ChE 344
Chemical Reaction Engineering
Winter 1999
Final Exam

Open Book, Notes, CD ROM, Disk, and Web

Name________________________________

Honor Code____

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1)	____/	25 pts
2)	____/	15 pts
3)	____/	10 pts
4)	____/	3 pts
5)	____/	6 pts
6)	____/	8 pts
7)	____/	8 pts
8)	____/	5 pts
9)	____/	20 pts
Total	____/	100 pts

(25 pts) 1) The gas phase irreversible reaction

$$A + B \rightarrow C$$

is elementary. The entering flow rate of A is 10 mol/min and is equal molar in A and B. The entering concentration of A is 0.4 mol/dm^3.

a) What is the CSTR reactor volume necessary to achieve 90% conversion?
b) What PFR volume is necessary to achieve 90% conversion?

Additional Information

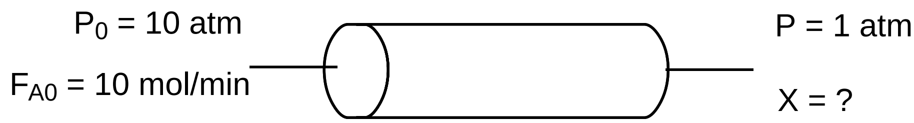
$k = 2\ dm^3/mol \bullet min$
$T_0 = 500\ K$

Note: You do not need to use POLYMATH, but if you do write your program below in case you do not obtain the correct answer.

(15 pts) 2) The irreversible zero order gas phase dimerization

$$2A \rightarrow A_2$$

is carried out in a packed bed reactor with 5 kg of catalyst. The entering pressure is 10 atm and the exit pressure is 1 atm. Pure A enters at a flow rate of 10 mol/min. The reaction is zero order in A.



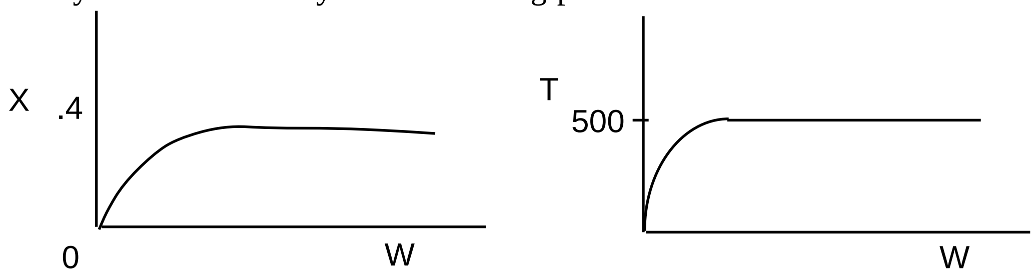
a) What is the pressure drop parameter α?
b) What is the exit conversion?

Additional Information

k = 1.5 mol/kg•min
T_0 = 500 K

Note: You do not need to use POLYMATH, but if you do write your program below in case you do not obtain the correct answer.

(10 pts) 3) The species A and B react to form species C, D, and E in a packed bed reactor. The catalyst does not decay. The following profiles were obtained



Circle the correct true (T) or False (F) answer for this system

T F a) The above profiles could represent an adiabatic system where the addition of inerts will increase the conversion.

T F b) The above profiles could represent a system where decreasing the flow rate will increase the conversion.

T F c) The above profiles could represent a system where if the feed temperature is increased, one cannot tell from the above profiles whether or not the conversion will increase or decrease.

T F d) There could be a heat exchanger on the reactor for which the heat flow is

$$\frac{d\dot{Q}}{dW} = \frac{1000 \text{ kJ}}{\text{kg s K}}(T - 500)$$

T F e) The above reaction may be an excellent candidate for reactor staging.

(3 pts) 4) The gas phase reaction

$$2A + B \longrightarrow C$$

is carried out in a PFR. The feed is equal molar in A and B and the entering temperature is 500K and the entering pressure is 16.4 atm. If the exit conversion is X, then the exit concentration of B (in mol/dm^3) is

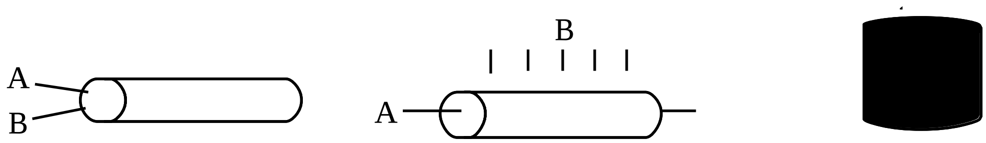
a) $C_B = 0.4(1 - X)/(1 - .5X)$
b) $C_B = 0.4(1 - X)(1 - 1.5X)$
c) $C_B = 0.4$
d) $C_B = 0.4(1 - 0.5X)/(1 - X)$
e) None of the above
f) Cannot be calculated without knowing the exit conversion.

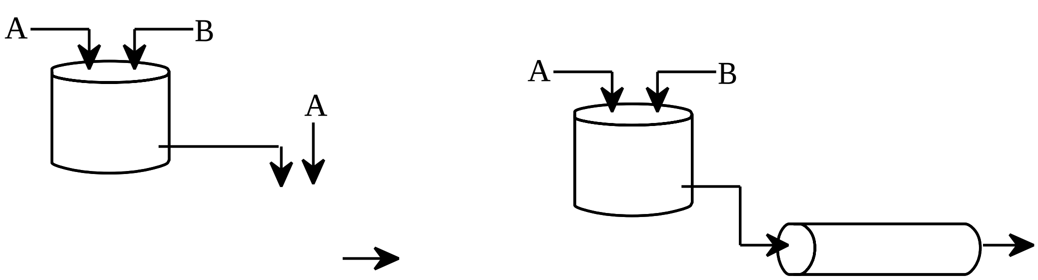
(6 pts) 5) a) The following elementary liquid phase reactions are to be carried out

$$A + B \rightarrow R$$

$$R + B \rightarrow S$$

Species R is the desired product. Which of the following schemes should be used?





