Reactor Calculation using Simulation Software

(Revised from Senior Project Report by Ryan P. Thibault 2001-02)

The PRO/II process simulation program performs rigorous mass and energy balances for a range of chemical processes from oil/gas separation to reactive distillation. The graphical user interface, Provision, provides a fully interactive, Windows based environment for the user. Many industries, such as Refining, Petrochemicals, and Polymers, can take advantage of PRO/II's usefulness. PRO/II also has many different applications. The user can design new processes, troubleshoot existing processes, evaluate alternate plant configurations, or optimize plant yield and efficiency to list a few.

The easy to use interface of Provision incorporates point-and-click and drag-and-drop functionality for defining streams and unit operations. This makes drawing Process Flow Diagrams (PFD's) very simple. Provision also incorporates many Microsoft standards, such as OLE Automation, enabling the user to quickly transfer graphics and process data to other Windows applications. It also allows you to configure the simulation environment to suit your preferences in areas such as units of measure and thermodynamics. PRO/II's interactive color-coded data entry and validation system guides you through simulation setup and execution.

Along with PRO/II's ease of use, it enables the user to successfully transfer important data to other engineering programs. Microsoft Excel and any other OLE compliant applications can be used to take data from PRO/II. A standard process engineering computing environment is desirable in any workplace. This reduces learning curves and increases software usage. PRO/II provides an environment where this happens and, in turn, produces engineers that spend less time simulating process problems and more time implementing process improvements.

In this example we will use conversion, equilibrium, and adiabatic Gibbs reactors, as well as heat exchangers and controllers. Consider a process stream at 39^{o}F and 390 psia shown as stream S1 in Figure 1. Table 1 lists the flow rates of all components in stream S1.

Table 1 Feed stream flow rate

Component	H_2	N_2	CO	CO_2
Flow rate, lbmol/h	10,000	5,000	50	5

We want to remove carbon monoxide and carbon dioxide in the feed by *methanation* reactions shown in equations (1) and (2). The product stream is then cooled to 25^{o}F using ammonia at – 25^{o}F and 20 psia.

$$4H_2 + CO_2 \Leftrightarrow CH_4 + 2H_2O \qquad (1)$$

$$3H_2 + CO \Leftrightarrow CH_4 + H_2O \qquad (2)$$

Since the methanation reactions are exothermic, the product stream leaving the reactor is used to preheat the feed stream before it transfers heat to the ammonia stream entering the heat exchanger E2 at – 25^{o}F and 20 psia.

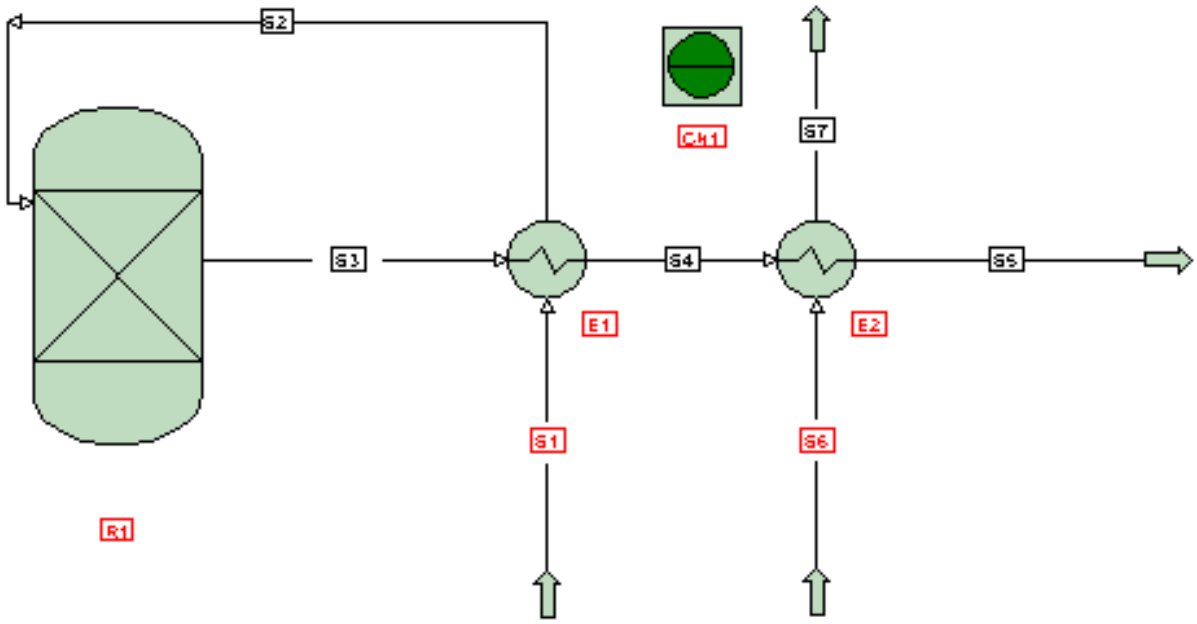
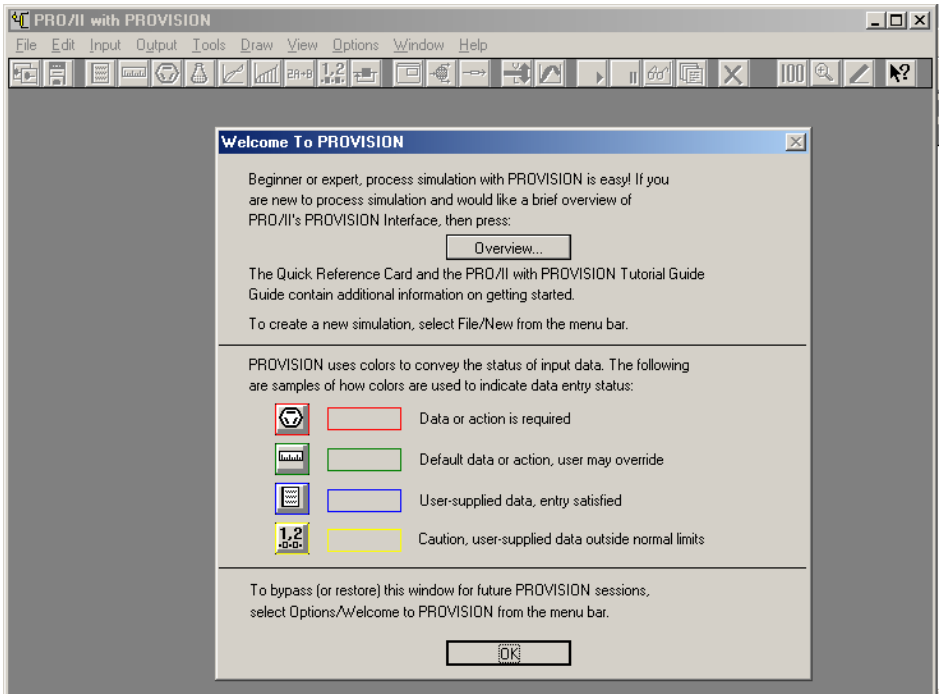


