HYSYS Design Tutorial for CHEE470

Queen's University Department of Chemical Engineering

2009

Introduction

UniSim or HYSYS are a program that can be used to design chemical plants. It is built around:

- a library of the physical properties of a large number of chemical species
- a set of subroutines to estimate the behavior of many types of plant equipment (heat exchangers, reactors, etc.)
- a graphical user interface to accept specifications for the case, and display results

The user describes the process in terms of pieces of equipment interconnected by process streams, and the program solves all the mass/energy/equilibrium equations, taking into consideration the specified design parameters for the units.

It is a very complex system, and there is no way that this tutorial is going to demonstrate all of the features. The features that will be shown are the ones that will prepare you to tackle the plant design assignment in CHEE470.

Like most programs of this type, operations can be done in different ways. In general, this tutorial will only describe one way. You will find other methods in the HYSYS documentation, but the ones shown here are best suited for people who are new to the program.

Hints for Success in Modeling

- 1. Build the model one step at a time. People new to this instinctively want to start by adding many streams and unit operations, and then try to get the whole mess working. This is futile. Add the elements one at a time. Get one working before you go on to the next one.
- 2. Save a whole series of backups, not just the latest working version. Disk space is cheap. If you get into trouble, you may find that it is difficult to restore the model to its previous state. Often you are better to retrieve a previous version and update it.
- 3. Put meaningful names on all streams and units. Debugging is difficult when you are trying to remember if stream S22 is the distillate or the bottoms in a distillation column.
- 4. If a piece of equipment does not work although the parameters all look reasonable, try deleting the unit and reconstructing it.

Steps in Developing a Model of a Chemical Process

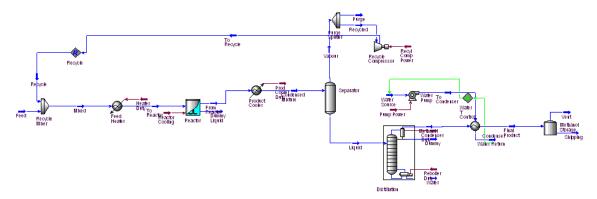
- 1. Select the units that you want to work with. Do you want kilograms and °C, or pounds and ° F?
- 2. Select the thermodynamic methods that will be used for predicting physical properties. The decision should be based on the type of chemical species involved.
- 3. Specify the chemical species that will be present in the process. At this stage you may be given some advice about the ability of the selected thermodynamic method to handle these chemicals.
- 4. If the process involves reactions, provide information such as stoichiometry and kinetic constants.
- 5. Build the model by adding streams and equipment one at a time.
- 6. If the process contains recycle loops, deal with closing them.
- 7. Use the HYSYS utilities to get additional information such as the mechanical design of distillation column trays.
- 8. Print a report describing the results of the simulation.

The Methanol Process

Methanol can be made from hydrogen plus carbon monoxide and/or carbon dioxide. 2 $H_2 + CO \Rightarrow CH_3OH$ 3 $H_2 + CO_2 \Rightarrow CH_3OH + H_2O$ Recent studies suggest that the first reaction actually proceeds as $CO + H_2O => H_2 + CO_2$ (the water gas shift reaction) followed by the second reaction.

For this exercise we will work with the simplest version – the second reaction only. By the way, running this reaction backwards provides a method of operating a hydrogen fuel cell with methanol as a feed.

The following diagram shows the process we will work on. It is important to recognize that this is not suggested as a good way to make methanol. The design has been formulated to demonstrate many key aspects of HYSYS, without getting overwhelmed by detail.



A mixture of H_2 and CO_2 is heated to the required temperature and fed to a stirred reactor. As noted above, the reaction is $3 H_2 + CO_2 => CH_2OH + H_2O$.

The product of the reaction is partially condensed. The vapour (mostly H_2 and CO_2) is compressed and recycled back to the beginning of the process. The liquid (mostly CH₂OH and H₂O) is fed to a distillation column.

The column produces a product stream (mostly methanol) and a waste stream (mostly water). The product is cooled to a temperature that is reasonable for storage. A pump is required provide cooling water for this heat exchanger.

Setting up Data for the Model

Open HYSYS.

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	UniSim Design R350.1

 \uparrow Click on the new file icon and get:

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Units

We will use the default SI units, so no action is required. In future cases you may want to use different units. See section 3.2.2 of "HYSYS Design Tutorials and Applications.pdf".

Thermodynamics

Click on the "''Fluid Pkgs" tab.

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<u>A</u> dd	Case (Main) <empty></empty>
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Сору	
Import Export	Default Fluid Pkg
	Use Default Fluid Pkg Use Parent's Fluid Pkg
Components Fluid Pkgs Hypotheticals Oil Man	ager Reactions Component Maps UserProperty
	Enter Simulation Environment

"Fluid Package" is HYSYS's terminology for a collection of data that includes all the thermodynamic, component, and reaction parameters required to run the model.

It is possible to have more than one package in a model. For example, it would be possible to use one thermodynamics model in the reactor, and another in the distillation column. We will just have one package.

Click on "Add" and scroll to find "SRK". This selects the Soave-Redlich-Kwong method, a popular equation of state model.

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D 🛩 🖬 🔺 🗷 🚭	Environment: Basis Mode: Steady State
🔺 👗 Fluid Package: Basis-1	
Property Package Selection OLL_Electrolyte Peng-Robinson PR-Twu PRSV Sour SRK Sour PR SRK. SRK SRK. Vapour Press Models C Vapour Press Models C Vapour Press Models C Miscellaneous Types UNIQUAC van Laar Component List Selection Component List - 1 View Set Up Parameters Binary Coeffs StabTest Phase D Delete	EDS Enthalpy Method Specification © Eguation of State © Lee-Kesler Use EDS Density ✓ Modify H2 Tc and Pc ✓ Smooth Liquid Density Advanced Thermodynamics Modify H2 Tc and Pc ✓ Smooth Liquid Density Advanced Thermodynamics Megression Import Export rder Rxns Tabular Notes SRK Edit Properties ment
	A V

Note that the default name "Basis-1" is given to the package, and our components will go into "Component List-1".

Components

Close the fluid package window and click on the "Components" tab of the "Simulation Basis Manager".

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Now, select "Component List – 1", click on "View" and enter "CO2" into field "Match".

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Add Component Selected Components	Components Available in the Component Library Match CO2 View Filters.
Traditional Hypo Components Other Comp Lists	C Sim Name I Full Name / Synonym C Formula
	<add pure<="" td=""> C2=G-2C2C6Er C2=Glycol2C2C6Ethr C10H2202 C1-1122-FC2 Chloro-1,1,2,2-Tetrafluoroethane C2HCIF4 C02 C02 C02 12-CIC6FCC4 Cyclobutane_1,2-Dichloro-1,2,3,3,4,4-Hexafluoro-1</add>
	C-Substitute-> 1234-T-M-CC6 Cyclohexane-1,2,3,4-Tetramethyl- C10H20 Inositol Cyclohexanhexol-(1r.2c.4t.5c.6t.) C6H1206 Remove>
	Sort List
	View Component
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Now click on "Add Pure", and do the same operation with "Hydrogen". Let's do methanol differently. Select the "Formula" option instead of "Full Name / Synonym" and enter "CH4O">

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Do the same with "H2O".

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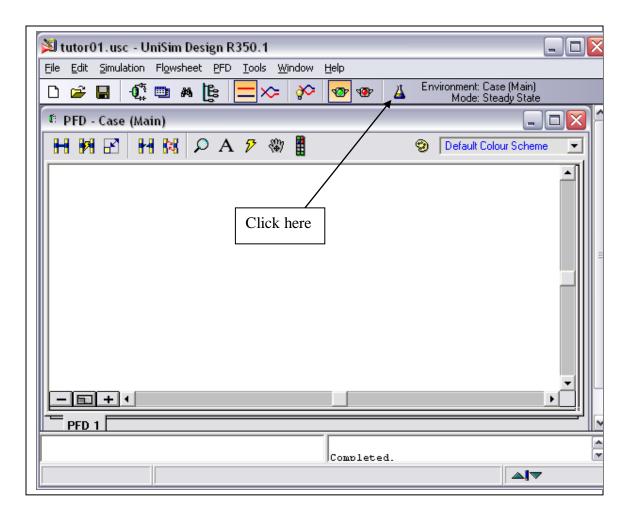
We now have all the components we need.

This would be a good time to save the case. Close the components window and click on the "Enter Simulation Environment" button of the "Simulation Basis Manager" window. Do the usual "File=>Save" operation and call the file tutor01.

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Reactions

Now we need to return to the Simulation Basis Environment. Click on the beaker.



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<u>File Edit Basis Tools Window H</u> elp	
	Environment: Basis Mode: Steady State
4 Simulation Basis Manager	
Rxn Components CO2 Hydrogen Add Bxn H2O Delete Rxn Copy Rxg Assoc. Fluid Pkgs Add Comgs Image: Copy Rxg	View Set Add Set Delete Set Copy Set Import Set Export Set Add to FP
Components Fluid Pkgs Hypotheticals Oil Manager Reactions Component Maps	UserProperty
	Return to Simulation Environment
Completed.	×
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In the "Simulation Basis Manager" window, select the "Reactions" tab.

Now, click on "Add Rxn". When the "Reactions" window appears, select "Kinetic" and click on the "Add Reaction" Button.

	🏁 Kinetic Reaction: Rxn-1 📃 🗖 🔀					
	Г	-Stoichio <u>m</u> etry and	Rate Info			
🔹 Reactions 🔤 🗖 🔀		Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
Conversion Equilibrium Heterogeneous Catalytic Kinetic Simple Rate		Balance	Balance Error Reaction Hea		0.00000 <empty></empty>	
		Stoichiometry	Basis Para	meters		
Add <u>Reaction</u>		Delete	Name Rxn-	1		Not Ready

A "Kinetic" reaction is one for which we will supply the kinetic constants that define the rate of reaction. This allows us to size the reactor. If we were only interested in simulating the heat and mass balances, we could use the simpler form, a "Conversion" reaction. Then we would only have to define the percent conversion.

Click on "**Add Comp" and select the components as shown.

×	Kinetic Reacti				
Г	Stoichio <u>m</u> etry and	Rate Info			
	Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
	C02	44.010	<empty></empty>	<empty></empty>	<empty></empty>
	Hydrogen	2.016	<empty></empty>	<empty></empty>	<empty></empty>
	Methanol	32.042	<empty></empty>	<empty></empty>	<empty></empty>
	H20	18.015	<empty></empty>	<empty></empty>	<empty></empty>
	**Add Comp*				
	B <u>a</u> lance	Balance Error Reaction Heal	t (25 C)	0.00000 <empty></empty>	
-	Stoichiometry	Basis Para	meters		
	Delete	Name Rxn-1			Not Ready

Now fill in the following data:

Kinetic Reaction: Methanol Reaction 📃 🗖 🔀					
-Stoichiometry and	Stoichiometry and Rate Info				
Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order	
C02	44.010	-1.000	1.00	0.00	
Hydrogen	2.016	-3.000	3.00	0.00	
Methanol	32.042	1.000	0.00	1.00	
H20	18.015	1.000	0.00	1.00	
**Add Comp*					
Balance Error 0.00000 Reaction Heat (25 C) -4.9e+04 kJ/kgmole					
Stoichiometry Basis Parameters					
Delete	<u>N</u> ame Metha	anol Reaction		Not Ready	

The significance of the numbers should be obvious from the definition of the reaction: $3 H_2 + CO_2 => CH_2OH + H_2O$. Note that "Rxn-1" has been replaced by a more meaningful name "Methanol Reaction".

Now look at the "Basis" tab.

Kinetic Reaction	🗏 Kinetic Reaction: Methanol Reaction 🛛 📃 🗖 🔀			
Basis				
Basis	Molar Concn			
Base Component	C02			
Rxn Phase	LiquidPhase			
Min. Temperature	-273.1 C			
Max Temperature	3000 C			
Dgsis Offics	kgmole/m3 💌 kgmole/m3-s 💌			
Stoichiometry Ba	asis Parameters			
DeleteN	ame Methanol Reaction	Not Ready		

Basis = Molar Concn means that the reaction rate equation uses concentrations of the reactants in moles/ m^3 .

Base Component = CO2 means that the reaction rate equation describes the rate of consumption of CO₂, not consumption of H₂ or production of Methanol (since CO₂ consumption = methanol production, methanol could be specified here).

Rxn Phase = LiquidPhase means that the reaction takes place in the liquid. Since we will not have any liquid in the reactor, this is not helpful. Change it to "VapourPhase".

