ChE 101 - Chemical Reaction Engineering
Problem Set 3
Winter 2017
Due 24 Jan 2017 at 5 pm to **caltech.che101@gmail.com**

Email Submission Instructions:
Email Subject: PS3_Your_Name_2017
File Name: PS3_Your_Name_2017.pdf
Note: State your assumptions and cite any external sources used for solving problems.

Reading

Finish Schmidt Chapter 3

Computational Problem Week 3: Reactors in Series

In this problem, we will be analyzing reactors in series and investigating how composition and reaction rate changes throughout these staged processes. We will write a MATLAB function that will create a $1/r$ plot for different sequences of reactors.

a) Write out a general expression for the output concentration CA,n of an irreversible first order reaction proceeding through a series of n reactors consisting of P PFTRs and R CSTRs. Be sure to take into account that the reaction rate coefficient k may be different in each reactor.

b) Create a function that generates a $1/r$ plot as a function of $C_{A,0}$–C_A. This function takes three arrays as inputs: array A indicating a sequence of reactors, array B representing respective residence times, and array B giving respective reaction rate coefficients. An example of array A for a CSTR to PFTR to 2 CSTRs to 2 PFTRs can be expressed as [1, 0, 1, 1, 0, 0] where 1 represents a CSTR and 0 represents a PFTR. Let $C_{A,0} = 5$ M. Comment on the features of the plot.

c) Using the function from part (b), plot the output for a CSTR, PFTR, CSTR, CSTR, PFTR, PFTR series of reactors with residence times of 10, 15, 5, 20, 7, and 7 minutes respectively and reaction rate coefficients in each reactor of 1, 5, 2, 4, 3, and 3 s^{-1} respectively.

d) For a constant reaction rate coefficient among all reactors in series, graphically show how a series of CSTRs will approximate a PFTR.

Hints:

- You may want to implement a loop that iterates through your series of reactors' array and distinguishes between a CSTR "procedure" and a PFTR "procedure" based on your model from part (a)
- Since the reactors are in series, each new iteration starts with the previous end value and calculates values through its own residence time ($C_{n,0} = C_{n-1,final}$).

Problem 1: Reactor Review

The aqueous reaction $A \rightarrow$ products has a rate of $r = 2C_A/(1 + C_A)^2$ (rate in moles/liter min), and is to be carried out in a continuous reactor system. We need to process 100 moles/h of 2 molar feed to 90% conversion. Calculate the reactor volumes required for the following:

a) a CSTR

b) a PFTR

c) two equal-volume CSTRs

d) Use plots of $1/r$ versus conversion to show these results

e) What is the ideal combination of reactors for total minimum volume for this reaction?

f) Show how you would solve problem (e) analytically. Set up equation and indicate the method of solution. You do not need to solve.

Problem 2: Autocatalytic Reactions

a) What is the optimum combination of ideal reactors for the reaction $A \rightarrow B$ if it is autocatalytic with $r = kC_AC_B$ and $C_A = C_{A\circ}, C_{B\circ} = 0$? What is the intermediate concentration between reactors?

b) Solve for 90% conversion if $C_{A\circ} = 1$ mole/liter and $k = 0.25$ liter/mole min.

Problem 3

The following reaction has variable order

$$\mathrm{A} \longrightarrow \mathrm{B} \qquad r = kC_A^n \tag{1}$$

You are given the following reactor configuration: a PFTR followed by a CSTR in series (PFTR + CSTR). In this reaction, the reactors are equal volume and operate at steady-state. The reaction proceeds to 90% conversion.

a) If $k = 0.500$ in the appropriate units, and $C_{A\circ} = 4.00$ moles/liter, determine the residence time τ for both reactor configurations, for $n_A = 1$.

b) Repeat part a), but for a 2nd order reaction ($n_A = 2$)

c) At your startup, your team has realized that the rate expression is much more complicated. Thankfully, you have the graphs of $1/r$ against conversion available on the next page (and printed by your TA). For the 3 different reaction rates, graphically show the optimal reactor configuration for 50% and 90% conversion.

Problem 4

The following aqueous, reversible reaction

$$\mathrm{A} \rightleftharpoons \mathrm{B} \qquad \mathrm{r} = k\,\mathrm{C_A} - \mathrm{k'C_B} \tag{2}$$

is to be carried out in a series of reactors with removal of product B between reactors. At each reactor, the reaction proceeds to 50% of the equilibrium composition. How many reactors are required for the final exit stream containing 90% conversion of the initial A for $k = 0.2 min^{-1}$, $K_{eq} = 1$ if ...

a) all B is extracted between reactors

b) 50% of B is extracted between reactors

c) Find τ for part a (all B is extracted between reactors) if the reactors are equal volume CSTRs

d) Find τ for part a if the reactors are equal volume PFTRs