-1})	4180	4180

ΔT_R(°C) =	50
ΔT_L(°C) =	30
LMTD(ºC) =	39.1523
S =	0.230769
R =	2.333333
F_T =	0.939183

Problem 2

Set up a second heat exchanger. Again we'll just use H_2O. Set the tube in temperature to be 25°C, pressure to be 300kPa, and flow rate to be 9000kg/hr. Set the shell flow in to be 90°C, pressure 200kPa, and flow rate to be 6000kg/hr.
Configure the heat exchanger to have a UA of 6000kJ^{0}C^{-1}hr^{-1} (you'll need to check the UA active box again to do this). Again set the Delta P to be 30kPa.
This gives the heat exchanger enough information to be solved. Record the values for the outlet temperatures and see if they are consistent with your calculations.

Problem 3

For our final heat exchanger we will configure inputs of H_2O at a temperature of 25°C and benzene at a temperature of 95°C. The pressures in all four streams are 101.3kPa. The flow rates are 9000kg/hr for the H_2O and 2000kg/hr for the benzene. The heat exchanger has a UA of 2x10^{4}kJ^{0}C^{-1}hr^{-1}.
There will be a phase change in the heat exchanger so this will dictate which fluid is in the shell and which in the tubes.
Make all the connections to solve the heat exchanger. Then plot a graph (performance plots) of temperature versus heat flow. Note how the phase change affects this graph. If you right click on the graph and choose *Graph Control* you can change the plot colours to something clearer.

Report

Your report should consist of the following:

- Screenshots of the PFD for all three systems **(1.5 marks)**
- Screenshots of the Worksheet for all three systems **(1.5 marks)**
- Calculations for the first two systems, showing if our sums agree with what is shown in UniSim. **(6 marks)**
- Screenshot of the graph from problem 3 **(1 marks)**

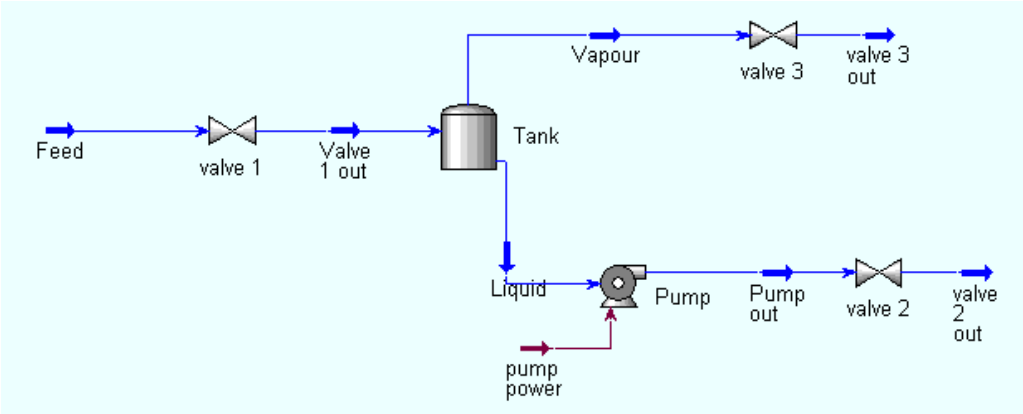
Dynamic Simulation of a Tank Separator System

Dynamic simulation enables us to see the effect of disturbances on a system. This is especially critical for batch systems, where steady state operation is the exception rather than the norm.
We will begin with a simple system involving a tank being fed by a single stream which separates into a liquid stream and a vapour stream. We will use three valves as controllers.

First we need to set up the steady state mode:

Create a fluid package containing ethane, propane, i-butane, and n-butane. Choose the Chao-Seader fluid package (this is a good choice for hydrocarbons and light gasses). You won't need to worry about binary coefficients here.
Create the pdf as shown below:

- The Feed stream composition is 10% ethane, 20% propane, 30% i-butane, and 40% n-butane
- The Feed stream flow rate is 100kgmolhr^{-1}
- The Feed stream temperature is 70^{o}C
- The Feed stream pressure is 2000kPa
- The pressure drop (DeltaP) across valve 1 is 1500kPa
- The pressure drops across valves 2 and 3 are 200kPa
- The pump has a pressure rise of 200kPa



Now we need to prepare our simulation for the switch into dynamics mode. This is important because some factors, like for instance the tank size, have no impact on the steady state conditions but are critical to know when it comes to the time response of the system, its dynamics.

- For each of the three valves, go to their dynamics tabs, set the Valve Opening % to 50%, check on the Check Valve box, and click on the Size Valve button
- For the pump, on its dynamics tab, ensure the pressure rise and efficiency buttons are clicked. This will ensure that the pump maintains the same pump pressure head as flowrates change during the dynamic simulation.
- The size of the tank is chosen to be 2.13m^3 with a diameter of 1.11m. This gives 10 minutes of hold-up (liquid flow rate is 3499kg/hr, liquid density is 547.7 kg/m^3, and the vessel is 50% full) and keeps the superficial vapour velocity below 0.187m/s.

At this point save your programme, including steady state in the name. Once we switch into dynamics mode UniSim will make changes to our programme that will be hard to reverse so it's good to keep a steady state copy, just in case.

Switch to dynamics mode by clicking on on the toolbar. Accept the changes that UniSim recommends. Make sure the dynamics mode button is depressed.

We want to include two control elements in our pdf:

1. flow control the feed with valve 1
2. control tank level with valve 2

- Click on the PID controller icon on the palette, drag it onto the pfd above valve 1.
- Click on Select PV and choose Feed, and Molar Flow.
- Click on Select OP then choose valve 1, and actuator desired position.