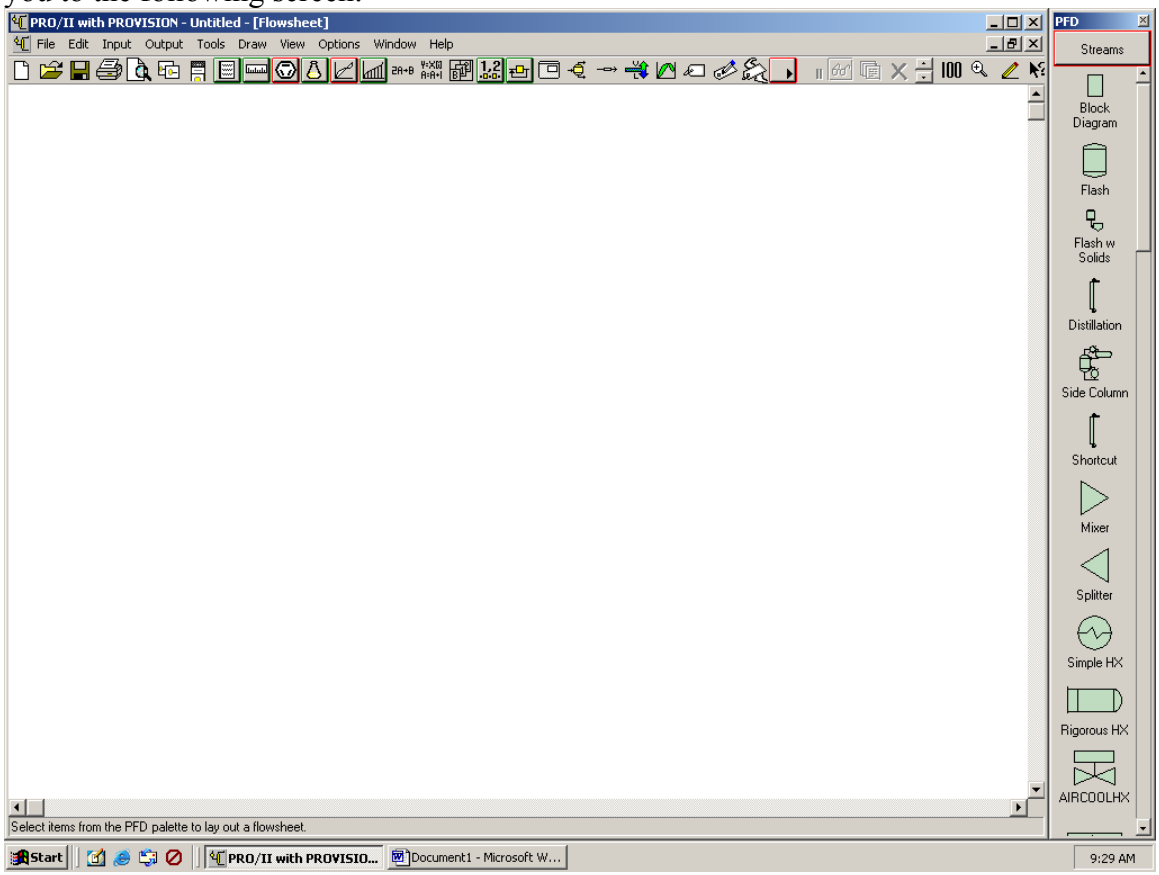
Figure 1 Schematic of the reactor setup.

