Chemical Reaction Engineering—Homework #2

Due: Online submission on Canvas, **Wednesday, January 22, 2020 at 11:59pm.**

No late submissions will be accepted.

You are encouraged to solve problems computationally, particularly with solving/evaluating difficult algebraic equations or integrals.

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

Let's look at the reaction A + 2B → C + D. The rate law expression is r = k c_A c_B. Assume that the reactors are isothermal and isobaric. k = 0.1 (1/M*min), v0 = 2 L/min, c_{A0} = 0.5M. Assume stoichiometric feed conditions.

a. Assume that the reaction occurs in the liquid phase. What are the expressions for the concentrations of A, B, C, and D. What is the volume of a CSTR that is needed to achieve 90% conversion of A? What is the volume of a PFR that is needed to achieve 90% conversion of A? [V_{CSTR} = 1800L, V_{PFR} = 180L]

b. Assume that the reaction occurs in the gas phase. What are the expressions for the concentrations of A, B, C, and D. What is the volume of a CSTR that is needed to achieve 90% conversion of A? What is the volume of a PFR that is needed to achieve 90% conversion of A? [V_{CSTR} = 900L, V_{PFR} = 100L]

c. Explain the difference in volumes needed between the liquid and gas phase reactions.

Problem 2: Multiple reactors in series with experimental data

Consider the exothermic, adiabatic reaction where we define the reaction event as:

A + B → C + D.

The following data were recorded for this reaction:

X	0	0.20	0.40	0.60	0.65	0.70	0.75	0.80	0.85	0.90
$-r_A$ (mol/(L*min)	2.00	2.73	4.29	10	10	10	6.67	5	4	3.33

The total entering molar flow rate is 4 mol/s, where the reactants are fed in the ratio of 3:1 (A:B).

a. What volume of CSTR and PFR are required to reach 60% conversion? [CSTR V = 3.6 L, PFR V = 10.8 L]
b. What conversion to you achieve if you use a 10.8 L PFR followed by a 3.6 L CSTR in series? [X = 0.85]
c. What if you instead begin with a 3.6 L CSTR and you follow it with a PFR. What volume of a PFR do you need to achieve 84% conversion? [2 L]
d. Is there a range of conversions over which we can use the same size PFR and CSTR to achieve the same conversion? If so, what is the range?
e. To achieve an overall conversion of 85%, what series of reactors will minimize the total required volume?

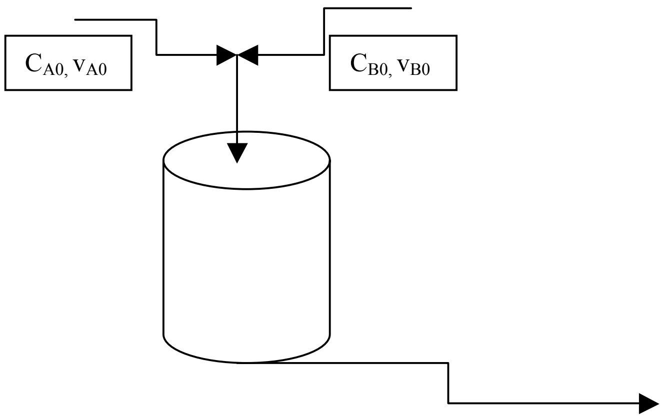
Problem 3: Digestion in cows

Farmer Michael is interested in the digestion capabilities of the the cows on his farm. Interestingly, cows have 4 stomachs that allow them to digest grass and can be modeled as isothermal liquid-phase CSTRs in series each with a volume of 20 L, given that these cows graze throughout the day. A 1000 lb cow will consume approximately 170 lbs (mass basis) of grass evenly over an 8 hour period of time. Enzymes in the cows' stomachs can convert the cellulose in grass to fatty acids that are used in metabolic pathways. The rate of cellulose consumption follows Michaelis-Menton Kinetics, which are typical for enzymatic reactions: $-r_A = \frac{k_{max} c_A}{K_M + c_A}$ where k_{max} = 2.8 mol/(L*hr) and K_M = 14 mol/L. Grass has a bulk density of 1.11 g/cm^3 and approximately 10.5% of the grass by weight is cellulose (molecular weight = 162 g/mol).

a. What conversion of cellulose do cows achieve by the exit of their fourth stomach? [78%]
b. What conversion would they achieve if they only had one stomach with the same total volume as the four stomachs combined? [65%]
c. What conversion would they achieve if their stomach was instead, more similar to a PFR? [83%]

Problem 4: Reactor decisions

A liquid-phase reaction 2A + B → C is conducted in an isothermal flow reactor with a reaction rate expression of $-r_A = k\, c_A^2$ where k = 0.07 L/(mol*min). You have 2 separated feed streams for A and B. The concentration of A in the feed stream is 2 M and the volumetric flow rate is 5 L/min. The concentration of B in the feed stream is 2 M and the volumetric flow rate is 3 L /min. These two feed streams combine to form a single feed stream into the flow reactor. You can choose to use either a 600 L PFR or a 400 L CSTR.



a. What is the conversion that can be obtained with each reactor? [CSTR, 0.62; PFR, 0.85]
b. For the reactor with the lower conversion, can we adjust the flow parameters in such a way to obtain the same conversion as the other reactor? To what values might the flow parameters be adjusted?

Problem 5: Economics of reactor sizing

Consider an isothermal, continuous flow reactor where the following reaction occurs in the liquid phase: $2A \rightarrow 3B + C$. You are to design the reactor to have 95% conversion of A at steady state. The initial concentration of A is 10 M and the volumetric flow rate is constant at 7 L/hr. For the following assumed rate equations (r_A), calculate the reactor volume required for both a CSTR and a PFR.

a. $-r_A = kC_A$ where $k = 0.9/h$ [CSTR, 150L; PFR, 25L]
b. $-r_A = kC_A^{-2}$ where $k = 0.6\ M^3/h$ [CSTR, 27L; PFR, 3900L]
c. $-r_A = k$ where $k = 0.4\ M/h$ [CSTR, 165 L; PFR, 165L]

d. In order to minimize capital costs, you need to decide which type of reactor to use for each set of kinetics listed in (a)-(c). Assume the volume is the only differing economic criteria and calculate the money saved for each if the cost is $750/L.