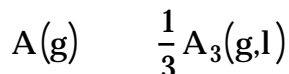


ChE 344
Chemical Reaction Engineering
Winter 1999
Exam I
Part 1 (80%)
Solution

(10 pts) 1) The trimerization



is carried out isothermally and without pressure drop in a PFR at 298 K and 2 atm. As the concentration of A_3 increases down the reactor and A_3 begins to condense. The vapor pressure of A_3 at 298 K is 0.5 atm. If an equal molar mixture of A and inert, I, is fed to the reactor at what conversion of A will A_3 begin to condense?



$$\text{Condensation begins at } y = \frac{P_V}{P_T} = \frac{0.5 \text{ atm}}{2 \text{ atm}} = 0.25$$

Species	Entering	Change	Before Cond.	After Cond.
A(g)	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$	$F_A = F_{A0}(1-X)$
I(g)	F_{A0}	---	$F_I = F_{A0}$	$F_I = F_{A0}$
$A_3(g,l)$	---	$\frac{F_{A0}X}{3}$	$F_{A_3} = \frac{F_{A0}X}{3}$	$F_{A_3} = y_{A_3,e} F_T$

$$F_T = F_{A0} \left(2 - \frac{2}{3} X \right)$$

$$y_{A_3,e} = \frac{F_{A_3}}{F_T} = \frac{F_{A0} \frac{X}{3}}{F_{A0} \left(2 - \frac{2}{3} X \right)} = 0.25$$

$$\frac{X}{6 - 2X} = \frac{1}{4}$$

$$4X = 6 - 2X$$

$$6X = 6$$

$$X = 1$$

(30 pts) 2) In order to study the photochemical decay of aqueous bromine in bright sunlight, a small quantity of liquid bromine was dissolved in water contained in a glass battery jar and placed in direct sunlight. The following data were obtained:



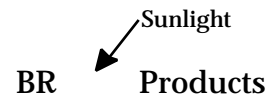
Time (min)	10	20	30	40	50	60
ppm Br	2.45	1.74	1.23	0.88	0.62	0.44

- a) Determine whether the reaction rate is zero-, first-, or second-order in bromine, and calculate the reaction rate constant in units of your choice.
- b) Assuming identical exposure conditions, calculate the required hourly rate of injection of bromine (in pounds) into a sunlit body of water 25,000 gal in volume in order to maintain a sterilizing level of bromine of 1.0 ppm.

(Note: ppm parts of bromine per million parts brominated water by weight. In dilute aqueous solutions, 1 ppm=1 milligram per liter, molecular weight of Br = 80 Daltons.)

1 gal 3.785 liters

1 lb 454 gms



Rate law: $-r_A = k C_A$

Experiment MB: $\frac{dC_A}{dt} = r_A$ (batch)

Experimental data provides C_A vs. time, thus $\frac{dC_A}{dt}$ can be calculated

Combine: $\frac{dC_A}{dt} = -k C_A$

$$\ln -\frac{dC_A}{dt} = \ln k + \ln C_A$$

See plot for $-\frac{y}{x}$ vs. t

Pick 2 points: 2.45, -0.080

at random and 0.88, -0.029

$$= \frac{\ln(+0.08) - \ln(+0.029)}{\ln(2.45) - \ln(0.88)}$$

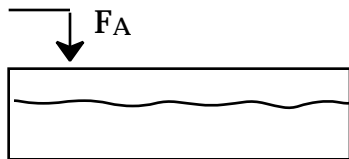
$$= 0.99 \quad 1$$

pick 0.88, - 0.029 $-3.54 = \ln k + (0.99)(-0.1278)$ $\ln k = -3.4134$

$$k = 0.033 \text{ min}^{-1}$$

						Chart Estimate
t	(C _A)					
<u>X</u>	<u>y</u>	<u>-y</u>	<u>-x</u>	<u>-y/x</u>		dy/dx
10	2.45					-0.080
		10	-0.71	-0.071		
20	1.74					-0.060
		10	-0.51	-0.051		
30	1.23					-0.042
		10	-0.35	-0.035		
40	0.88					-0.029
		10	-0.26	-0.026		
50	0.62					-0.020
		10	-0.18	-0.018		
60	0.44					-0.015