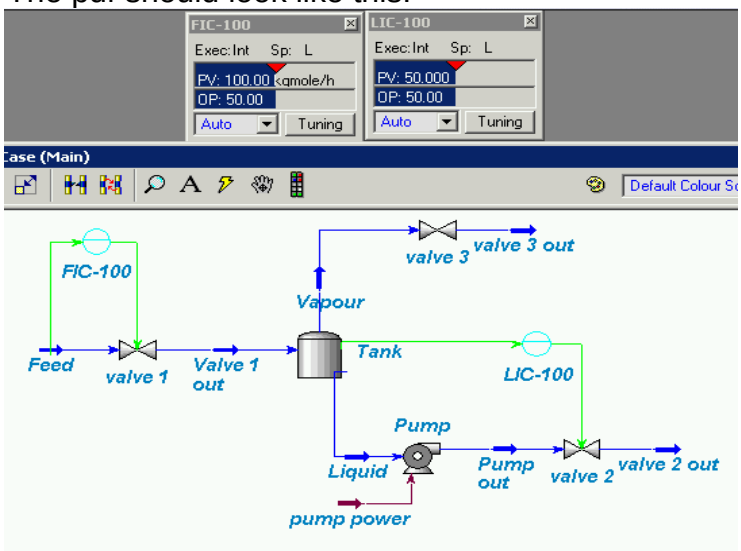
On the parameters tab of the controller

- Select reverse acting (increase in flow results in a closing of the valve).
- Set the range to be 0-200kgmolhr^{-1} (twice the steady state value).
- Select *Mode, Auto* (because the controller gets its set point from another controller.
- Set the PID constants to be K_c = 0.5 and T_i = 0.3minutes. Leave T_d empty.
- Click on the Faceplate button and drag the faceplate up above the pdf window

Add the tank level controller

- choosing *Tank, Liquid Percent Level* for the PV
- choose valve 2 for the OP
- choose a range of 0-100%
- choose direct action (an increase in tank level leads to an opening of the valve)
- Set K_c = 2 and leave T_i and T_d empty.
- Select *Mode, Auto*
- Again, click on the Faceplate button.

Save your work. The pdf should look like this:

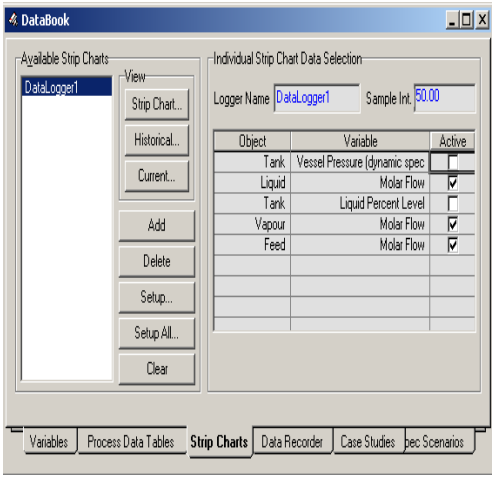


Your next job is to add a third controller to control the tank pressure level (called here *Vessel Pressure (dynamic specification)*). A range of 300-700kPa seems OK, and a K_c = 2 would work. We'll leave it a proportional only controller so leave T_i and T_d empty. But you'll need to find the correct PV, select the appropriate OP, and decide if it's direct or reverse acting.

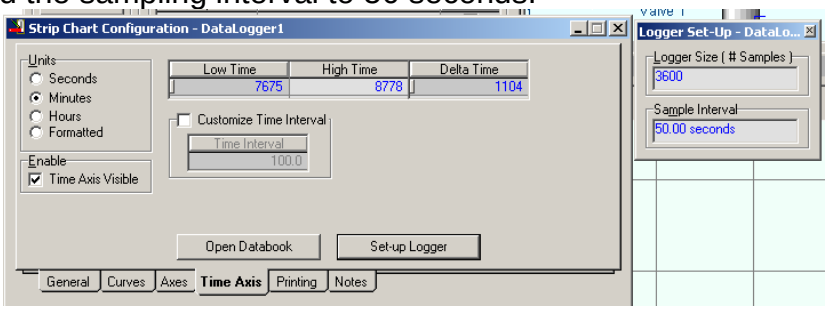
Installing Recorders

We need to be able to see how variables are changing with time, dataloggers and strip charts are useful for this. And even though the visualisation and analysis of data isn't that great in UniSim, it does let us export to other applications like Excel.

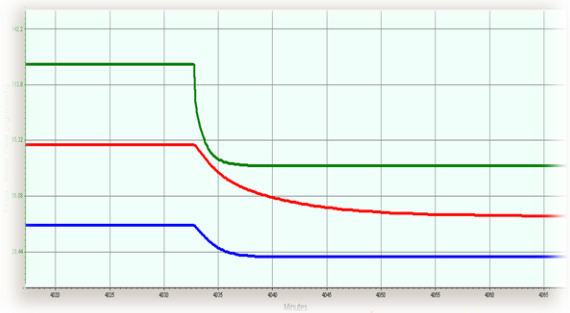
1. Open up the databook (from the Tools menu)
2. From the variables tab, click insert, then click Liquid, Molar Flow.
3. Click insert again and choose the Liquid percent level in the tank and then the tank vessel pressure (dynamic spec), the Feed molar flow and the Vapour molar flow.
4. Go to the strip charts tab. Click add to install a datalogger and click on the three molar flows to make them active
5. Click *View, StripChart*. Right click on the window that appears and choose *Graph Control*. Adjust the colours to something more appealing (and more printer friendly) than a black background. As well as *Graph control*, note the other options such as *Select Curve*, and the two *Autoscale*'s. These are useful.

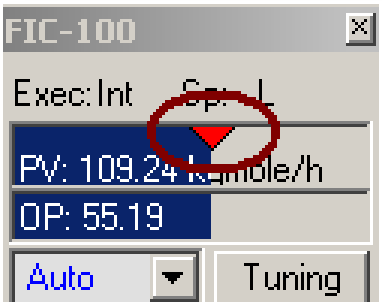


6. On the Time Axis tab click on Set Up Logger and change the number of samples to 3600 and the sampling interval to 50 seconds.

