

ChE 344
Chemical Reaction Engineering
Winter 2000

This questionnaire is to be removed from the exam and turned in before the exam begins.

In the first assignment you were asked to describe the goals of the course in terms of *critical thinking, creative thinking, and a fundamental understanding of CRE*. How well do you feel you made progress towards each of these goals?

- | | | | | | |
|---|---|---|---|---|-------------------|
| 1) I feel my critical thinking skills were increased
<u>Significantly</u> | | | | | <u>Not at All</u> |
| | 5 | 4 | 3 | 2 | 1 |
| 2) I feel my creative thinking skills were increased
<u>Significantly</u> | | | | | <u>Not at All</u> |
| | 5 | 4 | 3 | 2 | 1 |
| 3) I feel I learned how to ask critical questions
<u>Significantly</u> | | | | | <u>Not at All</u> |
| | 5 | 4 | 3 | 2 | 1 |
| 4) I expect to use the techniques discussed in creative thinking (e.g. vertical thinking, lateral thinking, ideas from Barkers videos).
<u>Often</u> | | | | | <u>Never</u> |
| | 5 | 4 | 3 | 2 | 1 |
| 5) I feel I met the goal of obtaining a fundamental understanding of CRE topics covered in the course.
<u>Definitely</u> | | | | | <u>Not at All</u> |
| | 5 | 4 | 3 | 2 | 1 |

Name (optional) _____

ChE 344
Chemical Reaction Engineering
Winter 2000

Final Exam

Open Book, Notes, and Web

Name _____ **SOLUTION** _____

Honor Code _____

Signed _____

1) ____/10 pts

2) ____/15 pts

3) ____/20 pts

4) ____/20 pts

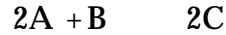
5) ____/15 pts

6) ____/15 pts

7) ____/ 5 pts

Total 100 pts

1) The gas phase reaction



is carried out isothermally and isobarically. The reaction is first order in B and first order in A. The feed is equal molar in A and B and the entering concentration of A is 0.5 mol/dm^3 . The specific reaction rate is $k = 4.0 \text{ dm}^3/\text{mol}\cdot\text{s}$.

- (8%) a) Write the rate of reaction, $-r_A$, solely as a function of conversion, evaluating all parameters.



$$-r_A = kC_A C_B$$

$$C_A = \frac{C_{A0}(1-X)}{(1+\epsilon X)}$$

$$C_B = \frac{C_{A0}(1-0.5*X)}{(1+\epsilon X)}$$

$$\epsilon = y_{A0}\delta = 0.5*(1-1-0.5) = -0.25$$

$$-r_A = \frac{kC_{A0}(1-X)C_{A0}(1-0.5*X)}{(1+\epsilon X)^2} = \frac{4.0 \frac{\text{dm}^3}{\text{mol s}} \cdot 0.5 \frac{\text{mol}}{\text{dm}^3}^2 (1-X)(1-0.5*X)}{(1-0.25*X)^2}$$

$$-r_A = \frac{(1-X)(1-0.5*X)}{(1-0.25*X)^2} \frac{\text{mol}}{\text{dm}^3 \text{ s}}$$

- (2%) b) Write an indepth question related to CRE that requires critical thinking and explain why it requires critical thinking. Be sure to be as specific as you can.

Must be related to Chemical Reaction Engineering and require critical thinking.

(15%) 2) The gas phase irreversible reaction is carried out isothermally in a PBR.



The reaction is zero order. The entering temperature is 400 K, and the entering pressure is 10 atm. The flow is turbulent. For a 10 kg PBR with a pressure drop parameter = 0.01 kg^{-1} , the exit conversion was found to be 0.4.

- a) What catalyst weight of the PBR will you require if you need an exit conversion of 0.8, assuming that the particle diameter is decreased by a factor of 2 so that the pressure drop parameter is now increased to 0.02? Assume all other operating conditions are the same as for the base case (i.e. $W = 10 \text{ kg}$).

$$\text{Mole Balance: } \frac{dX}{dW} = \frac{-r_A}{F_{A0}}$$

$$\text{Rate Law : } -r_A = k$$

$$\text{Combine: } \frac{dX}{dW} = \frac{k}{F_{A0}}$$

$$\text{Find } \frac{k}{F_{A0}} \text{ using the initial case}$$

$$W = \underline{20 \text{ kg}}$$

$$\int_0^{0.4} dX = \frac{k}{F_{A0}} \int_0^{10} dW \quad 0.4 = 10 \frac{k}{F_{A0}} \quad \frac{k}{F_{A0}} = 0.04$$

Now Find the new weight

$$\int_0^{0.8} dX = 0.04 \int_0^W dW \quad 0.8 = 0.04W \quad W = 20 \text{ kg}$$

- b) For the fixed inlet pressure of 10 atm, will the volumetric flow rate v , (dm^3/s), be greater, smaller, or remain the same when the particle diameter is decreased by a factor of 2?

