

ChE 344
Winter 2013
Final Exam

Thursday, May 2, 2013

Open Course Textbook Only
Closed everything else (i.e., 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)

The Basics

- 1) ____ / 2 pts
- 2) ____ / 5 pts
- 3) ____ / 5 pts
- 4) ____ / 5 pts
- 5) ____ / 5 pts
- 6) ____ / 5 pts
- 7) ____ / 8 pts

Applications

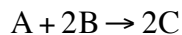
- 8) ____ / 10 pts
- 9) ____ / 10 pts

Professional

- 10) ____ / 20 pts
- 11) ____ / 25 pts
- Total ____ / 100 pts

(2 pts) 1) **Chapter 1 Mole Balances**

The reaction



takes place in a membrane reactor. The feed is only A and B in equimolar proportions. Which of the following set of equations gives the correct mole balances on A, B and C. Species A and B are disappearing and Species C is being formed and C is also diffusing out the sides of a membrane reactor.

Circle the correct answer where all 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)

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

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

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

(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 $A \rightleftharpoons \text{Product}$

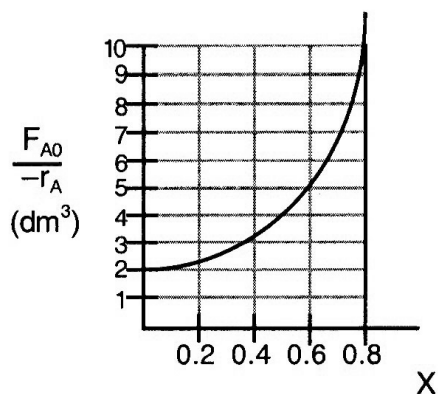


Figure 2-1

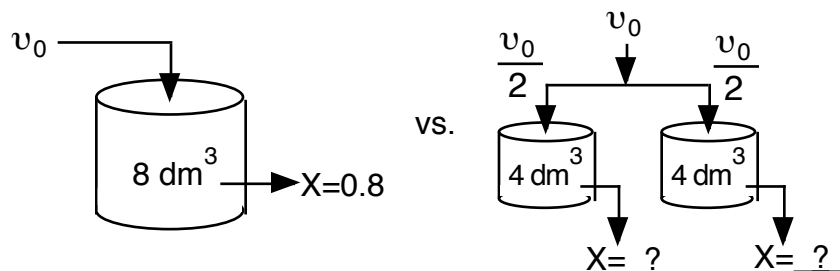
(1 pt) (a) The equilibrium conversion X_e in a 3 dm^3 reactor is

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

(1 pt) (b) The flow rate to an 8 dm^3 CSTR corresponding to Figure 2-1 where 80% conversion is achieved is

- (1) $F_{A0} = 0.8 \text{ mol/s}$ (2) $F_{A0} = 10 \text{ mol/s}$
 (3) $F_{A0} = 1 \text{ mol/s}$ (4) Can't tell from the information given

(1 pt) (c) 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).

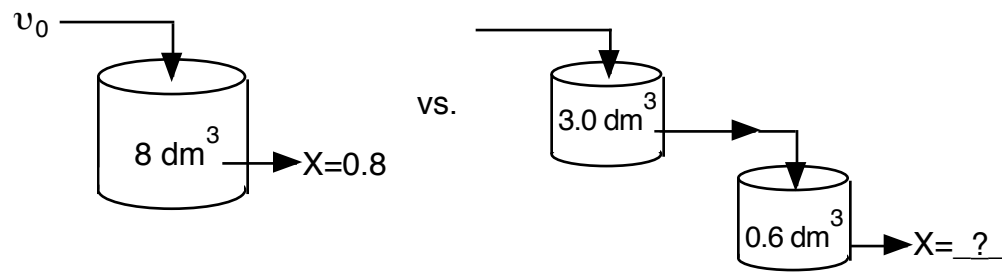


The total reactor volume is constant at 8 dm^3 .

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

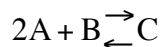
(2 pts) (d) If the conversion achieved in a single 8 dm^3 CSTR is 80%, what would the conversion be if two CSTRs are connected in series with first reactor having a volume of approximately 3.0 dm^3 and the second reactor having a volume of 0.6 dm^3 .