Problem 2, part b



M.B.: rate in - rate out + gen. = accum

$$\frac{dN_A}{dt} = F_A + r_A V$$

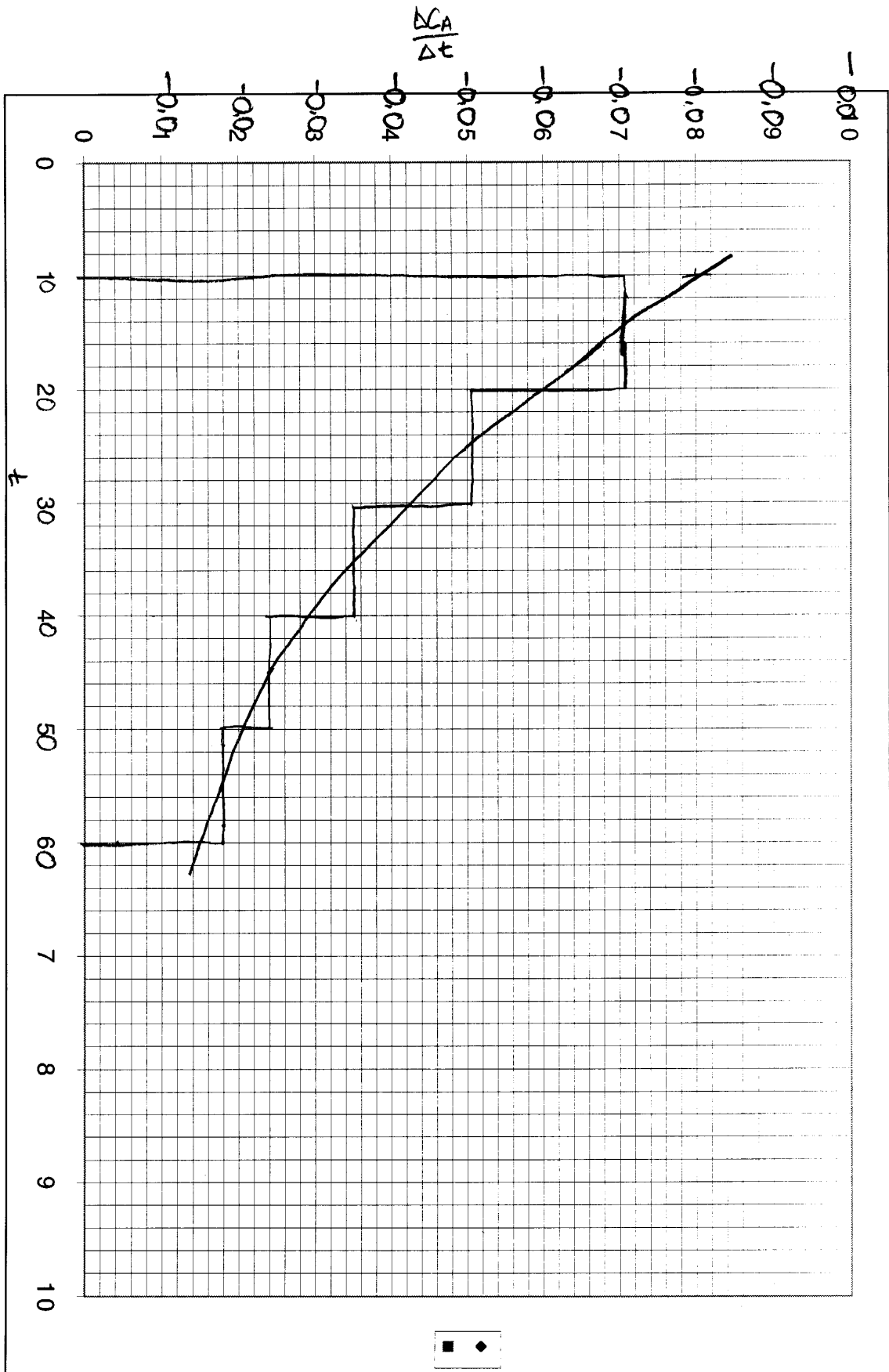
since the Br concentration is constant at 1 ppm, a steady state assumption is valid.

so $\frac{dN_A}{dt} = 0 \quad -r_A V = F_A \quad , \quad -r_A = kC_A$

$$F_A = \frac{0.033}{\text{min}} (1 \text{ ppm}) 25,000 \text{ gal}$$

$$F_A = 825 \frac{\text{ppm gal}}{\text{min}} \times \frac{60 \text{ min}}{1 \text{ hr}} \times \frac{3.785 \ell}{1 \text{ gal}} \times \frac{1 \text{ g}}{1000 \text{ mg}} \times \frac{\text{lb}}{454 \text{ g}}$$

$$F_A = 0.41 \text{ lb/hr}$$



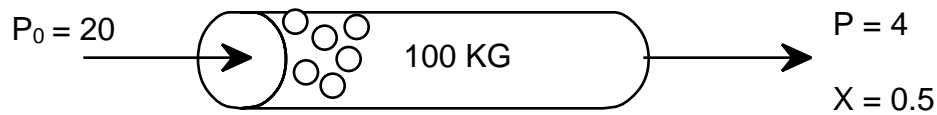
(20pts) 3) The irreversible elementary gas phase reaction