To open Provision, go to the *Start* menu, click on *Programs*, *Simsci*, and then *ProII 6*. The following screen should appear:

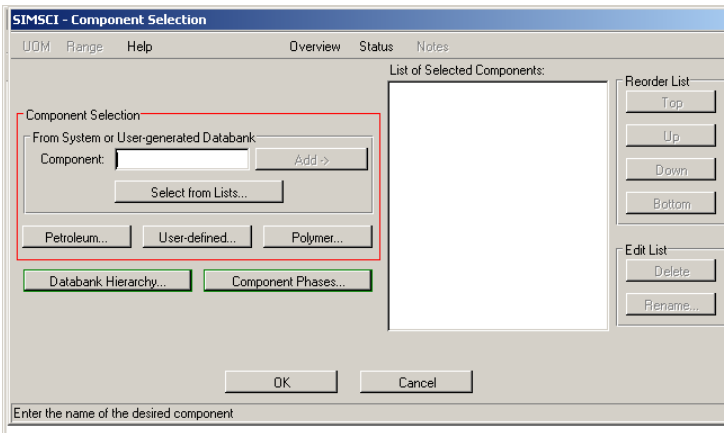


Note the different colored boxes and their meanings. They will be very important to remember later on in the simulation. Click on *OK* at the bottom of the box to continue

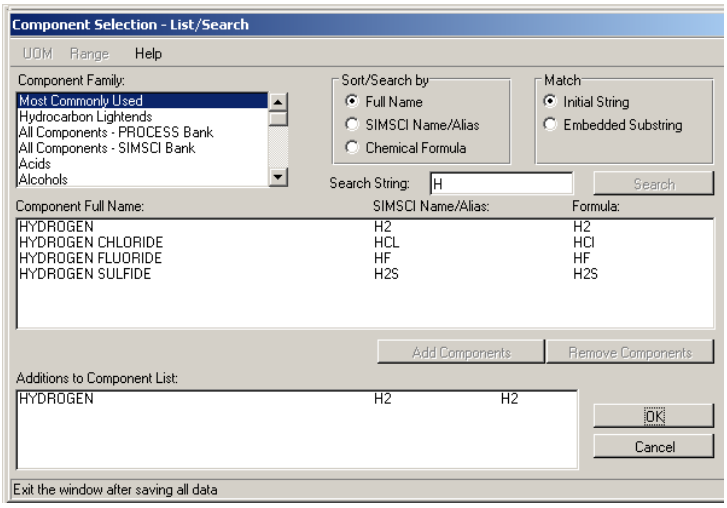
into the simulation environment. Next, click on *File* and then *New*. This should bring you to the following screen:



This is the basic simulation environment from which you will begin each time you use Provision. It is called the PFD screen. Before you begin with the procedure given to you in the assignment, you need to enter the components that you will be using and your equation of state. First click on the *Component Selection* button on the top toolbar. This button looks like this:  . The following screen should appear:



From here you can either type in the names of your desired components or you can select them from a list already inside Provision. We will select our components from a list by clicking on the *Select from Lists* button. The following screen should appear:



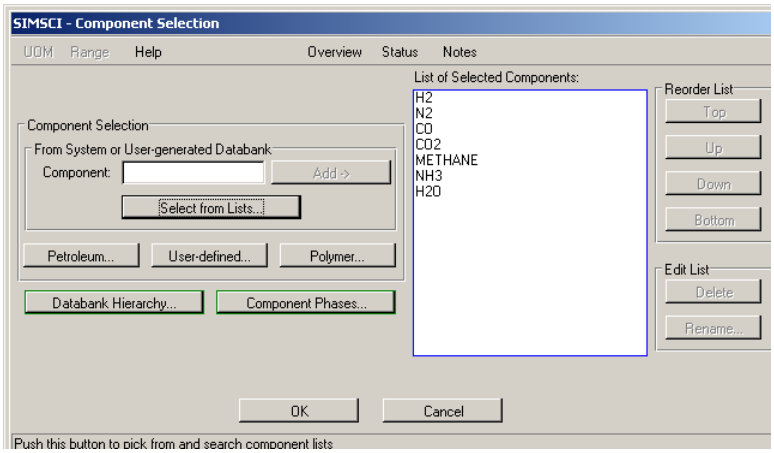
In this example, all of the needed components can be found in the *Most Commonly Used* file. Click on it and select each of the components listed in the first column of Table 2. After you click *Add Components*, the selected species will appear in the bottom text box *Additions to Component List*.

Table 2 Data for simulation

	Feed	
H_2	10000	Lb-Mol/Hr
N_2	5000	
CO	50	
CO_2	5	
CH_4	0	
NH_3	0	
H_2O	0	
Temp.	39	F
Pressure	390	Psia

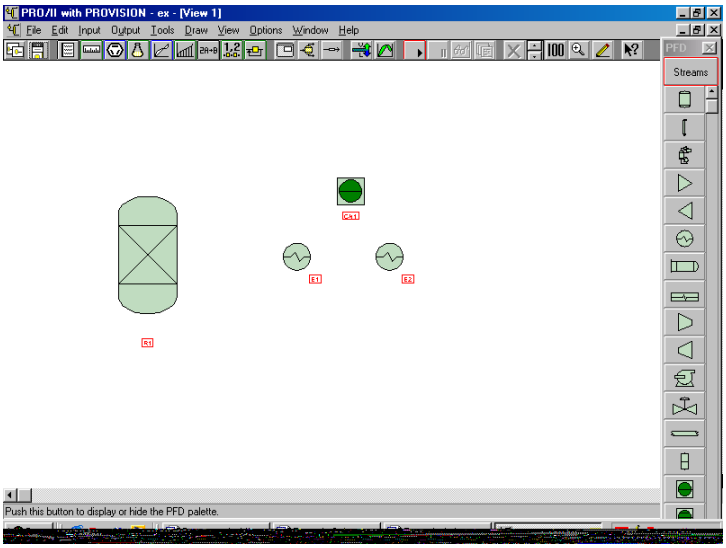
	Products	
Temp.	25	F
As little CO and CO2 as possible.		
You have an ample supply of ammonia at –25 F and 20.0 Psia. Pressure drop per side of exchanger/reactor = 3.0 Psia Temperature Rise in all equilibrium and conversion reactors = 10 F		

