HYSYS

James M. Lee

HYSYS is an interactive process engineering and simulation program. It is a powerful program that you can use to solve all kinds of process related problems. However, since you have to provide various conditions and choices in order to solve a problem, you cannot use it effectively unless you have good knowledge about the process and the solution procedures. The objective of this class is to introduce you to the program so that you can use it as you take core chemical engineering courses in the future.

You can find all kinds of documentation (tutorials, manuals, examples, etc) from the following web site:
http://www.hyprotech.com/hysys/support/index.html - HYSYS%20Documentation

You can find numerous other resources by searching the web. You search results will include many course web sites of other chemical engineering departments. Let’s start with simple examples to find out how HYSYS works.

Example 1: Flash Separation

We have a stream containing 15% ethane, 20% propane, 60% i-butane and 5% n-butane at 50°F and atmospheric pressure, and a flow rate of 100 lbmole/hr. This stream is to be compressed to 50 psia, and then cooled to 32°F. The resulting vapor and liquid are to be separated as the two product streams. What are the flow rates and compositions of these two streams?

Solution

This instruction is brief. You may not be able to understand it unless you see the classroom demonstration.

1. Start HYSYS
2. Go in the File menu to select New then Case.
3. Simulation Basis Manager will pop up. Click Add. Fluid Package window will be opened.
4. Choose Peng Robinson as Base Property Package
5. Open Component page of Fluid Package window and add components (ethane, propane, i-butane, n-butane) and close the Fluid Package.
6. Click Enter Simulation Environment at the bottom of Simulation Basis Manager.
7. Click Compressor in the Object Palette and click it on Process Flow Diagram (PFD). Do the same for the Cooler and Separator. See the figure next page for the shapes of compressor, cooler, and separator.
8. Click Compressor in PFD. Name the Inlet as Inlet Stream, the Outlet as Compressed, and the Energy as Comp Energy and close the window
9. Click Cooler in PFD. Choose the name of the Inlet as Compressed, the Outlet as Cooled, and the Energy as Cooling Energy. Close the window.
10. Click **Separator** in **PFD**. Choose the name of the **Inlet** as Cooled, the **Vapor** as Top, and the **Liquid** as Bottom. Close the window.

11. Arrange streams in **PFD** so that it looks orderly as shown in the figure below.

12. Now click [ ] at the top of the HYSYS window to open **Workbook**. Check the units to see if it is in English units. Otherwise, change the unit by clicking Tools/Preferences/Variables. Choose Field as your choice and close the window.

13. Now fill in the **Workbook** with all the given condition, starting from the inlet stream: temperature (50), pressure (14.7), and molar flow (100). Double click 100 (molar flow rate), and composition window will be opened. Fill in the composition and close. As you fill in the conditions, HYSYS will calculate the rest of the shell.

14. Continue to fill in the pressure (50) of the Compressed stream, temperature (32) and pressure (50) of the Cooled stream. Now the calculation is complete as shown in the table below. If you want to know the composition of the Top stream, double click 23.48 (molar flow rate of the Top stream.)

