ChE 344
Fall 2014
Exam I

Monday, October 20, 2014

Closed Book, Web, Notes, In-Class Problems and Home Problems

Name________________________________

Honor Code (Please sign in the space provided below)

"I have neither given nor received unauthorized aid on this examination, nor have I concealed any violations of the Honor Code."

____

(Signature)

1)	____/ 5 pts
2)	____/ 5 pts
3)	____/ 5 pts
4)	____/ 5 pts
5)	____/ 5 pts
6)	____/ 5 pts
7)	____/10 pts
8)	____/10 pts
9)	____/25 pts
10)	____/25 pts
Total	____/100 pts
Extra Credit:	
#)	____/5 pts

ChE 344 - Exam I Cribb Sheet

1. Simpson's Three-eighths rule (4 points)

$$\int_{X_0}^{X^3} f(X)dX = \frac{3}{8}h\left[f(X_0)+3f(X_1)+3f(X_2)+f(X_3)\right]$$

2. $y=(1-\alpha w)^{1/2}$

$$\frac{dy}{dW} = -\frac{\alpha(1+\varepsilon X)}{2y}\left(\frac{T}{T_0}\right) \quad \text{where } \alpha = \frac{2\beta_0}{A_C\ \rho_C(1-\phi)P_0}, \text{ and } \beta_0 = \frac{G(1-\phi)}{g_C\rho_0 D_p \phi^3}\left[\frac{150(1-\phi)\,\mu}{D_p}+1.75G\right]$$

$$\frac{dy}{dW} = -\frac{\alpha}{2y}\left(\frac{F_T}{F_{T0}}\right)\left(\frac{T}{T_0}\right) \quad , G=\dot{m}/A_C$$

3. Integrals

$$\int_0^X \frac{dX}{1-X} = \ln\frac{1}{1-X}$$

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

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

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

$$\int_0^X \frac{dX}{aX^2+bX+c} = \frac{-2}{2aX+b}+\frac{2}{b}$$

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

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

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

$$\int_0^X \frac{dx}{(1-X)(\theta_B-X)} = \frac{1}{\theta_B-1}\ln\frac{\theta_B-X}{\theta_B(1-X)} \quad \theta_B\neq 1$$

for $b^2=4ac$ where p and q are the roots of the equation.

$$aX^2+bX+c=0 \quad \text{i.e.,} p,q=\frac{-b\mp\sqrt{b^2-4ac}}{2a}$$

$$\int_0^X \frac{dX}{aX^2+bX+c} = \frac{1}{a(p-q)}\ln\left(\frac{q}{p}\ \frac{X-p}{X-q}\right) \quad \text{for } b^2>4ac, \quad \int_0^X \frac{a+bX}{c+gX}\ dX = \frac{bX}{g}+\frac{ag-bc}{g^2}\ln\left[\frac{(c+gX)}{c}\right]$$

4. Finite Difference

First Point:
$$-\left.\frac{dC_A}{dt}\right)_{t0} = -\left[\frac{-3C_{A0}+4C_{A1}-C_{A2}}{2\Delta t}\right]$$

Middle Points:
$$-\left.\frac{dC_A}{dt}\right)_{ti} = -\left[\frac{C_{A(i+1)}-C_{A(i-1)}}{2\Delta t}\right]$$

e.g.,
$$-\left.\frac{dC_A}{dt}\right)_{t3} = -\left[\frac{C_{A4}-C_{A2}}{2\Delta t}\right] = \frac{C_{A2}-C_{A4}}{2\Delta t}$$

Last Point:
$$-\left.\frac{dC_A}{dt}\right)_{t5} = -\left[\frac{C_{A3}-4C_{A4}+3C_{A5}}{2\Delta t}\right]$$