After you selected all species click *OK* to return to the following screen.

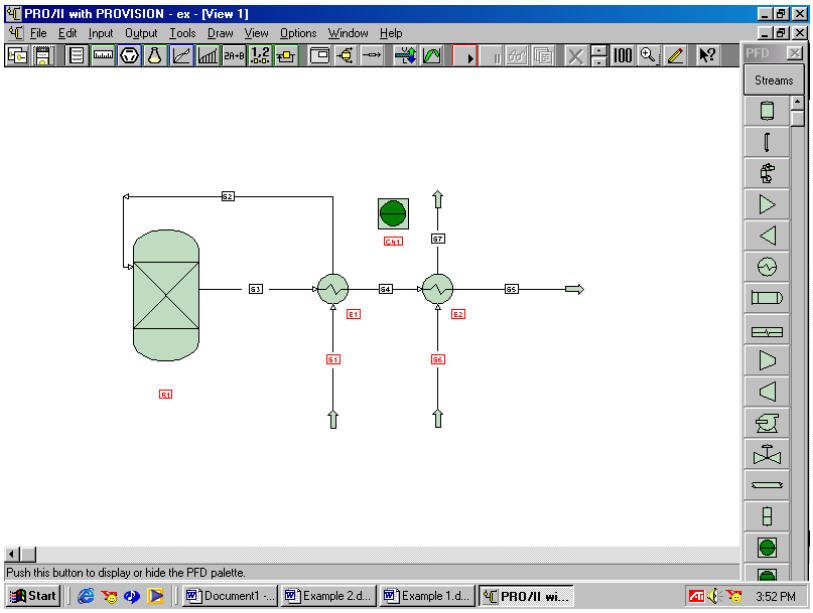


Click *OK* to return to the PFD screen. Next click on the *Thermodynamic Data* button,  . Once inside, click on *Most Commonly Used* and then click on *Peng-Robinson*. Then click *Add* and then *OK* to return back to the PFD screen. Now we are ready to begin inserting units and streams.

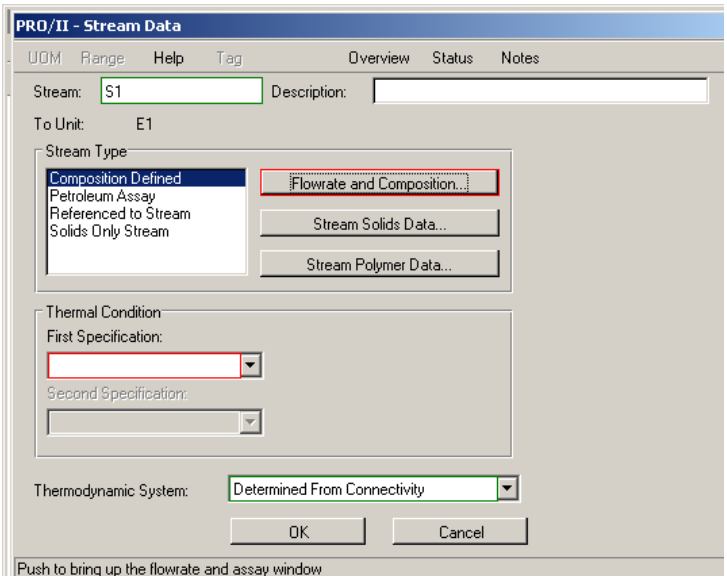
The first unit that we want to put in the simulation is the reactor. We will begin with the conversion reactor. Scroll down the toolbar until you see an icon that looks like this,  . There should be two in a row and then another, three icons later. The first one is the conversion reactor, the second is the equilibrium reactor, and the third is the Gibbs reactor. Choose the first one since we are using the conversion reactor first. The conversion reactor simulates a chemical reactor by solving the heat and material balances based on supplied reaction stoichiometry and fractional conversion. If there is not sufficient reactant to meet the specified conversions a few different things can happen. The calculation is terminated, the calculations are continued with no reaction taking place, makeup is added to satisfy the conversion, or the conversion is limited to the maximum possible amount with the available reactants. This reactor can support as many reactions as you would like and doesn't support modeling of two liquid phases. Next click on the heat exchanger icon,  and place two heat exchangers in series with the reactor. Finally, click on the controller button,  , and place the controller near the second heat exchanger. Your screen should now look similar to the following one:



Next click on *Streams*. First create a feed stream, *S1*, entering into the bottom of the first heat exchanger, *E1*. Next create stream *S2* from the top of *E1* to the left side of the reactor, *R1*. The next stream, *S3*, should go from the right side of *R1* to the left side of *E1*. The following stream, *S4*, should be placed from the right side of *E1* to the left side of the second heat exchanger, *E2*. The next one, *S5*, should go from the right side of *E2* to wherever you would like, as this will be the product stream. The next stream, *S6*, should go from wherever you would like into the bottom of *E2*. The final stream, *S7*, should go from the top of *E2* to wherever you would like. Streams *S6* and *S7* will constitute the stream that we will use to cool our product to its desired temperature. Your PFD should now look similar to the following one:



The next task at hand is entering the known data into the simulation. We will begin with the feed stream data. Double click on *S1* and the *Stream Data* screen should come up.



