ChE 344 **MIDTERM 1** Name:____________________

Tuesday, February 16th, 2016

9:30-11:30 AM

You may use a calculator and the provided notesheet.

Please sign the honor pledge (if applicable):

"I have neither given nor received aid on this exam, nor have I concealed any violation of the honor code."

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SCORE:

1. (15 points)	________________
2. (10 points)	________________
3. (20 points)	________________
4. (30 points)	________________
5. (25 points)	________________
TOTAL (100 points)	________________

Problem 1 (15 points)

The catalytic reaction

$$A \rightarrow B$$

to be carried out in a flow reaction system has the following rate law:

$$-r_A = \frac{kC_A}{(1+K_AC_A)^2}$$

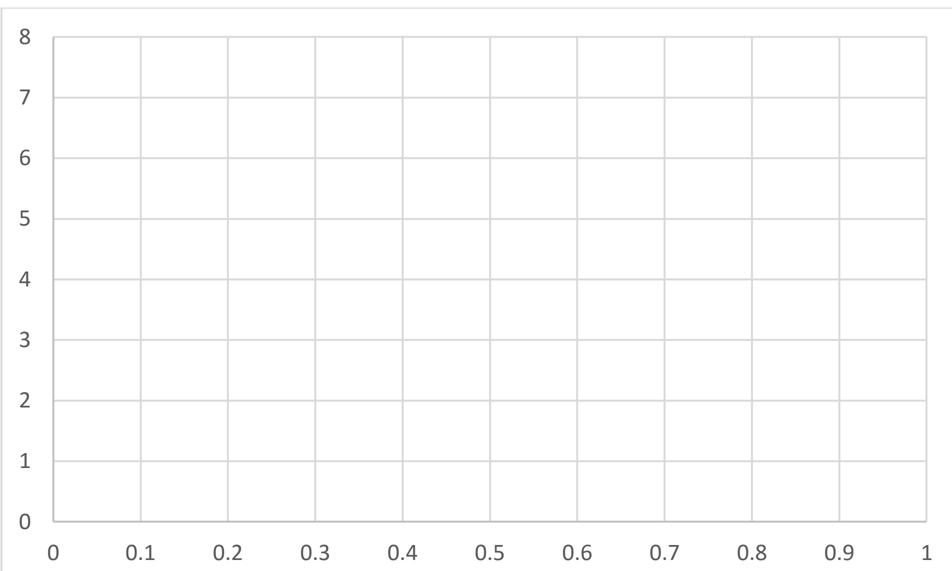
Where $k = 1\ min^{-1}$

$K_A = 1\ dm^3/min$

The entering concentration of A is 2 mol/dm^3. Sketch a Levenspiel plot to determine what type of reactor or combination of reactors would have the smallest volume to

a) achieve 50% conversion
b) achieve 80% conversion

You do not need to calculate the volume.



Problem 2 (10 points)

Determine whether the reversible, elementary, liquid phase reaction

$$A + B \rightleftharpoons 2C$$

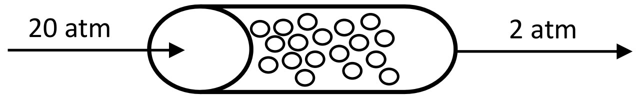
can be carried out in a flow reactor to obtain a conversion of 80% ($X = 0.8$) or greater. What conversion is achieved for this reaction? The feed is equimolar in A and B and the equilibrium constant $K_c = 8$.

Problem 3 (20 points)

The irreversible elementary gas-phase reaction

$$A + B \rightarrow C + D$$

Is carried out isothermally at 305 K in a packed-bed reactor with 100 kg of catalyst.



The entering pressure was 20 atm and the exit pressure is 2 atm. The feed is equal molar in A and B and the flow is in the turbulent flow regime, with F_{AO} = 10 mol/min and C_{AO} = 0.4 mol/dm^3. Currently 80% conversion is achieved. What would be the conversion if the catalyst particle size were doubled and everything else remained the same?

Problem 4 (30 points)

You are running a series of experiments for the generic, gas-phase reaction,

$$2A \rightarrow B$$

in a batch reactor run isothermally. You have carried out two experiments today at 400 °C and 500 °C. The time required to reach a conversion of 50% (X = 0.5) was 4 hr at 400 °C and 1 hr at 500 °C for an initial concentration of species A of C_{AO} = 0.5 mol/dm^3. You plan on running a reaction overnight at 200°C, but before you leave you want to make an estimate of what time you should come in the next morning. Assuming that the reaction is elementary, how long will it take to reach 50% conversion at 200°C?

Problem 5 (25 points)

The elementary, gas-phase reaction

$$A + B \rightarrow 3C$$

was carried out in batch reactor to achieve 50% conversion. The time required to reach this conversion for an initial charge of A and B at concentrations of C_{A0} = 0.75 mol/dm^3 and C_{B0} = 0.25 mol/dm^3 was 5 hours. Your job is to design a CSTR to obtain the same conversion of X = 0.5 for a feed stream containing A and B. The feed has a molar flow rate of 200 mol/hr of A and B at concentrations of C_{A0} = 0.75 mol/dm^3 and C_{B0} = 0.25 mol/dm^3. What volume of CSTR is required?