<table>
<thead>
<tr>
<th>Name</th>
<th>Inlet Stream</th>
<th>Compressed</th>
<th>Cooled</th>
<th>Top</th>
<th>Bottom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapour Fraction</td>
<td>1.0000</td>
<td>1.0000</td>
<td>0.2348</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Temperature [F]</td>
<td>50.00</td>
<td>135.6</td>
<td>32.00</td>
<td>32.00</td>
<td>32.00</td>
</tr>
<tr>
<td>Pressure [psia]</td>
<td>14.70</td>
<td>50.00</td>
<td>50.00</td>
<td>50.00</td>
<td>50.00</td>
</tr>
<tr>
<td>Molar Flow [lbmole/hr]</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td><strong>23.48</strong></td>
<td>76.52</td>
</tr>
<tr>
<td>Mass Flow [lb/hr]</td>
<td>5111</td>
<td>5111</td>
<td>5111</td>
<td>1018</td>
<td>4093</td>
</tr>
<tr>
<td>Liquid Volume Flow [barel/day]</td>
<td>665.1</td>
<td>665.1</td>
<td>665.1</td>
<td>147.4</td>
<td>517.6</td>
</tr>
<tr>
<td>Heat Flow [Btu/hr]</td>
<td>-5.244e+006</td>
<td>-5.075e+006</td>
<td>-5.924e+006</td>
<td><strong>-1.100e+006</strong></td>
<td>-4.824e+006</td>
</tr>
<tr>
<td>Molar Enthalpy [Btu/lbmole]</td>
<td>-5.244e+004</td>
<td>-5.075e+004</td>
<td>-5.924e+004</td>
<td><strong>-4.686e+004</strong></td>
<td>-6.304e+004</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Name</th>
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<th>Cooling Energy</th>
<th><strong>New</strong></th>
</tr>
</thead>
<tbody>
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<td>&lt;empty&gt;</td>
<td></td>
</tr>
<tr>
<td>Temperature [F]</td>
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<td></td>
</tr>
<tr>
<td>Pressure [psia]</td>
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<td>&lt;empty&gt;</td>
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</tr>
<tr>
<td>Molar Flow [lbmole/hr]</td>
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<td>&lt;empty&gt;</td>
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</tr>
<tr>
<td>Mass Flow [lb/hr]</td>
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<td></td>
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<tr>
<td>Liquid Volume Flow [barel/day]</td>
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</tr>
<tr>
<td>Heat Flow [Btu/hr]</td>
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<td>8.492e+005</td>
<td></td>
</tr>
<tr>
<td>Molar Enthalpy [Btu/lbmole]</td>
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<td>&lt;empty&gt;</td>
<td></td>
</tr>
</tbody>
</table>
Example 2: Process Involving Reaction and Separation

Toluene is produced from \( n \)-heptane by dehydrogenation over a \( \text{Cr}_2\text{O}_3 \) catalyst:

\[
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + 4\text{H}_2
\]

The toluene production process is started by heating \( n \)-heptane from 65 to 800°F in a heater. It is fed to a catalytic reactor, which operates isothermally and converts 15 mol\% of the \( n \)-heptane to toluene. Its effluent is cooled to 65°F and fed to a separator (flash). Assuming that all of the units operated at atmospheric pressure, determine the species flow rates in every stream.

Solution

1. Start HYSYS and File/New/Case
2. *Simulation Basis Manager* will pop up. Click *Add*. *Fluid Package* window will be opened. Choose *Peng Robinson* as Base Property Package
3. Open *Component* page of *Fluid Package* window and add components (toluene, \( n \)-heptane, and hydrogen) and close the *Fluid Package*.
4. Click *Enter Simulation Environment* at the bottom of *Simulation Basis Manager*.
5. Click *Heater* in the *Object Palette* and click it on *Process Flow Diagram (PFD)*. Click *General Reactor* \( \text{Re} \), three different reactors will pop up, click *conversion reactor* and click it on *PFD*. Do the same for the *Cooler* and *Separator*.
6. Name inlets and outlets of all process units as shown in *PFD* diagram on the next page (See the previous example if you don’t know how to do this.)
7. You will notice that the reactor is colored red with the error message, “Need a reaction set.” Now we need to input what the reaction is. Click Flowsheet/Reaction Package. Add Global Rxn Set. Then, click Add Rxn at the lower right side of the window and choose Conversion. Add three components (\( n \)-Heptane, Toluene, Hydrogen) and Stoich Coeff (-1, 1, 4). Click Basis page, and type 15 for Co (this is the conversion). Close windows until you see *PFD*.
8. Double click reactor. Choose Global Rxn Set as Reaction set and close the window.
9. Now, open worksheet \( \text{Re} \), and type in all the know conditions for the streams as shown in the worksheet below. Note that only blue colored fonts are the values that you specified. If you more information than the degree of freedom allows, it will give you error messages.
Example 3: Modification of Process for the Improvement

Inspection of the calculation results of Example 2 shows that the cooling duty is comparable to the heating duty, suggesting that the utility load can be reduced by preheating the feed stream with hot reactor product. Modify the process by adding a heat exchanger.