Increased

Decreased

Remain the Same

$$v = v_o \frac{P}{P_o} (1 + \epsilon X) \frac{T}{T_o}, \text{ isothermal so } \frac{T}{T_o} = 1$$

$$v \sim \frac{P}{P_o} \sim (1 - \alpha W)^{-0.5} \text{ because } \epsilon \text{ is zero}$$

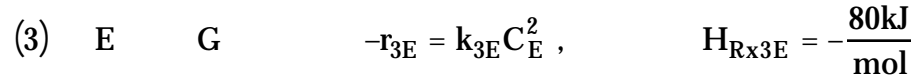
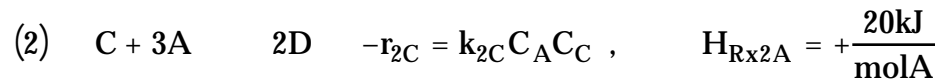
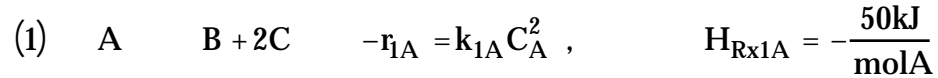
$$v_1 \sim (1 - 0.01 W)^{-0.5} \sim (1 - 0.01)^{-0.5} \sim (0.99)^{-0.5} \sim 1.005$$

$$v_2 \sim (1 - 0.02 W)^{-0.5} \sim (1 - 0.02)^{-0.5} \sim (0.98)^{-0.5} \sim 1.010$$

$$v_2 > v_1$$

(20%) 3)

The gas phase reactions



occur in a PBR with a heat exchanger. The PBR contains 500 kg of catalyst. The entering concentration of A is 0.8 mol/dm^3 and the entering concentration of E is 0.2 mol/dm^3 . The entering volumetric flow rate is $10 \text{ dm}^3/\text{s}$ at a temperature of 300K. It was found that the rate reaction for reactions (1) and (2) doubles for a 10 K increase from 300 to 310 in temperature while the rate of reaction (3) doubles for a 10 K increase from 500 K to 510 K. The entering pressure is 24.6 atm.

Additional Information

$$C_{P_A} = 60 \text{ J/mol K}$$

$$C_{P_B} = 20 \text{ J/mol K}$$

$$C_{P_C} = 20 \text{ J/mol K}$$

$$C_{P_D} = 100 \text{ J/mol K}$$

$$C_{P_E} = 50 \text{ J/mol K}$$

$$C_{P_G} = 50 \text{ J/mol K}$$

$$k_{1A} = 0.7 \text{ dm}^3/\text{mol s @300 K}$$

$$k_{2C} = 3.8 \text{ dm}^3/\text{mol s @300 K}$$

$$k_{3E} = 0.9 \text{ dm}^3/\text{mol s @500 K}$$

$$= .0001 \text{ kg}^{-1}$$

$$C_{T_0} = 1.0 \text{ mol/dm}^3$$

$$T_0 = 300 \text{ K}$$

$$T_a = 350 \text{ K}, \quad \frac{Ua}{b} = 20 \frac{\text{kJ}}{\text{s kg cat}}$$

Write a complete Polymath program to plot the temperature and species concentration as a function of catalyst weight. Including initial conditions.

$$\frac{dF_A}{dW} = -r_{1A} - 3r_{2C}$$

$$\frac{dF_B}{dW} = r_{1A}$$

$$\frac{dF_C}{dW} = 2r_{1A} - r_{2C}$$

$$\frac{dF_D}{dW} = 2r_{2E}$$

$$\frac{dF_E}{dW} = -r_{3E}$$

$$\frac{dF_G}{dW} = r_{3E}$$

$$r_{1A} = k_{1A} C_A^2$$

$$r_{2C} = k_{2C} C_A C_C$$

$$r_{3E} = k_{3E} C_E^2$$

$$\frac{dT}{dW} = \frac{20,000 (T_a - T) + [r_{1A}(50) + r_{2C}(-20) \cdot 3 + (r_{3E})(20)] \times 1000}{20 F_A + 20 F_B + 20 F_C + 100 F_D + 50 F_E + 50 F_G}$$