5. Ideal Gas Constant

$$R = \frac{8.309\ \text{kPa}\bullet\text{dm}^3}{\text{mol}\bullet\text{K}}$$

$$R = \frac{0.73\ \text{ft}^3\bullet\text{atm}}{\text{lb mol}\bullet\ {}^\circ\text{R}}$$

$$R = 0.082\frac{\text{liter}\bullet\text{atm}}{\text{mol}\bullet\text{K}} = \frac{0.082\,\text{m}^3\bullet\text{atm}}{\text{kmol}\bullet\text{K}}$$

$$R = \frac{1.987\ \text{BTU}}{\text{lbmol}\bullet\ {}^\circ\text{R}}$$

$$R = \frac{8.3144\,\text{J}}{\text{mol}\bullet\text{K}}$$

$$R = \frac{1.987\ \text{cal}}{\text{mol}\bullet\text{K}}$$

Volume of Ideal Gas
1 lb mol of an ideal gas at 32°F and 1 atm occupies 359 ft^3.
1 g mol of an ideal gas at 0°C and 1 atm occupies 22.4 dm^3.

Liquid
1 gal = 3.785 dm^3
1 ft^3 = 7.482 gal

(5 pts) 1) Chapter 1 Mole Balances

The reaction

$$A + 2B \rightleftarrows 2C$$

takes place in a membrane reactor. The feed is only A and B in equimolar proportions. Which of the following sets of equations gives the correct mole balances on A, B and C? Species A and B are disappearing and Species C is being formed $\left(-r_A = k_A\left[C_A C_B^2 - \frac{C_C^2}{K_C}\right]\right)$ and C is also diffusing out the sides of a membrane reactor.

Circle the correct answer where <u>all</u> the mole balances are correct

(a)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = r_B$$

$$\frac{dF_C}{dV} = -r_C - R_C$$

(b)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = 2r_B$$

$$\frac{dF_C}{dV} = 2r_C - 2R_C$$

(c)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = r_B$$

$$\frac{dF_C}{dV} = 2r_C - R_C$$

(d)

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = 2r_A$$

$$\frac{dF_C}{dV} = -2r_A - R_C$$

(e) None of the above

(5 pts) 2) Circle the correct answer.

Consider the following Levenspiel plot for a reversible reaction A $\rightleftarrows$ Product

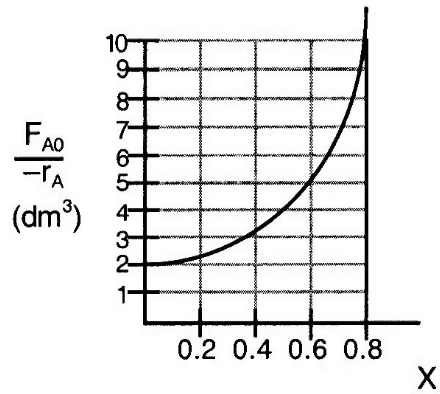
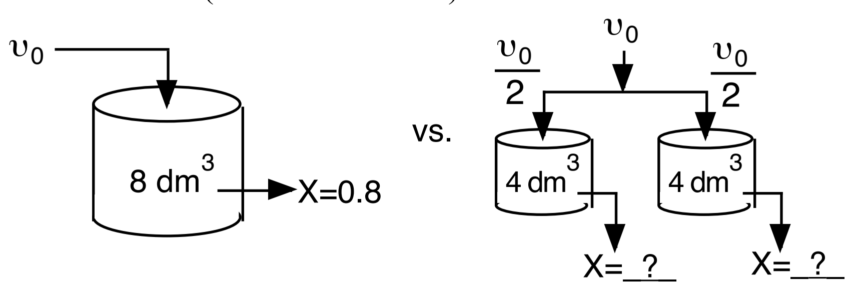


Figure 2-1

(1 pt) (a) The equilibrium conversion X_e in a 3 dm^3 reactor is

(1) $X_e < 0.6$ (2) $X_e = 0.6$ (3) $X_e > 0.6$ (4) Can't tell from the information given

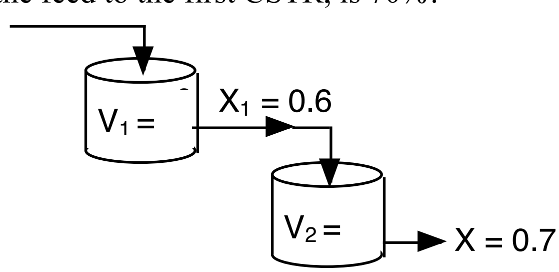
(2 pt) (b) If the conversion achieved in a single 8 dm^3 CSTR is 80%, what would the conversion be if the flow is equally divided into two CSTRs in parallel with each reactor having a volume of 4 dm^3 each (same total volume).



