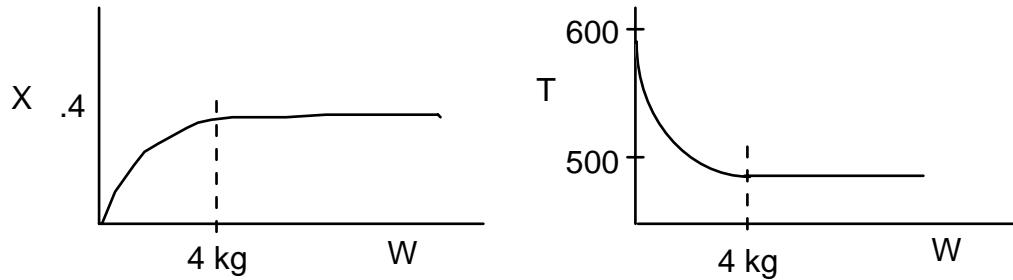


**ChE 344**  
**Chemical Reaction Engineering**  
**Winter 1999**  
Mid Term Exam

*Solution*

- (5 pts) 1) The isomerization of A to B was carried out 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

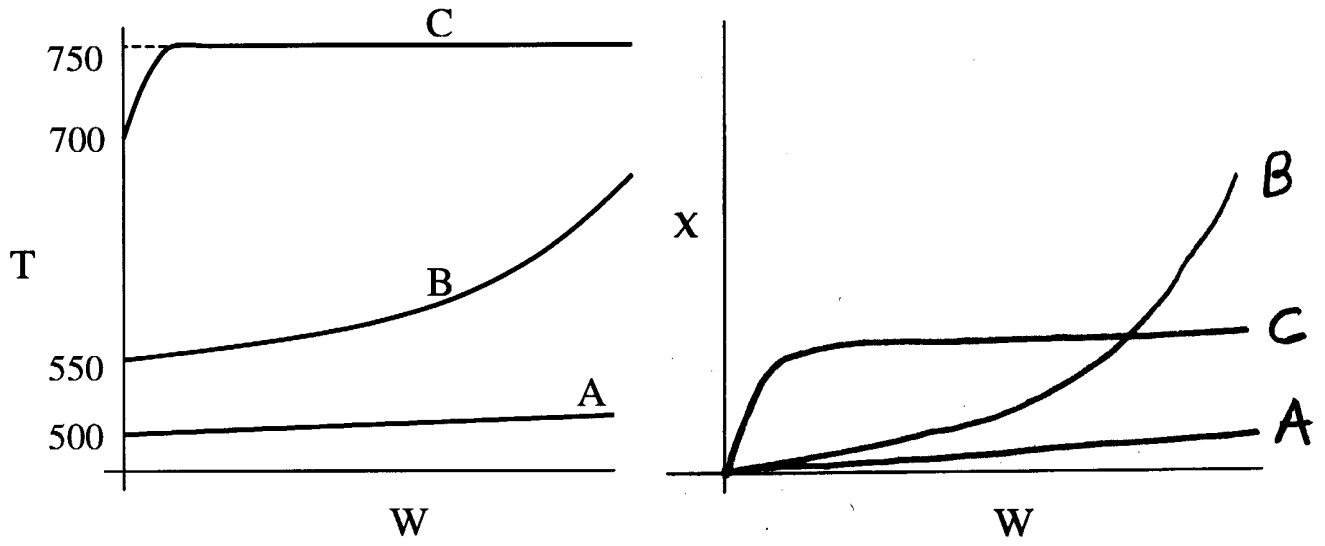
- F a) The above profiles could represent an adiabatic system where the addition of inerts to the feed stream will increase the conversion.
- T  b) A small decrease in the flow rate will produce a small increase in the conversion.
- T  c) An increase in the feed temperature will always increase the conversion.
- T  d) A decrease in feed temperature will always increase the conversion.
- T  e) There could be a heat exchanger attached to the reactor with the heat flow given by

$$\frac{d\dot{Q}}{dW} = \left( \frac{400 \text{ kJ}}{\text{kg min K}} \right) (T - 400)$$