Click on *Flowrate and Composition*, then *Individual Component Flowrates*, and then enter in all of the given feed flowrates.

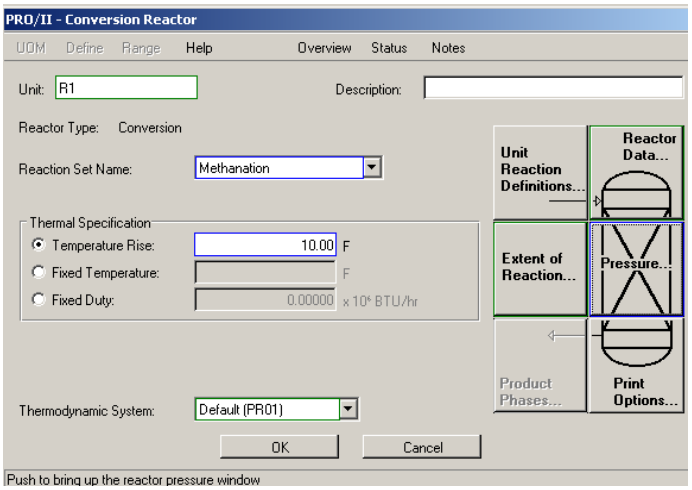
Table 1 Feed stream flow rate

Component	H_2	N_2	CO	CO_2
Flow rate, lbmol/h	10,000	5,000	50	5

Once that is done, click *OK* and the *Stream Data* screen should reappear with *Flowrate and Composition* now outlined in blue. Click on *First Specification* and choose *Temperature*. Enter in the given value, 39 F. Next click on *Second Specification* and choose *Pressure*. Enter in the given value, 390 Psia. Finally, click on *Thermodynamic System* and choose *Default(PRO1)*. Then click *OK* and return to the PFD screen.

Next double click on *E1*. In the *Hot Side* column, click on *Process Stream*. Make sure that *S3* and *S4* are the streams on the hot side and that *S1* and *S2* are on the cold side. If they are set correctly then click *OK* and return to the previous screen. Click on *Specification* and then click the button *Specification* on the new screen and select *Cold Product Temperature*. Enter in the value of 150 F. This is a randomly chosen value. The purpose of this exchanger is to preheat the feed so that the reaction takes place faster and a higher conversion is reached. The value of 150 F was chosen because it is small enough to where a relatively small exchanger can be used. Click *OK* to return you to the previous screen. Click on each of the *Pressure Drop* boxes and enter 3 (psi). Next click *OK* to return you to the PFD screen.

Now double click on *R1*. The following screen should appear:

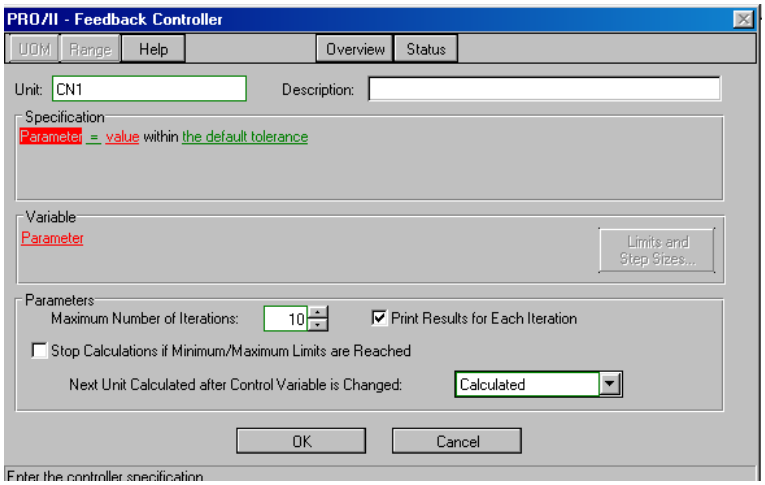


Click on the button *Reaction Set Name* and choose *Methanation*. Then, in the *Thermal Specification* area, click in the box *Temperature Rise* and enter 10 (F). Next click on *Pressure* and then click in the box *Pressure Drop*. Enter in the given pressure drop value (3 psi). Then click *OK* twice to return to the PFD screen.