The total reactor volume is constant at 8 dm^3.
The conversion for the two reactors in parallel is

(1) $X > 0.8$ (2) $X < 0.8$ (3) $X = 0.8$ (4) Can't tell from the information given

(2 pts) (c) What would be the reactor volumes V_1 and V_2, for two CSTRs connected in series with first reactor having a conversion of 60% and the overall conversion of the second reactor, based on the feed to the first CSTR, is 70%?



(5 pts) 3) Consider the following reaction

$$2A + B \rightleftarrows C$$

Write the rate law in terms of the specific reaction rate and species concentration when

(1 pt) (a) The reaction is elementary and reversible

$-r_A =$ ________________

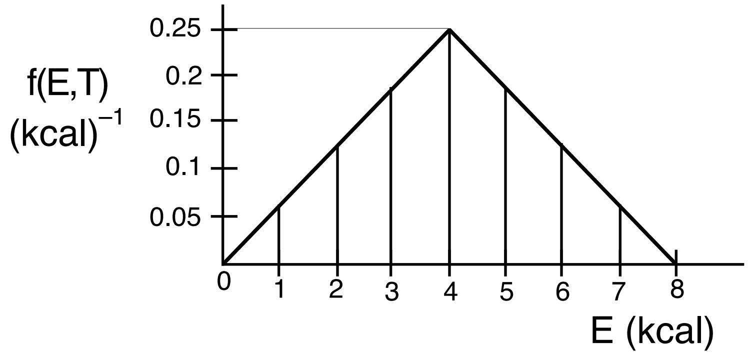
(2 pt) (b) The reaction is irreversible and second order in A, and independent of the concentration of C, and overall first order.

$-r_A =$ ________________

(2 pt) (c) Now consider the case when the reaction is irreversible and it is first order in A and first order in B at high concentrations of A and B and is first order in A and second order in B at low concentrations of B. The rate law is

$-r_A =$ ________________

(5 pts) 4) The following figure shows the energy distribution function at 300 K for the reaction $A + B \rightarrow C$

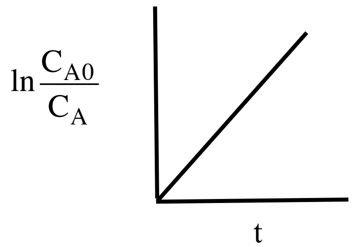


(a) What fraction of the collisions have energies between 4 and 5 kcal?
(b) What fraction of collisions have energies greater than 6 kcal?

(5 pts) 5) Write the rate law for the following plots for the irreversible isothermal isobaric reaction, $C_{B0} = 0$.

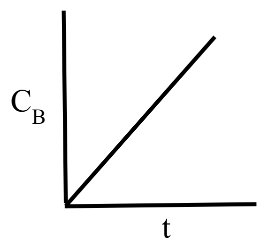
$$A \rightarrow B$$

(1 pt) (a)



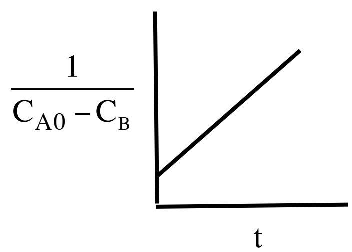
$-r_A =$ ________

(2 pt) (b)