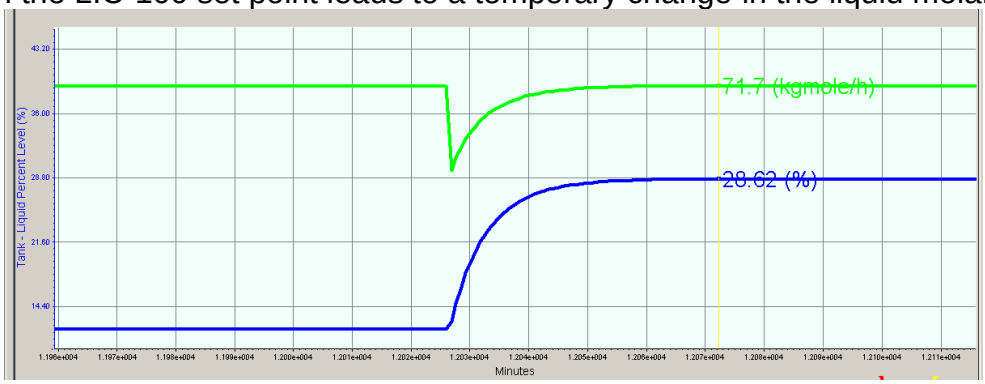


7. This is a good time to save your simulation (give it a file name with dynamic in the title this time). Once we start playing around with set points it is possible to make it unstable and we might need to start again.
8. Run the simulation by clicking the integrator active button  on the toolbar.
9. See how changes in Feed flow effect the flows in the vapour and liquid streams. Adjust the set point on the Feed flow rate by dragging the red arrow on the FIC-100 Faceplate. Note the changes in the flow rates in the liquid and vapour streams. Which one responds more rapidly?

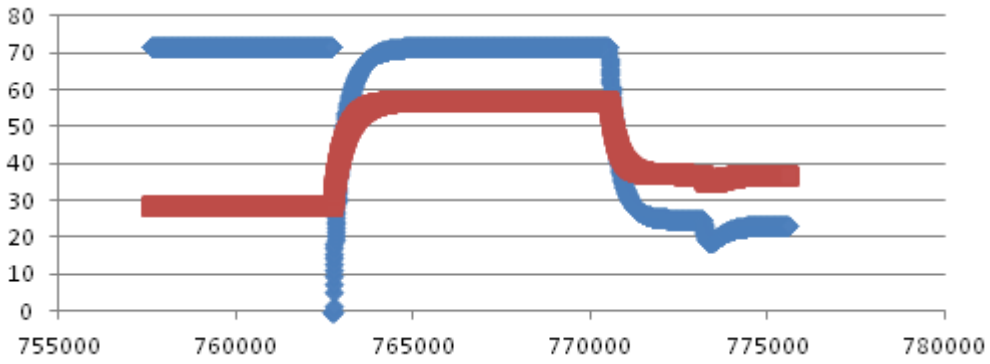




10. We can also examine other dependencies. For example, note how a change in the LIC-100 set point leads to a temporary change in the liquid molar flow.



11. To export data to another application, go back to the databook, highlight the datalogger you used, and click historical. The file can be exported to a .csv file which can be opened by Excel for example.



Report

In your report include the following:

- A screenshot of the pdf, also detail the steps you took to include the tank pressure controller (3 marks)

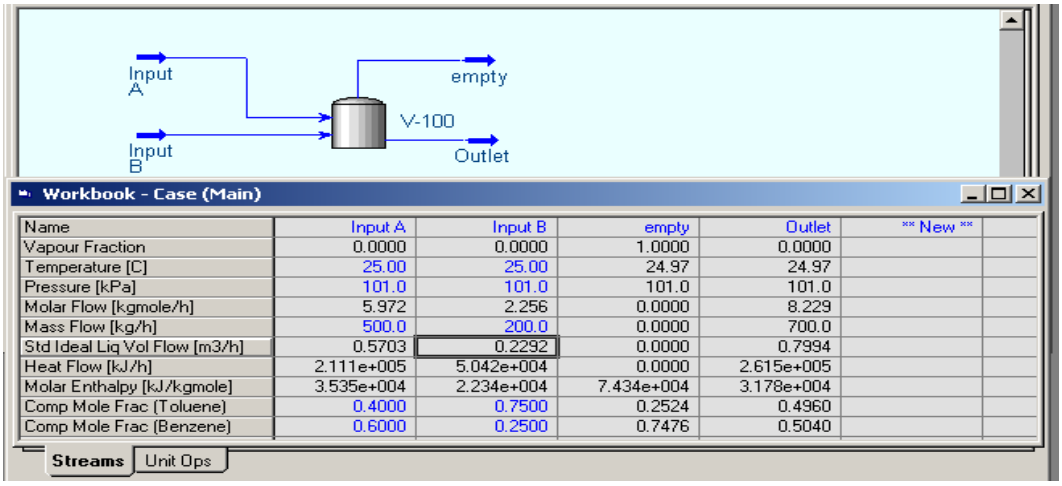
- A screenshot of a strip chart showing the response of the system to a step change in the feed flow rate. Use this chart to explain the connections between changes in the flow rates of the three streams. (2 marks)
- A screenshot of a strip chart showing the response of the system to a step change in the tank fill level set-point. Use this chart to explain the connection between fill and liquid flow rate (2 marks)
- A screenshot showing data exported to Excel (1 marks)
- Justify the choice of 2.13m^3 for the tank size. (2 marks)

Mixing Dynamics

This lab sets out to examining the dynamic behaviour of a mixing system in response to a change in one of the input streams. We will be setting up and running a mixing system in UniSim, exporting its results into ExCel, and analysing these results with mathematical modelling.

