Introduction to Reactor Design, 3K4
Assignment 2

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Assignment objectives:

- To refresh concepts from your math and chemistry pre-requisites
- Learn how to work with conversion to size a reactor
- To demonstrate that you understand material on design reactors, and know what rate laws and stoichiometric tables are used for.

Question 1 [4]

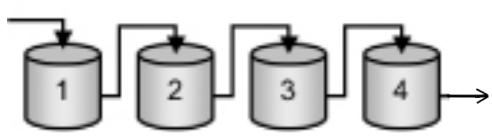
Make sure you can do these in a test/exam (i.e. without internet access). Let X be conversion; find:

1. $\displaystyle\int \frac{1}{(1-X)^2}\,dX =$
2. $\displaystyle\int_{X_1}^{X_2} \frac{1}{(1-X)^2}\,dX =$
3. And in general, what is: $\displaystyle\int \frac{a+x}{bx}\,dx =$

Question 2 [10]

For the question we covered in the end of class last week (see last page of this tutorial), we showed the volume of a PFR required is the area under the curve. The volume required was $2.16\,\text{m}^3$ to obtain 80% conversion.

If we used 4 CSTRs in series:



1. What would be the size of each reactor if we wanted 20% conversion in each reactor?
2. What is the total volume of these 4 reactors?
3. How does this total CSTR volume compare with (a) the single CSTR volume and (b) the single PFR volume?
4. What is the reaction rate in each reactor?

Question 3 [20]

The following reaction rate, $-r_A$ measured in units of $\left[\dfrac{\text{kmol}}{\text{hr.m}^3}\right]$ is observed at a particular conversion, X:

Reaction rate	Conversion
78	0.0
106	0.2
120	0.4
70	0.6

We showed in class that the area under this curve is related to volume of the plug flow reactor.

1. Start from the general mol balance and derive the equation that shows the area is equal to the plug flow reactor's volume; clearly state all assumptions used in your derivation.
2. Assuming these assumptions are all met, calculate the plug flow reactor's volume to achieve a 60% conversion given a feed rate of $15\,\text{mol.s}^{-1}$ to the reactor.
3. If there is zero conversion at the entry to the PFR and 60% at the exit; what is the conversion half-way along the reactor?
4. What is the reaction rate at the entry of the reactor?
5. And at the midpoint?
6. And at the exit?

Question 4 [12]

A new drug is being prototyped in a batch reactor; as is becoming common-place now, this drug is grown *inside* a cell as a by-product of the regular cellular processes. So far, experiments have shown the rate of consumption of the starting material, an animal-derived cell A, is the only concentration in the rate expression.

$$-r_A = \frac{5.5C_A}{20 + C_A}$$

where $-r_A$ has units of $\left[\dfrac{\text{mol}}{\text{day.m}^3}\right]$

1. Why is a batch reactor suitable for this type of testing?
2. 30 mols of cellular material are added to a batch reactor of $0.5\,\text{m}^3$; the liquid food source is added at the same time to the reactor, in excess. Calculate the amount of cellular material remaining in the tank after 10 days.
3. How many days are required to convert 80% of the starting cellular material.
4. Show a plot of the concentration in the tank over time until there is almost 100% conversion.

Note: in tutorial 1 you solved a similar problem, but for a CSTR and PFR.

Question 5 [5]

For the elementary liquid-phase reaction, $A + B \rightleftharpoons C$ with $C_{A0} = C_{B0} = 2\,\text{mol.L}^{-1}$ and $K_C = 10\,\text{L.mol}^{-1}$

1. What is the equilibrium concentrations of all the species?
2. Does it matter in which reactor this occurs? Explain your answer.
3. What is the equilibrium conversion of A?

Question 6 [10]

Set up a stoichiometric table for the isothermal, isobaric gas-phase pyrolysis of ethane, and express the concentration of each species in the reaction as a function of conversion.

1. Set up the table for a *flow reactor* at 6 atm and 1110K for the reaction: $C_2H_6 \longrightarrow C_2H_4 + H_2$

Question 7 [10]

For the system considered in class previously (see last page of this tutorial's PDF) we have designed a single CSTR to achieve a conversion of 80%. I will teaching in you the 4N4 course how to estimate the capital cost of the CSTR vessel. For now, please use this formula to estimate the capital cost in dollars, in 2011 prices:

$$\text{Cost} = 2800 \cdot \left(\frac{V}{100}\right)^{0.53} \cdot 4 \cdot \left(\frac{1490}{300}\right)$$

where V is the CSTR tank volume, in US gallons (these reason for the formula structure will become clear in the 4N4 course).

1. Estimate the price of a single CSTR to obtain 80% conversion.
2. Estimate the price of two equally-sized CSTR's to obtain 80% conversion. Also write down the reaction rate in each tank, and the conversion leaving each tank.
3. Would it be more economically viable to purchase 3 equally-sizes CSTR's, ordered in series, than to buy a single large CSTR? Show your calculations and explain.

Table 2-2. Processed Data

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{\text{m}^3\cdot\text{s}}{\text{mol}}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$(F_{A0}/-r_A)(\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0