The conversion for the two reactors in series is

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

(5 pts) 3) Consider the following reaction for parts (a), (b) and (c)



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

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

$$-r_A = \underline{\hspace{2cm}}$$

- (1 pt) (b) The reaction is elementary and reversible

$$-r_A = \underline{\hspace{2cm}}$$

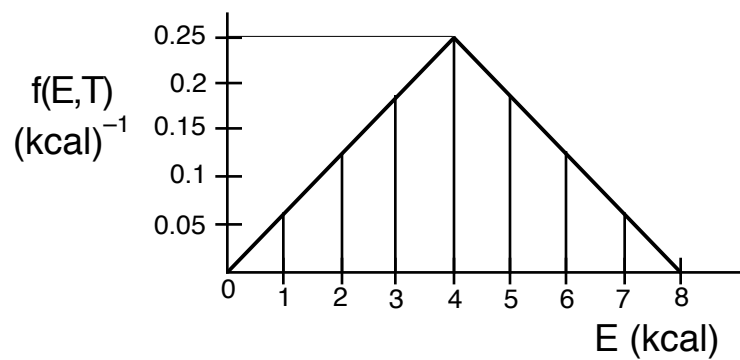
- (1 pt) (c) Now consider the case when the reaction is first order in A and first order in B at high concentrations of A and B and is first order in A and second order in B at low concentrations of B. The rate law is

$$-r_A = \underline{\hspace{2cm}}$$

- (2 pt) (d) The irreversible reaction is catalyzed on a Pt surface where surface reaction limits and B is not adsorbed on the surface but reacts with adsorbed A on the surface.

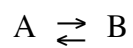
$$-r_A = \underline{\hspace{2cm}}$$

- (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 3 and 5 kcal?
(b) What fraction of collisions have energies greater than 5 kcal?

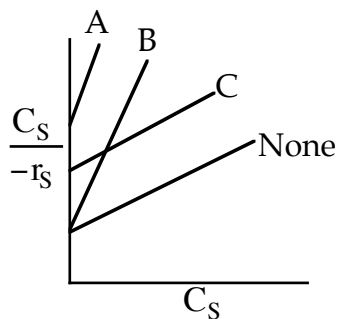
(5 pts) 5) For elementary reaction



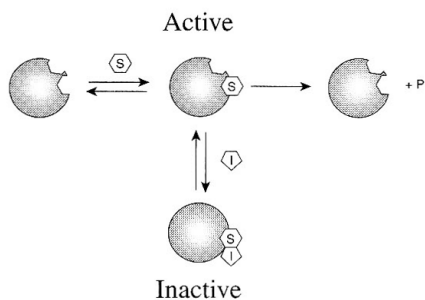
the equilibrium conversion is 0.8 at 127°C and 0.5 at 227°C. What is the heat of reaction?

$\Delta H_{R_x} =$ _____ cal/mole A

- (5 pts) 6) A **Hanes-Woolf** plot is shown below for the different types of enzyme inhibition. Match the line with the type of inhibition.

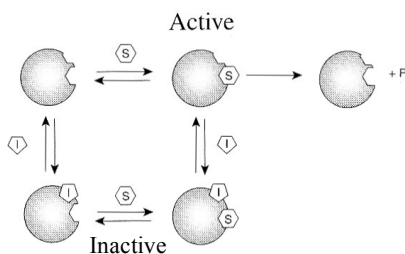


(a) Inhibition Mechanism



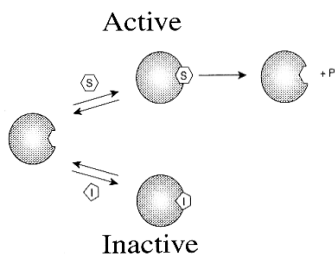
Ans: _____

(b) Inhibition Mechanism



Ans: _____

(c) Inhibition Mechanism



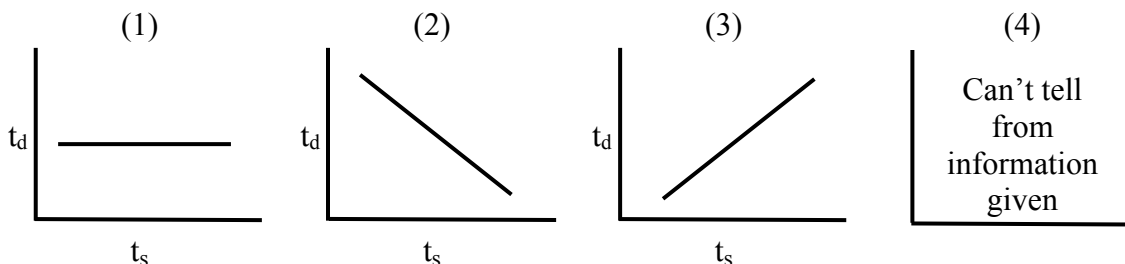
Ans: _____

(8 pts) 7)

- (2pt) (a) Keeping in mind the explosions we discussed this term, suggest at least one possible cause of the West, Texas fertilizer plant explosion on April 15, 2013 that resulted in 14 fatalities.

