<u>ASSIGNMENT 2</u>   CHE 4273

Submit all files directly to the TA through e-mail (including simulation files). Make sure they can be opened before you submit. Sometimes students inadvertently submit corrupted files. Copy what you plan to submit in a new directory and make sure they open there.

DUE: March 5, no later than 5:00 pm.

<u>PROBLEM #1:</u> *Designed to familiarize you with the use of column tolerances and the use of the Optimizer features in Pro II.*

Part a) Set up in Pro II a column to distill a mixture of 23 mole % n-butane, 53 mole % i-pentane and 24 mole % n-hexane at atmospheric pressure and 100 ^{o}F. A 97% recovery of n-butane in a form of a 99% n-butane stream is desired. Determine column diameter and provide details of sieve trays. Use the column hydraulics design mode in Pro II. Justify your choice of thermodynamic system (there is a tutorial to choose it) and show how much the results change with your second best choice.

Part b) Add an OPTIMIZER and set it up to search for the best feed tray location. Your objective is to minimize the reboiler duty. Reset the column to the initial values you provided, rather than the values from the previous run. This is done in the Initial Estimates menu . There is a box there that say use "Use product rates calculated in the last iteration".

1. What is the new feed tray location?
2. What is the new reboiler duty?

The OPTIMIZER starts from a converged solution, takes a small step in feed tray location, and converges the COLUMN using the previous solution as an initial estimate. For this particular column, the convergence tolerances may be loose enough so that PRO/II converges the COLUMN almost immediately; both feed tray locations may result in essentially the same solution. Because the change in the objective function (reboiler duty) could be below the current tolerance setting, the OPTIMIZER may discontinue the search for a better feed tray location.

Change the following convergence tolerances on the COLUMN:

- The relative tolerance for both column specifications to 1 E-05.
- The Bubble Point tolerance to 1 E-06.
- The Enthalpy Balance tolerance to 1 E-06.
- The Equilibrium K-value tolerance to 1 E-06.

Rerun the problem with the new tolerances. Make sure that you still have the initial estimates Use product rates calculated in the last iteration" box unchecked.

1. What are the new feed tray location and reboiler duty?
2. By approximately what percentage did the reboiler duty decrease?

We saw that changing the COLUMN convergence tolerances had a significant impact on the calculated optimum feed tray location.

Change the following OPTIMIZER parameters:

- Set the absolute maximum step size to 5.

- Set the defined absolute step size to 1.
- Set the minimum relative change for the objective function to 0.0001.

Rerun the problem with the new parameters. Double-click on the COLUMN and reset the initial feed tray location to its original tray. Retain the tightened tolerances of the last problem.

1. What is the new feed tray location?
2. How big an effect does changing the OPTIMIZER parameters have on the feed tray location when compared to the effect of changing the COLUMN convergence tolerances?

PROBLEM #2: *This exercise is for sharpening your optimization skills in a simulator.*

Download the Cyclohexane production plant simulation file. The reactor is a PFR containing 30 tubes, 30 ft long and 6" diameter. Assume the reactor is operating at a fixed temperature (320 ^oF, not a bad approximation). The reactr has a bed of catalysts, but you do not need to worry about it for the time being. This only affects superficial velocity, so at the end, the length of the ractor will have to be proportionally longer than what the calculations in Pro II indicate. Use the following kinetic constant $k=4.78\ 10^5 \exp(-9000\ (Btu/lbmol)/RT)$. Use first order in benzene and zero order in Hydrogen. These, you have to make sure you input, as the simulator picks the stoichiometric coefficients by default. The flash should be set at 115 ^oF and a fixed split ratio (15%) should be used for the splitter.

1) Include a calculator to evaluate your profit (profit=Revenue-raw material cost-operating costs). Don't forget to include the cost of compressing. The reactor will produce extra heat that can be used to produce steam by adding water to its jacket. Use the heat duty of the reactor to calculate a revenue based on selling the steam produced. You should pick the pressure and the quality of the steam produced, as price will vary for different options. The flash in the simulation is not adiabatic. If it were adiabatic, what additional piece of equipment would need to be added before the flash to obtain the same product results? Based on this answer, assume that cooling water is required for the operation of that piece of equipment, determine the cooling water requirement, and add the cooling water cost to the operating expenses. All these calculations can be done inside the Calculator by just using the heat duties as parameters. There is no need to include new streams. Make sure you also include the cost of compressing. To do this, you need to assess somehow what is the pressure drop you will have, which in turn means you need to have some idea of the distances and the diameters of your piping. Peters and Timmerhaus has some simple formulas to obtain "economical pipe diameters" as a function of flowrate and other properties. In other words, do what you can with the little time you have to make a good assessment of cost. Run the problem again and determine the profit for the set of parameters that you have.

2) Include an optimizer and maximize the profit by varying the reactor temperature. Re-run the simulation a couple of times to verify that it stays at the same value. Truncation errors and convergence tolerances may change the results. It is a fact you need to be aware of. Be careful with the limits you put in the variables. If they are too wide, the optimizer may take a step that is too large and the flow sheet become infeasible and the simulation may not converge. Don't know what the limits could be? Start with small intervals and keep enlarging them. Use your judgment as of when to stop. Since the reverse reaction is not there, establish a reasonable limit for the upper bound. Explain what are the effects of varying the temperature and why the optimizer behaved the way it did.

3) Add the heat exchanger area to the variables varied by the optimizer. Make sure first that the exchanger has an area You pick a U and a maximum value of this area. Report the results. Tighten the optimizer tolerances (Click in Options and change the Relative change in the Objective function to ten times lower) and tighten convergence tolerances. Explain the results. Why did you have to tighten convergence tolerances?

4) Add the splitter specification to the variables varied by the optimizer. Use 0.1 and 0.25 as limits. Report the results. You are told now that the molar flowrate of hydrogen into the reactor has to be at least 9 times larger than the molar flowrate of benzene. Explain where this specification might come from. Introduce this constraint into the optimizer and re-run the problem. Explain the result.

5) Add the flash temperature as variable. Be careful with the lower bound. It cannot be lower than what cooling water can cool. Upper bound has its problems too. Report and explain the results.

6) Add a constraint requesting the cyclohexane in the product should have a molar fraction larger than 0.975. Be careful with the tolerances. This may or may not converge, depending on the limits you used for other variables. If successful, explain the results, if not, explain why it cannot reach the desired concentration. Why is this constraint needed?

Grading on this exercise: 1) through 5): 15% each, 6): 25%.

Points for problem 1: 35
Points for problem 2: 65