Finally, change "Rate Units" from "kgmole/m3-s" to "kgmole/m3-h". Since everything else in the model is in units of hours, it is best to be consistent.

The important consideration is to ensure that the treatment here is compatible with what was used in generating the constants describing the reaction rate (probably from lab data).

洋 Kinetic Reaction	: Methanol Reaction	
Basis		
Basis	Molar Concn	
Base Component	C02	
Rxn Phase	VapourPhase	
Min. Temperature	-273.1 C	
Max Temperature	3000 C	
Dasis Offics	kgmole/m3 💌	
<u>R</u> ate Units	kgmole/m3·h 📃 💌	
StoichiometryBa	asis Parameters	
Delete <u>N</u> a	me Methanol Reaction	Not Ready

Now go to the "Parameters" tab and enter the following values"

Forward ReactionA1.0400e+022E1.7000e+005B <empty>Reverse Reaction<empty>A'2.6000e+028E'2.2000e+005B'<empty></empty></empty></empty>	🎽 Kinetic Reaction: Methanol Reaction 🛛 📃 🗖 🔀				
	A 1.0400e+022 E 1.7000e+005 B <empty> Reverse Reaction A' A' 2.6000e+028 E' 2.2000e+005</empty>	r = k*f(Basis) - k**f'(Basis) k = A * exp { -E / RT } * T ^B k' = A' * exp { -E' / RT } * T^B'			
Delete Name Methanol Reaction Ready		arameters			

These are the kinetic constants for an Arrhenius equation: $k = A e^{(-E/RT)}$ Note that the bar in the lower right has turned green and says "Ready". This means that all the necessary data have been supplied, and are valid (that does not necessarily mean correct).

Close the window and return to the Simulation Basis Manager. Note that "Methanol Reaction" has been added to the list of reactions.

Click on "Reaction Set" in the configuration window

Configuration	Reaction <u>S</u> ets			
Reactions	Global Rxn Set	⊻iew Set		
Reaction Set		Add Set		
Shemistry Set		Delete Set		
		Copy Set		
	Assoc. Fluid Pkgs	Import Set		
		Export Set		
		Add to FP		
Components FI	uid Pkgs Hypotheticals	Oil Manager Reactions	Component Maps User P	roperties

HYSYS has put together data for a set of reactions for us called "Global Rxn Set". It only contains one reaction, "Methanol Reaction", but we could add others (e.g. side reactions that produced small quantities of ethanol and acetone). If our model contained an unrelated group of reactions (e.g. if we put a water gas shift reactor on the front of the process) we could create another Reaction Set. In this way we could model different reactors using different reactions.

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Eile Edit Basis Iools Window Help				
🗅 😅 🖬 👗 🕂 🗢 Environment: Basis Mode: Steady Stat	e			
▲ Simulati Reaction Set: Global Rxn Set				
Components Fluid Pkgs Hypotheticals Oil Manager Reactions Component Maps UserProperty	,			
Return to Simulation Environment				
	>			
View / Edit the selected Reaction Set	7			

To see what is in our Reaction Set, click on "View Set".

This does not tell us anything that we do not already know, but it confirms that our reaction is really there.

The next step is very important, and it is easy to forget to do it. If you find yourself unable to model a reactor because the reactions you need do not exist, it is probably because you forgot this step.

At this point HYSYS has put "Methanol Reaction" in "Global Rxn Set", but it has not put "Global Rxn Set" in "Basis-1". When building the reactor it will look in "Basis-1" for the reaction data.

Back in "Simulation Basis Manager" click on "Add to FP".

🖄 Add	'Global F	Rxn Set'	_ 🗆 🗙
Basis-1	NC: 4	PP: SRK	
	Add Set to) Fluid Pacl	kage

Now click on "Add Set to Fluid Package".

A Simulation Be	asis Manager		
Configuration Reactions Reaction Set Chemistry Set	Reaction <u>S</u> ets Global Rxn Set Assoc. Fluid Pkgs Basis-1	View Set Add Set Delete Set Copy Set Import Set Export Set	
Components Enter <u>P</u> VT F	Fluid Pkgs Hypotheticals	Dil Manager Reactions Component Maps Extend Simulation Basis Manager	User Properties Enter Simulation Environment

Note that "Basis-1" is now listed in "Assoc. Fluid Pkgs".

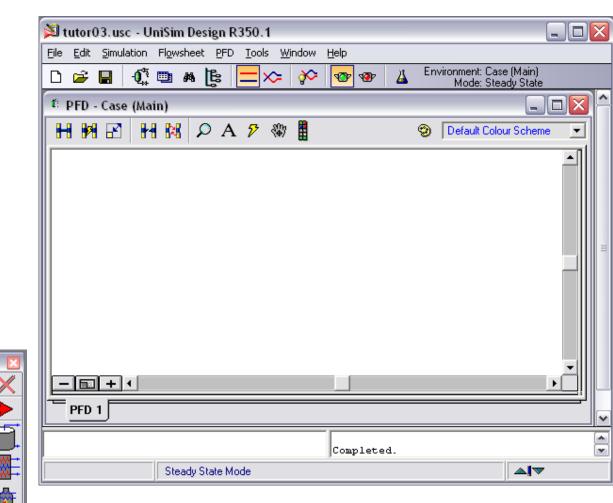
We have now finished the job of supplying the data for physical properties, components, and reactions. Note that we have left the names "Global Rxn Set", "Component List-1" and "Basis-1" with their default values. If we had more than one basis, component list, or reaction set, we would have been wise to change the names to something more meaningful, just like we changed "Rxn-1" to "Methanol Reaction". But if there is only one of each, we are not going to get confused about which one we are dealing with in the model, and this is unnecessary.

To proceed with building the process model, click on "Return to Simulation Environment".

Building the Process Flow Diagram

Always save the case at this point in the development. In this way, regardless of how screwed up the model gets, you can always go back to a valid case

Do a "Save" followed by "Save As tutor03".



We now have a blank screen on which we can start to build a PFD (Process Flow Diagram) that will define the process.

Feed Section

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Case (Main)

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While we are working on the PFD we will require the use of the unit operations palette as shown on the left. If it is not present, do "Flowsheet=>Palette".

Material Stream

The first thing we want to do is create the feed to the system. Double click on the blue material stream icon to bring up an empty stream window.

	Stream Name	1	
Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters	Vapour / Phase Fraction Temperature [C] Pressure [kPa] Molar Flow [kgmole/h] Mass Flow [kg/h] Std Ideal Liq Vol Flow [m3/h] Molar Enthalpy [kJ/kgmole] Molar Entropy [kJ/kgmole-C] Heat Flow [kJ/h] Liq Vol Flow @Std Cond [m3/h] Fluid Package	<empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	
Worksheet Attachments Dynamics			

Note that this is reminding us that the properties are being estimated with the Basis-1 package.

Enter the following data:

- Stream Name = Feed
- Temperature = $40 \, ^{\circ} \text{C}$
- Pressure = 4000 kPa
- Mass Flow = 1000 kg/h

Feed		_ 🗆 🗙	
Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters	Stream Name Vapour / Phase Fraction Temperature [C] Pressure [kPa] Molar Flow [kgmole/h] Mass Flow [kg/h] Std Ideal Liq Vol Flow [m3/h] Molar Enthalpy [kJ/kgmole] Molar Entropy [kJ/kgmole-C] Heat Flow [kJ/h] Liq Vol Flow @Std Cond [m3/h] Fluid Package	Feed <empty> 40.00 4000 <empty> 1000 <empty> <empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	
Worksheet Attachments Dynamics			
Unknown Compositions			

To finish the stream definition, we need to specify the composition. Click on "Composition" at the left side of the window.

➡ Feed _ D K			
Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters	Mole Fractions C02 <empty> Hydrogen <empty> Methanol <empty> H20 <empty> H20 <empty> Total 0.00000 Edit Edit Properties Basis</empty></empty></empty></empty></empty>		
Worksheet Attachments Dynamics			
Unknown Compositions			

We want to specify a stoichiometric ratio, so mole fraction is the correct units.

Specify:

- CO2 = .25
- H2 = .75
- "Normalize"

🎽 Input Composi	tion for Stream: Feed	
CO2 Hydrogen Methanol H2O	MoleFraction 0.2500 0.7500 J 0.0000 0	Composition Basis Composition Basis Mole Fractions Composition Eractions Composition Controls Erase Composition Controls Composition Controls Composition Controls Composition Controls Composition Controls Concel
Total	1.0000	ОК

Go back to the "Conditions" window.

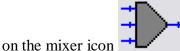
🕈 Feed		_ 🗆 🔀
Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters	Stream Name Vapour / Phase Fraction Temperature [C] Pressure [kPa] Molar Flow [kgmole/h] Mass Flow [kg/h] Std Ideal Liq Vol Flow [m3/h] Molar Enthalpy [kJ/kgmole] Molar Entropy [kJ/kgmole-C] Heat Flow [kJ/h] Liq Vol Flow @Std Cond [m3/h] Fluid Package	Feed 1.0000 40.00 4000 79.91 1000 2.795 -9.806e+004 110.7 -7.836e+006 <empty> Basis-1</empty>
Worksheet Att	achments Dynamics	
	OK	

Note that the stream is now fully defined, and HYSYS has calculated the variables that you did not specify. From now on we will only be able to change the blue values, not the black ones.

You may have notices that there were two stream icons on the palette.

The first (blue) is a material stream going from one piece of equipment to another. The second (red) is an energy stream. These will be handled by HYSYS. The energy used or generated by equipment will be displayed in these streams. This information will be useful in costing the utilities (steam, electricity etc.) used by the process.

Now let us add a mixer to combine the feed with the recycle stream. In most cases, but not all, a mixer is not a piece of equipment - just two pipes coming together.Double click



in the palette.

₱ WIX-100		
Design	<u>N</u> ame MIX-100	
Connections		
Parameters		
User Variables		
Notes		
	Injets Outlet	•
	Fluid <u>P</u> ackage Basis-1	-
Design Rating	Worksheet Dynamics	,I
Delete	Requires a feed stream	📕 🗌 Ignored

For "Name", specify "Recycle Mixer". Then click on "<<Stream>>" in the "Inlets" list. You will be presented with a list of acceptable streams.

₱ Recycle Mixer		
Design Connections Parameters User Variables Notes	Name Recycle Mixer	Outlet Fluid Package Basis-1
Design Rating	Worksheet Dynamics	
Delete	Requires a feed s	tream 🗌 🗌 Ignored

Select the only item in the list: "Feed".

Now we want a second input stream, so enter "Recycle" in the line below "Feed".

Next, click on $\mathbf{\nabla}$ in the "Outlet" box, and you will see that there are no candidate streams. So enter the name "Mixed".

♣ Recycle Mixer		
Design Connections Parameters User Variables Notes	Name Recycle Mixer	O <u>u</u> tlet Mixed Fluid <u>P</u> ackage Basis-1
Design Rating	Worksheet Dynamics	
Delete	Not Solved	🔽 Ignored

Why is it "Not Solved"? Because we have not described the other input stream "Recycle". To do this, go to the "Worksheet" tab because it will allow access to all the streams connected to the mixer.

Worksheet	Name	Feed	Recycle	Mixed
Conditions	Vapour	1.0000	<empty></empty>	<empty></empty>
	Temperature [C]	40.00	<empty></empty>	<empty></empty>
Properties	Pressure [kPa]	4000	<empty></empty>	<empty></empty>
Composition	Molar Flow [kgmole/h]	79.91	<empty></empty>	<empty></empty>
PF Specs	Mass Flow [kg/h]	1000	<empty></empty>	<empty></empty>
rr opees	Std Ideal Lig Vol Flow [m3/h]	2.795	<empty></empty>	<empty></empty>
	Molar Enthalpy [kJ/kgmole]	-9.806e+004	<empty></empty>	<empty></empty>
	Molar Entropy [kJ/kgmole-C]	110.7	<empty></empty>	<empty></empty>
	Heat Flow [kJ/h]	-7.836e+006	<empty></empty>	<empty></empty>
Design Rating	Worksheet Dynamics			

At this point we need an estimate of the recycle stream. How this is arrived at will be different for every process, but usually requires knowing what the conversion per pass in the reactor will be. For this exercise, use the following values.

- Temperature & pressure = same as stream "Feed"
- Molar Flow = 200 kgmole/h

Next, go to the "Composition" window and enter the following values.

₱ Recycle Mixer					_ 🗆 🗙
Worksheet		Feed	Recycle	Mixed	
Conditions	CO2	0.2500	0.1000	0.1428	
	Hydrogen	0.7500	0.9000	0.8572	
Properties	Methanol	0.0000	0.0000	0.0000	
Composition	H20	0.0000	0.0000	0.0000	
PF Specs					
	Worksheet Dynamics]			
Delete		OK			Ignored

Now HYSYS has sufficient data to do the necessary calculations. Let us look at the main screen.