In the following, circle the correct answer below.

- (2 pt) (b) Which of the following figures best represents the relationship between the amount of down time, t_d , and the time the heat exchanger failed after start up, t_s for which the ONCB/ammonia reactor would not explode



- (2 pt) (c) Currently 50% conversion is being achieved in an endothermic liquid phase reaction $A + B \rightarrow C + D$ in a CSTR when the reaction is carried out adiabatically and the feed is stoichiometric. If the reaction molar flow rate of B is doubled with everything else held constant, the exit temperature will

Increase

Decrease

Remain the same

Insufficient
information to tell

- (2 pt) (d) A co-current heat exchanger with a variable ambient temperature will always have a greater equilibrium conversion than a heat exchanger with a constant ambient temperature when an exothermic reversible reaction is taking place.

True

False

Insufficient information to tell

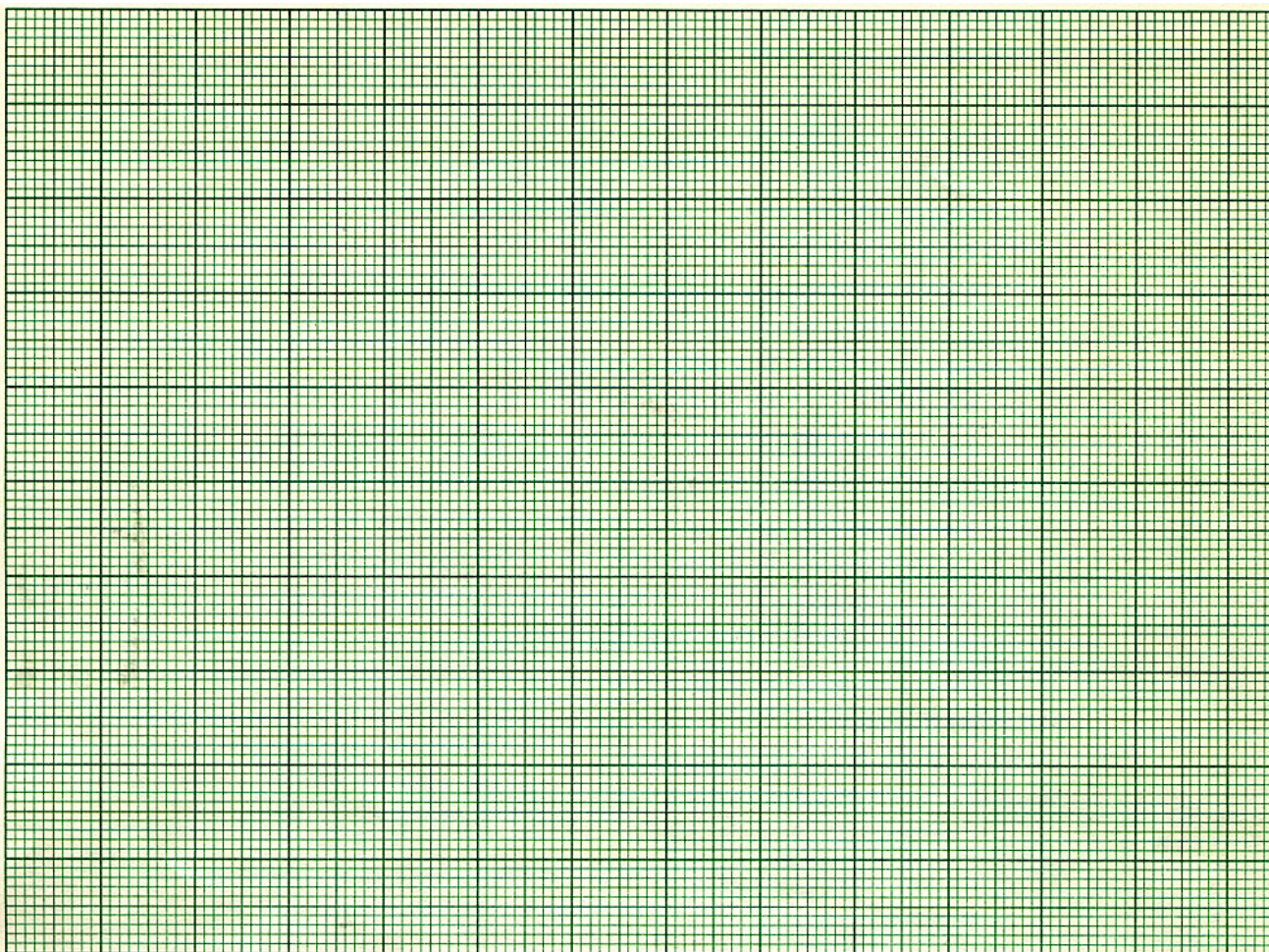
(10 pts) 8) Experimental data for the gas phase catalytic reaction