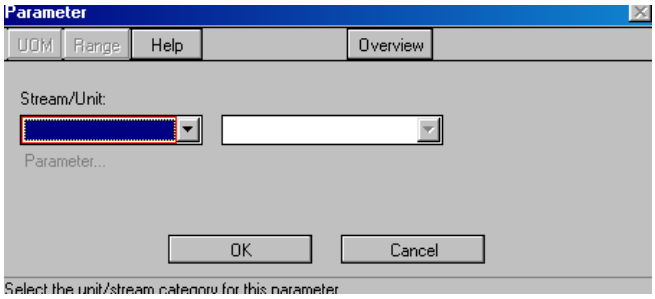
Now double click on *E2*. The purpose of this exchanger is to continue the cooling of the product stream to its final temperature. The same screen that appeared when you double clicked on *E1* should appear. In the *Hot Side* column, click on *Process Stream*. Make sure that *S4* and *S5* are the streams on the hot side and that *S6* and *S7* are on the cold side. Click *OK* to return to the previous screen. Click on each of the *Pressure Drop* boxes and enter in the given values (3 psi). Click on *Specification* and then click the button *Specification* on the new screen and select *Cold Product Temperature*. Enter in the temperature, 15 F. We choose this temperature so that the temperatures of the two streams do not cross over but we still get the most heat transfer out of our ammonia supply. Finally, click *OK* twice in a row to return to the PFD screen.

Now double click on *S6* and the *Stream Data* screen should appear. Click on *Flowrate and Composition* and then *Individual Component Flowrates*. Next click in the box next to NH_3 and enter the value 10 into the box. The value that you enter here does not matter as the controller will change it when you run the simulation. Click *OK* to return to the *Stream Data* screen. In the *Thermal Condition* group, click on *First Specification* and choose *Temperature*. Enter the given value (–25 F). Now click on *Second Specification* and choose *Pressure*. Enter the given value (20.0 psia) and then click *OK* to return to the PFD screen.

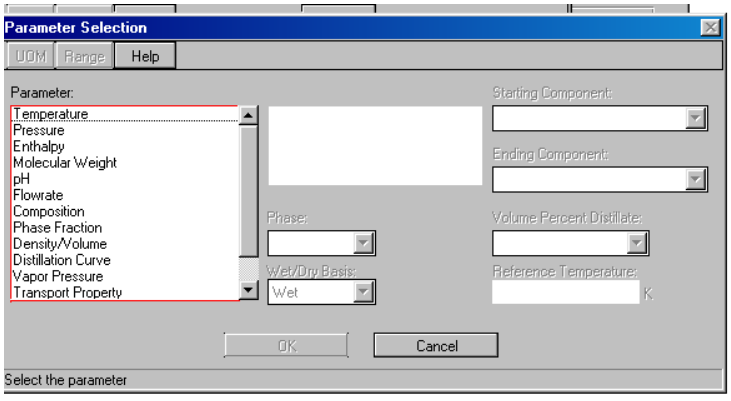
The only thing left to do now is enter the known data into the controller. The controller is used to manipulate one specification by changing a different variable. In this case we will use the controller to control the temperature of our product stream, *S5,* out of *E2* by changing the flowrate of the ammonia, *S6*, into the exchanger. Double click on the controller, *CN1*, and the following screen should appear:



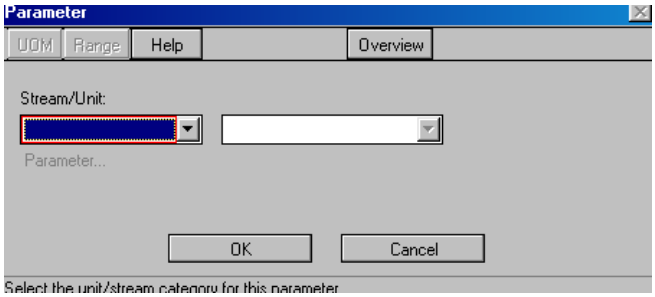
Under *Specification* click *Parameter* and the following screen should appear:



Click *Stream/Unit* and choose *Stream*. Then click *Stream Name* and choose *S5*. Click on *Parameter* and the following screen should appear:



In the *Parameter* group, choose *Temperature* and then click *OK*. Then click *OK* again to return to the first screen. Next click on *Value* and enter the given value (25 F). Now, in the *Variable* group, click on *Parameter* and the following screen should appear again:



Now click on the *Stream/Unit* button and choose *Stream*. Click on the *Stream Name* button and choose *S6*. Now click on *Parameter* and choose *Flowrate* from the list that pops up. Now click *OK* three times to return to the PFD screen. Now it's time to run the simulation. Click on the run button on the toolbar,  , and your simulation should turn blue. If it does not, you can double click on the controller and then increase the number of iterations until it converges. Otherwise, you should retrace your steps to find your error and fix it. The next thing to do is to view the results. The important results for this example come from streams *S5* and *S6*. To view the results from each of these streams right-click on the stream and then choose *View Results*. Sample results can be seen below.

STREAM 'S5'

	TOTAL	VAPOR	DECANT H2O
RATE, LB-MOL/HR	14955.0000	14907.5486	47.4514
TEMPERATURE, F	25.00	25.00	25.00
PRESSURE, PSIA	378.00	378.00	378.00
MOLECULAR WEIGHT	10.8222	10.7993	18.0150
FRACTION		.9968	3.1729E-03
ENTHALPY, BTU/LB-MOL	284.0087	285.3183	-127.4180
CP, BTU/LB-F	.6475	.6464	1.0100

	TOTAL	VAPOR	DECANT H2O
MOLAR FLOWRATES, LBMOL/HR			
1 - H2	9850.0000	9850.0000	
2 - N2	5000.0000	5000.0000	
3 - CO	.0000	.0000	
4 - CO2	5.0000	5.0000	
5 - METHANE	50.0000	50.0000	
6 - NH3	.0000	.0000	
7 - H2O	50.0000	2.5486	47.4514