€ PFD - Case (Main)		_ 🗆 🛛
H M 🗹 H 🕅	🛛 🔎 A 🦻 🏶 🚦	🧐 🛛 Default Colour Scheme 💽
	Recycle Recycle Mixer	
PFD 1		

Since all of the streams are dark blue, HYSYS is happy.

Before proceeding with the model a warning is in order. Notice the set of green and red traffic lights on the top toolbar. The green light at the left should have a

peach coloured square around it to indicate that it is turned on. There are some situations in which you make a mistake and HYSYS stops calculating. To indicate this, it turns off

the green light and turns on the red one. In many cases this is the only indication that something is wrong. After correcting the mistake you can waste a frustrating few minutes wondering why HYSYS does not work when all the parameters are OK. If you find yourself in this situation, check the red light. If it is on, just click on the green light and HYSYS will proceed.

The next step is to heat the mixed stream up to reactor temperature. In the palette, double



click on the heater icon.

🚿 E-100		
Design	Name E-100	
Connections		
Parameters User Variables	Injet Energy	
Notes	Fluid Package	
Design Rating	Worksheet Performance Dynamics	
Delete	Requires a feed stream	<u>I</u> gnored

Note that the Basis-1 properties package will be used here. If another one was available we could select it.

Enter the following data:

- Name = "Feed Heater"
- Inlet = "Mixed" (from dropdown list)
- Energy = "Heater duty"
- Outlet = "To Reactor" (a new stream)

🚿 Feed Heater		_ 🗆 🗙
Design	Name Feed Heater	
Connections		
Parameters	Injet Energy	
User Variables	Mixed 💌 Heater Duty 💌	
Notes	Outlet Fluid Package Basis-1	
Design Rating	Worksheet Performance Dynamics	
Delete	Unknown Delta P	📕 🔲 Ignored

Next, go to the "Parameters" window and enter a value for the pressure drop across the heater. 50 kPa is a reasonable number.

An alternative would be to leave this empty and specify the pressure of the output stream in the next step. But it makes more sense to specify the pressure drop rather than the output pressure. Consider what would happen if the upstream pressure changed.

Do not enter a value for duty. In a moment we are going to specify the output temperature, and it is not possible to specify both. Of course, there are situations in which we might want to define duty rather than temperature, but this is not one of them.

If you have used other process simulators such as PRO/II you will remember that the output temperature specification is treated as a parameter of the heat exchanger rather than the output stream. You will need to reorient your thinking.

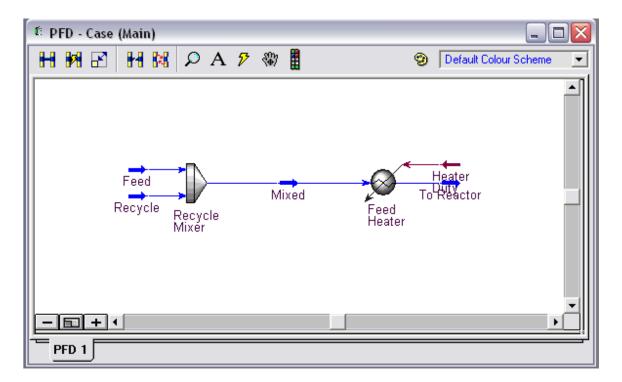
🚿 Feed Heater		- 🗆 🛛
Design Connections Parameters User Variables Notes	Delta P 50.00 kPa	
Design Rating	Worksheet Performance Dynamics	
Delete	Unknown Duty	☐ <u>I</u> gnored

To specify the temperature we need to go to the "Worksheet" tab. Enter a value of 200°C.

Worksheet	Name	Mixed	To Reactor	Heater Duty
Conditions	Vapour	1.0000	<empty></empty>	<empty></empty>
Conditions	Temperature [C]	39.81	<empty></empty>	<empty></empty>
Properties	Pressure [kPa]	4000	3950	<empty></empty>
Composition	Molar Flow [kgmole/h]	279.9	279.9	<empty></empty>
	Mass Flow [kg/h]	2243	2243	<empty></empty>
PF Specs	Std Ideal Liq Vol Flow [m3/h]	9.056	9.056	<empty></empty>
	Molar Enthalpy [kJ/kgmole]	-5.580e+004	<empty></empty>	<empty></empty>
	Molar Entropy [kJ/kgmole-C]	104.2	<empty></empty>	<empty></empty>
	Heat Flow [kJ/h]	-1.562e+007	<empty></empty>	<empty></empty>
Design Rating	Worksheet Performance Dyna	amics		

Now everything can be calculated.

Worksheet	Name	Mixed	To Reactor	Heater Duty
Conditions	Vapour	1.0000	1.0000	<empty></empty>
Conditions	Temperature [C]	39.81	200.0	<empty></empty>
Properties	Pressure [kPa]	4000	3950	<empty></empty>
Composition	Molar Flow [kgmole/h]	279.9	279.9	<empty></empty>
•	Mass Flow [kg/h]	2243	2243	<empty></empty>
PF Specs	Std Ideal Liq Vol Flow [m3/h]	9.056	9.056	<empty></empty>
	Molar Enthalpy [kJ/kgmole]	-5.580e+004	-5.088e+004	<empty></empty>
	Molar Entropy [kJ/kgmole-C]	104.2	117.0	<empty></empty>
	Heat Flow [kJ/h]	-1.562e+007	-1.424e+007	1.377e+006
Design Rating	Worksheet Performance Dyna	mics		



Before proceeding to tackle the reactor, it would be good idea to save the case again. Do "Save" followed by "Save As tutor04".

Reaction Section

We will model the reactor as a stirred vessel with sufficient cooling to maintain the output temperature at the same value as the input. On the palette, double click on the



CSTR-100		
Design	Name CSTR-100	
Connections Parameters User Variables Notes	Injets Vapour Outlet	
Design Reaction	Energy (Optional)	
Delete	Requires a feed stream	<u>Ig</u> nored

Fill in the data, using the same techniques that were used in previous units. Although we will not have any liquid leaving the reactor, UnSim requires a liquid stream just in case some is generated. The flow rate will be set to zero.

Reactor		
Design	Name Reactor	
Connections Parameters User Variables Notes	Injets To Reactor Keactor Control C	
	Fluid <u>Package</u> Basis-1	
Design Reaction	ns Rating Worksheet Dynamics	,
Delete	Requires a Reaction Set	☐ <u>I</u> gnored

Note the message about the need for reaction data. Go to the "Reactions" tab and select the reaction set from the dropdown list (only one option exists).

🔨 Reactor - Globa	l Rxn Set			_ 🗆 🔀
Reactions	Reaction Information			-
Details	Reaction <u>S</u> et Global Rxn Set	<u>R</u> eacti	ion Methanol Reactior 💌	
Results	Specifics 💿 Stoichio <u>m</u> etry	⊙ <u>B</u> asis	⊻iew Reaction	
	Stoichiometry			
	Component	Mole Wt.	Stoich Coeff	
	C02	44.010	-1.000	
	Hydrogen	2.016	-3.000	
	Methanol	32.042	1.000	
	H20	18.015	1.000	
	Add Comp**			
	B	alance Error	0.00000	
		eaction Heat (25°C)	-4.9e+04 kJ/kgmole	
Design Reaction	ns Rating Worksheet Dynar	mics		
Delete	Volun	ne not specified		🔲 Ignored

Now we need to specify the size of the reactor. At this stage we do not know how big the reactor should be. The best thing to do is set the dimensions unreasonably large. This will

drive the reaction close to the equilibrium point, and provide a stable environment when we come to deal with the recycle. Go to the "Rating" tab, and enter numbers like the following.

🔨 Reactor - Glob	al Rxn Set	
Rating Sizing Heat Loss	Geometry Orientation: Vertical Horizontal Cylinder Volume [m3] 785.4 Diameter [m] 10.00 Height [m] 10.00	
DesignReaction	ons Rating Worksheet Dynamics	
Delete	Unknown Duty	🔲 🗌 Ignored

We also have the ability to specify a pressure drop across the reactor. That is done in the "Parameters" section of the "Design" tab.

🔨 Reactor - Globa	l Rxn Set	_ 🗆 🗙
Design Connections Parameters User Variables Notes	Delta P 100.0 kPa 1.000 bar 14.50 psi Hegting Cooling Duty	
Design Reaction	ns Rating Worksheet Dynamics	
Delete	Unknown Duty	☐ <u>I</u> gnored

Now it is complaining that it does not have enough data to calculate duty (the cooling rate). We have two choices:

- Specify a cooling rate in kJ/h (the "Duty" field in the window shown above)
- Specify the outlet temperature (we will do this in the "Worksheet" tab)

🗄 Reactor - Global Rxn Set 📃 🗖 🔀					
	Name	To December	Dummer Constal	From Reactor R	
Worksheet		To Reactor	Dummy Liquid		
Conditions	Vapour	1.0000	0.0000	1.0000	
Conditions	Temperature [C]	200.0	200.0	200.0	
Properties	Pressure [kPa]	3950	3850	3850	
Composition	Molar Flow [kgmole/h]	279.9	0.0000	244.9	
	Mass Flow [kg/h]	2243	0.0000	2243	
PF Specs	Std Ideal Lig Vol Flow [m3/h]	9.056	0.0000	7.627	
	Molar Enthalpy [kJ/kgmole]	-5.088e+004	-2.521e+005	-6.227e+004	
	Molar Entropy [kJ/kgmole-C]	117.0	93.81	122.9	
	Heat Flow [kJ/h]	-1.424e+007	0.0000	-1.525e+007	
_Design _ Reacti	Design Reactions Rating Worksheet Dynamics				
Delete		DK		Ignored	

Worksheet		To Reactor	Dummy Liquid	From Reactor
	C02	0.1428	0.0127	0.0917
Conditions	Hydrogen	0.8572	0.0129	0.7653
Properties	Methanol	0.0000	0.3012	0.0715
Composition	H20	0.0000	0.6732	0.0715
PF Specs				
- Design React	ions Rating Worksheet Dyna	mics		

Now it is happy. If you want to see what is happening in the reactor, look at the "Composition" section. The output has more methanol and less $CO_2 \& H_2$ than the feed.

Recycle System

The next step is to condense the methanol and water, and return the gases as recycle.

First, we need a cooler to condense the liquid by cooling it to 40°C. We will do this in the

same way that we defined the feed heater, but will select a cooler heater from the palette. Assume a pressure drop of 50 kPa.

instead of a

🥬 Product Cooler		_ 🗆 🔀
Design	Name Product Cooler	
Connections		
Parameters	Injet Energy	
User Variables	From Reactor Prod Cooler Duty	
Notes	Outlet Fluid Package Basis-1	
Design Rating	Worksheet Performance Dynamics	
Delete	Unknown Delta P	☐ <u>I</u> gnored

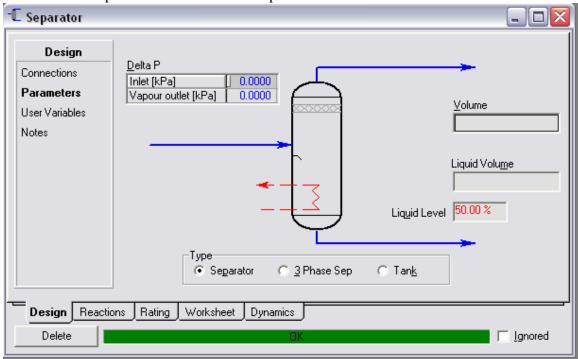
🚿 Product Cooler		
Design Connections Parameters User Variables Notes	Delta P Duty	
Design Rating	Worksheet Performance Dynamics	
	Unknown Duty	lgnored

Worksheet	Name	From Reactor	Condensed Mi:	Prod Cooler Du	
Conditions	Vapour	1.0000	0.8606	<empty></empty>	
conditions	Temperature [C]	200.0	40.00	<empty></empty>	
Properties	Pressure [kPa]	3850	3800	<empty></empty>	
Composition	Molar Flow [kgmole/h]	244.9	244.9	<empty></empty>	
•	Mass Flow [kg/h]	2243	2243	<empty></empty>	
PF Specs	Std Ideal Lig Vol Flow [m3/h]	7.627	7.627	<empty></empty>	
	Molar Enthalpy [kJ/kgmole]	-6.227e+004	-7.303e+004	<empty></empty>	
	Molar Entropy [kJ/kgmole-C]	122.9	94.61	<empty></empty>	
	Heat Flow [kJ/h]	-1.525e+007	-1.788e+007	2.635e+006	
Design Rating Worksheet Performance Dynamics					

Note that the output, "Condensed Mixture", is two phase. We need a separator to isolate

the two phases. Select a "Separator" from the palette and attach the streams as shown.