$-r_A =$ ________

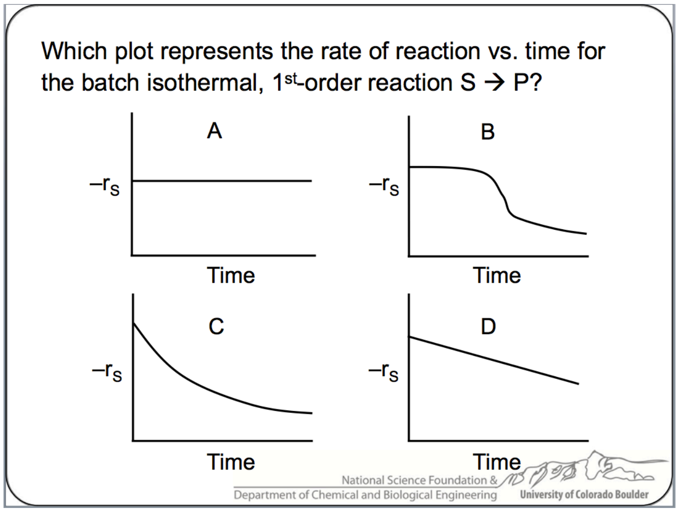
(2 pt) (c)



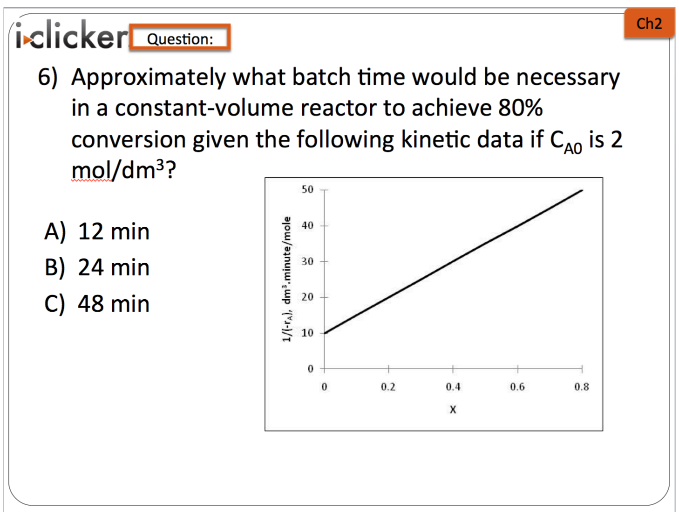
$-r_A =$ ________

(5 pts) 6) i>clickers. Circle answers on i>clicker graphs.

(2 pt) (a)



(3 pt) (b)



(10 pts) 7) Study Problem 4-4.

$P4\text{-}4_B$ Stoichiometry. The elementary gas reaction

$$2A + B \rightarrow C$$

is carried out isothermally in a PFR with no pressure drop. The feed is equal molar in A and B and the entering concentration of A is 0.1 mol/dm^3.

(1 pt) (a) What is the entering concentration (mol/dm^3) of B?

C_{B0} = _______

(2 pt) (b) What are the concentrations of A and C (mol/dm^3) at 25% conversion of A?

C_A = _______ C_C = _______

(2 pt) (c) What is the concentration of B (mol/dm^3) at 25% conversion of A?

C_B = _______

(2 pt) (d) If at a particular conversion the rate of formation of C is 2 mol/min/dm^3, what is the rate of formation of A at the same conversion?

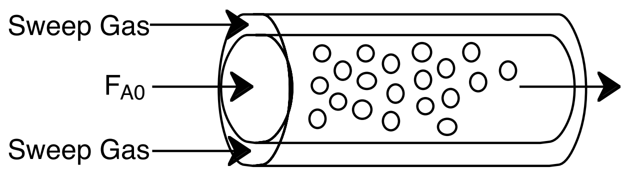
r_C = _______

(3 pt) (e) Write $-r_A$ solely as a function of conversion (i.e., evaluating all symbols) when the reaction is an elementary, reversible, gas phase, isothermal reaction with no pressure drop with an equal molar feed and with C_{A0} = 2.0 mol/dm^3 at, k_A = 2 dm^6/mol•s to find the rate at X = 0.25.

r_A = _______

(10 pts) 8) The following elementary reaction is carried out in a membrane reactor packed with 100 kg of catalyst. The reaction is carried out isothermally and there is no pressure drop.