Explanation:

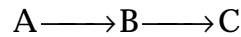
- a) If it is an adiabatic system then it has to be endothermic. Increasing inerts increases the exit temperature and hence the conversion is higher.
- b) The exit condition is an equilibrium condition and small change in the flow rate will not affect the equilibrium condition. Hence, it will not change the conversion.
- c) One possibility is that the reaction has zero heat of reaction and there is a heat exchanger present. In this case the increase in feed temperature will not increase the conversion.
- d) Same as (c) if  $\Delta H \approx 0$ . Otherwise if it is an endothermic reaction then it should have smaller equilibrium conversion at low temperature.
- e) Because final temperature is 500 and reaction is in equilibrium. Hence, the ambient temperature of the heat exchanger cannot be 400.

- (6 pts) 2) The isomerization of A to B was carried out adiabatically in a packed bed reactor. The catalyst does not decay.

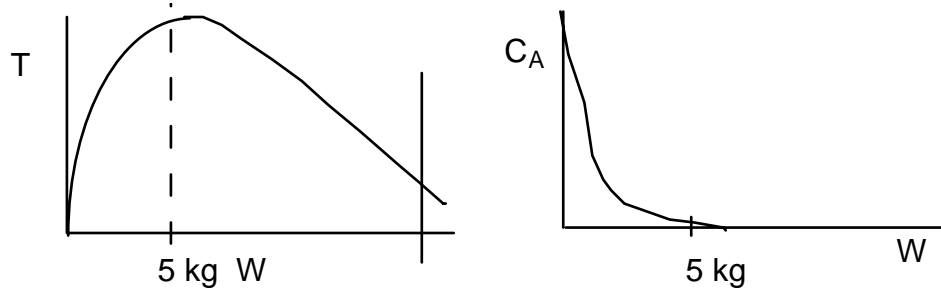


Sketch the corresponding conversion profiles for A, B, and C.

(6 pts) 3) The series reaction



is carried out in a packed bed reactor. The following profiles were obtained.



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

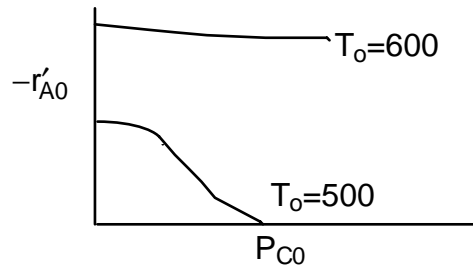
- T  F a) The above profiles could represent a system where the reactions are carried out adiabatically.
- T  F b) The above profiles could represent a system where there is a heat exchanger attached to the system.
- T  F c) The above profiles could represent an adiabatic system where both of the reactions could be endothermic.
- T  F d) The above profiles could represent an adiabatic system where only one of the reactions is exothermic
- T  F e) The above profiles could represent a system where the addition of inerts could decrease the exit molar flow rate of the desired product, B.
- T  F f) The above profiles could represent an adiabatic system where increasing the feed temperature will increase the concentration of B in the exit stream.

Explanation:

- a) Possible if  $A \rightarrow B$  is exothermic and  $B \rightarrow C$  is endothermic.
- b) Possible when either  $A \rightarrow B$  is exothermic or  $B \rightarrow C$  is endothermic or both.
- c) Not possible because the temperature is initially increasing.
- d) Same as (a)
- e) Addition of inerts could decrease the temperature which reduces the reaction rate of  $A \rightarrow B$  and hence decreases the exit molar flow of B.
- f) Increasing the feed temperature will increase the rate of reaction of both  $A \rightarrow B$  and  $B \rightarrow C$ . Hence, exit concentration of B could decrease.

- (4 pts) 4) The irreversible gas phase reaction of A and B to form C and D was carried out in a packed bed reactor in which there is no catalyst decay.