UniSim Steady State

Create a component list including toluene and benzene. Use Peng-Robinson as the fluid package. Set up the following pfd and worksheet as shown below. Note, you should set the Tank to have a volume of 0.05m^3:



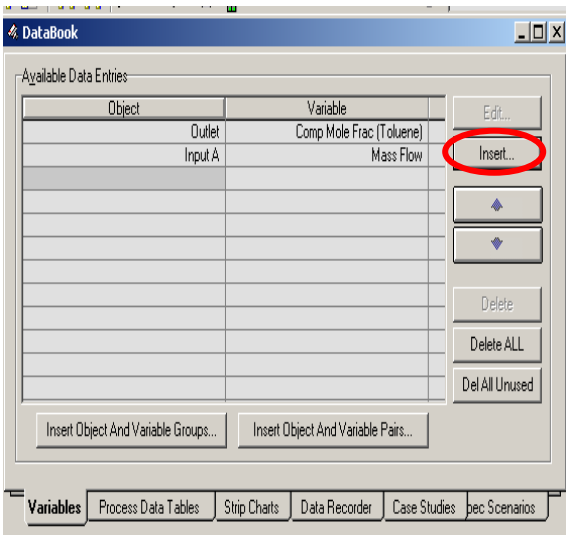
Name	Input A	Input B	empty	Outlet	*** New ***
Vapour Fraction	0.0000	0.0000	1.0000	0.0000	
Temperature [C]	25.00	25.00	24.97	24.97	
Pressure [kPa]	101.0	101.0	101.0	101.0	
Molar Flow [kgmole/h]	5.972	2.256	0.0000	8.229	
Mass Flow [kg/h]	500.0	200.0	0.0000	700.0	
Std Ideal Liq Vol Flow [m3/h]	0.5703	0.2292	0.0000	0.7994	
Heat Flow [kJ/h]	2.111e+005	5.042e+004	0.0000	2.615e+005	
Molar Enthalpy [kJ/kgmole]	3.535e+004	2.234e+004	7.434e+004	3.178e+004	
Comp Mole Frac (Toluene)	0.4000	0.7500	0.2524	0.4960	
Comp Mole Frac (Benzene)	0.6000	0.2500	0.7476	0.5040	

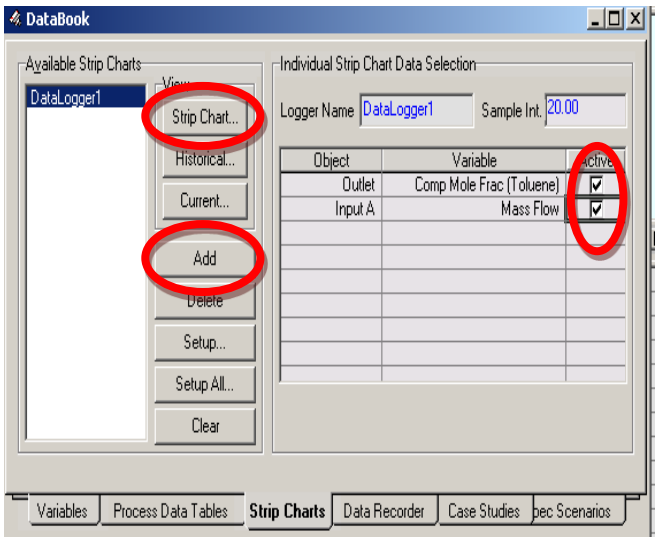
Save your file.

UniSim Dynamics

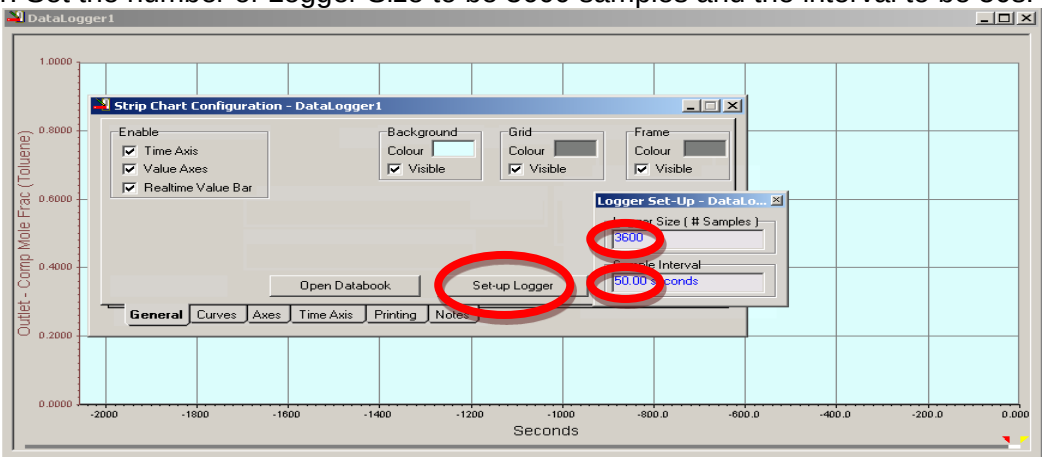
Switch to Dynamic Mode () and accept the change that UniSim proposes. You might need to click the dynamic mode button a second time for these to take effect. Note that on the worksheet, the molar flow values for Input A, Input B and Output are now in blue, meaning they can be adjusted.

We want to examine the composition of the Outlet stream as we change the inlet streams, so add a Strip Chart tracking the mole fraction of toluene in the outlet along with the flow rate of Input A. Click on Tools, then Databook and set up the variables as shown below. Go to the strip charts tab, Add a Datalogger, and click on our two variables to make them active. The click on Strip Chart.