-C Separator		_ 🗆 🔀
Design Connections Parameters User Variables Notes	Name Separator	T
	Vessel Fluid Package Liquid Outlet	•
Design Reaction	ons Rating Worksheet Dynamics OK	

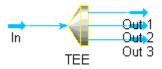


Note that this is all that HYSYS wants from us. But we have made an unconscious decision to accept a default. Look in the "parameters" section.

This is telling us that both outputs are at the same pressure as the input. There are other parameters we could specify, but they are not necessary for our case.

Before we recycle the vapour, we need to split off a small purge stream to prevent buildup of noncondensible gases in the loop. In the palette, the device we need is a "Tee".

Note that a Tee has a different shape in the PFD than in the palette



Give it the following parameters.

🗏 Purge Splitter		
Design Connections Parameters User Variables Notes	Name Purge Splitter Inlet Outlets Vapour Fluid Package Basis-1	
Design Rating	_Worksheet _DynamicsOK	Ignored

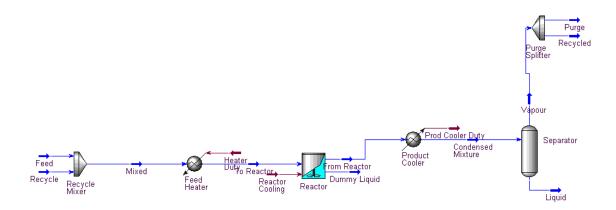
In the following window, the "Warn on Negative Flow" checkbox may not appear.

🖶 Purge Splitter			
Design Connections Parameters User Variables Notes	Splits Purge Recycled	Flow Ratios 0.000 1.000	
Design Rating	Worksheet Dynamics		
Delete		OK	🔲 Ignored

This may look like it is putting nothing into the purge stream. The problem is too few digits in the display. Look in the "Worksheet" tab.

Worksheet	Name	Vapour	Purge	Recycled		
C (1)(Vapour	1.0000	1.0000	1.0000		
Conditions	Temperature [C]	40.00	40.00	40.00		
Properties	Pressure [kPa]	3800	3800	3800		
Composition	Molar Flow [kgmole/h]	210.8	2.108e-002	210.7		
-	Mass Flow [kg/h]	1386	0.1386	1385		
PF Specs	Std Ideal Lig Vol Flow [m3/h]	6.629	6.629e-004	6.629		
	Molar Enthalpy [kJ/kgmole]	-4.204e+004	-4.204e+004	-4.204e+004		
	Molar Entropy [kJ/kgmole-C]	102.6	102.6	102.6		
	Heat Flow [kJ/h]	-8.861e+006	-886.1	-8.860e+006		
Design Rating Worksheet Dynamics						

This would be a good point to see what the process looks like. It should look something like this.



If the equipment has got pushed around on the screen do a "PFD=>Auto Position All" operation and the units will be arranged in a logical order.

The stream "Recycled" is at a lower pressure than the feed, so we need a compressor



to get it back to the mixer.

🏴 Recycle Compressor	
Design Name Recycle Compressor Connections Inlet Recycled Fluid Package Links User Variables Basis-1 Image: Comp Power Outlet Notes Energy Recycle Outlet To Recycle	
Design Rating Worksheet Performance Dynamics Delete Unknown Duty Unknown Duty	🔽 On 🔲 Ignored

In the "Parameters" section, accept the default efficiency of 75%.

🔎 Recycle Compr	essor 💷 🗖 🔀
Design Connections Parameters Links User Variables Notes	Efficiency Adiabatic Efficiency Polytropic Efficiency Cempty>
Design Rating	Operating Mode Curve Input Option Image: Constraint of the
	Unknown Duty

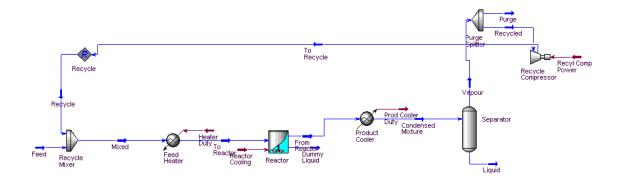
Then, set the output pressure in the "Worksheet" tab.

Vapour 1.0000 Temperature [C] 40.00 Properties Pressure [kPa] 3800 Composition Molar Flow [kgmole/h] 210.7 Mass Flow [kg/h] 1388 PF Specs LiqVol Flow [m3/h] 6.629 Molar Entropy [kJ/kgmole] -4.204e+004 Molar Entropy [kJ/kgmole] -8.860e+006 — — — — — — — — —	46.06 4000 210.7 1385 6.629 -4.186e+004 102.8	<empty> <empty> <empty> <empty> <empty> <empty> <empty> <empty> 3.859e+004</empty></empty></empty></empty></empty></empty></empty></empty>
Properties Pressure [L] 40.00 Properties Pressure [kPa] 3800 Composition Molar Flow [kgmole/h] 210.7 Mass Flow [kg/h] 1388 LiqVol Flow [m3/h] 6.629 Molar Enthalpy [kJ/kgmole] -4.204e+004 Molar Entropy [kJ/kgmole-C] 102.6	4000 210.7 1385 6.629 -4.186e+004 102.8	<emply> <emply> <emply> <emply> <emply> <emply></emply></emply></emply></emply></emply></emply>
CompositionMolar Flow [kgmole/h]210.7PF SpecsMass Flow [kg/h]1385LiqVol Flow [m3/h]6.625Molar Enthalpy [kJ/kgmole]-4.204e+004Molar Entropy [kJ/kgmole-C]102.6	210.7 1385 6.629 -4.186e+004 102.8	<empty> <empty> <empty> <empty> <empty></empty></empty></empty></empty></empty>
PF Specs Mass Flow [kg/h] 1385 LiqVol Flow [m3/h] 6.625 Molar Enthalpy [kJ/kgmole] -4.204e+004 Molar Entropy [kJ/kgmole-C] 102.6	1385 6.629 -4.186e+004 102.8	<empty> <empty> <empty> <empty></empty></empty></empty></empty>
PF Specs Mass Flow [kg/h] 138t LiqVol Flow [m3/h] 6.625 Molar Enthalpy [kJ/kgmole] -4.204e+004 Molar Entropy [kJ/kgmole-C] 102.6	6.629 -4.186e+004 102.8	<empty> <empty> <empty></empty></empty></empty>
Molar Enthalpy [kJ/kgmole] -4.204e+004 Molar Entropy [kJ/kgmole-C] 102.6	-4.186e+004 102.8	<empty> <empty></empty></empty>
Molar Entropy [kJ/kgmole-C] 102.6	102.8	<empty></empty>
191 2 1		
Heat Flow [kJ/h] -8.860e+000	-8.821e+006	3.859e+004
Design Rating Worksheet Performance Dynamics		

We are about to close the recycle loop. In doing this, it is not uncommon to end up with an unworkable model. Always save the case before closing the loop. Do a "File Save" and "File Save As tutor05".

e	cle" unit from the palette	and specify the two com	
Recycle			
Connections	Name Recycle	Fluid <u>P</u> ackage Basis-1	
Notes	Injet To Recycle	Oytlet Recycle	
Connections	Parameters Worksheet Monitor	User Variables	
		OK	
Delete	Continue	<u>R</u> ecycle Assistant	Ignored

The PFD should now look something like this:



Before we finish with the reaction section there is one more job to do. Earlier we had set aside the question of how big the reactor should be and just set it very big. For all practical purposes the stream leaving the reactor is at the equilibrium concentration. There is a tradeoff here between reactor size and the size of the rest of the equipment in the recycle loop. If we reduce the size of the reactor, the conversion per pass will fall. This will require a higher recycle rate, leading to larger heat exchangers compressor separator etc. Somewhere there will be an minimum equipment cost (operating costs will also be an issue).

For this exercise we will say that previous designs have shown the optimum is about 90% of the equilibrium conversion, and the height of the reactor should be twice the diameter.

Reactions	Reaction Results Sum Extents		ion <u>B</u> alance		
)etails		Act. % Cnv.	Base Comp	Rxn Extent	-
esults	Methanol Reaction	46.03	CO2	19.75	-
					-
					-
					_
					_
					-
					-

Look at the "Results" section of the "Reactions" tab.

We should aim for a conversion of 46.03 * .9 = 41.4

Vary the reactor size and see what happens to the conversion.

壁 Reactor - Globa	ıl Rxn Set			_ 🗆 🖂
Rating Sizing Heat Loss	<u>G</u> eometry	Orientation: Volume [m3] Diameter [m] Height [m] as a boot	C Horizontal 3.142 2.000 1.000	
DesignReaction	ns Rating Wo	rksheet Dynamics		
Delete		OK		🔲 🗌 Ignored

<u>Diameter</u>	<u>Heigh</u> t	Conversion
1	2	42.65
.9	1.8	41.54
.89	1.78	41.40

Depending upon what numbers you enter, you may encounter unusual results. The conversion you observe may depend upon, not only the values of the dimensions that you have specified, but also the values you specified in preceding runs. This results from the fact that essentially all of the calculations done by a process simulator are trial-and-error sequences. The system has to decide when to quit. Sometimes it makes a good decision, sometimes it stops too soon. This is most likely to occur in models with recycle loops.

In most cases of adjusting parameters like this you will sneak up on the correct values, the last few runs will have similar values, and error will be small. But there are times in which you will want to run the case a few times to let it settle out.

We will end up with something like this.

🖲 Reactor - Global	Rxn Set				
Reactions Details Results	Reaction Results Sum		ion <u>B</u> alance Base Comp CO2	Rxn Extent 19.27	
Design Reaction	ns Rating Workshe	et Dynamics			J
Delete		OK			🔲 Ignored

🤨 Reactor - Globa	ıl Rxn Set			_ 🗆 🖂
Rating Sizing Heat Loss	<u>G</u> eometry ● <u>C</u> ylinder ● Sghere ■ This reactor h	Orientation: Volume [m3] Diameter [m] Height [m]	 Horizontal 2.215 1.780 0.8900 	
Design Reactio	ns Rating Wo	orksheet Dynamics		
		OK		☐ <u>I</u> gnored

Do a "File Save" and "File Save As tutor06".

Product Separation Section

All of the equipment simulations we have done so far have been ones in which any reasonable set of parameters would lead to a calculation that works. For example, as long as we did not do anything ridiculous like specify a temperature of -500C, we would get a valid heat exchanger design. The answer might not be what we wanted, but we would get an answer.

With a distillation column we might not even get an answer. You may recall from earlier courses in distillation that some separations are only possible with a number of equilibrium stages above a certain value, or a reflux ratio above a certain value. Some configurations just do not work.

In most cases we want to design a column to meet certain concentration specifications. In our case they are:

- 97% of the methanol entering the column leaves in the product
- The methanol product contains 1% (by mass) water

There are two specifications because a simple column with two products and feed, pressure, number of stages, location of feed tray specified has two degrees of freedom.

In some cases we could go directly to a model with these specs. In general, it is safer to start by creating a case that works (even though it is not what we want) and then migrate to the case we want. The configuration most likely to work is specifying:

- The flow from either the top or the bottom of the column
- The reflux ratio

We will do it this way.

With HYSYS you must have certain information lined up before you start putting the column together. You will be taken through a series of windows that you must complete. You cannot break out and come back later. We will need the following information:

- Name of feed stream ("Liquid")
- Number of stages (this separation is easy so try 10)
- Location of feed (we have nothing to base this on so put it in the middle stage 5)
- Pressure in the condenser (use 1000 kPa)
- Pressure in the reboiler (use 1015 kPa)
- Will we take the product off as a liquid or vapour (vapour, do you think it would be a good idea to attempt to condense hydrogen?)
- A starting value for reflux ratio (3 is suggested most cases will end up between .5 and 10)
- A starting value for the distillate rate (19.729 kgmoles/hr see the chart below)

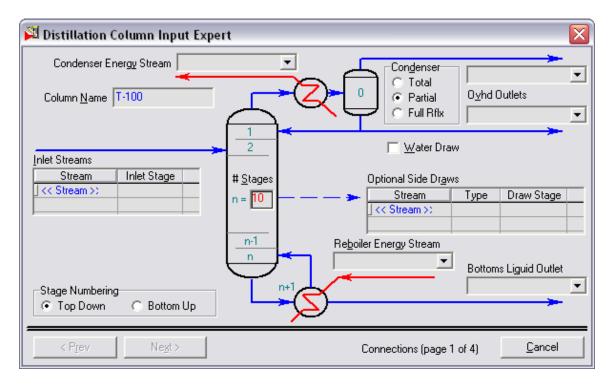
➡ Liquid	
Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters	Molar Flows C02 0.45603 Hydrogen 1.5758e-002 Methanol 19.257 H2O 19.265 Image: Strate Stra
Worksheet At	achments Dynamics
Delete	Define from Other Stream 🔶 🗭 🔿

What we expect to happen here is for most of the CO2, hydrogen and methanol to come out the top of the column, and most of the water out the bottom. So the sum of the first three components is a good guess for the distillate rate.