$$T_0 = 300$$

$$\frac{dP}{dW} = \frac{-\alpha}{Z} \left(\frac{I}{T_0} \right) \left(\frac{P_0}{P} \right)^2 \left(\frac{F_T}{F_{T0}} \right)$$

$$P_0 = 24.6$$

$$P_0 = 24.6$$

$$T_0 = 300$$

$$\alpha = 0.0001$$

$$F_T = F_A + F_B + F_C + F_D + F_E + F_G$$

$$F_{T0} = 10 \times (0.8 + 0.2)$$

$$C_A = \left(\frac{F_A}{F_T} \right) \left(\frac{P}{RT} \right)$$

$$C_C = \left(\frac{F_C}{F_T} \right) \left(\frac{P}{RT} \right)$$

$$C_E = \left(\frac{F_E}{F_T} \right) \left(\frac{P}{RT} \right)$$

$$\text{or } C_i = C_{T0} \frac{F_i}{F_T} \frac{P}{P_0} \frac{T_0}{T}$$

$$\text{where } C_{T0} = 1.0$$

IC

$$F_{A0} = (10 \times 0.8) = 8$$

$$F_{B0} = 0$$

$$F_{C0} = 0$$

$$F_{D0} = (10 \times 0.2) = 2$$

$$F_{E0} = (10 \times 0.2) = 2$$

$$F_{G0} = 0$$

$$k_{1A} = 0.7 \exp \left[6446 \left(\frac{1}{300} - \frac{1}{T} \right) \right]$$

$$k_{2C} = 3.8 \exp \left[6446 \left(\frac{1}{300} - \frac{1}{T} \right) \right]$$

$$k_{3E} = 0.9 \exp \left[17675 \left(\frac{1}{500} - \frac{1}{T} \right) \right]$$

obtain $\frac{E}{R}$ values

for k_{1A} and k_{2C}

$$k_1(310) = k(300) \exp \left[\frac{E}{R} \left(\frac{1}{300} - \frac{1}{310} \right) \right]$$

$$2 = \exp \left[\frac{E}{R} \left(\frac{1}{300} - \frac{1}{310} \right) \right]$$

$$\frac{E}{R} = \frac{\ln 2}{\left(\frac{1}{300} - \frac{1}{310} \right)} = 6446$$

for k_{3E}

$$\frac{E}{R} = \frac{\ln 2}{\left(\frac{1}{500} - \frac{1}{510} \right)} = 17675$$

(20%) 4) The following reversible, elementary, liquid phase reaction occurs in a PFR:



The entering flow rate is $10 \text{ dm}^3/\text{s}$ with an entering concentration of 2 M of A and the feed temperature is 310 K .

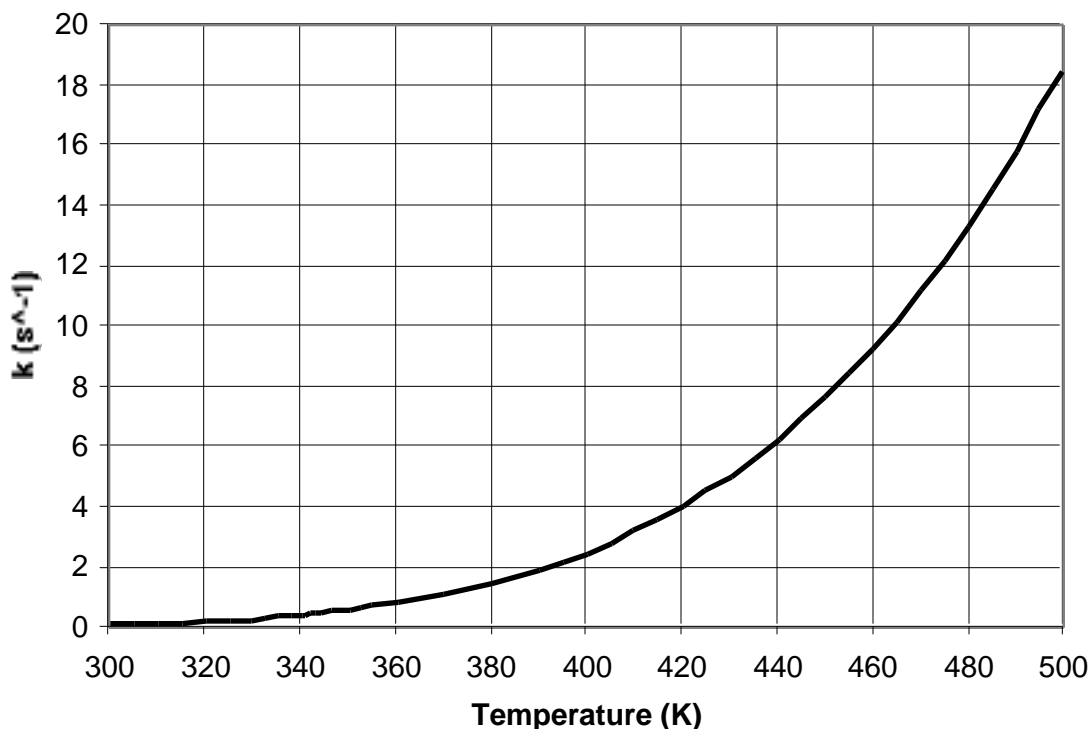
- a) What is the reactor volume necessary to achieve 90% of the adiabatic equilibrium conversion in one PFR operated adiabatically? **$V \sim 12.34 \text{ dm}^3$ (see below)**
- b) Now consider a series of reactors with interstage cooling so that the temperature is cooled to 300 K in each interstage cooler. How many reactors are necessary to achieve 95% conversion assuming 99.9% of the equilibrium conversion is achieved in each reactor? **3 Reactors (see Xequil. vs. T graph below)**