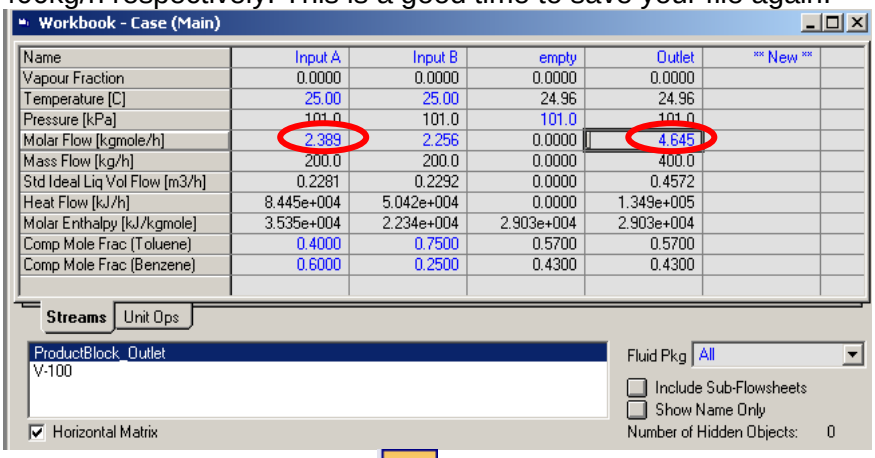




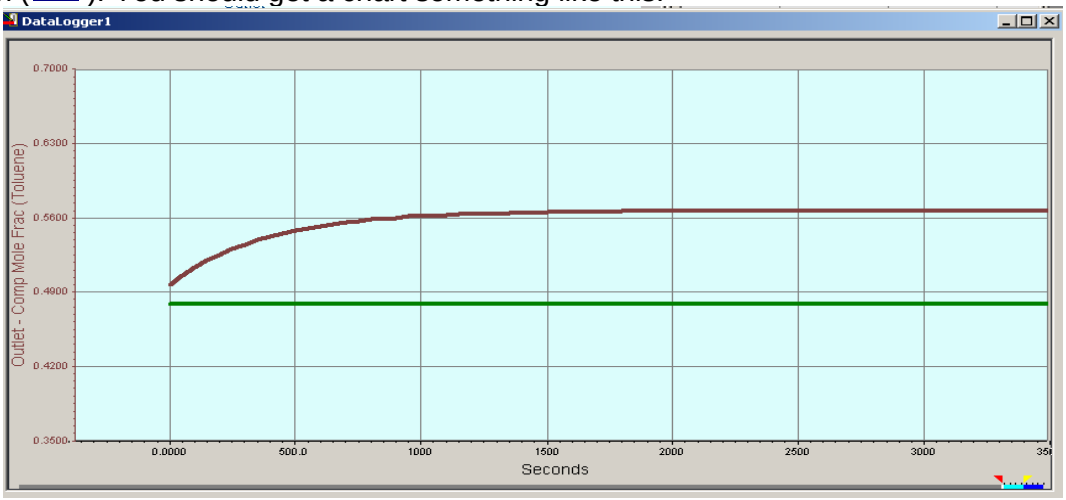
Right click on the Strip Chart. Make the colour scheme more attractive. And Click on Set-up Logger. Set the number of Logger Size to be 3600 samples and the interval to be 50s.



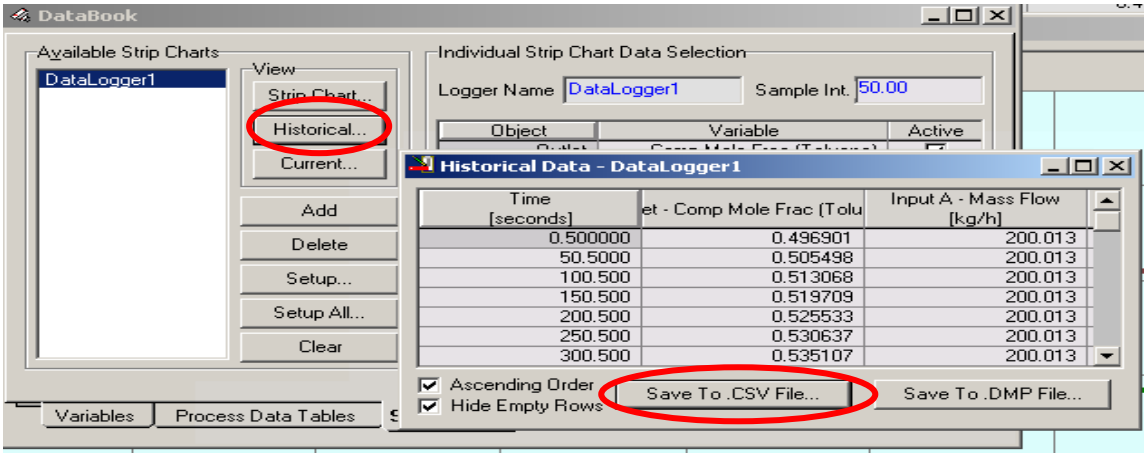
Now, go back to the workbook and set the Molar Flow rate of Input A to be 2.389kgmol/h and the Molar Flow of the Outlet to be 4.645kgmol/h. This should make the mass flow rates 200kg/h and 400kg/h respectively. This is a good time to save your file again.



Now click on the Integrator Active button () and choose 100% Liquid. Let the integrator run for a couple of seconds (but no more, otherwise the amount of data becomes huge) until the Comp Mole Fraction (Toluene) line levels off and then stop it with the integrator holding button (). You should get a chart something like this:

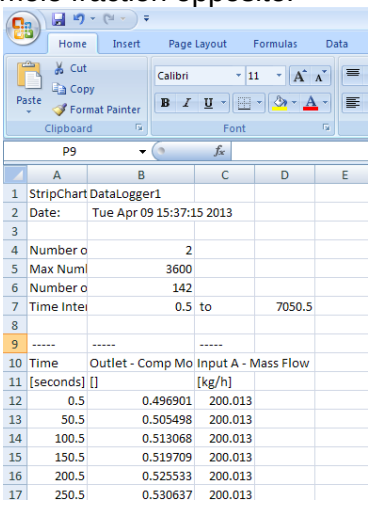


Export the data to an excel compatible format by clicking on the Historical button of the Databook and choosing the .csv format (which can be opened by excel):