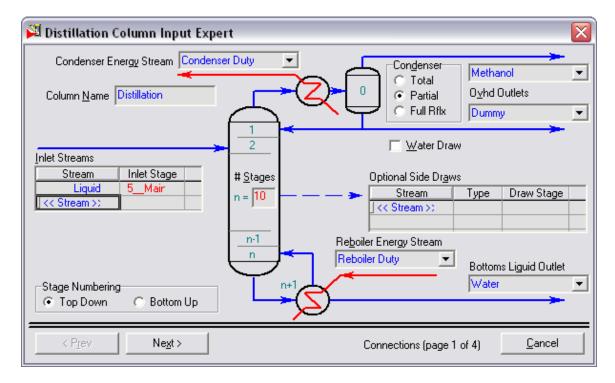
Double clicking on the "Distillation Column" icon up this:



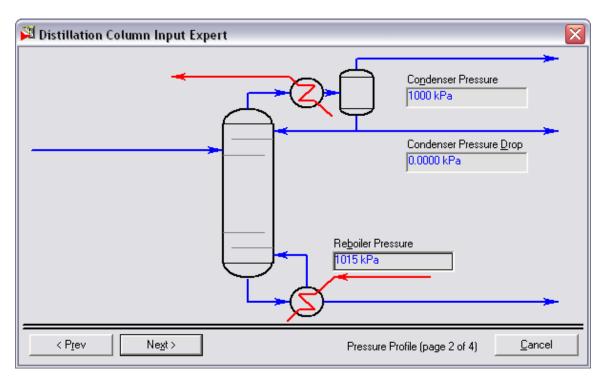
• on the palette will bring



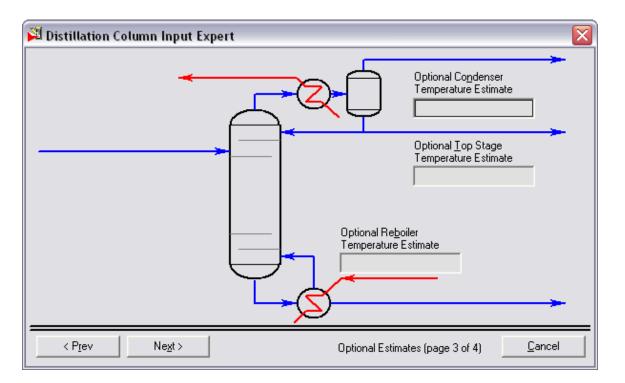
Enter the following data:



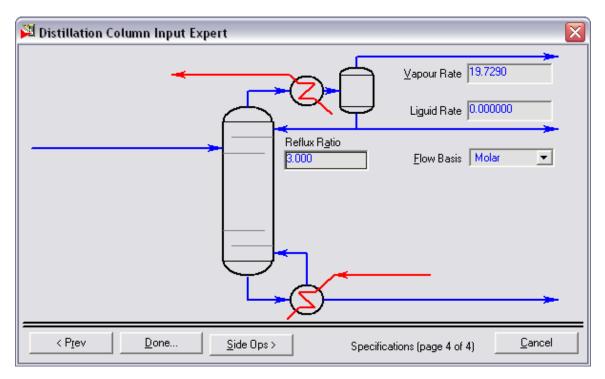
We want to take all of the top product as a vapour. A partial condenser allows both liquid and vapour. We have specified two streams, but will set the flow of "Dummy" to zero at a later step. Note that the addition of this third output stream increases the degrees of freedom by 1. At the same time a constraint (flow = 0) is added and the net effect is that we still need to provide two specifications. Another way of looking at it is that a stream with zero flow does not really exist.



Next, specify the pressure profile.



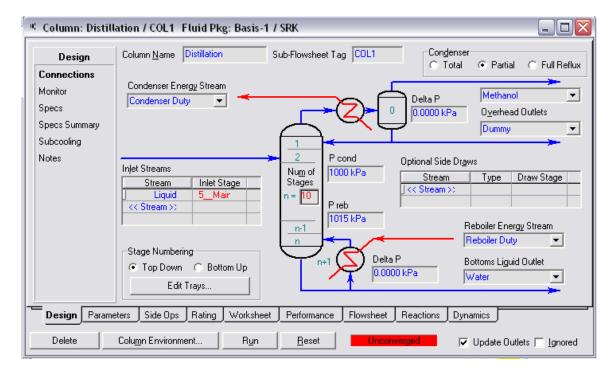
In case with complex vapour-liquid equilibrium relationships, estimating the temperature profile can help the program to converge on the right answer. Our case does not require this.



Note that we have set "Dummy" to zero as we will not take any liquid off the top of the column.

By supplying Vapour rate and Reflux Ratio values here we are asking HYSYS to set up two specifications that will generate a solution that matches these values. But we don't want this solution, we want one that matches composition specs. My experience has been that, if I start to model a column without having prior experience to tell me what is reasonable, I have less than a 50% chance of getting a composition spec case to work.

Our strategy will be to develop a case that we don't want (vapour rate – reflux ratio) and then modify it to get the case we do want (compositions). This is an example of a technique that can be very useful in modeling. Start by getting something that works, even if it is not what you want. Then, by changing parameters, migrate to the case you want. At each step in the process you have a case that works. This is much better than taking a case that does not work and trying to make it work.



We now have all the parameters specified. Click on "Done".

Click on run and get a valid case (but not the right case).

🤻 Column: Distill	ation / COL1 Fluid Pkg: Basis-1	/ SRK	_ 🗆 🗙
* Column: Distill Design Connections Monitor Specs Specs Summary Subcooling Notes		Sub-Flowsheet Tag COL1	Condenser Total Partial Full Reflux Delta P Overhead Outlets Dummy
	Stream Inlet Stage	Num of Stages n = 10 P reb 1015 kPa n+1 Delta P 0.0000 kJ	Stream Type Draw Stage < Stream >: Image: Stream Reboiler Energy Stream Image: Stream Reboiler Duty Image: Stream Bottoms Liguid Outlet Image: Stream Pa Image: Stream
Design Parame	Edit Trays eters Side Ops Rating Worksheet Column Environment	Performance Flowsheet R	eactions Dynamics

To complete the job, go to the "Specs" section.

🖲 Column: Distilla	ation / COL1 Fluid Pkg: Basis-1 / SRK	
Design Connections Monitor Specs Specs Summary Subcooling Notes	Column Specifications Reflux Ratio Ovhd Vap Rate Distillate Rate Reflux Rate Btms Prod Rate Delete	Specification Details Spec Name Reflux Ratio Converged ? Yes Yes Current Dry Flow Basis Spec Type Fixed/Ranged Spec Fixed/Ranged Spec Primary/Alternate Spec
	Update Specs from Dynamics Default Basis Molar Degrees of Freedom Switch To Alternate Specs	Values Specification Value 3.000 Current Calculated Value 3.000 Errors Weighted Tolerance 1.000e-002 Weighted Calculated Error -7.067e-005 Absolute Tolerance 1.000e-002 Absolute Calculated Error 2.120e-004
Design Parame	eters Side Ops Rating Worksheet Performan	ance Flowsheet Reactions Dynamics
Delete	Colu <u>m</u> n Environment <u>Run <u>R</u>eset</u>	t Converged 🔽 Vpdate Outlets 🥅 Ignored

If you examine the "Column Specifications" you will see that the first three are "Active" (the calculations force them to be met) and the last two are alternatives that are "Inactive" (ignored). We will leave "Distillate Rate" alone (the dummy liquid stream) while we replace "Reflux Ratio" and "Ovhd Vap Rate" by our two composition specs.

First, create the two new specs but leave them inactive. Under "Column Specifications" click on the "Add" button and start on the methanol recovery spec.

🏁 Add Specs - Distillati 🔀
Column Specification Types
Column Cold Properties Spec Column Component Flow Column Component Fraction Column Component Ratio Column Component Recovery Column Cut Point Column Draw Rate Column DT (Heater/Cooler) Sper Column DT (Heater/Cooler) Sper Column DT Spec Column Dt Spec Column Duty Column Duty Ratio Column Duty Ratio Column Feed Ratio Column Feed Ratio
Column Physical Properties Spec Column Pump Around Column Reboil Ratio Spec Column Recovery Column Reflux Feed Ratio Spec
Add Spec(s)

Select "Component Recovery" and click on "Add Spec(s)...".

🎽 Comp Recov Spec: Comp 🗐 🗆 🔀	🏁 Comp Recov Spec: Comp 📃 🗆 🔀	
Name Comp Recovery Draw << Stream >> Spec Value <empty></empty>	Name Comp Recovery Draw Methanol @COL1 Spec Value 0.9700	
Components:	Components: <u>Methanol</u> << Component >>	
Target Type 💿 Stream 🔿 Stage	Target Type 💿 Stream 🔿 Stage	
Parameters Summary Spec Type	Parameters Summary Spec Type	

"Recovery" means the fraction of the component in the feed that goes to the specified stream. You should select "Stream" for "Target Type", not "Stage". The "Stage" option allows you to specify a condition within the column.

Now do the methanol concentration in water spec.

🏁 Add Specs - Distillati 🔀	
Column Specification Types	
Column Cold Properties Spec	
Column Component Fraction Column Component Ratio	🏁 Comp Frac Spec: Comp Fr 🖃 🗆 🔀
Column Component Recovery Column Cut Point Column Draw Rate	Name Comp Fraction Draw Methanol @COL1
Column DT (Heater/Cooler) Spei [≡] Column Dt Spec Column Duty	Basis Mass Fraction Spec Value 1.000e-002
Column Duty Ratio Column Feed Ratio Column Gap Cut Point Column Liquid Flow Column Physical Properties Spec	Components: H20 << Component >>
Column Pump Around Column Reboil Ratio Spec Column Recovery	Target Type 💿 Stream C Stage
Column Reflux Feed Ratio Spec	Parameters Summary Spec Type
Add Spec(s)	Delete

The "Spec Values" we have entered are the ones that we will end up using, but now we want to synchronize them with the vapour rate – reflux ratio case. First, select the "Comp Fraction" spec.

🤻 Column: Distilla	ntion / COL1 Fluid Pkg: Basis-1 / SRK	
Design Connections Monitor Specs Specs Summary Subcooling Notes	Column Specifications Reflux Ratio View	Specification Details Spec Name Comp Fraction Image: Comp Fraction Converged ? Inactive Image: Comp Fraction Spec Type Image: Comp Fraction Image: Comp Fraction Spec Type Fixed/Ranged Spec Fixed * Primary/Alternate Spec Primary
	Update Specs from Dynamics Default Basis Molar Degrees of Freedom 0	Values 1.000e-002 Current Calculated Value 2.365e-002 Errors
	Switch To Alternate Specs	Absolute Tolerance 1.000e-003 Absolute Calculated Error 1.365e-002
Design Paramet	ters <u>Side Ops</u> Rating Worksheet Performan	ce Flowsheet Reactions Dynamics
Delete	Colu <u>m</u> n Environment R <u>u</u> n <u>R</u> eset	Converged Vpdate Outlets 🗐 Ignored

Change the "Specification Value" to the value that "Current Calculated Value" has in the current case , and make the spec active.

Note that "Degrees of Freedom" has changed from zero (the correct number of specs are active) to -1 (too many are active). Deactivate "Ovhd Vap Rate" and look at "Comp Recovery".

🖲 Column: Distillation / COL1 🛛 Fl	uid Pkg: Basis-1 /	SRK		
Default Basis		ew	Specification Details Spec Name Comp Recovery Converged ? Yes Spec Type Fixed/Ranged Spec Primary/Alternate Spec Values Specification Value Current Calculated Value Errors Weighted Tolerance Weighted Tolerance Absolute Tolerance Absolute Calculated Error	✓ Active ✓ Use As Estimate ✓ Current Dry Flow Basis Fixed Primary 0.9574 0.9574 0.9574 1.000e-002 1.686e-005 1.000e-003 3.301e-005
Design Parameters Side Ops	Rating Worksheet	Performance	Flowsheet Reactions Dynam	ics
DeleteColu <u>m</u> n Environmen	it R <u>u</u> n	<u>R</u> eset	Unconverged 🔽 U	pdate Outlets 🥅 Ignored

Now do the same with this spec. Put the "Current Calculated Value" in "Specification Value" and activate the spec.

