CHE 201 CHEMCAD Exercise 1

Goals for this exercise:

- Introduce the ChemCAD flowsheet simulator.
- Reinforce key concepts of sensible and latent heat and vapor-liquid equilibrium.

Problem Statement 1:
100 mol/min of benzene at 120 °C and 1 atm enters a condenser. (A condenser is a heat exchanger that cools a vapor stream until some of it (or all of it) condenses, and then lets the liquid drain off separate from the vapor.) The normal boiling point of benzene is 80.10 °C.

- If you cool the mixture to 100 °C in the condenser,
  - what will the composition and flow rate of the gas be?
  - what will the composition and flow rate of the liquid be?
  - how much heat must be transferred to/from the utility stream to accomplish this?
- If you cool the mixture to 15 °C in the condenser,
  - what will the composition and flow rate of the gas be?
  - what will the composition and flow rate of the liquid be?
  - how much heat must be transferred to/from the utility stream to accomplish this?

Problem Statement 2:
100 mol/min of 50 mol % benzene and 50 mol % toluene at 120 °C and 1 atm enters a condenser. The normal boiling point of toluene is 110.62 °C.

- If you cool the mixture to 100 °C in the condenser,
  - what will the composition and flow rate of the gas be?
  - what will the composition and flow rate of the liquid be?
  - how much heat must be transferred to/from the utility stream to accomplish this?
- If you cool the mixture to 15 °C in the condenser,
  - what will the composition and flow rate of the gas be?
  - what will the composition and flow rate of the liquid be?
  - how much heat must be transferred to/from the utility stream to accomplish this?

Problem Statement 3:
100 mol/min of a contaminated air stream at 120 °C containing 10 mol % benzene and 10 mol % toluene enters a condenser.

- If you cool the mixture to 100 °C in the condenser,
  - what will the composition and flow rate of the gas be?
  - what will the composition and flow rate of the liquid be?
  - how much heat must be transferred to/from the utility stream to accomplish this?
- If you cool the mixture to 15 °C in the condenser,
  - what will the composition and flow rate of the gas be?
  - what will the composition and flow rate of the liquid be?
  - how much heat must be transferred to/from the utility stream to accomplish this?

CHEMCAD Solution Procedure – Use ChemCAD to calculate heat duty and compositions of product streams

1) *Start ChemCAD.* Double click on the CHEMCAD icon on the desktop. Click on File > New Job. Pick a name for your job and save it. Save your job periodically.

2) *Get ready to draw your process flow sheet.* Click on "Edit Flowsheet" if you see it on the toolbar. You need that spot to say "Run Simulation" in a pale font. An equipment module palette should appear.

3) *Select the modules you need and place them on the drawing one at a time.* The module names appear under the icons in the palette when you move the cursor there. Modules are in alphabetical order. Left click the module you want in the palette and then left click on the spot in the drawing field where you want the symbol placed. Right click on a module in the palette to get different configurations. Right click in the drawing field to select modules to delete, rotate or flip. For this exercise, select a "Flash", a "Feed" (red arrow) and two "Products" (purple arrows). (A condenser looks to us like a heat exchanger, but the "Flash" module is the signal to ChemCAD that vapor-liquid equilibrium (VLE) is involved here. Use a flash module to simulate flash tanks and partial and total condensers. Pick the configuration that looks most like what you want. I like Flash #3 for a condenser.)

4) *Connect the modules with streams.* Left click on the stream icon (a line with a red and a blue end) in the module palette. Draw streams between the modules as needed. Start and end each stream using the left mouse button. Use the left mouse button to mark any corners you want in the streams. Use a right click to erase a line or line segment. Each line should begin on a red circle and end on a blue circle.

5) *Get ready to run the flowsheet simulator.* Left click on "Run Simulation" if you see it on the toolbar. You need that spot to say "Edit Flowsheet."

6) *Specify the units you want to use*. Click on Format > Engineering Units. You can use the buttons at the bottom of the screen, or use the drop-down menus for individual quantities. You can change the units later, and ChemCAD will automatically convert all of your values to the new units.

7) *Input the list of components you will use in your simulation.* Left click on Thermophysical > Component List. The computer may hesitate here. Use the search field to find the components you need. Add them to the component list with the "Add" button. Left click on "OK" when you're done. For this exercise, select "Benzene", "Toluene" and "Air". You can add or delete components later.

8) *Choose your thermodynamics*. ChemCAD can use any of several models to calculate vapor-liquid equilibrium (VLE) and enthalpies. (It uses models instead of huge tables of real values.) Different models work better for different chemical systems, and changing models can sometimes change your results by a lot. ChE students learn about these models as juniors in Thermodynamics. As sophomores, the only VLE calculations you understand are ideal ones, based on Raoult's Law and Henry's Law, so for this exercise we will use those. Left click on Thermophysical > K-values. Select "Ideal Vapor" from the drop-down menu. To set the model used to calculate enthalpies,

left click on Thermophysical > Enthalpy. Select SRK.