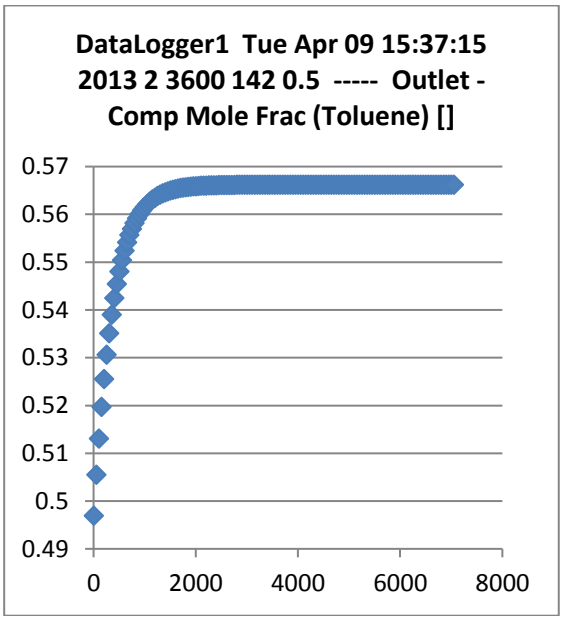


Excel

Open up Excel and open up the .csv file you just created. It should look a bit like the image below, with a plot of the comp mole fraction opposite.



	A	B	C	D	E
1	StripChart	DataLogger1			
2	Date:	Tue Apr 09 15:37:15 2013			
3					
4	Number o	2			
5	Max Numl	3600			
6	Number o	142			
7	Time Inte	0.5	to	7050.5	
8					
9	-----	-----	-----		
10	Time	Outlet - Comp Mo	Input A - Mass Flow		
11	[seconds]	[]	[kg/h]		
12	0.5	0.496901	200.013		
13	50.5	0.505498	200.013		
14	100.5	0.513068	200.013		
15	150.5	0.519709	200.013		
16	200.5	0.525533	200.013		
17	250.5	0.530637	200.013		



Note that the Time column begins at 0.5s. This is important. If you have a time offset in your excel data you will need to recalibrate this by subtracting the ~initial time from all the values in the Time column.

Mathematical Analysis

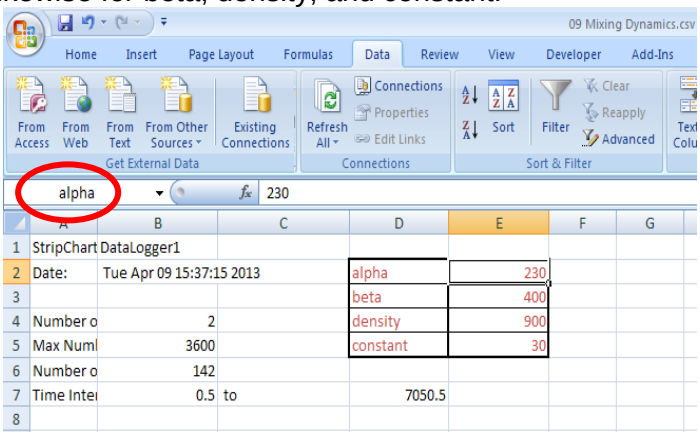
The Comp Mole Fraction curve, we'll call it x(t), should follow an equation like:

$$x(t) = \frac{1}{\beta}\left[\alpha - Ke^{-\lambda t}\right]$$

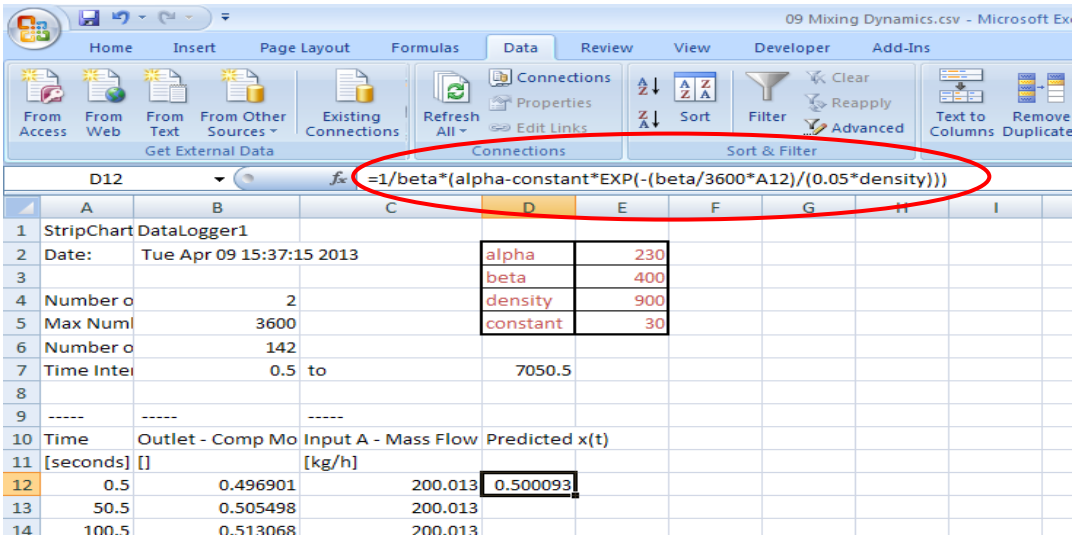
Where β is the outlet mass flow (=400kg/h), α is the total inlet mass flow of toluene (=200*0.4+200*0.75=230kg/h), and λ = β/[(volume of tank)*density]. K is a constant of integration that we can estimate from the value of x(0) =0.5.

We are going to fit our data in excel to this curve to get values for α, β, and the density ρ.