🦉 Column: Distilla	ation / COL1 Fluid Pkg: Basis-1 / SRK	
Design Connections Monitor Specs Specs Summary Subcooling Notes	Column Specifications Reflux Ratio View Ovhd Vap Rate Add Distillate Rate Add Btms Prod Rate Delete Comp Recovery Delete Comp Fraction Delete Update Specs from Dynamics Default Basis Default Basis Molar Switch To Alternate Specs -2	Specification Details Image: Agtive Spec Name Comp Fraction Image: Use As Estimate Converged ? Yes Image: Use As Estimate Spec Type Image: Dry Flow Basis Spec Type Fixed Primary Fixed/Ranged Spec Fixed Primary Values Primary Primary Current Calculated Value 2.365e-002 Errors Weighted Tolerance 1.000e-002 Weighted Tolerance Weighted Calculated Error 8.451e-005 Absolute Tolerance Absolute Calculated Error 3.742e-006
Design Parame	ters Side Ops Rating Worksheet Performan	ce Flowsheet Reactions Dynamics
Delete	Colu <u>m</u> n Environment R <u>u</u> n <u>R</u> eset	Unconverged Vpdate Outlets 🔽 Ignored

We now have two too many specs. Deactivate "Reflux Ratio" and "Ovhd Vap Rate" and the case will run.

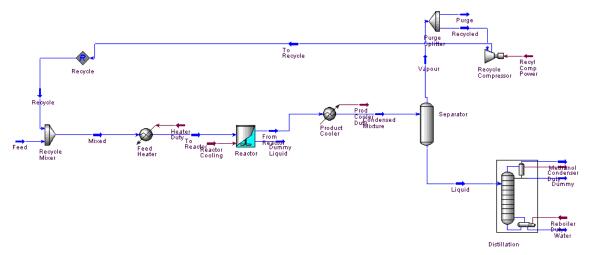
🕷 Column: Distilla	ntion / COL1 Fluid Pkg: B	asis-1 / SRK		
Design Connections Monitor Specs Specs Summary Subcooling Notes	Column Specifications Reflux Ratio Ovhd Vap Rate Distillate Rate Btms Prod Rate Comp Recovery Comp Fraction Update Specs from Default Basis Molar Degrees of f		Specification Details Spec Name Comp Recovery Converged ? Yes Spec Type Fixed/Ranged Spec Frixed/Ranged Spec Primary/Alternate Spec Values Specification Value Specification Value I Current Calculated Value Errors Weighted Tolerance I Weighted Calculated Error I	I Active I Use As Estimate I Current Dry Flow Basis Fixed Primary 0.9574 0.9574 1.000e-002 -3.983e-006
	Switch To Alterna	te Specs	Absolute Tolerance Absolute Calculated Error	1.000e-003 7.796e-006
Design Paramet	ters Side Ops Rating Wo	rksheet Performance	e Flowsheet Reactions Dynami	
Delete	Colu <u>m</u> n Environment	R <u>u</u> n <u>R</u> eset	Converged 🔽 Up	odate Outlets 🥅 Ignored

We have switched to a new set of specs, but the case has not really changed. All of the concentrations, temperatures etc. are the same as before. This makes the transition more or less foolproof.

🤘 Column: Distilla	ation / COL1 Fluid Pkg: Basis-1 / SRK		
Design Connections Monitor Specs Specs Summary Subcooling Notes	Column Specifications Reflux Ratio View Ovhd Vap Rate Add Distillate Rate Add Btms Prod Rate Delete Comp Recovery Delete Comp Fraction Delete Update Specs from Dynamics Default Basis Default Basis Molar Switch To Alternate Specs O	Specification Details ✓ Agtive Spec Name Comp Recovery ✓ Use As Estimate Converged ? Yes ✓ Eurrent Dry Flow Basis ✓ Dry Flow Basis Spec Type Fixed Primary/Alternate Spec Fixed Primary/Alternate Spec Primary Values Specification Value 0.9700 Current Calculated Value 0.9701 Errors Weighted Tolerance 1.000e-002 Weighted Calculated Error 2.663e-005 Absolute Tolerance 1.000e-003 Absolute Calculated Error 5.258e-005	
Design Parame Delete	ters Side Ops Rating Worksheet Performance Column Environment Run <u>R</u> eset Ation / COL1 Fluid Pkg: Basis-1 / SRK	Flowsheet Reactions Dynamics	
Design Connections Monitor Specs Specs Summary Subcooling Notes	Column Specifications Reflux Ratio Ovhd Vap Rate Distillate Rate Reflux Rate Btms Prod Rate Comp Recovery Comp Fraction Update Specs from Dynamics Default Basis	Specification Details ✓ Active Spec Name Comp Fraction ✓ Use As Estimate Converged ? Yes ✓ Lurrent Dry Flow Basis ✓ Dry Flow Basis Spec Type Fixed/Ranged Spec Fixed * Primary/Alternate Spec Primary Values 1.000e-002 Current Calculated Value 9.999e-003 Errors Errors	
Degrees of Freedom 0 Weighted Tolerance 1.000e-002 Weighted Calculated Error -4.772e-005 Absolute Tolerance 1.000e-003 Absolute Tolerance 1.000e-003 Absolute Tolerance 1.009e-006 Design Parameters Side Ops Rating Worksheet Performance Flowsheet Reactions Dynamics Delete Column Environment Run Reset Converged Update Outlets Ignored			

The final step is to change the values of the specs to what we really want.

The PFD should now look like this:



Now do a "File Save" and "File Save As tutor07".

Before leaving the column simulation, let us review the steps we went through to get the case we wanted.

- 1. Estimate the distillate rate from the feed composition and a knowledge of which components are to go out the top.
- 2. Pick a starting value for reflux ratio. Other programs use a default of 3, and that works most of the time.
- 3. Build a model with distillate rate and reflux ratio specs.
- 4. Get this model to converge. It may be necessary to change parameters such as number of stages, feed location, reflux ratio etc.
- 5. Build the specs that you really want and set their values to those in the working case.
- 6. Activate these new specs and deactivate the distillate/reflux ones. The model should converge.
- 7. Change the values of the new specs to match what you want in the column. If there is a large change, you may want to do it in stages.

Product Finishing

The final step in the process is to condense the methanol product and prepare it for storage. Before we start on the condenser, we need a source of cooling water. It will be taken from a storage tank and pumped to 600 kPa. Initially, we will set the flow rate very high (100,000 kg/hr) to ensure that we have enough for the heat exchanger. During the heat exchanger design we will reduce this to a reasonable value.

Set up stream "Water Source" in the same way that we created "Feed".

🔫 Water Source		_ 🗆 🔀
Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters	Stream Name Vapour / Phase Fraction Temperature [C] Pressure [kPa] Molar Flow [kgmole/h] Mass Flow [kg/h] Std Ideal Liq Vol Flow [m3/h] Molar Enthalpy [kJ/kgmole] Molar Entropy [kJ/kgmole-C] Heat Flow [kJ/h] Liq Vol Flow @Std Cond [m3/h] Fluid Package ◀	Water Source 0.0000 30.00 150.0 5551 1.000e+005 100.2 -2.851e+005 54.63 -1.583e+009 98.54 Basis-1 ▶
Worksheet Att	achments Dynamics	
Delete	OK Define from Other Stream	← ⇒

🔫 Water Source		_ 🗆 🔀
Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters	CO2 Hydrogen Methanol H2O J Total 1.00000 E_dit Edit Properties	Fractions 0.000000 0.000000 1.000000 ■ ■ ■ ■ Basjs
Worksheet Att	achments Dynamics	
Delete	OK Define from Other Stream	\



Now add a pump.

🕿 Water Pump		
Design	Name Water Pump	
Connections		
Parameters	Outlet	
Curves	Injet To Condenser 💌	
Links	Water Source	
User Variables		
Notes		
	Energy Fluid <u>P</u> ackage	
Design Rating	Worksheet Performance Dynamics	
Delete	Unknown Duty 🔽 On 🔲 Igne	ored

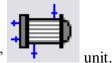
As with the compressor, we set the output pressure in the output stream. Use a value of 600 kPa.

🖉 Water Pump				_			
Worksheet	Name	Water Source	To Condenser	Pump Power			
	Vapour	0.0000	0.0000	<empty></empty>			
Conditions	Temperature [C]	30.00	30.03	<empty></empty>			
Properties	Pressure [kPa]	150.0	600.0	<empty></empty>			
Composition	Molar Flow [kgmole/h]	5551	5551	<empty></empty>			
· ·	Mass Flow [kg/h]	1.000e+005	1.000e+005	<empty></empty>			
PF Specs	Std Ideal Lig Vol Flow [m3/h]	100.2	100.2	<empty></empty>			
	Molar Enthalpy [kJ/kgmole]	-2.851e+005	-2.851e+005	<empty></empty>			
	Molar Entropy [kJ/kgmole-C]	54.63	54.63	<empty></empty>			
	Heat Flow [kJ/h]	-1.583e+009	-1.583e+009	5.979e+004			
Design Rating Worksheet Performance Dynamics							
Delete OK On I Ignored							

Now we can start on the heat exchanger.

HYSYS provides three levels of detail for heat exchanger design:

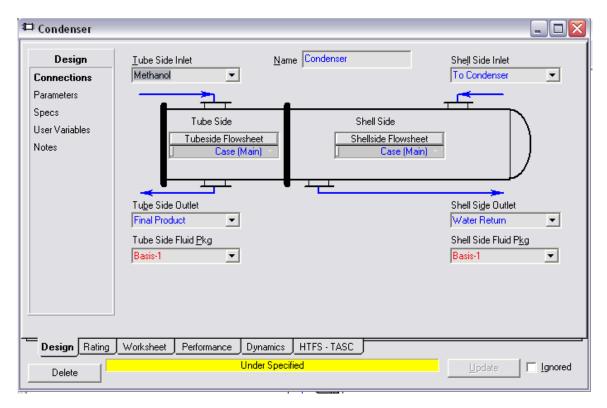
- 1. The simple method, using a "Heater" or "Cooler" just does the heat balance necessary to take a stream to a specified temperature.
- 2. The intermediate method deals with transfer of heat between two streams. A value of UA (overall heat transfer coefficient * heat transfer area) is specified and HYSYS calculates the two output temperatures. If an estimate of U is available, the area can be calculated and used for a crude cost estimate. The recommended procedure is "Exchanger Design (Weighted)".
- 3. The most rigorous method is "Steady State Rating". With this procedure the mechanical design is specified (tube number/dimensions/spacing, shell number and configuration, etc.), HYSYS estimates U and calculates the two output temperatures. We will defer the use of this method until we have learned more about heat exchanger design.



Let us design the condenser by method 2, using the "Heat Exchanger"

There are two requirements for the design. The process stream should exit at 40°C, and the cooling water at 45°C.

Start by specifying the following data. Note that the process stream is going through the tubes and the cooling water through the shell.

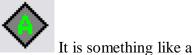


In the "Parameters" section select the "Exchanger Design (Weighted)" method and supply pressure drop estimates. Then adjust the UA value so that the stream "Final Product" has a temperature near the target of 40°C, as seen in the Workshop tab.

🕮 Condenser		X
Design Connections Parameters	Heat Exchanger Model Exchanger Design (Weighted) ▼	
Specs User Variables Notes	Tube Side Shell Side Delta P Delta P 50.00 kPa UA 1.200e+004 kJ/C-h	
	Pass Name Intervals Dew/Bubble Pt Step Type Pressure Profile Methanol-Final Pr 5 I Equal Enthalpy Const dPdH To Condenser-W 5 I Equal Enthalpy Const dPdH	
Design Rating	Worksheet Performance Dynamics HTFS - TASC	

	Name	Methanol	Final Product	To Condenser	Water Return
Worksheet					
Conditions	- Vapour	1.0000	0.0007	0.0000	0.0000
	Temperature [C]	138.1	39.22 950.0	30.03 600.0	31.94 550.0
Properties	Pressure [kPa]	19.50	950.0	5551	5551
Composition	Molar Flow [kgmole/h]	624.9	624.9	1.000e+005	1.000e+005
PF Specs	Mass Flow [kg/h] Std Ideal Lig Vol Flow [m3/h]	0.7832	0.7832	100000000000000000000000000000000000000	100000000000000000000000000000000000000
rr specs		-2.022e+005	-2.454e+005	-2.851e+005	-2.850e+005
	Molar Enthalpy [kJ/kgmole] Molar Entropy [kJ/kgmole-C]	133.6	-2.4048+000	54.63	55.13
	Heat Flow [kJ/h]	-3.942e+006	-4.784e+006	-1.583e+009	-1.582e+009
Design Rating	Worksheet Performance Dyna	amics _ HTFS - TASC OK	:	Update	e 🗖 Ignored

We are not finished because the cooling water exit temperature is too low because of the



high flow rate. HYSYS has a unit called an adjust.

process controller in a plant, but it manipulates the model, not the process. It tells us nothing about the dynamics of the process. Like a controller, it changes the value of one parameter in order to bring another parameter to a specified value.