This can be accomplished in the PFD using the following steps:

1. Click Heater of PFD and change the name of the feed stream to Pre-Heat. Close the window.

2. Click the R-Prod stream of PFD. Worksheet of the outlet stream will pop up. Change the name of the Reactor effluent stream to R-Prod1.

3. Click Cooler of PFD and change the name of the feed stream to R-Prod2.

4. Install the Pre-Heater unit, using the Heat-exchanger model, with Feed and Pre-Heat as the tube-side inlet and outlet streams, and with R-Prod1 and R-Prod2 as the shell-side inlet and outlet streams. Click Parameter at the left side of the window. Specify Delta p as 0 for both tube side and shell side. Choose Weighted Exchanger as Model. Close the window.

5. You still need to specify one more condition. Open the Worksheet and specify the temperature of Pre-Heat stream to 600°F. You may change this temperature to see how it affects the Heat-duty.
6. You can change the Pre-Heat stream temperature and see how it affects the H-Duty and UA (heat transfer coefficient × interfacial area). Increasing Pre-Heat temperature can reduce the H-Duty, but it will increase UA, which means that you need a heat exchanger with more interfacial area (bigger and with more inner pipes). Obviously, there will be upper limit of Pre-Heat temperature no matter how good your heat exchanger is. You can see this effect by changing the temperature and recording the change of other values. This can be done by using Databook function (under the Tools pull down menu.). The process can be described as follows:

   a. Open Tools/Databook. Click Insert button and choose Pre-Heat as object, Temperature as Variable and click Add button. Do the same for Heat-Duty as object, Heat Flow as Variable and Heat Exch as object, UA as Variable. Close the window.

   b. Go to the Case Studies page and click Add. Check Ind (Independent variable) for Pre-Heat and check Dep (Dependant variable) for Heat-Duty and Heat Exch. Click View. Type in 500 for Low Bound, 620 for High Bound, and 10 for Step Size.

   c. Click Start. After a few seconds, click Results.
Example 4: Processes Involving Recycle

Ethyl chloride will be produced by the gas-phase reaction of HCl with ethylene over a copper chloride catalyst supported on silica as

$$\text{C}_2\text{H}_4 + \text{HCl} \rightarrow \text{C}_2\text{H}_5\text{Cl}$$

The feed stream is composed of 50 mol% HCl, 48 mol% C\textsubscript{2}H\textsubscript{4}, and 2 mol% N\textsubscript{2} at 100 kmol/hr, 25°C, and 1 atm. Since the reaction achieves only 90 mol% conversion, the ethyl chloride product is separated from the unreacted reagents, and the latter is recycled. The separation is achieved using a distillation column, where it is assumed that a perfect separation is achievable. The process is operated at atmospheric pressure, and pressure drops are ignored. To prevent the accumulation of inerts in the system, 10 kmol/hr is withdrawn in a purge stream, W. Show the effect of the flowrate of the purge stream W on the recycle R and on the composition of the reactor feed.

Solution

This instruction is brief. You may not be able to understand it unless you see the classroom demonstration.

1. Start HYSYS and choose Peng Robinson as Base Property Package. Open Component page of Fluid Package window and add components (ethylene (or ethene), hydrogen_chloride, ethyl_chloride, and nitrogen) and close the Fluid Package.

2. Click Enter Simulation Environment and click Mixer in the Object Palette and click it on Process Flow Diagram (PFD). Do the same for the Conversion Reactor, Component Splitter, Tee (Tee is at the right side of mixer in Object Pallette), and Recycler as shown in the figure below.

3. Name all streams as shown in the figure below.

4. Click Flowsheet/Reaction Package. Add Global Rxn Set. Then, click Add Rxn at the lower right side of the window and choose Conversion. Add three components (ethylene, hydrogen_chloride, and ethyl_chloride) and Stoich Coeff (−1, −1, 1). Click Basis page, and type 90 for Co for Ethylene as a basis. Close windows until you see PFD.