	TOTAL	VAPOR	DECANT H2O
MOLAR COMPOSITIONS			
1 - H2	.6586	.6607	
2 - N2	.3343	.3354	

3 - CO	.0000	.0000	
4 - CO2	3.3434E-04	3.3540E-04	
5 - METHANE	3.3434E-03	3.3540E-03	
6 - NH3	.0000	.0000	
7 - H2O	3.3434E-03	1.7096E-04	1.0000

STREAM 'S6'

	TOTAL	LIQUID
RATE, LB-MOL/HR	321.8646	321.8646
TEMPERATURE, F	-25.00	-25.00
PRESSURE, PSIA	20.00	20.00
MOLECULAR WEIGHT	17.0310	17.0310
FRACTION		1.0000
ENTHALPY, BTU/LB-MOL	-1226.8087	-1226.8087
CP, BTU/LB-F	1.0605	1.0605

	TOTAL	LIQUID
MOLAR FLOWRATES, LBMOL/HR		
1 - H2	.0000	.0000
2 - N2	.0000	.0000
3 - CO	.0000	.0000
4 - CO2	.0000	.0000
5 - METHANE	.0000	.0000
6 - NH3	321.8646	321.8646
7 - H2O	.0000	.0000

	TOTAL	LIQUID
MOLAR COMPOSITIONS		
1 - H2	.0000	.0000
2 - N2	.0000	.0000
3 - CO	.0000	.0000
4 - CO2	.0000	.0000
5 - METHANE	.0000	.0000
6 - NH3	1.0000	1.0000
7 - H2O	.0000	.0000

The most important information to be obtained from these results is the flow rate of ammonia and the fact that all of CO was reacted but the CO_2 didn't react at all. Keep these facts in mind as we will now run the simulation with the two other types of reactors and then compare the results of each of the simulations.

The next reactor that we will deal with is the equilibrium reactor. The equilibrium reactor simulates a chemical reactor by solving the heat and material balances based on supplied reaction equilibrium data. The reaction stoichiometry must be defined in the *Reaction Data Sets* window before the reactor performance can be specified. Equilibrium equation data may be entered in the reaction set or in the reactor unit operation. This reactor only supports a single reaction. There are two ways to replace the reactor. The first way is to begin with a new simulation and input everything again with the new reactor this time. This is the long way. The easier way to do this is to right-click on the reactor and choose *Delete*. Next click on the second reactor button,  , and click in the empty space where the old reactor used to be. Now click on *Streams* on the side toolbar so that you can connect the existing streams to your new equilibrium reactor. To do this, click and hold on the arrow at the end of the stream, and drag it to the side of the reactor that you want it to connect to, and then let it go. The data entry for this reactor is the same as for the conversion reactor. Run the simulation again and see if it converges. If it doesn't converge then follow the previously given instructions for that situation. If it does converge then you can right-click and view the results for streams *S5* and *S6*. Sample results for the equilibrium reactor can be found below.

STREAM 'S5'

	TOTAL	VAPOR	DECANT H2O
RATE, LB-MOL/HR	14955.0000	14887.5456	57.4544
TEMPERATURE, F	25.00	25.00	25.00
PRESSURE, PSIA	378.00	378.00	378.00
MOLECULAR WEIGHT	10.8294	10.8017	18.0150
FRACTION		.9962	3.8444E-03
ENTHALPY, BTU/LB-MOL	281.6221	283.2004	-127.3471
CP, BTU/LB-F	.6476	.6462	1.0100

	TOTAL	VAPOR	DECANT H2O
MOLAR FLOWRATES, LBMOL/HR			
1 - H2	9830.0000	9830.0000	
2 - N2	5000.0000	5000.0000	
3 - CO	2.4512E-08	2.4512E-08	
4 - CO2	1.6256E-06	1.6256E-06	
5 - METHANE	55.0000	55.0000	
6 - NH3	.0000	.0000	
7 - H2O	60.0000	2.5456	57.4544

	TOTAL	VAPOR	DECANT H2O
MOLAR COMPOSITIONS			
1 - H2	.6577	.6603	
2 - N2	.3346	.3359	
3 - CO	1.6401E-12	1.6465E-12	
4 - CO2	1.0877E-10	1.0919E-10	
5 - METHANE	3.6802E-03	3.6944E-03	
6 - NH3	.0000	.0000	
7 - H2O	4.0147E-03	1.7099E-04	1.0000

STREAM 'S6'

	TOTAL	LIQUID
RATE, LB-MOL/HR	339.6185	339.6185
TEMPERATURE, F	-25.00	-25.00
PRESSURE, PSIA	20.00	20.00
MOLECULAR WEIGHT	17.0310	17.0310
FRACTION		1.0000
ENTHALPY, BTU/LB-MOL	-1226.8087	-1226.8087
CP, BTU/LB-F	1.0605	1.0605

	TOTAL	LIQUID
MOLAR FLOWRATES, LBMOL/HR		
1 - H2	.0000	.0000
2 - N2	.0000	.0000
3 - CO	.0000	.0000
4 - CO2	.0000	.0000
5 - METHANE	.0000	.0000
6 - NH3	339.6185	339.6185
7 - H2O	.0000	.0000