♦ Water T Contro		
Connections	Adjust <u>N</u> ame Water T Control	
Connections	Adjusted Variable	
Notes	Object:	Select <u>V</u> ar
	Variable:	
	Target Variable	
	Object:	Select Va <u>r</u>
	Variable:	
	Target Value Source Surce Specified Target Value Another Object SpreadSheetCell Object	
	arameters Monitor User Variables	
	Requires an Adjust connection	
Delete	Start	Ignored

First, under "Adjusted Variable" click on "Select Var" and specify that we want it to manipulate the cooling water flow.

Select Adjusted Value	* Select Adjusted Variable ForWater T Control					
Flowsheet Case (Main) Distillation (COL1)	Object Mixed Prod Cooler Duty Pump Power Purge Reactor Cooling Reboiler Duty Recycle Recycled Recycled Recycled Recycled Recycled Vapour Vapour Water Water Return Water Source	⊻ariable BO Std Vol Flow - Gas BO Std Vol Flow - Oil BO Std Vol Flow - Overall BO Std Vol Flow - Vater BO Std Vol Flow - Water BO Surface Tension BO Viscosity Coefficient A BO Water Oil Ratio Mow Flow Molar Enthalpy Molar Flow PHValue Processes	Variable <u>Specifics</u>	<u>D</u> K Object <u>F</u> ilter C All C Streams C UnitOps C Logicals C Utilities C ColumnOps C Custom Custom Disconnect		
Variable <u>D</u> escription	Mass Flow			<u>C</u> ancel		

Then, under "Target Variable" click on "Select Var" and specify that we want to control the outlet water temperature.

Flowsheet	<u>0</u> I	bject	<u>V</u> ariable	Variable <u>Specifics</u>	ОК
	ain) Mixed DL1) Prod Coo Purge Reactor I Reboiler Recycleo Recycleo To Cond To Reac To Reac Vapour Water Water Re Water So	wer Cooling Duty f mp Pow enser tor cle	Power Pressure Product Nozzle Elevation Specific Gravity Specific Gravity rel Air Std Gas Flow Std Ideal Lig Mass Densi Std Ideal Lig Vol Flow Std Lig Vol Flow Spec Steady State Specs Surface Tension Temperature Thermal Conductivity Total Component Liquid V Total Component Mass F Total Component Mole Fl		Dbject <u>F</u> ilter C All Streams C UnitOps C Logicals C Utilities C ColumnOps C Custom <u>Custom</u>
Variable <u>D</u> escriptior	n Temperat	ure			Cancel

The value we want it to settle out at is 45°C.

🔷 Water T Contro	ıt				
Connections	Adjust <u>N</u> ame Water T Control				
Connections	Adjusted Variable				
Notes	Object: Water Source	Select <u>V</u> ar			
	Variable: Mass Flow				
	Target Variable				
	Object: Water Return	Select Va <u>r</u>			
	Variable: Temperature				
	Target Value Source Surce Specifie <u>d</u> Target Value Another Object SpreadSheetCell Object				
Connections F	Parameters Monitor User Variables				
	Unknown Maximum				
Delete	Start	☐ <u>I</u> gnored			

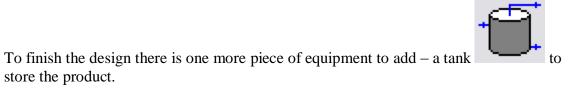
Ignore the warning about "Unknown Maximum". If there is a problem in converging, changing the values in the "Parameters" tab may help.

ĺ	UniSim I	Design 🛛 🔀
	2	Adjust Water T Control is at maximum iterations. Do you wish to continue for another 10 iterations?
		<u>Y</u> es <u>N</u> o

This message is common the first time the model is run. Click on "Yes".

Now look at the condenser worksheet tab and verify that both outlet temperatures are correct.

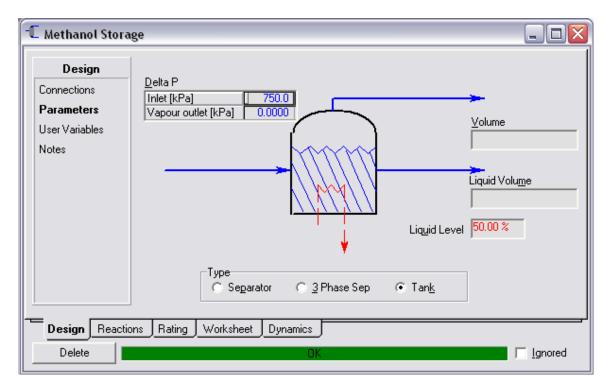
Worksheet	Name	Methanol	Final Product	To Condenser	Water Return
a r.:	Vapour	1.0000	0.0007	0.0000	0.0000
Conditions	Temperature [C]	138.1	42.06	30.03	45.05
Properties	Pressure [kPa]	1000	950.0	600.0	550.0
Composition	Molar Flow [kgmole/h]	19.50	19.50	697.2	697.2
	Mass Flow [kg/h]	624.9	624.9	1.256e+004	1.256e+004
PF Specs	Std Ideal Liq Vol Flow [m3/h]	0.7832	0.7832	12.59	12.59
	Molar Enthalpy [kJ/kgmole]	-2.022e+005	-2.450e+005	-2.851e+005	-2.839e+005
	Molar Entropy [kJ/kgmole-C]	133.6	24.78	54.63	58.49
	Heat Flow [kJ/h]	-3.942e+006	-4.778e+006	-1.988e+008	-1.980e+008
Design Rating	Worksheet Performance Dyna	amics HTFS - TASC	:		
		OK		Update	e 📃 📃 Ignore



Connect the input stream "Final Product" and supply names for liquid and vapour outputs.

🕂 Methanol Stora	ge	- 🗆 🛛
Design Connections Parameters User Variables Notes	Name Methanol Storage Inlets Vapour Outlet < Vent Liquid Outlet Shipping Vessel Fluid Package	
Design Reaction	ons Rating Worksheet Dynamics	
Delete	OK	Ignored

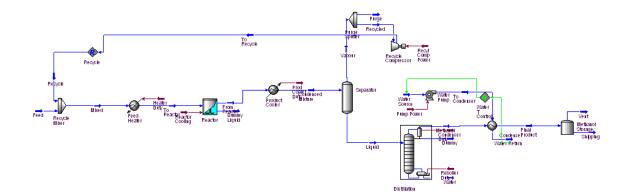
Also, you can specify the pressure in the tank.



Note that there is some vapour (mostly CO_2 and hydrogen) that will be vented from the tank. "Final Product" was a two phase mixture.

Worksheet	Name	Final Product	Shipping	Vent
PP1	Vapour	0.0007	0.0000	1.0000
Conditions	Temperature [C]	39.85	38.55	38.55
Properties	Pressure [kPa]	950.0	200.0	200.0
Composition	Molar Flow [kgmole/h]	19.50	19.24	0.2630
-	Mass Flow [kg/h]	624.9	614.4	10.47
PF Specs	Std Ideal Lig Vol Flow [m3/h]	0.7832	0.7701	1.315e-002
	Molar Enthalpy [kJ/kgmole]	-2.453e+005	-2.440e+005	-3.429e+005
	Molar Entropy [kJ/kgmole-C]	23.94	22.20	165.6
	Heat Flow [kJ/h]	-4.783e+006	-4.693e+006	-9.018e+004
Design React	ions Rating Worksheet Dynami			

The final model should look like this.



Now do a "File Save" and "File Save As tutor08".

Modeling Tools

Having completed the process model we will now take a look at some of the facilities in HYSYS that allow us to generate reports, do additional design tasks, and help with model development.

Reports

It is possible to generate, view, and print reports on the whole model or specific pieces of equipment. Let us get an overall view of the streams in the model. The "Tools" menu has a "Reports" item.

)	Tools	Window Help			
		<u>W</u> orkbooks	Ctrl+W		
	- 0 **	PFDs	Ctrl+P		
-		Summarjes	-		
•	<u>i</u> T	<u>U</u> tilities	Ctrl+U		
		<u>R</u> eports	Ctrl+R		
	<u>^</u>				
6	📜 Re	eport Manager			
Γ	Ava	ilable <u>R</u> eports			Printing
	[Cr <u>e</u> ate	<u>P</u> rint
				Edjt	Text to <u>F</u> ile
				Delete	🗖 Delimited
				Dejete	Pre <u>v</u> iew
					Format/Layout
					Print Setup
11					

Click on "Create" to generate a new report.

🎽 Report	Manager					
Available <u>F</u>	<u>eports</u>		Printing		9	Default Colour Sci
Report1		<u>Create</u> Edit Dejete	Print Text to File Delimited			
	💐 Report Builder - Repor	t1				
	Report Name Report1		Size: 0 Pages			
	Report Datasheets			Printing	Reo/I Comp	
	[] (🛱 Select Datablocks for	Datasheet			_ 🗆 🛛
Feed	Insert Datasheet	Source for Datablocks Pick a Specific Object Elowsheets Case (Main) Distillation (COL1)	by Name C Pick All C Objects Cworkbook - CDL1> Cworkbook - Main> Condensed Mixture Condensed Mixture Condensed Duty Dummy Liquid Feed Final Product From Reactor Heater Duty Liquid Methanol	Dijects of a Given Type Filter All UnitOps C UnitOps C Logicals C Reactions C Other C Custom Setup Custom	Available Datablocks	

🚰 Report Builder - Report1	
Report Name Report1 Size: 2 Pages	
Report Datasheets	Printing
Case (Main) (Workbook): All Pages	<u>P</u> rint
	Text to <u>F</u> ile
	🔽 Delimited
	Pre <u>v</u> iew
	Format/Layout
Insert Datacheet Edit Datacheet Bernove Datacheet	Print Setup
Insert Datasheet Edit Datasheet Remove Datasheet 🐟 🔹	Print Setup

This is the result of "Create", "Insert Datasheet". A report on the whole model is selected.

To view the report click on "Preview". Here are some samples of what is in the report.

1			1	Case Name:	C:\Program Files\Honeywa	IIVUniSim Design R350.1 Bu	ild 11051\Cases\tutor08.u
3	Honeywell Calgary, Alberta CANADA			Unit Set:	nit Set: SI		
4				Date/Time:	Wednesday Mar 22 2006,	9:16:27	
6	Work	booki	Case (Main)				
8	Workbook: Case (Main)						
9 10	H Material Streams Fluid Pkg: All				All		
11	Name		Feed	Recycle	Mixed	To Reactor	From Reactor
12	Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
13	Temperature	(C)	40.00 ×	46.09 ×	44.54	200.0 *	200.0 ×
14	Pressure	(kPa)	4000 ×	4000 ×	4000	3950	3850
15	Molar Flow	(kgmole/h)	79.91	287.2 *	367.1	367.1	328.6
16	Mass Flow	(kg/h)	1000 ×	1743	2743	2743	2743
17	Liquid Volume Flow	(m3/h)	2.795	8.950	11.74	11.74	10.17
18	Heat Flow	(kJ/h)	-7.836e+006	-1.066e+007	-1.849e+007	-1.675e+007	-1.785e+007

51 52		Fluid Pkg:	All			
53	Name	Feed	Recycle	Mixed	To Reactor	From Reactor
54	Comp Mole Frac (CO2)	0.2500 ×	0.0925 ×	0.1268	0.1268	0.0830
55	Comp Mole Frac (Hydrogen)	0.7500 ×	0.9012 *	0.8683	0.8683	0.7942
56	Comp Mole Frac (Methanol)	× 00000 ×	0.0049 *	0.0038	0.0038	0.0629
57	Comp Mole Frac (H2O)	0.0000 ×	0.0015 ×	0.0011	0.0011	0.0599
58	Name	Dummy Liquid	Condensed Mixture	Vapour	Liquid	Purge
59	Comp Mole Frac (CO2)	0.0138	0.0830	0.0926	0.0117	0.0926
60	Comp Mole Frac (Hydrogen)	0.0162	0.7942	0.9011	0.0004	0.9011
61	Comp Mole Frac (Methanol)	0.3145	0.0629	0.0049	0.4938	0.0049
62	Comp Mole Frac (H2O)	0.6555	0.0599	0.0015	0.4941	0.0015
63						
64						
65	Honeywell International Inc.	UniS	Gim Design (R350.1 Buil)	d 11051)		Page 1 of 2