5. Double click the Conversion Reactor. Choose Global Rxn Set as Reaction set and close the window.
6. Double click the Recycle and set your Parameter/Tolerance to be all “1.”

7. Since it was assumed that the components were separated perfectly, ethyl chloride was recovered in the bottom at 100% purity, with the other three components in the overhead product. This can be specified by double clicking Component Splitter and Clicking Splits (Under Design) and filling in 0 for ClC2 and 1’s for other three components.

8. Now open Workbook. Check the units to see if it is in SI units. Otherwise, change the unit by clicking Tools/Preferences/Variables. Choose SI and click Clone and change the units so that it is most convenient to you.

9. Fill in the Workbook with all the given condition, starting from the Feed stream: temperature (25°C), pressure (1 atm), and molar flow (100 kmol/hr). Double click 100 (molar flow rate), and fill in the composition and close.

10. Continue to fill in the Workbook for the R* stream with the flow rate of zero and the condition and composition equal to those of the feed, to allow computations to proceed. Fill in the temperature (25 °C) of the streams S3, S4, and P. Fill in the pressure (1 atm) of the streams S4 and P.

11. Specify the molar flow rate of the stream of W to be 10 kmol/hr. Now you can open the Worksheet to see the result of the calculation as shown below.

12. As in Example 3, the Case Study option in the Datebook can be used to investigate the impact of the purge flow rate on the recycle flow rate, reactor feed composition, and amount of unused reactants in W stream.
Example 5: Distillation

We need to separate a mixture of five paraffins into light and heavy fraction by using multistage distillation column with 12 ideal trays, a total reflux condenser, and a reboiler. The feed stream (1000 lbmols/hr) consists of 3% (mole %) ethane, 20% propane, 37% n-butane, 35% n-pentane, and 5% n-hexane at 225 °F and 250 psia, which enters the column on the seventh tray, counting from the top. The condenser and reboiler pressures are 248 and 252 psia, respectively. The preliminary design specifications require a reflux ratio of 6.06 and a vapor overhead product of 226 lbmol/hr. Subsequently, the design is modified to ensure propane overhead recovery of 191 lbmol/hr and butane bottom recovery of 365 lbmol/hr.

Solution

1. Start HYSYS and choose SRK as Base Property Package. Open Component page of Fluid Package window and add components and close the Fluid Package.

2. Click Enter Simulation Environment and click Distillation Column in the Object Palette and click it on Process Flow Diagram (PFD). Double click Distillation Column, and fill in the stream names as C-Duty, R-Duty, F for Feed, D for Distillate), and B for Bottom. Fill in # Stages = 12 and Inlet Stages 8_Main. Choose the condenser type as Full Reflux. Click Next.

3. Fill in Condenser and Reboiler pressures as given in the problem and click Next.

4. Fill in Optional Condenser and Reboiler Temperature Estimate. Good estimates are 100 °F for Condenser and 240 °F for Reboiler. The HYSYS will calculate the correct values. Click Next.

5. Fill in Vapor Rate of 226 and Reflux Ratio of 6.06. Click Done and close Distillation Input Expert window.

6. Open Worksheet and fill in F stream as given in the problem.

7. Double click the column on PFD and click Run. If you followed all the direction correctly, it should converge. Now you can turn various pages to see the results of the calculation.

8. Now, as stated in the problem, we need to ensure that propane overhead recovery must be 191 lbmol/hr and butane bottoms recovery must be 365 lbmol/hr. This can be done by clicking Monitor at the left side of the window and clicking Add Spec at the bottom of the window. Click Column Component Flow and fill in the condition for the D stream. Close the window. Repeat this for the B stream.

9. After adding the two new specifications, the list of active specifications must be updated. This is carried out in the Monitor page, where the two original specifications are deactivated and the two new specifications are activated.