Ch En 386

**Winter 2014 Homework**

**Homework #8 (20 points)**

**Due Friday, February 28**

Note: Anytime you solve a problem with Polymath or MathCad, you must print a copy of the report (Polymath) or the page with equations (MatchCad).

*Conditioning Problems (0.5 points each- you may not work with other students):*

1. What solving variable must be used for solving non-steady state CSTR equations? Why?
2. If you have a non-steady state CSTR where the volume is changing with time due to inlet *v0* being different than outlet *v*, show the relationship between dNA/dt and dCA/dt. You may assume a liquid reaction with constant density.

Magnitude and Reasonableness Problems *(0.5 points each)*

1. If you have A 🡪 B 🡪 C, what must be true about the rate constants for B to stay very low in concentration compared to A and C?
2. For Problem 6-9c, what would you recommend for a reactor type and temperature to maximize the selectivity of D relative to U. Answer in qualitative terms.

*Lesson 19: Reactors with mass transfer*

1. (3 points) Fogler P4-23 a, c, d. Note that this is a semi-batch reactor. During the process, you should assume that CO2 leaves the solution via mass transfer through the gas-liquid interface. The tank is open to the atmosphere and you may assume that CO2 in the surroundings (CCO2,S) is zero. For CO2, k’c = 10 cm/hr and AS = 6000 cm2. For part a, only plot the information until the tank is full (2500 dm3). The conversion refers to sodium bicarbonate. For part d, discuss what you learned between parts a and c as to how to obtain the best conversion by the time the reactor is filled. Use N for your solving variable. Be careful of your units.
2. (3 points) The aqueous elementary reaction A 🡪 2B occurs in a PFR that has a membrane permeable to B. For example, B may be ethanol in solution that goes through the membrane wall. You may assume *v = v0* since the loss of B does not affect the liquid flow rate. kA = 0.5 min-1. CA0 = 2 M and v0 = 1 liter/min. No B enters the reactor. CBS = 0 and k’c*a* = 0.4 min-1. What is the concentration of B exiting the 1.5 liter reactor? What would the concentration be if B did not go through the membrane? Solve by hand. You will need to use the integrating factor.

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*Lesson 20: Series and parallel reactions*

1. (3 points) Batch reactor problem: Fogler P6-10 d, e. Use polymath. For part e, choose k1 =300 and k2 = 0.05 and answer the question for the three scenarios of a) k-1= 0 and k-2 = 0, b) k-1= 0 and k-2 = 1 h-1 and c) k-1= 0 and k-2 = 0.25 h-1.
2. (3 points) Plug flow problem: Fogler P6-16 a. In addition to plotting species flow rates, plot the yields of all products and the conversion of coal as a function of space time. At what volume do you obtain 90% conversion? To input yields into polymath, you need to do a slight trick. For example, the yield of P is YP = (FP-FP0)/(FC0-FC). The problem is that at the PFR entrance, FC0 = FC and Polymath will blow up when it tries to solve. Therefore, input YP = (FP-0)/(20.0001-FC) for this example and then when your inlet is FC = 20 you can still get a solution that is pretty accurate. Do the same things for the other yields.

*Lesson 21: Multiple reactions*

1. (3 points) Steady state CSTR problem: Fogler 6-14b. You will need to solve using Polymath or MathCad since you will have multiple algebraic equations that need to be solve simultaneously.
2. (3 points) Non-steady state CSTR problem: Using the kinetic information in Fogler P6-12, plot the concentrations of all species with time for a 3000-liter constant volume CSTR. Only A enters the reactor at 100 liter/min and an inlet concentration of 3 M. At t=0, the reactor is initially filled with water, following which the inlet and outlet flows begin. Remember to pay particular attention to the rate constants (i.e. k2D refers to the rate constant for reaction 2 based on D. At approximately what time do you reach 99% of the steady state concentrations?