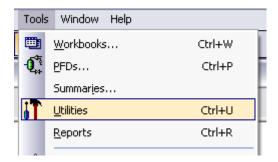
32 33			Unit Ops			
34	Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
35 36	Recycle Mixer	Mixer	Feed	Mixed	No	500.0 ×
36	Recycle Mixer	Mixer	Recycle		NO	500.0 *
37	Feed Heater	Heater	Mixed	To Reactor	No	500.0 ×
38	i eeu i leatei	Tieatei	Heater Duty		140	500.0
39			To Reactor	Dummy Liquid		
40 41	Reactor	actor Cont. Stirred Tank Reactor	Reactor Cooling	From Reactor	No	500.0 ×
41				Reactor Cooling		
42	Product Cooler	Cooler	From Reactor	Condensed Mixture	No	500.0 ×
43	Froduct Cooler	Cooler		Prod Cooler Duty	NO	500.0 **
44 45	Separator	Separator	Condensed Mixture	Liquid	No	500.0 ×
45	Separator	Separator		Vapour	140	
46 47	Purge Splitter	Тее	Vapour	Purge	No	500.0 ×
47	Furge Spitter	Tee		Recycled	NU	
48 49	Recycle Compressor	Compressor	Recycled	To Recycle	No	500.0 ×
49	Recycle compressor	Compressor	Recyl Comp Power			
50	Recycle	Recycle	To Recycle	Recycle	No	3500 *
51			Liquid	Methanol		
52	Distillation	Distillation	Reboiler Duty	Dummy	No	2500 ×
53	Distilation	Distilation		Water	NU	2000 "
54				Condenser Duty		
55 56	Water Pump	Pump	Water Source	To Condenser	No	500.0 ×
56	water Fump	Fanp	Pump Power		NO	500.0 **
57 58	Condenser	Heat Exchanger	Methanol	Final Product	No	500.0 ×
58	Condenser	Heat Exchanger	To Condenser	Water Return	NU	500.0 *
59	Water T Control	Adjust			No	3500 *
60	Methanol Storage	Tank	Final Product	Shipping	No	500.0 ×
61	meurarior storage	T CALLIN.		Vent		500.0 *
62						
63						
64	•					
65	Honeywell International Inc.		UniSim Design (R350.1 B)	uild 11051)		Page 2 of 2

If you click on "Print" you can print a copy.

Later, after modifying the model, you can come back through the "Tools=>Report" route and print an updated copy. You do not have to redefine the report content at that time.

Column Tray Design

HYSYS has a utility to do a mechanical design of distillation columns, both trayed and packed. Go to the "Tools" menu and select "Utilities".



🕂 Available Utilities	
	Boiling Point Curves CO2 Freeze Out Cold Properties Composite Curves Utility Critical Properties Data Recon Utility Depressuring - Dynamics Derivative Utility Envelope Utility FRI Tray Rating Hydrate Formation Utility Master Phase Envelope Utility Parametric Utility Pipe Sizing Property Balance Utility Property Table Tray Sizing User Property Vessel Sizing
⊻iew Utility	Add Utility
Delete Utility	

We want the "Tray Sizing" utility.

-	71	-
	71	

Design	Name Tray Section Tray Sizing-1 Main TS	n [Select TS]
Setup	, , , , , , , , , , , , , , , , , , ,	
Specs	Setup Sections	
Tray Internals	Section Name	
Notes	Start	
NOIG2	End Internals	
	Mode	
	Active	
	Status	
	Design Limit	
	Limiting Stage	
	Add Section	Copy Section
	<u>A</u> uto Section	Bemove Section
	% Liquid Draw 0.00 % Use T	ray Vapour to Size Ask Each Time 💌
Design Perfor	mance Dynamics	
Delete	No Sections	

To specify which section of which column to do, click on "Select TS", and select the column to be sized.

* Select Tra	ay Sectio	n	$\overline{\mathbf{X}}$
Flowsheet		<u>O</u> bject	
Case Distillation	(Main) (COL1)	Main TS	0 <u>K</u>
	()		Object Filter
			🖲 All
			C Streams
			◯ UnitOps
			C Logicals
			🔿 ColumnOps
			C Custom
			Custom
			<u>D</u> isconnect
			<u>C</u> ancel

Now click on "Auto Section" and let HYSYS decide what needs to be done.

- 72 -

Design	Name	Tray Section	
Design	Tray Sizing-1	Main TS	Select TS
Setup	1	Main 15	
Specs	Setup Sections		
Tray Internals	Section Name	1	(***
· ·	Start	1Main TS	🏁 Auto Section Information
Notes	End	10Main TS	
	Internals	Valve	Internal Type
	Mode	Design	C Sieve 💿 Valve C Bubble Cap C Packed
	Active		
	Status	Needs Calculatir	
	Design Limit		
	Limiting Stage	<empty></empty>	
			Area Tolerance
			When the ratio between the current calc'd area and either of min/max previous areas for the
	Add S	ection	0.6000 section exceeds this tolerance, a new diameter
			section is started.
	<u>Auto</u> S	Section	Higher more sections; lower fewer sections.
			NFP Diam Factor
	% Liquid Draw 0.00 %	Use Tray Va	
			When a new number of flow paths will result in a diameter diff >= diam fact * old diameter, a new
Design Perfo	rmance Dynamics		0.1500 NFP section is started.
			Not required for packed columns.
Delete		Calculate	Lower more sections; higher fewer sections.
			Cancel Next >

Here we have selected valve trays. In this utility there are a lot of parameters that can be specified, but we will just accept the defaults.

Tray Section Informat	tion [
Internals	
C Sieve 💽 Valve	🔿 Bubble 🛛 🔿 Packed
_ <u>V</u> alve Tray	
Orifice Type	Straight
Design Manual	Glitsch
Valve Mat'l Density	8220 kg/m3
Valve Mat'l Thickness	1.524 mm
Hole Area (% of AA)	15.30 %
Common Tray Properties	
Tray Spacing	609.6 mm
Tray Thickness	3.175 mm
Tray Foaming Factor	1.000
Max Tray dP (ht of liquid)	152.4 mm
Max Tray Flooding	85.00 %
DC/Weir Info	
Weir Height	50.80 mm
Max Weir Loading	89.42 m3/h-m
Downcomer Type	Vertical
Downcomer Clearance	38.10 mm
Maximum DC Backup	50.00 %
[*	
Delete	Complete AutoSection

👫 Tray Sizing: Tr	ay Sizing-1						
Design	<u>N</u> ame Tray Sizing-1	Tray Section Main TS		Select TS			
Setup		Main 13					
Specs	Set <u>up</u> Sections						
Tray Internals	Section Name	Section_1 Section					
-	Start	1Main TS	9Main TS				
Notes	End	8Main TS	10Main TS				
	Internals	Valve	Valve				
	Mode	Design	Design				
	Active						
	Status	Complete	Complete				
	Design Limit	Flooding	Flooding				
	Limiting Stage	1Main TS	9Main TS				
		ection	Copy Sectio	ion			
% Liquid Draw 0.00 % Use Tray Vapour to Size Ask Each Time Design Performance Dynamics							
Delete		OK		Ignored			

Click on "Complete AutoSection".

Note that HYSYS has decided to do the design in two parts. "Section_1" is the trays above the feed tray, "Section_2" is below. Because the flow rates are different in the two sections, one part can be made smaller than the other, if desired.

Look at the "Results" section of the "Performance" tab.

Performance	Section Results	Export P	ressures	View Warnings
Results				
rayed	Tray Results			
	Section	Section_1	Section_2	-
able	Internals	Valve	Valve	
Plot	Section Diameter [m]	0.6096	0.4572	
	Max Flooding [%]	54.40	76.59	
	X-Sectional Area [m2]	0.2919	0.1642	
	Section Height [m]	4.877	1.219	
	Section DeltaP [kPa]	4.188	1.874	
	Number of Flow Paths	1	1	
	Flow Length [mm]	444.5	330.2	
	Flow Width [mm]	550.1	413.6	
	Max DC Backup [%]	26.07	34.34	
	Max Weir Load [m3/h-m]	18.39	16.66	
	Max DP/Tray [kPa]	0.561	1.007	
	Tray Spacing [mm]	609.6	609.6	
	Total Weir Length [mm]	417.2	316.2	
	Weir Height [mm]	50.80	50.80	
	Active Area [m2]	0.2445	0.1366	•
Design Perfor	mance Dynamics			

This shows the recommended design. Note that the lower section could be made with a smaller diameter than the top. Building a top-heavy column is not a good idea, although the reverse is sometimes done. The best thing to do here is to build the whole column at the larger diameter. (.6096 m = 2 feet).

Note that the dimensions, although displayed in metres, are actually selected from standard sizes in feet.

Useful Techniques in Developing a Model

Here are a couple of techniques that can make it easier to develop models.

Suppose we are told that, over the lifetime of the catalyst in the reactor, its activity can fall as much as 20%. And we are asked the question "Will this affect the concentration of the feed to the distillation column". It would be helpful if we could work on the reactor and the column feed stream at the same time so that we would not have to flip back and forth between them.

Double click on the reactor icon and move to the "Sizing" section of the "Rating" tab. Double click on the stream "Liquid" and move to the "Composition" section. Select "Mole Fraction" as the basis.

Reactor - Glo	bal Rxn Set	🔁 Liquid	
Rating Sizing Heat Loss	Geometry Orientation:	C Horigontal 2.215 1.780 0.8900 Conditions Properties Composition K Value User Variables Notes Cost Parameters	rogen 0.000404 hanol 0.493846
Design Read	stions Rating Worksheet Dynamics	Worksheet Attachme	ents Dynamics

If you minimize the PFD window, you should get something like this.

Looking at the dimensions of the reactor, something seems wrong. The height/diameter ratio is $\frac{1}{2}$ when it should be 2. Although it does not affect the reaction calculations (only the volume is significant), we should fix this before proceeding.

We want to change two numbers, but we do not want HYSYS to recalculate the model until both numbers are changed. The intermediate case with one number changed would send the model off into unexplored territory and might not converge.

At the top of	the main w	indow you wi	ill find this:	10	The left	(green) light
indicates that	t calculation	is activated.	Click on the	right (red)) light to a	deactivate

calculation.

10 7	۹ و ه	

Now change the numbers. A little arithmetic shows that we want D=1.121, H=2.242 to get the same volume. Change both of these and then click on the green light.

HINT: In working with HYSYS and the program seems to seize up, check to make sure that the red light is not on.

At this point we should have something like this:

Reactor - Glo Rating Sizing Heat Loss	Geometry C Dvlinder Sphere	Orientation: Orientation: <u>Veltical</u>	► Liquid		Mole Fractions 0.011595 0.000404 0.433845 0.494056 0.4940
Design Read	tions Bating Wor	ksheet Dynamics CK		uttachments Dynamics	

Now, reduce the height 20% (to 1.794) to simulate the effect of catalyst decay.

😨 Reactor - Glol	bal Rxn Set			➡ Liquid		
Rating Sizing Heat Loss	©eometry ← Cylinder ← Sphere ← This reactor h	Orientation:	contal 1.771 1.121 1.794	Worksheet Conditions Properties Composition K Value User Variables Notes Cost Parameters		Mole Fractions 0.011848 0.000404 0.433856 0.433856 0.433892 0.493892 0.0000 0.000 0.0000 0.0000 0.0000 0.000 0.0000 0.0000 0.0000 0.000
Design Reac	tions Rating W	orksheet Dynamics		Worksheet Att	achments Dynamics	
Delete		OK.		Delete	DK Define from Other Stre	am 🔶 🖨

Here we have our answer. There is no significant change in composition.

Change the height back to its original value, close the two windows, and restore the PFD window.

We are now finished with the development of the model. Save the file (it should be "tutor08") and exit HYSYS.

Appendix

HYSYS Customization

In Tools=>Preferences=>Resources=>Colours

- Set "PFD Background" to white
- Set "PFD Label Text" to black
- Set "PFD Annotation" to black

In Tools=>Preferences=>Simulation=>Options

- Uncheck "Confirm Before Adding if Active Correlations are Present"
- Uncheck "Enable Cross Hairs on PFD"