The following figure shows the rate of reaction at the reactor entrance as a function the partial pressure of C for various entering temperatures,  $T_o$ .



Circle the correct answer T (True), F (False), or CT (Cannot Tell) from the information given for the above system

- T F  CT a) The reaction is exothermic.  
 T F  CT b) The reaction is endothermic.  
 T F CT c) Species C is adsorbed on the catalyst surface at 400°K.  
 T  F CT d) Species C is adsorbed on the catalyst at 700°K.

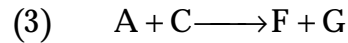
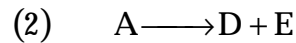
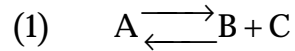
Explanation:

- c) Because at 500K,  $-r'_{A0}$  depends on  $P_{C0}$  but at 600K, it is nearly independent. Hence, the adsorption reaction of C is exothermic.  
 d) Same as (c).

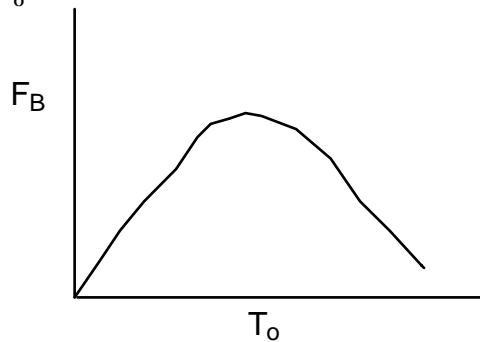
(5 pts) 5) Circle the correct true (T) or False (F) answer

- T  F a) Multiple steady states can exist for an irreversible endothermic first order reactions.
- T  F b) Multiple steady states can only exist for reversible reactions.
- T  F c) Multiple steady states can only exist for adiabatic reactions.
- T  F d) Reactor staging is used for irreversible reactions.
- T  F e) The effects of pressure drop are more pronounced for adiabatic-exothermic reactions than for adiabatic endothermic reactions.

(5 pts) 6) The reactions



are carried out in a packed bed reactor where B is the desired product. The flowrate of species B exiting the reaction is shown below as a function of the entering temperature,  $T_0$ .



Circle the correct true (T) or False (F) answer

- F a) The above figure could represent an adiabatic system where the reaction 1 is adiabatic exothermic and reversible.
- F b) The above figure could represent an adiabatic system where the reaction 1 is adiabatic, endothermic and reversible.
- F c) The above figure could represent an adiabatic system where all reactions are endothermic.
- F d) The above figure could represent a system where the reactions 1 and 3 are endothermic and reaction 2 is exothermic.
- F e) The above figure could represent a system where the reactions 1 and 2 are endothermic and reaction 3 is exothermic.

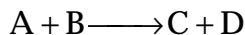
Explanation:

- a) Possible because if reaction (1) is exothermic, at low  $T_0$ , rate of forward reaction (1) is low and at high  $T_0$ , equilibrium conversion is low.
- b) Possible because if reaction (1) is endothermic, at low  $T_0$ , rate of forward reaction (1) is low and at high  $T_0$ , reaction (1) and (2) can take over.
- c) Same as (b)
- d) & e) Possible