	TOTAL	LIQUID
MOLAR COMPOSITIONS		
1 - H2	.0000	.0000
2 - N2	.0000	.0000
3 - CO	.0000	.0000
4 - CO2	.0000	.0000
5 - METHANE	.0000	.0000
6 - NH3	1.0000	1.0000
7 - H2O	.0000	.0000

Notice from this simulation how all of the CO_2 reacts as well as all of the CO. Also, more decant water is formed as a result of the methanation reactions. The amount of cooling ammonia increased as well. The final reactor that we want to compare is the Gibbs reactor. The Gibbs Reactor simulates a chemical reactor by solving the heat and material balances based on minimizing the free energy of the components in the reaction. The Gibbs reactor determines the distribution of components, which is expected at chemical equilibrium for the system. No prior knowledge of the chemistry of the system is required and the reaction stoichiometry doesn't need to be defined. All the components in the reactor are considered as reactants. The calculation determines the distribution of the components, which gives the minimum free energy for the system. Reaction stoichiometry may be defined in the *Reaction Data Sets* window and used in the Gibbs reactor. In this case, the calculations will be limited to these defined reactions. This reactor supports single or double liquid phases.

Using the same procedure as when you replaced the reactor before, place a Gibbs reactor in the space where the equilibrium reactor was before. The button for the Gibbs reactor looks the same as that of the other reactors only it is located 3 spots below the other two reactor buttons on the side toolbar. Now double-click the reactor and the data entry screen should appear. Click on *Pressure* and enter in the pressure drop. Click on *Reaction Set Name* and notice that there is no reaction set listed. Do not worry about this. Next move down to the *Thermal Specification* section. Click on *Fixed Duty* and let the value equal 0, as it is an adiabatic reactor. Now click *OK* to return to the PFD screen. Your simulation should be ready to run now so click the run button and see if it converges. If it doesn't, you may want to increase the number of iterations in the particular unit that doesn't converge. Sample results for streams *S5* and *S6*, for the Gibbs reactor can be found below.

STREAM 'S5'

	TOTAL	VAPOR	LIQUIQ	DECANT H2O
RATE, LB-MOL/HR	12775.6298	12601.3006	116.4840	57.8452
TEMPERATURE, F	25.00	25.00	25.00	25.00
PRESSURE, PSIA	378.00	378.00	378.00	378.00
MOLECULAR WEIGHT	12.6684	12.6036	17.0168	18.0150
FRACTION		.9864	9.1177E-03	4.5278E-03
ENTHALPY, BTU/LB-MOL	1625.0888	1650.7315	-278.7059	-127.3430
CP, BTU/LB-F	.5935	.5869	1.1049	1.0100

	TOTAL	VAPOR	LIQUID	DECANT H2O
MOLAR FLOWRATES, LBMOL/HR				
1 - H2	6575.9447	6575.7933	.1514	
2 - N2	3915.3149	3915.2578	.0570	
3 - CO	2.8890E-08	2.8888E-08	1.2528E-12	
4 - CO2	1.8387E-08	1.8301E-08	8.6404E-11	
5 - METHANE	55.0000	54.9960	4.0185E-03	
6 - NH3	2169.3702	2053.0988	116.2714	
7 - H2O	60.0000	2.1547	1.1648E-04	57.8452

	TOTAL	VAPOR	LIQUID	DECANT H2O
MOLAR COMPOSITIONS				
1 - H2	.5147	.5218	1.2997E-03	
2 - N2	.3065	.3107	4.8965E-04	
3 - CO	2.2613E-12	2.2925E-12	1.0755E-14	
4 - CO2	1.4393E-12	1.4523E-128	7.4177E-131	
5 - METHANE	4.3051E-03	4.3643E-03	3.4498E-05	
6 - NH3	.1698	.1629	.9982	
7 - H2O	4.6964E-03	1.7099E-04	1.0000E-06	1.0000

STREAM 'S6'

	TOTAL	LIQUID
RATE, LB-MOL/HR	4902.6204	4902.6204
TEMPERATURE, F	-25.00	-25.00
PRESSURE, PSIA	20.00	20.00
MOLECULAR WEIGHT	17.0310	17.0310
FRACTION		1.0000
ENTHALPY, BTU/LB-MOL	-1226.8087	-1226.8087
CP, BTU/LB-F	1.0605	1.0605

	TOTAL	LIQUID
MOLAR FLOWRATES, LBMOL/HR		
1 - H2	.0000	.0000
2 - N2	.0000	.0000
3 - CO	.0000	.0000
4 - CO2	.0000	.0000
5 - METHANE	.0000	.0000
6 - NH3	4902.6204	4902.6204
7 - H2O	.0000	.0000

	TOTAL	LIQUID
MOLAR COMPOSITIONS		
1 - H2	.0000	.0000
2 - N2	.0000	.0000
3 - CO	.0000	.0000
4 - CO2	.0000	.0000
5 - METHANE	.0000	.0000
6 - NH3	1.0000	1.0000
7 - H2O	.0000	.0000

As you can see all of the CO and CO_2 have been reacted. This time, however, the N_2 and H_2 have reacted together as well to form NH_3. This is acceptable if there is a desire for ammonia in the stream. If not, there is now a need for some sort of separator to remove this component from the stream. The other noticeable difference form the previous two reactors was the fact that a much larger quantity of cooling ammonia was needed. This was caused by the large rise in temperature due to the exothermic reaction.