Hint: Recall Chapter 2 and/or appendix A.4 and make a rough estimate.

Additional information:

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

$$H^\circ_{\text{rxn}} = -10,000 \text{ cal/mol A}$$



Answer (for solution see table and graphs below) : $V_{\text{PFR}} \sim \underline{12.34} \text{ dm}^3$

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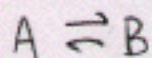
Problem 4 continued

$$X_{EB} = \frac{C_{PA} (T - T_0)}{-\Delta H_{EB}(T_R)} = \frac{50(T - 310)}{10000} = 0.005 (T - 310)$$

$$T = 310, X_{EB} = 0$$

$$T = 410, X_{EB} = 0.5$$

X	T	K _c	k	-r _A	$\frac{1}{r_A}$
0	310	50	0.1	0.2	5
0.1	330	20	0.5	0.895	1.12
0.2	350	8	0.8	1.24	0.8
0.3	370	3	1.2	1.44	0.69
0.4	390	2	2	1.6	0.625
0.5	410	1	3	0.27	3.7



liquid phase, elementary

$$-r_A = k C_{A0} \left[(1 - X) - \frac{X}{K_c} \right]$$

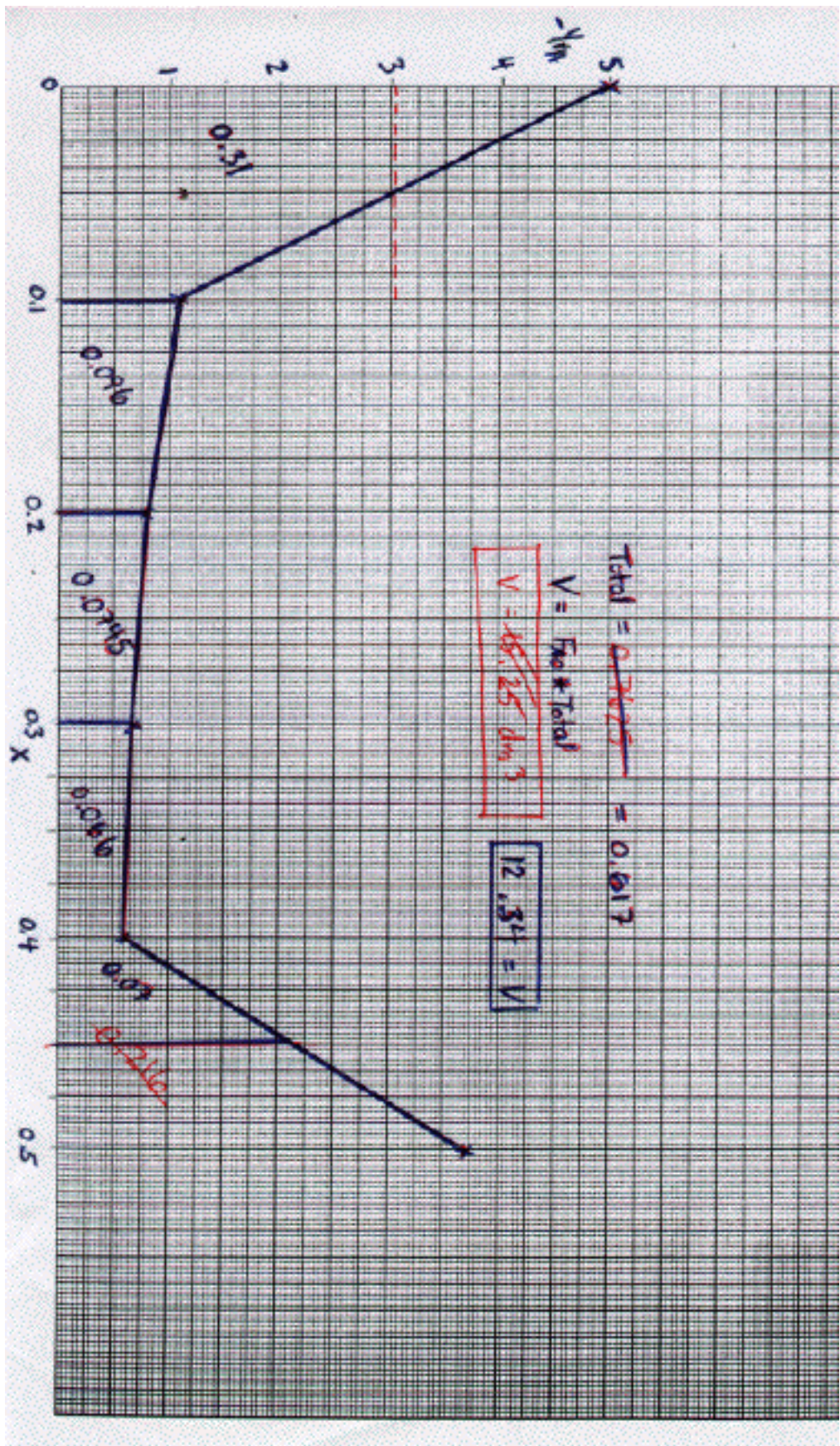
$$C_{A0} = 2 \text{ M}$$

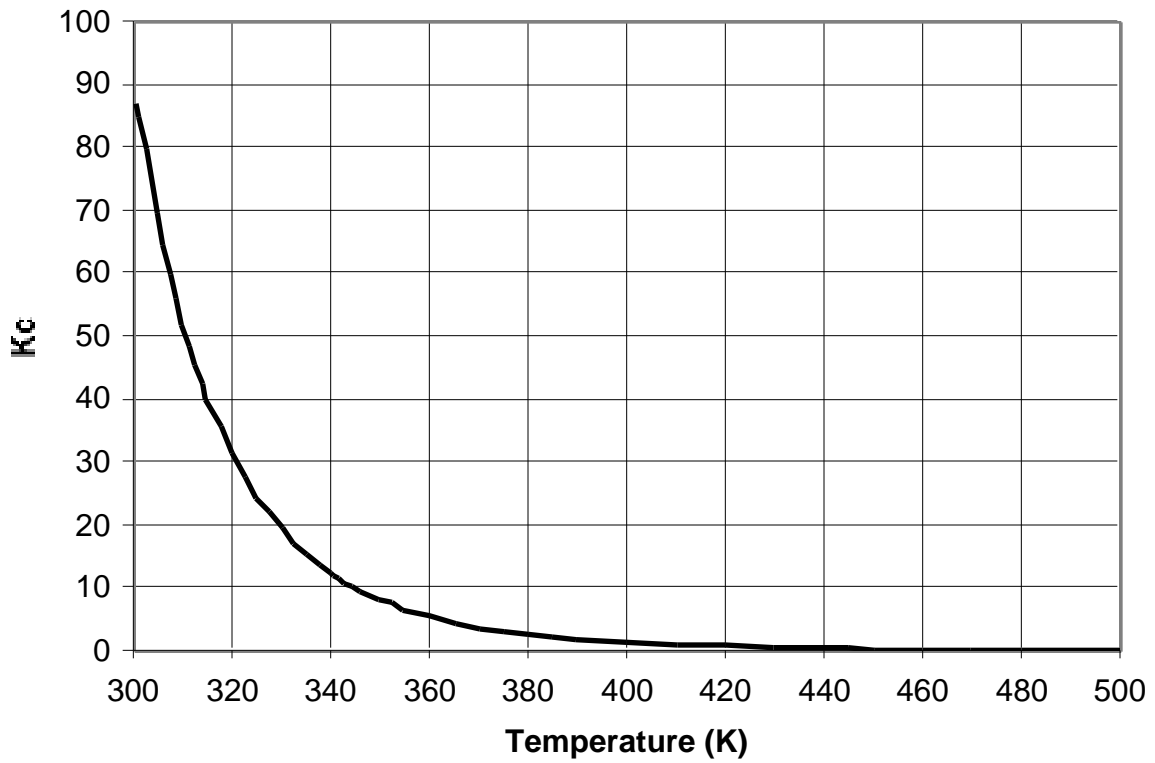
See pg. 453

-7 for not varying k, K_c

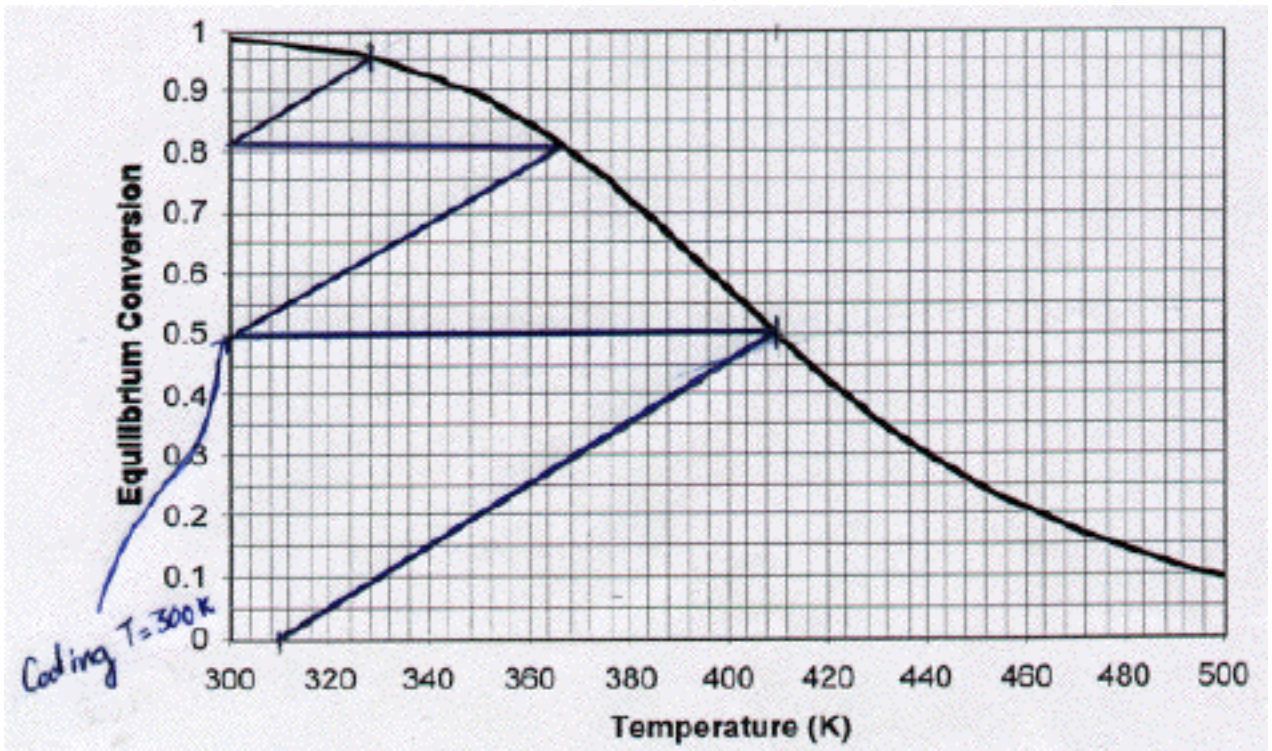
344/W'00 Final Exam

$$\dot{F}_{A0} = \frac{2 \text{ mol}}{\text{dm}^3} \bigg| \frac{10 \text{ dm}^3}{\text{s}} = 20 \text{ mol/s}$$



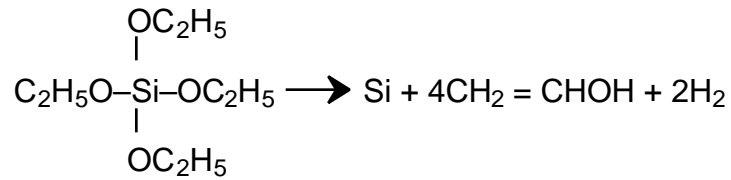


Solution to Part (b)