$$A \rightleftarrows 2B + D$$



The following is a sketch of the concentration profile in a conventional PBR

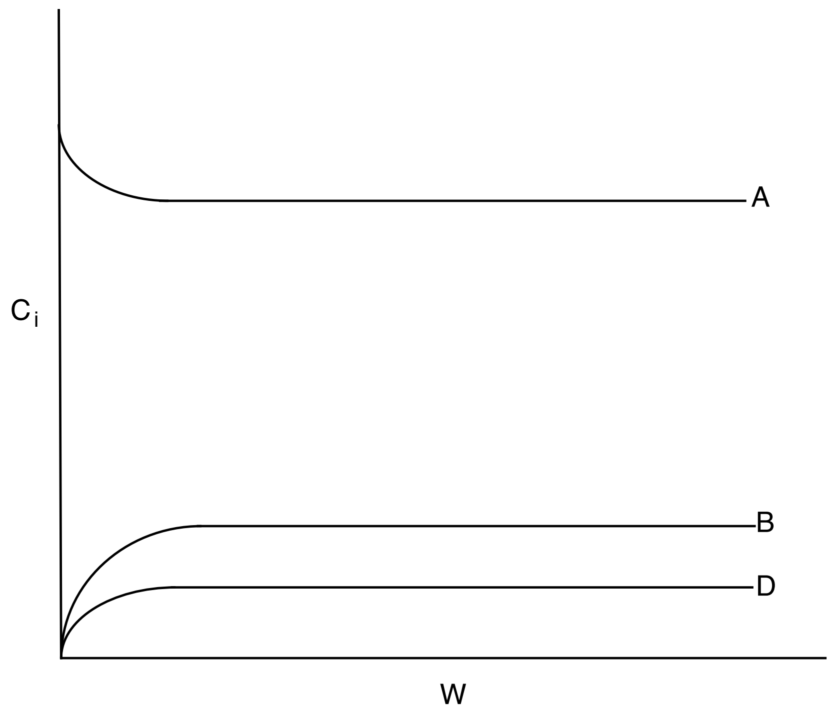


Figure 8-1

(a) Suppose B diffuses out through the membrane. Using a dashed line (-----) sketch and label the concentration profiles for A, B, and D in a membrane reactor for a moderate value of the mass transfer coefficient for B, k_{CB}, on Figure 8-1.
Why?

(b) Now suppose that both B and D can diffuse out of the reactor. Use a solid line (——) to sketch and label the profiles of A, B, and D on Figure E9-1. Assume the mass transfer coefficients of B and D are the same, $k_{CB} = k_{CD}$.
Why?

(25 pts) 9) The elementary irreversible gas phase reaction

$$2A \rightarrow B$$

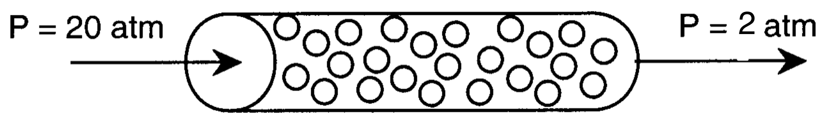
is carried out in a constant volume batch reactor where 50 % conversion is achieved in 1 hour. Pure A was charged to the reactor at an initial concentration of 0.2 mol/dm^3. If the same reaction is carried out in a CSTR, what volume would be necessary to achieve 50 % conversion for a feed molar flow rate of 500 mol/h and an entering concentration of A of 0.2 mol/dm^3.

V_{CSTR} = ___________dm^3

(25 pts) 10) The irreversible elementary gas phase reaction

$$A + B \longrightarrow C + D$$

is carried out isothermally at 300 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_{A0} = 10 mol/min and C_{A0} = 0.4 mol/dm^3. Currently 80% conversion is achieved. If the specific reaction rate at 400 K is $\left[25 \frac{dm^6}{gcat \bullet mol \bullet min}\right]$ what is the activation energy?

E = __________

Extra Credit:

(5 pts) #) For elementary reaction

$$A \rightleftarrows B$$

where Pure A is fed to a reactor the equilibrium conversion is 0.8 at 127°C and 0.5 at 227°C. What is the heat of reaction?

ΔH_{Rx} = ___________cal/mole A

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