9) *Set the conditions of the feed streams.* Left click on Specifications > Feed Streams. Enter the temperature, pressure, and flow rate of each component from the problem statement. Note that you also have the option to enter the vapor fraction (0 – 1). You can only enter two of the following three parameters: temperature, pressure, vapor fraction. Specifying any two along with the stream composition automatically fixes the third. (You should understand why.) Also, note that ChemCAD uses a 0 to mean "no entry", which sometimes leads to trouble when you want the value to **be** 0. If you want a value of 0, you may need to enter a small number like 0.000000001 to get it to work correctly.

10) *Set the operating characteristics of the modules.* Left click on Specifications > Selected Units and then left click on the module you want to work with, or just double click on the module itself. The different calculations that ChemCAD can perform on a flash module are shown in a drop-down menu. For this problem, select "Specify T and P, calculate V/F and heat". After you select this option, new boxes will appear where you should enter the operating (outlet) temperature and pressure of the condenser.

11) *Run the simulation.* Left click on Run > Run All. (If you have a more complex flow sheet, you may choose to run only selected modules.)

12) *Look at your results.* Left click on Results, and then choose what you want to look at. You can look at the streams (to see flow rates and compositions) or at the units (to see heat duty). The results are in Rich Text Format, so they can be imported directly into word documents.

Discussion of the Problems

Problem Statement 1

This is the simplest kind of VLE problem you can have: a pure compound that is volatile (can be vaporized) and condensable. At 100 °C and 1 atm (above the boiling point), benzene is all vapor. The vapor stream exiting the condenser is of the same composition and molar flow rate as the vapor stream entering. There is no liquid stream exiting. At 15 °C and 1 atm (below the normal boiling point), the benzene is all liquid. The liquid stream exiting the condenser is of the same composition and molar flow rate as the vapor stream entering the condenser. There is no vapor stream exiting.

Problem Statement 2

This is a more complex VLE problem. Here, you have a mixture of volatile, condensable components. At 100 °C and 1 atm, you are between the boiling points of the two compounds. Your exiting streams could be all vapor (same composition and flow rate as the inlet vapor), all liquid (same composition and flow rate as the inlet vapor), or a liquid stream and a vapor stream in equilibrium with each other (at the same temperature, but different compositions). To see what situation we will be in, let's look at a Txy diagram.

Drawing a T-xy Diagram with ChemCAD

1) Select Plot > Tpxy.
2) Choose the two components from the drop-down menus. Select "constant pressure" mode. Enter the pressure. No need to estimate temperature. Ask for mole fractions from 0 to 1.
3) A table may appear. If it does, close it or move it to see the T-xy diagram.

The T-xy diagram for the benzene-toluene system shows that a 50/50 molar mixture of the two is all vapor at 100 °C and 1 atm. If you want to produce both a vapor and a liquid stream from your condenser, pick a temperature within the two-phase region. Play with different temperatures and observe how the compositions and flow rates of the vapor and liquid streams change. At 15 °C and 1 atm (below the normal boiling points of both components), the mixture is all liquid, of the same composition and flow rate as the inlet vapor stream.

Problem Statement 3

Often, we think of air as being "non-condensable". In other words, we assume that 100 % of the air always stays in the vapor phase. That assumption simplifies this type of VLE problem. At temperatures below the saturation point, we have a liquid mixture of benzene and toluene, and a vapor phase mixture of all three. In this case, at 100 °C and 1 atm, the material exiting the condenser is all vapor with the same composition and flow rate as the inlet vapor. Try different operating temperatures with ChemCAD until you get condensate (liquid out). How does this temperature compare with the dew point temperature from the T-xy diagram for the benzene-toluene system?

Even at 15 °C and 1 atm, below the boiling point of both benzene and toluene, there is still benzene and toluene in the vapor stream. (Remember, there is water (humidity) in the air even at temperatures below 100 °C.) The mole fraction of organics in the vapor phase may surprise you. A condenser probably wouldn't be enough to help you meet EPA emissions regulations in a situation like this. In the presence of a non-condensable component, NEVER assume that 100 % of the condensables go out with the condensate.

Another useful way to look at this problem is to think of it as just like Problem 2. The only way to get all of the benzene and toluene into the liquid phase is to condense the whole mixture, and that won't happen until you get below the boiling point of **all** components, including air (nitrogen and oxygen).

If it is just like Problem 2, then why isn't there air in the liquid phase at 15 °C? There is. If you calculated it by hand, you would probably assume that there wasn't, but ChemCAD doesn't assume that. There is a little bit of air dissolved in the liquid benzene and toluene. In some cases, that little bit can be important. The little bit of oxygen found in liquid water is very important to fish, for example. The idealized way to handle vapor-liquid equilibrium when you have a vapor (air) that is only slightly soluble in the liquid (benzene-toluene), and you want to know how much of the vapor is in the liquid, is Henry's Law.