3 Reactors are needed to achieve 95% conversion

(15%) 5) The chemical vapor deposition of silica from TEOS (tetrethyl othosilicate)



is carried out in a batch from the gas phase. The following data were obtained.

r_{Dep} Rate (nm/s)	P_{TEOS} (atm)	P_{H_2} (atm)	$P_{\text{CH}_2 = \text{CHOH}}$
.1	.1	0	0
.4	.2	0	0
1.5	.4	0	0
9.1	1	5	10
9.1	1	0	0
500	10	0	10
500	10	0	0
4167	50	50	50
9091	100	0	50
19048	200	0	50
39024	400	1	50
99010	1000	100	50

a) Suggest a rate law from the above data.

$$r_{\text{Dep}} = \text{function}(P_{\text{H}_2})$$

$$r_{\text{Dep}} = \text{function}(P_{\text{CH}_2 = \text{CHOH}})$$

$$r_{\text{Dep}} = \text{function}(P_{\text{TEOS}})$$

Initially,

$$\frac{r_2}{r_1} = \frac{0.4}{0.1} = \frac{0.2^2}{0.1^2} = \frac{P_2^2}{P_1^2} \quad r_{\text{Dep}} \sim P_{\text{TEOS}}^2$$

Finally,

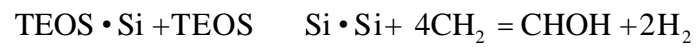
$$\frac{r_2}{r_1} = \frac{99010}{39024} \quad (2.5) = \frac{P_2}{P_1} \quad r_{\text{Dep}} \sim P_{\text{TEOS}}$$

Combining,

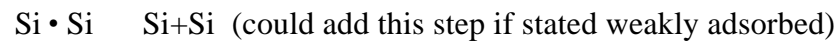
$$r_{\text{Dep}} = \frac{kP_{\text{TEOS}}^2}{1 + K_1 P_{\text{TEOS}}}$$

b) Suggest a mechanism and rate limiting step consistent with the rate law.

Eley-Rideal Mechanism:



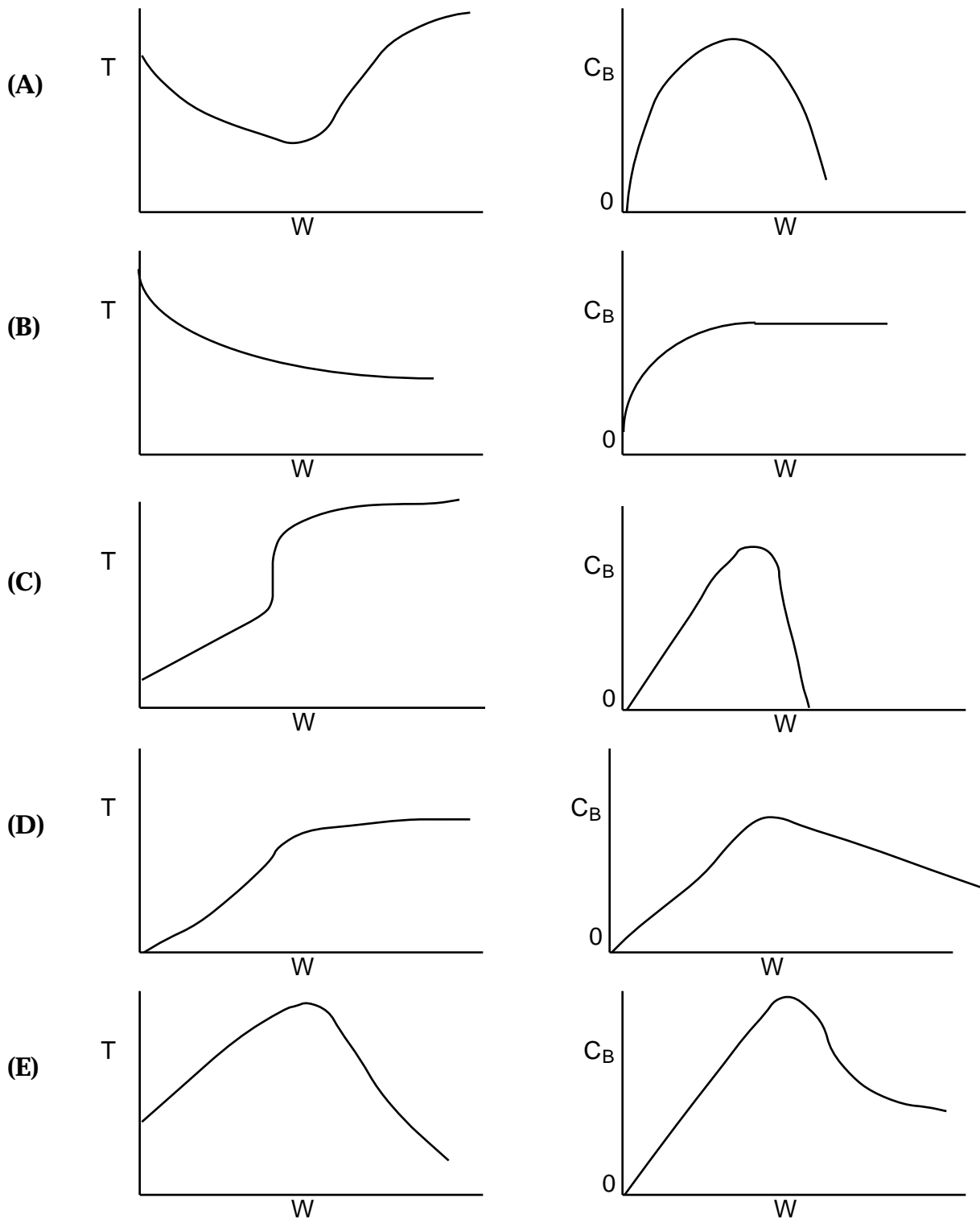
The above is the rate limiting step



(15%) 6) A number of irreversible elementary series reactions (e.g. $X \xrightarrow{A} Y \xrightarrow{B} Z, D \xrightarrow{E} E \xrightarrow{F} F$) all follow the sequence

A B C

were carried out adiabatically in a PBR. The following plots were obtained for the different reactions. (E.g. Case A represents the reaction $X \xrightarrow{A} Y \xrightarrow{B} Z$, Case B represents $D \xrightarrow{E} E \xrightarrow{F} F$, etc.)



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- a) Which case or cases could represent a reaction in which the second reaction in series (B → C) has a very very low frequency factor and a very very high activation energy when compared to the first (A → B)?

Ans. B and C

Explain B because the reaction stops (only first reaction occurs due to low frequency factor and high activation energy) C because high activation energy will cause the second reaction to be very temperature sensitive

- b) Which case or cases could represent a situation where both reactions are exothermic?

Ans. C and D

Explain The temperature goes up for both reactions (formation of B and destruction of B to form C)

- c) Which case could represent a situation in which the first reaction is endothermic and the second is exothermic?

Ans. A

Explain The temperature goes down for the first reaction (formation of B) and goes up for the second reaction (formation of C from B)

- d) Which case could represent a situation in which the first reaction is exothermic and the second is endothermic?

Ans. E

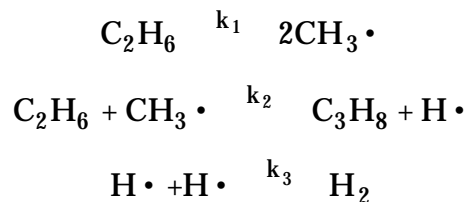
Explain The temperature goes up for the first reaction (formation of B) and goes down for the second reaction (formation of C from B)

- e) Which case could represent a situation in which absolute value of the heat of reaction of the second reaction is greater than the first?

Ans. C

Explain The rate temperature increase for the second reaction is greater than that for the first reaction (indicative of a more exothermic heat of reaction for the second reaction)

(5%) 7) The following sequence is believed to occur for the decomposition of ethane



Develop a rate law for the rate of formation of propylene in terms of the concentration of ethane.

Note: there was a typo in the exam. The chemical formula for propylene is C_3H_6 , not C_3H_8 as given above.

$$r_{\text{prop}} = k_2 [\text{C}_2\text{H}_6][\text{CH}_3\cdot]$$

Apply the PSSA to $\text{CH}_3\cdot$

$$r_{\text{CH}_3\cdot} = 0 = -k_2 [\text{C}_2\text{H}_6][\text{CH}_3\cdot] + k_1 [\text{C}_2\text{H}_6]$$

$$k_2 [\text{C}_2\text{H}_6][\text{CH}_3\cdot] = k_1 [\text{C}_2\text{H}_6]$$

$$[\text{CH}_3\cdot] = \frac{k_1}{k_2}$$

Now substitute back into r_{prop}

$$r_{\text{prop}} = k_2 [\text{C}_2\text{H}_6] \frac{k_1}{k_2}$$

$$r_{\text{prop}} = k_1 [\text{C}_2\text{H}_6]$$