Work continued from ___

Formula Sheet

Fundamental Equation

$$\frac{dN_A}{dt} = F_{A0} - F_A + \int^{V} r_A dV$$

Design Equations

	Conversion Basis	Molar Basis
Batch	$N_{A0}\frac{dX}{dt} = -r_A V \qquad t_1 = N_{A0}\int_0^X \frac{dX}{-r_A V}$	$\frac{dN_A}{dt} = r_A V \qquad t_1 = \int_{N_{A_1}}^{N_{A_0}} \frac{dN_A}{-r_A V}$
CSTR	$V = \frac{F_{A0}(X_{out} - X_{in})}{-r_{A_{out}}}$	$V = \frac{F_{Ain} - F_{Aout}}{-r_{A_{out}}}$
PFR	$F_{A0}\frac{dX}{dV} = -r_A \qquad V_1 = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r_A}$	$\frac{dF_A}{dV} = r_A \qquad V_1 = \int_{F_{A_1}}^{F_{A_0}} \frac{dF_A}{-r_A}$
PBR	$F_{A0}\frac{dX}{dW} = -r_A' \qquad W_1 = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r'_A}$	$\frac{dF_A}{dW} = r_A' \qquad W_1 = \int_{F_{A_1}}^{F_{A_0}} \frac{dF_A}{-r'_A}$

Ideal gas law: $pV = nRT \qquad R = 8.314\,\frac{J}{mol.K} = 1.987\,\frac{cal}{mol.K}$

Arrhenius Equation: $k_A(T) = A \cdot \exp\left[\frac{E_A}{-RT}\right] \qquad k_A(T) = k_A(T_0)\cdot \exp\left[\frac{E_A}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$

$$K_C(T) = K_C(T_0)\cdot \exp\left[\frac{\Delta H^o_{rxn}}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

Stoichiometry:

For Reaction: $aA + bB \rightarrow cC + dD$ Liquid Phase: $C_i = C_{A0}(\Theta_i - v_i X)$

Gas Phase: $C_i = \frac{C_{A0}(\Theta_i + v_i X)}{1+\varepsilon X}\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right) \qquad v = v_0(1+\varepsilon X)\left(\frac{T}{T_0}\right)\left(\frac{P_0}{P}\right)$

$$\Theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}} \qquad \delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \qquad \varepsilon = y_{A0}\delta$$

Packed Beds:

laminar turbulent

$$\frac{dP}{dz} = -\frac{G}{\rho g_c D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right] \qquad \frac{dP}{dW} = -\frac{\alpha}{2}\frac{P_0}{P/P_0}\left(\frac{T}{T_0}\right)(1 + y_{A0}\delta X)$$

$$\beta_0 = -\frac{G}{\rho_0 g_c D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right] \qquad \alpha = \frac{2\beta_0}{A_C\rho_c(1-\phi)P_0} \qquad dW = (1-\phi)A_C\rho_c\,dz$$

If isothermal and $\delta = 0$ or X is very small: $\frac{P}{P_0} = (1-\alpha W)^{1/2} = \left(1 - \frac{2\gamma W}{P_0}\right)^{1/2}$

Integrals:

$$\int_0^X x^a dx = \frac{x^{a+1}}{a+1}, \qquad a \neq -1$$

$$\int_0^X \frac{dX}{1+\varepsilon X} = \frac{1}{\varepsilon}\ln(1+\varepsilon X)$$

$$\int_0^X x^{-1} dx = \ln(x)$$

$$\int_0^X \frac{1+\varepsilon X}{1-X} dX = (1+\varepsilon)\ln\left(\frac{1}{1-X}\right) - \varepsilon X$$

$$\int_0^X \frac{dX}{1-X} = \ln\left(\frac{1}{1-X}\right)$$

$$\int_0^X \frac{1+\varepsilon X}{(1-X)^2} dX = \frac{(1+\varepsilon)\mathrm{X}}{1-X} - \varepsilon\ln\left(\frac{1}{1-X}\right)$$

$$\int_0^X \frac{dX}{(1-X)^2} = \frac{X}{1-X}$$

$$\int_0^W (1-\alpha W)^{1/2} dW = \frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right]$$

$$\int_0^X \frac{(1+\varepsilon X)^2}{(1-X)^2} dX = 2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X}$$

$$\int_0^X \frac{dX}{(1-X)(\Theta_B - X)} = \frac{1}{\Theta_B - 1}\ln\left(\frac{\Theta_B - X}{\Theta_B(1-X)}\right), \qquad \Theta_B \neq 1$$

$$\frac{dx}{dt} + P(t)y = Q(t), \qquad I(t) = e^{\int P(t)}, \qquad \frac{d\big(yI(t)\big)}{dt} = Q(t)I(t),$$

$$y = \frac{1}{I(t)}\int Q(t)I(t)dt$$

Roots for: $ax^2 + bx + c$ $\quad \dfrac{-b \pm \sqrt{b^2 - 4ac}}{2a}$