Chemical Engineering 142

Chemical Kinetics and Reaction Engineering

Midterm 1

Tuesday, October 8, 2013

8:10 am-9:30 am

The exam is 100 points total. Please read through the questions very carefully before answering. Make sure to show all your work.

Name:________________________________

Student ID: ______________________________

Problems	Points (Max.)	Points Received
1	25	
2	25	
3	25	
4	25	

Total:____________

You are allowed one 8.5”×11” sheet of paper with your notes on it and a calculator for this exam. A list of (possibly) useful integrals and constants is provided on the last page of this exam.

1. Consider the overall reversible formation of hydrobromic acid from hydrogen and bromine whose mechanism is given below:

$$Br_2 \rightleftharpoons^{k_1}_{k_{-1}} 2Br$$
$$Br + H_2 \rightleftharpoons^{k_2}_{k_{-2}} H + HBr$$
$$H + Br_2 \rightarrow^{k_3} HBr + Br$$

Note that all rate constants in the first reaction are given in terms of Br_2. The active intermediates are H and Br. This problem has parts a. through e. (25 points)

a. Write rate expressions for the two intermediates. (4 points)

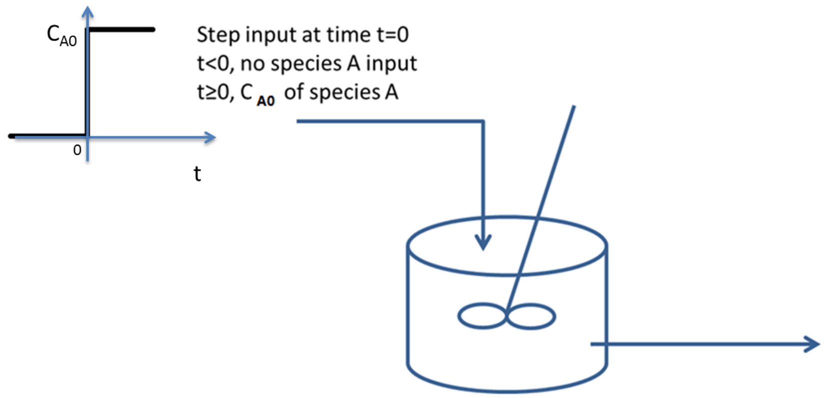
b. Write a rate expression for the formation of HBr. (2 points)

c. Using a pseudo-steady-state assumption determine the rate expression for the formation of HBr in terms of rate constants and concentrations of non-intermediate species. (10 points)

d. Repeat part c. using a quasi-equilibrium assumption instead of a pseudo-steady-state assumption. (8 points)

e. Do you prefer quasi-equilibrium or pseudo-steady-state? No need to explain. (1 point)

2. Consider constant ν (m^3/s) of water flowing through an ideal, isothermal, isobaric and liquid phase CSTR of volume V (m^3). Now at time t=0 switch from pure water to an aqueous solution of species A at a concentration C_{A0} (mol/m^3). (25 points)



(a) If the species A is inert, please write the general mole balance of species A and derive the outlet concentration of species A C_A versus t ($t \geq 0$)   (8 points)

(b) If a 0^{th} order reaction A(l) $\rightarrow$B(l) with rate constant k (mol/(m^3*s)) is carried out in the CSTR once species A enters the reactor, please derive the outlet reactant concentration C'_A versus t ($t \geq 0$) (10 points)

(c) Calculate the time to reach 99% of the steady state concentration in the CSTR with and without the 0^{th} order reaction A(l) $\rightarrow$ B(l). Comment on whether the presence of the reaction doesn't change/shortens/lengthens this time. (4 points)

(d) Please qualitatively plot C'_A versus t ($t \geq 0$) and label the maximum and minimum values clearly on the plot. (3 points)

3. Consider the following elementary reaction taking place in a steady-state CSTR under isothermal and isobaric conditions:

$$2\ A\ (g) \rightarrow B(g,l) + C(g)$$

The feed consists of species A and an inert species I in equimolar amounts. The total feed rate is 10 mol/min and the total volumetric flow rate into the reactor is 1 liter/min. The saturation mole fraction of B is 0.2. Assume that the gas phases are all ideal. Use k =1 liter/(mol-min) (25 points)

a) Construct a stoichiometric table in terms of the molar feed rates and account for all possible conversion regimes. (5 points)

b) At what conversion does condensation begin? Show your calculation. (5 points)

c) Write down the expression for the reaction rate r_A (mol/liter-min) as a function of initial concentrations of A and the conversion of A. Account for all possible conversion regimes. (5 points)

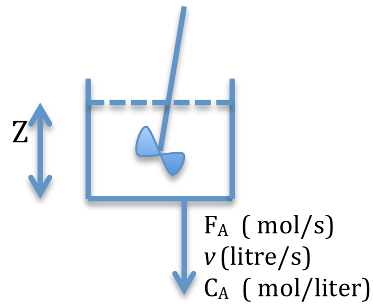
d) Find out the CSTR volume needed to achieve a conversion X_A=0.95. (5 points)

e) What is the mole fraction of different components in the gaseous phase at the CSTR outlet for a conversion X_A =0.95? (5 points)

4. (25 points)

$$A \rightarrow 2B\ ,\ r_A = -k\ C_A$$

Consider the elementary liquid-phase reaction above, which is being carried out in the leaking cylindrical batch reactor. This reactor is defective and has a small hole of area a in the base. As a result, reactor contents leak continuously at a volumetric flowrate $v = a\ (2gz)^{0.5}$ where z is the height of liquid in the reactor and g is the acceleration due to gravity. The cross-sectional area of the reactor is A_C. The initial concentration is C_{AO} and height of liquid is z_o. Assume that density ρ remains constant.



a) Express the volume of the liquid in the reactor explicitly as a function of time t and other constants. (5 points)

b) Obtain an equation for $\frac{dC_A}{dt}$. Hint: Write the general mole balance equation and simplify it. Express your answer in terms of C_{AO}, k and t. (10 points)

c) Express C_A explicitly as a function of t and other known constants. Is your answer going to be same or different for a batch reactor without any leak? Please explain physically why it is different or same? Answers without explanation will receive no credit. (4 points)

d) Find out the number of moles of A in the reactor, N_A (t). (3 points)

e) Find out the ratio of number of moles of B obtained in the leaky batch reactor after a time t to the number of moles of B obtained when there is no leakage. Assume that the lost liquid, which has leaked from the reactor, cannot be recovered and has no commercial value. Your final answer should contain time t and known constants only. (3 points)