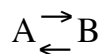
is shown below. The limiting step in the reaction is known to be irreversible, so that the overall reaction is irreversible. The reaction was carried out in a differential reactor (i.e., virtually no concentration gradient down the reactor) to which A, B, and C were all fed.

Run Number	P_A (atm)	P_B (atm)	P_C (atm)	Reaction rate (mol)/(gcat • s)
1	1	1	2	0.114
2	1	10	2	1.140
3	10	1	2	0.180
4	1	20	2	2.273
5	1	20	10	0.926
6	20	1	2	0.186
7	0.1	1	2	0.0243

- (a) Suggest a rate law consistent with the experimental data. (Hint: Sketch $(-r'_A)$ as a function of P_A , as a function of P_B , and as a function of P_C .)
- (b) From your rate expression, which species can you conclude are adsorbed on the surface?
- (c) Suggest a mechanism that is consistent with the rate law in part (a).



(10 pts) 9) The reversible liquid phase reaction



is carried out in a 12 dm^3 CSTR with heat exchange. Both the entering temperature, T_0 , and the heat exchange fluid, T_a , are at 330 K. An equal molar mixture of inerts and A enter the reactor.

- (6 pt) (a) What product of the heat transfer coefficient and heat exchange area would give the maximum conversion?

Ans: $UA = \underline{\hspace{2cm}} \text{ cal/h/K}$

- (4 pt) (b) Using UA from part (a), what is the maximum conversion that can be achieved in this reactor?

Ans: $X_{\max} = \underline{\hspace{2cm}}$

Additional Information

The $G(T)$ curve for this reaction is shown below

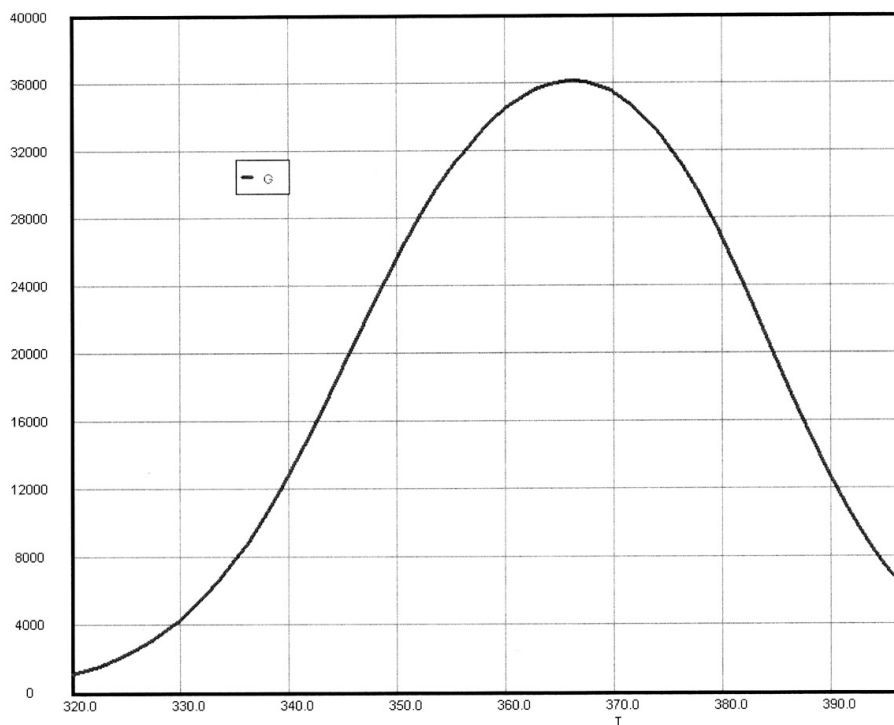
$$C_{P_A} = C_{P_B} = 100 \text{ cal/mol/K}, \quad C_{P_I} = 150 \text{ cal/mol/K}$$

$$F_{A0} = 10 \text{ mol/h}, \quad C_{A0} = 1 \text{ mol/dm}^3, \quad v_0 = 10 \text{ dm}^3/\text{h}$$