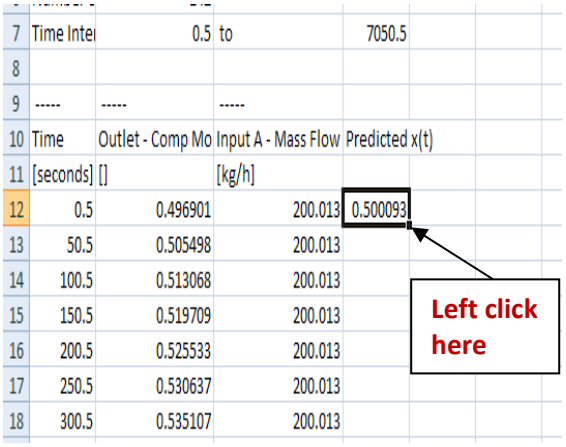
On our excel sheet, create a little table of values that we will use to fit our data to the formula above. Give these values names so we can use them more easily in the formula. This is shown below, click on the cell that contains the value for alpha (e.g. the cell E2 below which has the value 230 in it rather than D2 which has the name alpha in it), and type in alpha into the Name Box. Do likewise for beta, density, and constant.

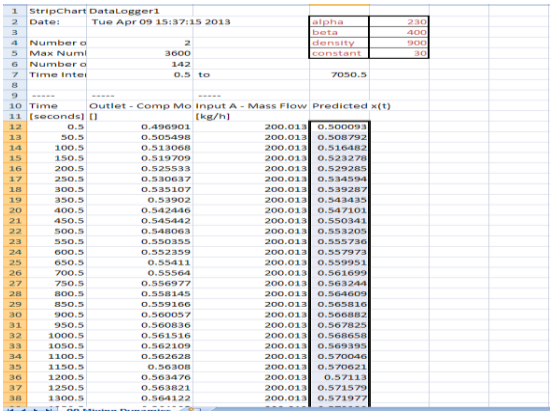


We are now going to create a new column in our excel sheet for the predicted value of x(t) and fill it out with values based on our equation. Do this as shown below. Note, the 0.05 refers to the tank volume and the 3600 is to convert from hours to seconds.

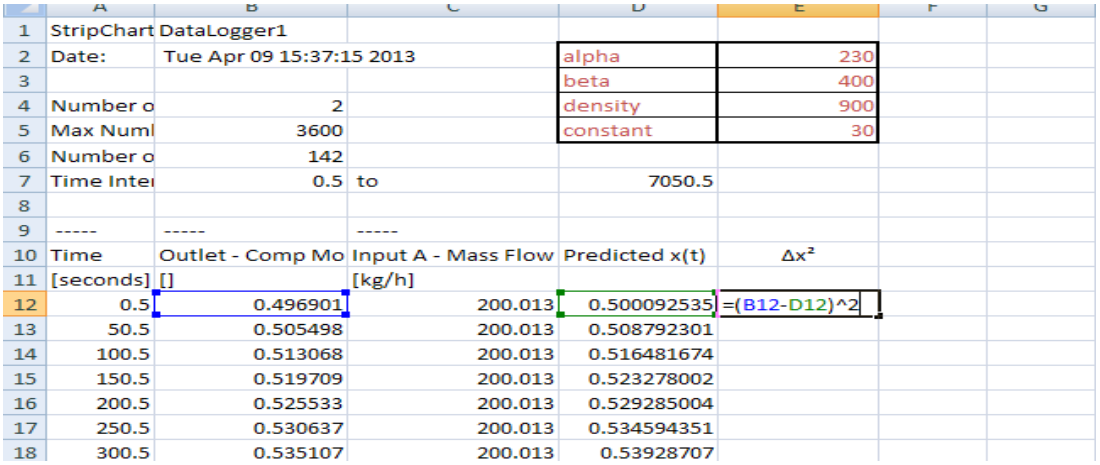


Having done this for one cell, you can copy this formula for every subsequent cell (i.e. *Fill, Down*). The fastest way to do this is to left click the bottom right corner of the first cell, drag down over the column, and then chose copy cell. See the diagrams below for before and after.



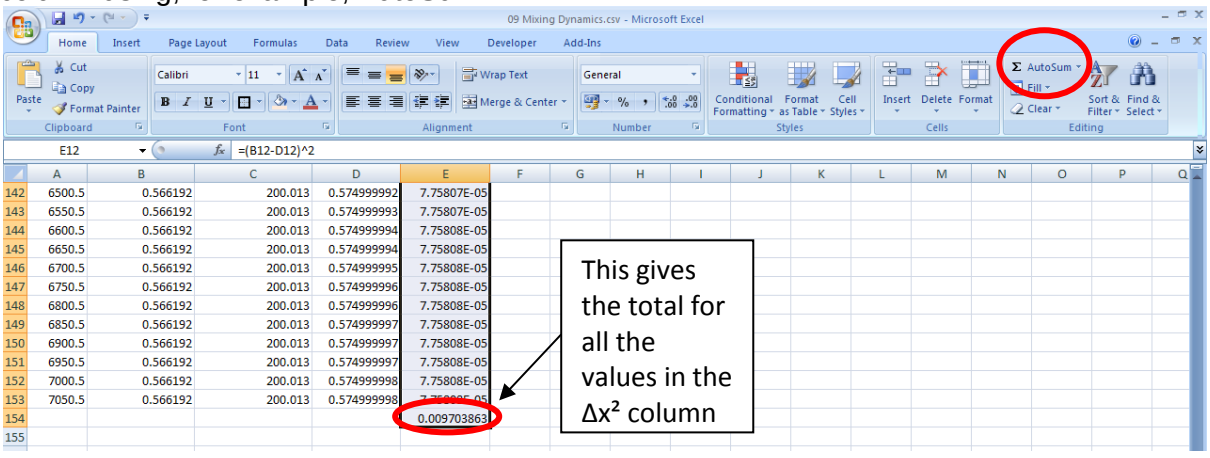


Now we have the predicted composition for all values of time. We can take the difference between the actual and predicted values and calculate the square of the difference.