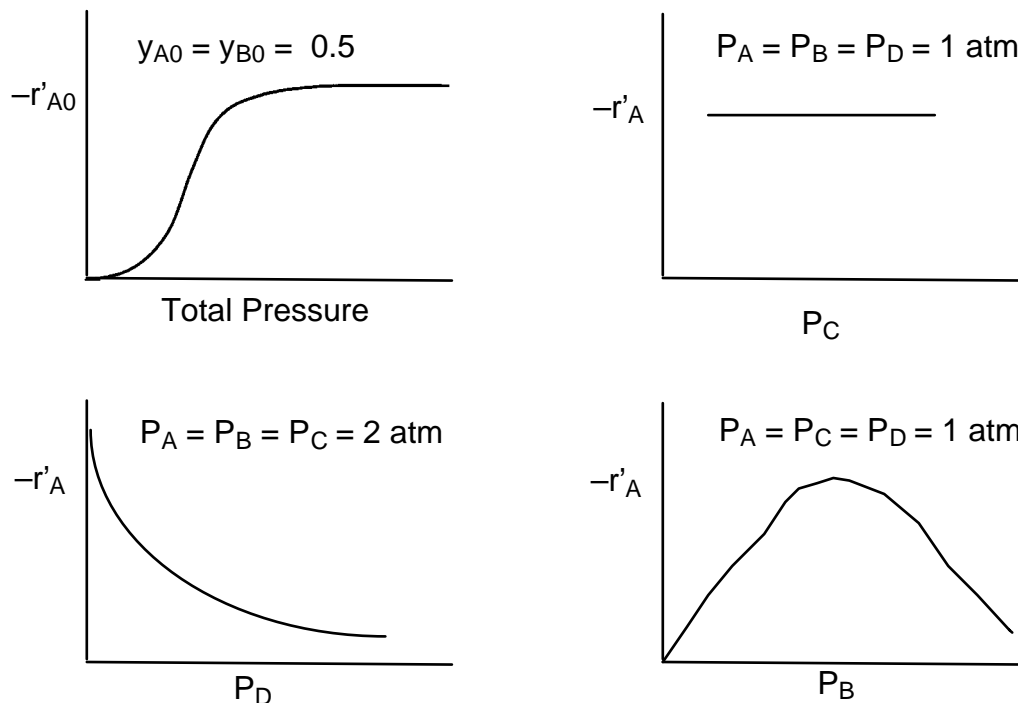




(15 pts) 7) The catalytic reaction



was carried out in a differential reactor with the following results



- What is the rate law consistent with the experimental data?
- What is the mechanism and rate limiting step consistent with the rate law? (Can be done by inspection).

### Solution

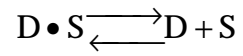
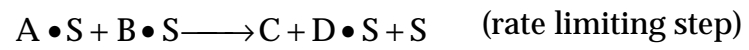
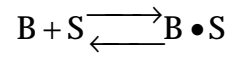
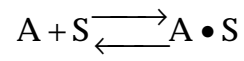
#### Interpretation of graphs.

- $-r'_A$  is independent of  $P_C$
- $-r'_A$  monotonically decreases with  $P_D$ . Hence,  $P_D$  has to be only in the denominator.
- $-r'_A$  linearly increases with  $P_B$  for low  $P_B$ . This means that  $-r'_A$  is first order with  $P_B$  for low  $P_B$ . For high  $P_B$ ,  $-r'_A$  linearly decreases with  $P_B$ . This means that  $-r'_A$  has  $P_B$  in the denominator and the exponent of denominator is 2.
- $-r'_A$  quadratically increases with total pressure for lower total pressure and hence  $-r'_A$  is second order.