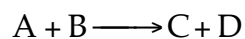
$$\Delta H_{R_x} = -42,000 \text{ cal/mol}$$

$$k = 0.001 \text{ h}^{-1} \text{ at } 300\text{K} \text{ with } E = 30,000 \text{ cal/mol}$$

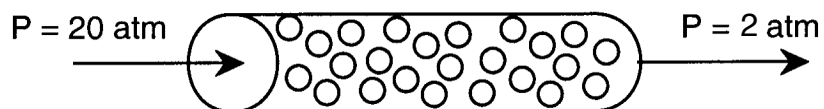
$$K_C = 5,000,000 \text{ at } 300\text{K}$$



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



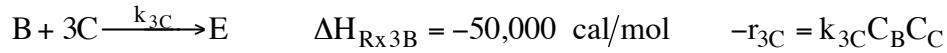
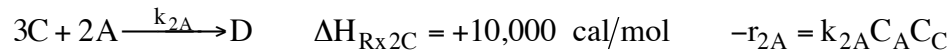
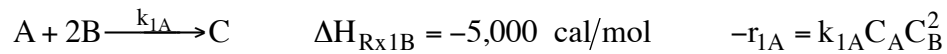
is carried out isothermally at 305 K in a packed bed reactor with 100 kg of catalyst.



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 $F_{A0} = 10$ mol/min and $C_{A0} = 0.4$ mol/dm³. Currently 80% conversion is achieved. What would be the conversion if the catalyst particle size were doubled and everything else remained the same?

X = _____

(25 pts) 11) The following reactions are taking place in a 2,000 dm³ liquid phase batch reactor under a pressure of 400 psig



The initial temperature is 450 K and the initial concentrations of A, B and C are 1.0, 0.5 and 0.2 mol/dm³ respectively. The coolant flow rate was at its maximum value so that $T_{a1} = T_{a2} = T_a = 400 \text{ K}$ so that the product the exchange area and overall heat transfer coefficient, UA, is $UA = 100 \text{ cal/s}\cdot\text{K}$.

(2 pt) (a) If $Q_r > Q_g$ at time $t = 0$, and there is no failure of the heat exchange system, is there any possibility that reactor will run away? Explain_____

(4 pt) (b) What is Q_r at $t = 0$?

(10 pt) (c) What is Q_g at $t = 0$?

(3 pt) (d) What is the initial rate of increase in temperature, (dT/dt) at $t = 0$?

$$\frac{dT}{dt} = \underline{\hspace{2cm}}$$

(3 pt) (e) Suppose that the ambient temperature T_a is lowered from 400 K to 350 K, what is the initial rate of reactor temperature change?

$$\frac{dT}{dt} = \underline{\hspace{2cm}}$$

(3 pt) (f) A suggestion was made to add 50 moles of inerts at a temperature of 450 K. Will the addition of the inerts make runaway more likely or less likely? How? Show quantitatively.

Additional information

As a first approximation, assume all heats of reaction are constant (i.e., $\Delta C_{P_{ij}} \approx 0$)

Specific reaction rates at 450 K are

$$k_{1A} = 1 \times 10^{-3} \left(\text{dm}^3/\text{mol} \right)^2 / \text{s}$$

$$C_{PA} = 10 \text{ cal/mol/K}$$

$$C_{PD} = 80 \text{ cal/mol/K}$$

$$k_{2A} = \frac{1}{3} \times 10^{-3} \left(\text{dm}^3/\text{mol} \right)^2 / \text{s}$$

$$C_{PB} = 10 \text{ cal/mol/K}$$

$$C_{PE} = 50 \text{ cal/mol/K}$$

$$C_{PC} = 50 \text{ cal/mol/K}$$

$$k_{3C} = 0.6 \times 10^{-3} \left(\text{dm}^3/\text{mol} \right)^2 / \text{s}$$

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