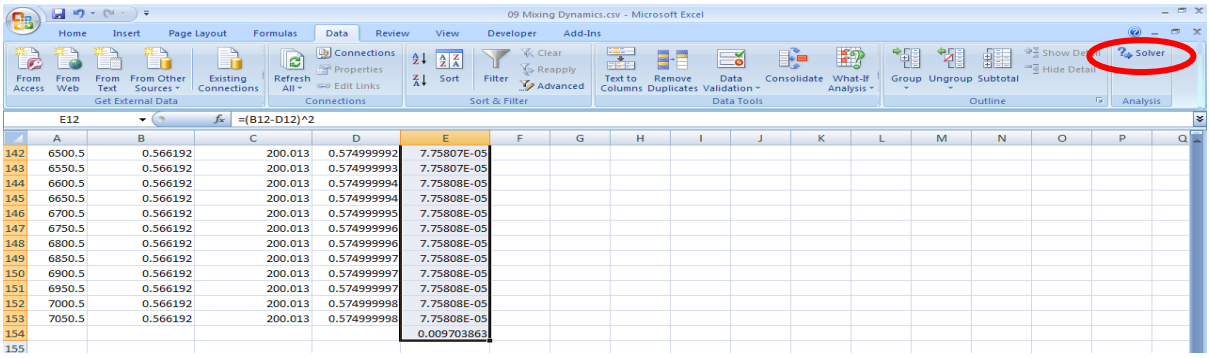


	A	B	C	D	E
1	StripChart	DataLogger1			
2	Date:	Tue Apr 09 15:37:15 2013		alpha	230
3				beta	400
4	Number o	2		density	900
5	Max Numl	3600		constant	30
6	Number o	142			
7	Time Inte	0.5	to	7050.5	
8					
9	-----	-----	-----		
10	Time	Outlet - Comp Mo	Input A - Mass Flow	Predicted x(t)	Δx²
11	[seconds]	[]	[kg/h]		
12	0.5	0.496901	200.013	0.500092535	=(B12-D12)^2
13	50.5	0.505498	200.013	0.508792301	
14	100.5	0.513068	200.013	0.516481674	
15	150.5	0.519709	200.013	0.523278002	
16	200.5	0.525533	200.013	0.529285004	
17	250.5	0.530637	200.013	0.534594351	
18	300.5	0.535107	200.013	0.53928707	

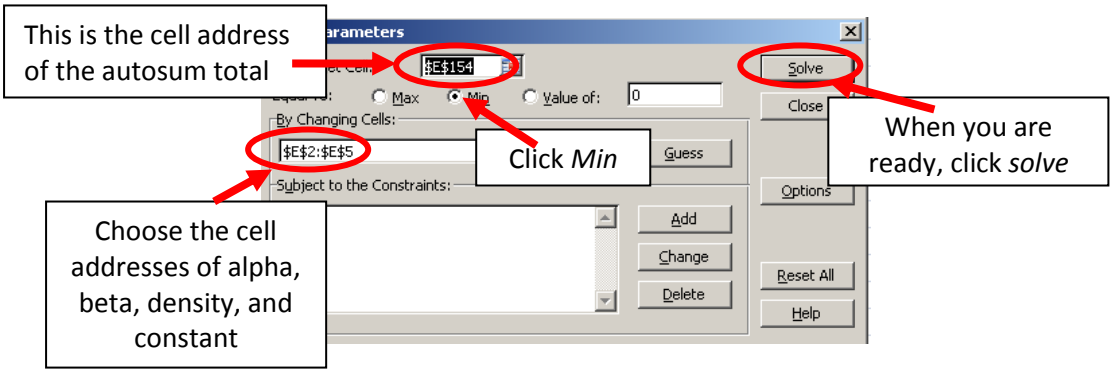
Again, we fill down the entire column, and then we take the sum of all the values in the column using, for example, AutoSum.



Now for the analysis. Launch Solver from the Data menu (you might need to install solver from excel add-ons. If so, consult http://office.microsoft.com/en-us/excel-help/load-the-solver-add-in-HP010021570.aspx):

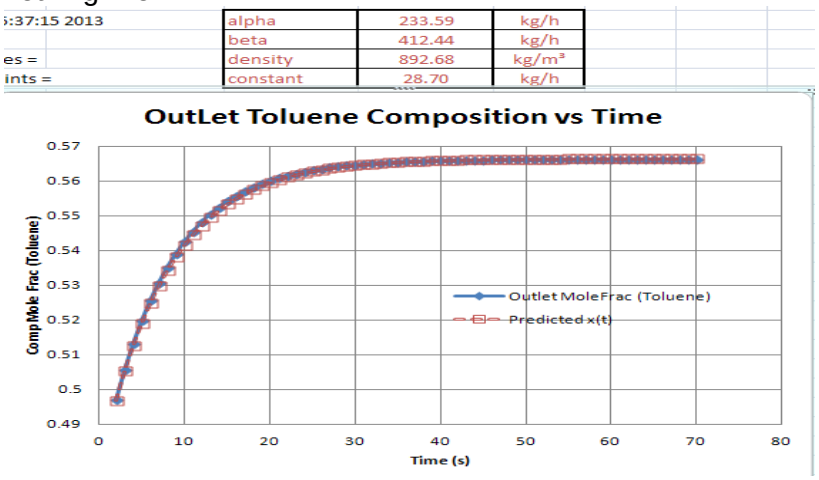


Solver brings up a dialog box that you can fill out as shown below:



When this is done, choose to keep Solver solution and click OK.

Now plot a graph in Excel of the new predicted values for Δx^2 and the UniSim values. It should look something like:



15. Report

Your report will consist of:

- A screenshot of your PFD **(1 marks)**
- A screenshot of the workbook **(1 marks)**
- A screenshot of the strip chart from UniSim **(2 marks)**
- A screensot of the fitted parameters alpha, beta, density, and constant from the excel workbook. **(3 marks)**
- A screenshot of the fitted curve from excel **(3 marks)**
- And you'll get extra marks if you can justify the equation

$$x(t) = \frac{1}{\beta}\left[\alpha - Ke^{-\lambda t}\right]$$

(we'll talk about this equation in class)