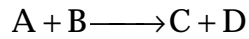
a) Hence,

$$-r'_A = \frac{k' P_A P_B}{(1 + K_A P_A + K_B P_B + K_D P_D)^2}$$

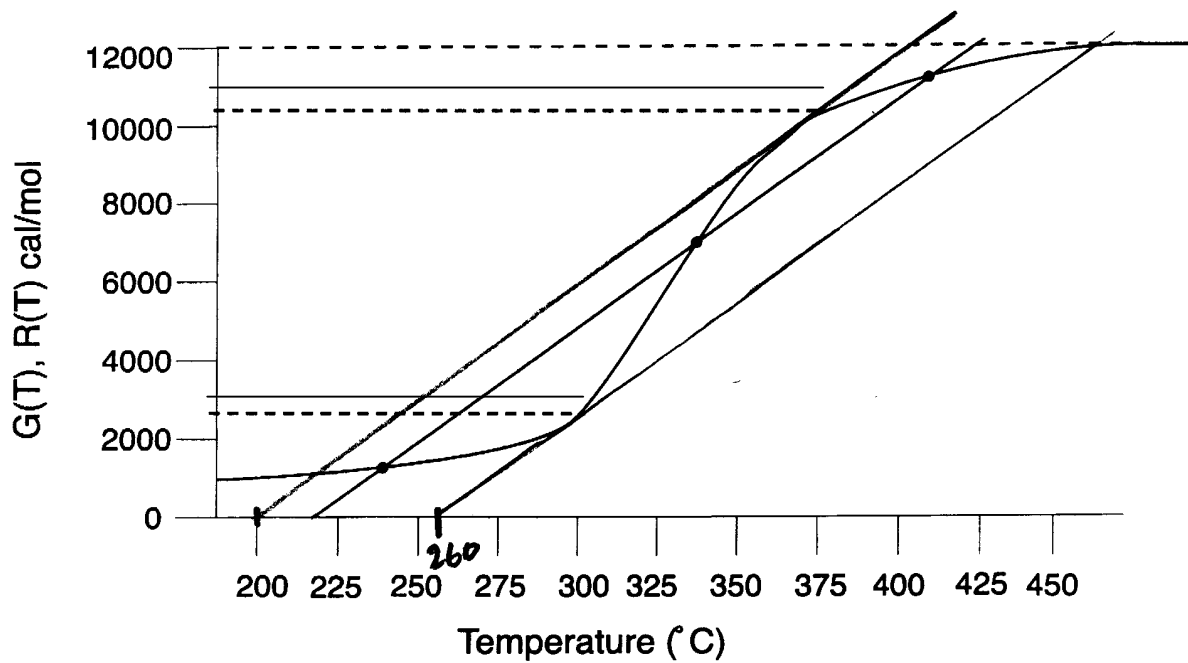
b) Possible mechanism



(10 pts) 8) The irreversible reaction



is carried out in a CSTR. The “heat generated” [G(T)] and the “heat removed” [R(T)] curves are shown below



Assume Adiabatic

a) What is the  $\Delta H_{R_x}$  of the reaction?

$$\Delta H_{R_x} = \underline{\quad -12000 \quad} \text{ cal/mol}$$

b) What are the ignition and extinction temperatures?

$$\begin{aligned} \text{Ignition} &= \underline{\quad 260 \quad} \text{ }^\circ\text{C} \\ \text{Extinction} &= \underline{\quad 200 \quad} \text{ }^\circ\text{C} \end{aligned}$$

c) What are the conversions just before the ignition and extinction temperatures?

$$X_{\text{ignition}} = \frac{2500}{12000}$$

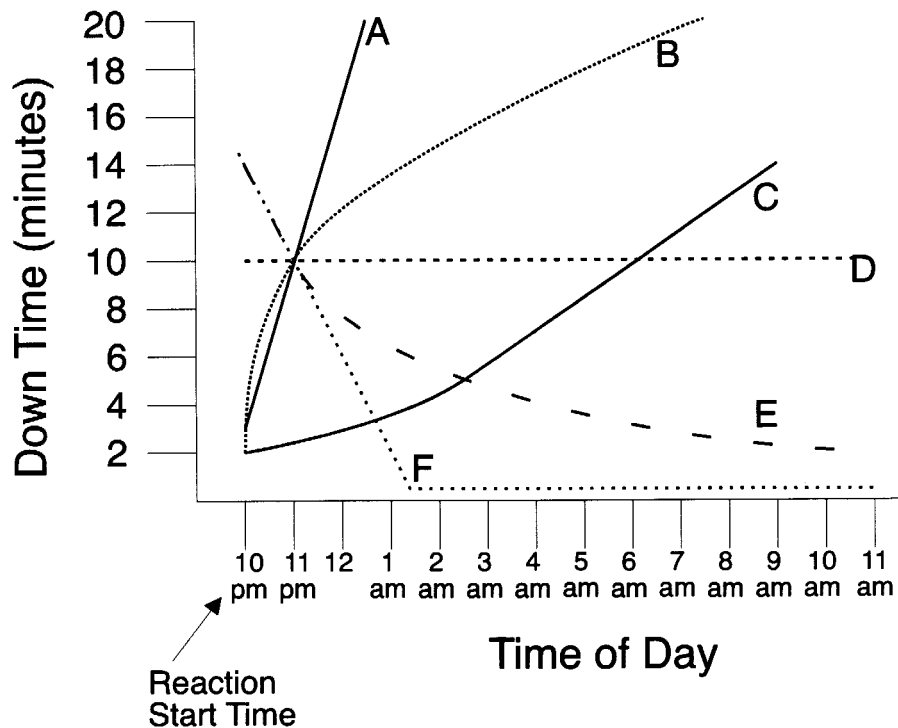
$$X_{\text{extinction}} = \frac{10300}{12000}$$

