Chemical Reaction Engineering—Homework #1

Due: Online submission on Canvas, **Wednesday, January 15, 2020 at 11:59pm.**

No late submissions will be accepted.

Problems that require a numeric answer should have 3 significant figures.
Units, where required, are shown in blue. Please use these units.

Problem 1: Basics

Consider a continuous flow reactor where the first order irreversible reaction A→ B is performed. If the feed only contains A with volumetric flow rate of 10 L/s and the first order rate constant is 0.05 s^{-1}, what are the conversions in a 100L CSTR and a 100L PFR? What is the reaction time needed in a batch reactor to reach the same conversion as in a PFR? [X_{CSTR} = 0.33, X_{PFR} = 0.4, t = 10s]

Problem 2: Rate Laws and Units

Determine the units of all constants (rate constants (k) and equilibrium constants (K)) in the following rate expressions. Please follow the nomenclature found in Appendix F of your textbook. Use meters for length, moles for amounts, seconds for time, Pascals for pressure, and grams for mass.

a. $$-r_A = \frac{k_1 c_A c_B^2}{c_C^2}$$

b. $$-r'_A = \frac{k_1\left(P_A - \frac{P_B P_C}{K_3}\right)}{1 + K_2 P_B^2 + K_4 P_C}$$

c. $$-r_N" = \left(\frac{k_N k_S K_P}{k_{-N} + k_S}\right) \frac{c_N c_P}{\left(1 + \frac{k_N}{k_{-N}+k_S}\left(1 + \frac{k_S}{k_I}\right) c_N + k_I c_I^{0.5}\right)^2}$$

Problem 3: CSTR vs. PBR for a catalyzed reaction

You are given the rate equation, $-r_A'' = k_A'' c_A$ for the reaction A→ B. The inlet flow rate is 200 mol/s of pure A. Pure A has a density of 500 kg/m^3 and a molar mass of 500 g/

mol. The rate constant is 10^{-6} m/s. The reactor has a catalyst of surface area S_g of 5 m^2/g, and the catalyst density in the reactor is 30 kg/m^3.

a. To achieve 40% conversion in an isothermal, steady-state, liquid phase CSTR, what is the volume required? [0.9 m^3]

b. What volume is required for the same conversion in an isothermal, steady-state, liquid phase PBR? [0.7 m^3]

c. What is the residence time in a CSTR vs. a PBR? Calculate a residence time with units of catalyst weight/volumetric flow rate as well as the usual reactor volume/volumetric flow rate. The former does not have the convenient units of time, but physically expresses the residents time accurately in a reaction catalyzed by a solid catalyst in a reactor. Explain in a single sentence, why the residence time for the CSTR is different from the PBR. [τ_{CSTR} = 4.5 s, τ_{PBR} = 3.5 s, $\tau_{w,CSTR}$ = 130 kg*s/m^3, $\tau_{w,PBR}$ = 100 kg*s/m^3]

d. It is decided to decrease the residence time by a factor of 2 by doubling the flow rates. What happens to the conversion in a PBR and CSTR. Support your conclusions with calculations. [X = 0.25]

Problem 4: Residence time

You are asked to select and size reactors to isothermally carry out a liquid phase, irreversible, reaction A → B with the following kinetics: $-r_A = kc_A^2$ where k = 0.2 L/(mol*min).

a. Starting with a mole balance (and assumptions), calculate the time that it would take a batch reactor to process your feed to achieve 95% conversion. The batch reactor is initially charged with 10 mol of pure A and the reactor size is 2L. [20 min]

b. Starting with a mole balance (and assumptions), calculate the residence time it would take a PFR to process your feed to 95% conversion. The PFR has an inlet feed of pure A at a rate of 10 mol/min and the volumetric flow rate is 2L/min. [20 min]

c. Compare your results in parts A and B and explain their relationship.

d. Starting with a mole balance (and assumptions), calculate the volume it would take for a CSTR to process your feed (from part B) to achieve 95% conversion. [800 L]

e. Calculate the residence time for the CSTR in part D and compare it with part B. Which reactor will you use and why? Which reactor yields the higher conversion given the same residence time. [400 min]

f. If the reaction exhibited negative second-order kinetics, does this change your reactor decision and why?

g. If the given reaction exhibited zero-order kinetic behavior, does this influence your decision from part E? Why?

Problem 5: CSTR with more complex rate law expression

The reaction A → B occurs in a steady state CSTR with a volume of 10L, an inlet flow rate of 5 mol/min of pure A and a conversion of 90%. The rate equation is of the form:

$$-r_A = \frac{k_1 c_A}{\left(1 + k_2\sqrt{c_A}\right)^2}$$

where k_1 = 2 min^{-1} and k_2 is 2(L/mol)$^{0.5}$. Solve for the steady state concentration of A in this reactor. [85 mol/L]