(g)

b) In the reactors

$$A \rightarrow B \qquad r_B = k_B C_A^2$$

$$A + B \rightarrow 2C \qquad r_C = k_C C_A C_B$$

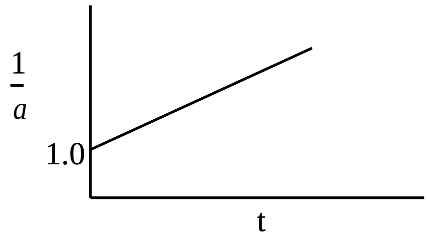
What is the instantaneous selectivity of C to B? Which reactor or combination of reactors and at what temperatures would you use for the following reaction system?
C is the desired product.

<u>Data for Part (b)</u>

$C_{A0} = 4\ mol/dm^3$ $k_B = 1\ dm^3/mol\ \ min$ at 300K with E = 4000cal/mol

$k_C = 1\ dm^3/mol\ \ min$ at 300K with E = 12000cal/mol

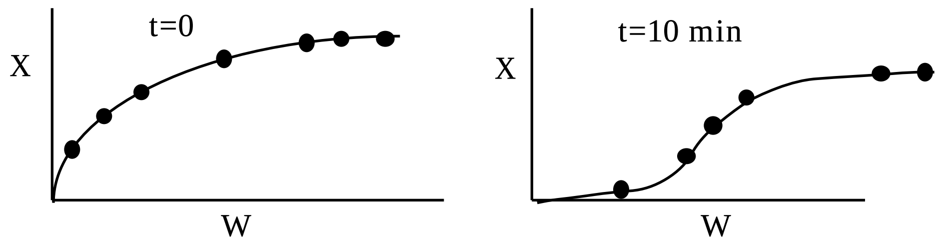
(8 pts) 6) a) The following plot of activity as a function of time was obtained.



What type of decay would best describe to data? (circle the correct answer)

1) Poisoning
2) Sintering
3) Coking
4) None of the above

b) The following profiles were measured in a PBR



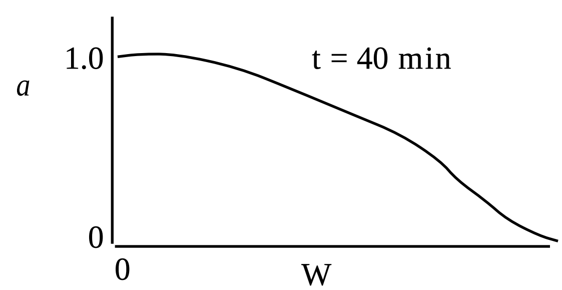
The type of catalyst decay can best be described by (circle the correct answer)

1) Poisoning
2) Sintering
3) Coking
4) None of the above

c) The following catalyst activity profile was measured in a PBR for the isomerization of A to B.

The decay law that best describes this data is (circle the correct answer)

1) $\frac{da}{dt} = -ka$
2) $\frac{da}{dt} = -ka^2$
3) $\frac{da}{dt} = -ka\ C_A$
4) $\frac{da}{dt} = -ka^2\ C_B$
5) None of the above



(8 pts) 7) (P10-4) The rate law for the hydrogenation (H) of ethylene (E) to form ethane (A) over a cobalt-molybdenum catalyst [*Collection Czech. Chem. Commun.*, 51, 2760 (1988)] is

$$-r'_E = \frac{kP_E P_H}{1 + K_E P_E}$$

Suggest a mechanism and rate-limiting step consistent with the rate law. (Can be done by inspection.)

(5 pts) 8) Suppose the heat exchanger in Example E8-12 became fouled so that the overall heat transfer coefficient was reduced by 50%?
What would be the new steady state temperatures inside the reactor?

(20 pts) 9) The elementary liquid phase reactions

(1) $A \longrightarrow B$

(2) $2A \longrightarrow C$

are carried out in a 100 dm^3 PFR where species B is the desired product. Pure A enters at a molar flow rate of 40.0 mol/min and at a concentration of 4.0 mol/dm^3.

Additional Information

$C_{P_A} = C_{P_B} = 20$ cal/mol/K

$C_{P_C} = 40$ cal/mol/K

$\Delta H_{Rx1A} = +10{,}000$ cal/mol

$\Delta H_{Rx2A} = -20{,}000$ cal/mol

$Ua = 100 \dfrac{\text{cal}}{\text{dm}^3 \text{ min K}}$ with $T_a = 400K$

$k_{1A} = 0.05\ \text{min}^{-1}$ at 400K with $E = 10{,}000$ cal/mol

$k_{2C} = 0.0005\ \text{dm}^3/\text{mol}/\text{min}$ at 400K with $E = 19{,}000$ cal/mol

a) For a feed temperature of 450K, what are the exit concentrations and temperature

C_A = ______, C_B = ______, C_C = ______, T = ______K

b) The feed temperature can be varied between 400 and 700. What feed temperature do you recommend to maximize the exit molar flow rate of B?

75% Marks for setting up the problem correctly with all correct equations and numbers in POLYMATH Notation

25% Final Answer