$$\begin{aligned} X(\text{Ignition}) &= \underline{\quad 0.21 \quad} \\ X(\text{Extinction}) &= \underline{\quad 0.86 \quad} \end{aligned}$$

(9 pts) 9) Reconsider the example 9-2

- a) Which of the following curves best describes the correlation between the shortest length of time the heat exchange stopped functioning (i.e.  $\dot{Q} = 0$ ) (down time) and the time in the evening at which the malfunction occurred that will cause an explosion.

Ans \_\_\_\_\_ B



- b) If 10% more water had been added to the mixture in the reactor the explosion would not have occurred that evening.

True

False

### Solution

- a) The concentrations of reactants decrease with the time in the evening. Hence, rate of reaction decreases with the time in the evening. Hence, the shortest length of time the heat exchanger stopped functioning, which will cause an explosion, will increase with the time in the evening.

b) 10% more water added

$$\begin{aligned}V &= V_{\text{others}} + 1.1 V_{\text{water}} \\ &= 3.269 + 1.1 \times 1.854 \\ &= 5.3084 \text{ m}^3\end{aligned}$$

$$\begin{aligned}NC_P &= \sum N_i C_{P_i} = (9.0448 \times 40) + (103.7 \times 18) \times 1.1 + 33 \times 8.38 \\ &= 2691.592 \text{ kcal/K}\end{aligned}$$

A. Isothermal Operation up to 45 mins

$$45 = \left( \frac{5.3084}{0.0001167 \times 9.044} \right) \left( \frac{1}{1.64} \right) \ln \frac{3.64 - 2x}{3.64(1 - X)}$$

$$\Rightarrow x = 0.0318$$

B. Adiabatic operation for 10 mins

See POLYMATH

At t = 55 mins

$$T = 465.477$$

$$x = 0.0406$$

$$Q_g = 5959.35$$

$$\begin{aligned}Q_r &= 35.83 (465.477 - 298) \\ &= 6000.7\end{aligned}$$

Example 9-2

Equations:

$$d(T)/d(t) = (Qg - Qr) / NCp$$

$$d(X)/d(t) = (-ra) * V / Nao$$

$$NCp = 2691.592$$

$$V = 3.265 + 1.854 * 1.1$$

$$Nao = 9.0448$$

$$UA = 0$$

$$dH = -590000$$

$$Nbo = 33$$

$$k = .00017 * \exp(11273 / (1.987) * (1/461 - 1/T))$$

$$Qr = UA * (T - 298)$$

$$Theata = Nbo / Nao$$

$$ra = -k * Nao * 2 * (1 - X) * (Theata - 2 * X) / V * 2$$

$$rate = -ra$$

$$Qg = ra * V * (dH)$$

$$t_0 = 45, \quad t_f = 55$$

Initial values:

