Problem Set 3

This problem set explores simulation of batch distillation with ABACUSS. .

Problem 1: Binary Batch Distillation (50 Points)

A process produces a waste stream of 4500 kg of a 55 mass% methanol/ethanol mixture (per batch). The sales department believes it could sell methanol recovered from this waste stream, provided that its concentration is increased to 80 mass%. The plant manager would like you to study the feasibility of recovering methanol of the desired purity. A batch rectifier is available for the solvent recovery operation. It takes 2.1 hours to charge, preheat, discharge, and clean the column for each batch (the still is used for other separations between solvent recovery batches). The still is normally operated at a constant boilup rate of 50 kmol/h. The fractionating capability is equivalent to 9 theoretical stages (including the reboiler). A suitable model has been prepared in a file stored in the course locker: /mit/10.490/Public/ABACUSS/include/DistHW.ABACUSS

The mixture can be considered to have a constant relative volatility of 1.72. The sales office suggests that you evaluate the column productivity, P, through the simple formula:

$$P = \frac{D_w}{t_{dist} + t_{change}}$$

where D_w is the mass of on-specification methanol product collected in the accumulator, t_{dist} is the distillation time, and t_{change} is the changeover time (2.1 h). To avoid simulation failures, initialize the accumulator with 1 mole of methanol (models cannot predict mole fractions when holdups are zero).

   (a) Provide a derivation of the model in DistHW.ABACUSS, detailing the consequences of all assumptions.
   (b) Run a series of simulations with different constant reflux ratios. Plot column productivity vs. reflux ratio. What is the optimum reflux ratio?
   (c) Can you improve the productivity further by designing a time-varying reflux policy?
   (d) What factors does the productivity metric not measure?

Hand in ABACUSS input files for your optimal policies in parts (b) and (c).

Problem 2: Multicomponent Distillation with ABACUSS (50 points)

The first distillation task in the Lucretex process separates a mixture of six components. Suppose 20 kmol of product from the second reaction task is charged to a batch rectifier. The molar composition of the feed (on a catalyst-free basis) is:

Component	Mole fraction
A	0.15
E	0.12
I2	0.02
MeOH	0.24
Allyl Alcohol	0.19
Toluene	0.28

Problem Set 3

The packing height can be considered to be equivalent to ten equilibrium stages. The distillation is conducted in the following way:

1. Atmospheric distillation:
   - (a) Pres-Profile: Atmospheric pressure, zero pressure drop in the column.
   - (b) Col-Specs: Vapor rate from reboiler is 15 kmol/h; reflux ratio is 8.0.
   - (c) Stop-Crit: Since the Pt catalyst slurry catalyzes unwanted side reactions above 140ºC, distillation should be stopped when the reboiler temperature reaches 130ºC.
2. Vacuum distillation:
   - (a) Pres-Profile: Pressure of 150 mm Hg is applied to the column. The rate of vacuum application is linear, and it takes 30 minutes to go from 760 mm to 150 mm Hg. Pressure drop in the column is zero.
   - (b) Col-specs: Vapor rate from reboiler is 15 kmol/h; reflux ratio is 8.0.
   - (c) Stop-Crit: Stop when reboiler temperature reaches 135ºC.

Use ABACUSS to simulate this sequence of operating tasks. For physical properties, use the Wilson activity coefficient model and the ideal gas equation of state. The property file should be included from the course locker as you did for the tutorial. Switch the distillate to the second accumulator between the two tasks.

- (a) Give the amount and composition of the material in the first accumulator after the atmospheric distillation step.
- (b) Determine the amount and composition of the material in the second accumulator after vacuum distillation. What is left in the reboiler?
- (c) Calculate the total amount of (A+E) lost in the distillation, if only the second cut (overhead from the vacuum distillation) is passed to the downstream process.
- (d) What is the total time of operation of the column?
- (e) Record the instantaneous distillate composition for each of the six components as a function of time. Print out a plot of these compositions versus time and point out where the vacuum distillation cut is made.
- (f) Plot the temperature profile in the column at a number of equally spaced points in time during the course of the operation.

NB: the reflux ratio values stated above are according to the usual definition, i.e., $R = L/D$, which can vary between zero and infinity (total reflux). ABACUSS cannot deal with infinity as a number, so the reflux ratio used in the ABACUSS model is a normalized reflux ratio defined between zero and unity (total reflux).

$$R_{norm} = \frac{L}{L+D} = \frac{R}{R+1}$$