448

0.0318

Example 9-2

<u>Variable</u>	<u>Initial value</u>	<u>Maximum value</u>	<u>Minimum value</u>	<u>Final value</u>
t	45	55	45	55
T	448	465.477	448	465.477
X	0.0318	0.0406151	0.0318	0.0406151
NCp	2691.59	2691.59	2691.59	2691.59
V	5.3044	5.3044	5.3044	5.3044
Nao	9.0448	9.0448	9.0448	9.0448
UA	0	0	0	0
dH	-590000	-590000	-590000	-590000
Nbo	33	33	33	33
k	0.000118948	0.000191362	0.000118948	0.000191362
Qr	0	0	0	0
Theata	3.64851	3.64851	3.64851	3.64851
ra	-0.0012004	-0.0012004	-0.00190419	-0.00190419
rate	0.0012004	0.00190419	0.0012004	0.00190419
Qg	3756.76	5959.35	3756.76	5959.35

$$Q_g = 5959.35$$

$$Q_r = 6000.7$$

$$Q_g < Q_r \text{ (hence, no explosion)}$$

(10 pts) 10) The vapor-phase cracking of gas-oil in Example 10-7 is carried out isothermally over a different catalyst, for which the rate law is

$$-r'_A = a(t)k'P_A^2 \quad \text{with } k' = 1.0 \times 10^{-5} \frac{\text{kmol}}{\text{kgcat} \cdot \text{s} \cdot \text{atm}^2} \text{ at } 400^\circ\text{C} \text{ and with } E_A = 5000 \frac{\text{cal}}{\text{mol}}$$

The decay law is

$$-\frac{da}{dt} = k_d a^2 P_B$$

with  $k_d = 0.002 \text{ s}^{-1} \text{ atm}^{-1}$  at  $400^\circ\text{C}$  and with  $E_D = 35000 \text{ cal/mol}$

Assuming that you can vary the entering temperature between  $200^\circ\text{C}$  and  $700^\circ\text{C}$ , what entering temperature would you recommend? ( $\pm 25^\circ\text{C}$ )

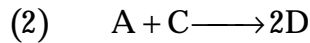
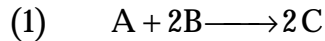
$T_o = \underline{\hspace{2cm} 500 \hspace{2cm}} ^\circ\text{C}$
--

You can make any assumptions that were made in the example problem.

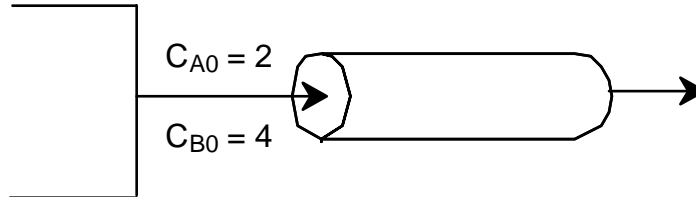
<u>T</u>	<u>X</u>
400	0.48
500	0.56
600	0.48
475	0.549
525	0.551



(25 pts) 11) The elementary liquid phase reactions



are carried out adiabatically in a  $10 \text{ dm}^3$  PFR. After streams A and B mix, species A enters the reactor at a concentration of  $C_{A0} = 2 \text{ mol/dm}^3$  and species B at a concentration of  $4 \text{ mol/dm}^3$ . The entering volumetric flow rate is  $10 \text{ dm}^3/\text{s}$ .



Assuming you could vary the entering temperature between 300K and 600 K, what entering temperature would you recommend to maximize the concentration of species C exiting the reactor? ( $\pm 25^\circ\text{K}$ ).

$T_o = \underline{\quad 325 \text{ (}^\circ\text{C)} \quad} X_C$
--

Assume all species have the same density.

Additional Information

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

$$C_{P_C} = 60 \text{ cal/mol/K}$$

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

$$\Delta H_{R_{x1A}} = 20,000 \text{ cal/mol A}$$

$$\Delta H_{R_{x2A}} = -10,000 \text{ cal/mol A}$$

$$k_{1A} = 0.001 \frac{\text{dm}^6}{\text{mol}^2 \cdot \text{s}} \text{ at } 300\text{K with } E = 5000 \text{ cal/mol}$$

$$k_{2A} = 0.001 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}} \text{ at } 300\text{K with } E = 7500 \text{ cal/mol}$$

Note:

Before beginning write your POLYMATH program below in POLYMATH NOTATION

1. \_\_\_\_\_

2. \_\_\_\_\_

*Continue*

(10)

Example 10-7 STTR: Langmuir-Hinshelwood Kinetics

Equations:

$$d(a)/d(z) = -kd \cdot a^2 \cdot P_b / U$$

$$d(X)/d(z) = -ra / U / C_{ao}$$

$$K_a = 0.05$$

$$K_b = 0.15$$

$$P_{ao} = 12$$

$$\epsilon = 1$$

$$A = 7.6$$

$$R = 0.082$$

$$T = 500 + 273$$

$$\rho = 80$$

$$D = 1.5$$

$$U_o = 2.5$$

$$K_c = 0.1$$

$$kd = 0.002 \cdot \exp(-35000 / 1.987 \cdot (1/T - 1/673))$$

$$k_{prime} = 1.0 \cdot 10^{-5} \cdot \exp(-5000 / 1.987 \cdot (1/T - 1/673))$$

$$U = U_o \cdot (1 + \epsilon \cdot X)$$

Initial values:

1

0

$$P_b = P_{ao} \cdot X / (1 + \epsilon \cdot X)$$

$$P_a = P_{ao} \cdot (1 - X) / (1 + \epsilon \cdot X)$$

$$v_o = U_o \cdot 3.1416 \cdot D \cdot D / 4$$

$$C_{ao} = P_{ao} / R / T$$

$$K_{ca} = K_a \cdot R \cdot T$$

$$P_c = P_b$$

$$r_{a_{prime}} = a \cdot (-k_{prime} \cdot P_a^2)$$

$$r_a = \rho \cdot r_{a_{prime}}$$

$$z_0 = 0, \quad z_f = 10$$

(11)

<u>T(K)</u>	<u>C<sub>C</sub></u>
800	0.92
700	1.06
600	1.0755
500	0.78
650	1.1025
625	1.099
675	1.088

Ans: In the range between 300K to 600K, answer is

600K

Equations:

$$d(Ca)/d(V) = (r1a+r2a)/vo$$

$$d(Cb)/d(V) = 2*r1a/vo$$

$$d(Cc)/d(V) = (-2*r1a+r2a)/vo$$

$$d(Cd)/d(V) = -2*r2a/vo$$

$$d(T)/d(V) = (r1a*dh1a+r2a*dh2a) / ((Ca+Cb+3*Cc+4*Cd)*vo*Cpa)$$

$$vo=10$$

$$dh1a=20000$$

$$dh2a=-10000$$

$$Cpa=20$$

$$k1a=0.001*\exp(-5000/1.987*(1/T-1/300))$$

$$k2a=0.001*\exp(-7500/1.987*(1/T-1/300))$$

$$r1a=-k1a*Ca*Cb^2$$

$$r2a=-k2a*Ca*Cc$$

$$V_0 = 0, \quad V_f = 10$$

Initial values:

2

4

0

0

800

<u>Variable</u>	<u>Initial value</u>	<u>Maximum value</u>	<u>Minimum value</u>	<u>Final value</u>
V	0	10	0	10
Cb	4	4	2.17095	2.17095
Ca	2	2	0.165608	0.165608
Cc	0	0.923461	0	0.909182
Cd	0	1.83973	0	1.83973
T	800	800	735.817	736.409
vo	10	10	10	10
dh1a	20000	20000	20000	20000
dh2a	-10000	-10000	-10000	-10000
Cpa	20	20	20	20
k1a	0.189125	0.189125	0.143745	0.144141
k2a	2.6009	2.6009	1.72341	1.73053
r1a	-6.052	-0.112504	-6.052	-0.112504
r2a	-0	-0	-1.80756	-0.260564