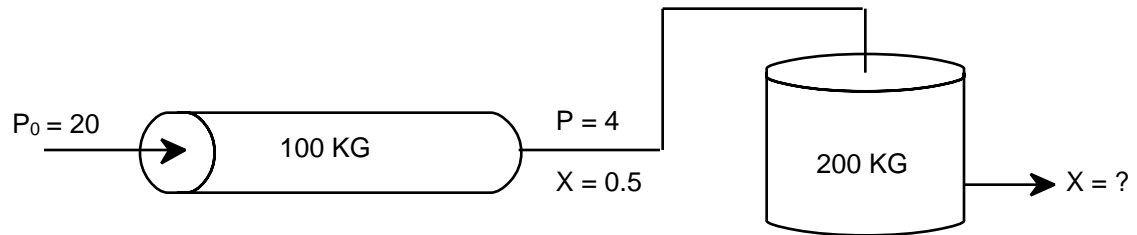
is currently carried out in a packed bed reactor containing 100 kg of catalyst. The entering pressure is 20 atm and the exit pressure is 4 atm. Currently 50% conversion is achieved. It is proposed to add a CSTR with 200 Kg of catalyst downstream of the PBR. There is no pressure drop in the CSTR. The flow rate and temperature remain unchanged.

- What would be the overall conversion in such an arrangement?
- Is there a better way to carry out the reaction, and if so what is it?

Current



Proposed



a) CSTR: $-r_{A_{out}} = \frac{F_{A0}(X_{out} - X_{in})}{w}$

MB

PBR: $-r_A = F_{A0} \frac{dX}{dw}$

RL

$$-r_A = kC_A^2$$

$$A \rightarrow \frac{1}{2}B + \frac{1}{2}C$$

ST

$$C_A = C_{A0} \frac{(1-X) \frac{P}{P_0} \frac{T_0}{T}}{(1+X)}$$

Since $\frac{P}{P_0} = 0$, $\frac{P}{P_0} = (1-w)^{1/2}$

$$\frac{P}{P_0}^2 = 1-w$$

$$\begin{aligned} &= \frac{1 - \frac{P}{P_0}^2}{w} = \frac{1 - \frac{4}{20}^2}{100} \\ &= 0.0096 \end{aligned}$$

Combine: $kC_{A0}^2(1-X)^2 \frac{P}{P_0}^2 = F_{A0} \frac{dX}{dw}$

$$= y_{A0} \quad , \quad y_{A0} = 1 \quad , \quad = 0$$

$$= 0$$

$$\frac{kC_{A0}^2}{F_{A0}} \frac{P}{P_0} dw = \frac{dX}{(1-X)^2}$$

$$C_A = C_{A0}(1-X) \frac{P}{P_0}$$

$$\frac{kC_{A0}^2}{F_{A0}} (1-w)dw = \frac{dX}{(1-X)^2}$$

Integrate

$$\frac{kC_{A0}^2}{F_{A0}} w - \frac{w^2}{2} \Big|_0^{100} = \left| \frac{1}{(1-X)} \right| \Big|_0^{0.5}$$

$$\frac{kC_{A0}^2}{F_{A0}} (100 - 48) = 2 - 1$$

$$\frac{kC_{A0}^2}{F_{A0}} = \frac{1}{52}$$

For CSTR $kC_{A0}^2(1-X)^2 \frac{P}{P_0} = (X_2 - 0.5)F_{A0}/w$

$$\frac{wkC_{A0}^2}{F_{A0}} \frac{P}{P_0} (1-X_2) = X_2 - 0.5$$

$$\frac{200}{52} (0.04)(1-X_2)^2 = X_2 - 0.5$$

$$\frac{2}{13} (1 - 2X_2 + X_2^2) = X_2 - 0.5$$

$$\frac{2}{13} - \frac{4}{13}X_2 + \frac{2}{13}X_2^2 = X_2 - 0.5$$

$$\frac{2}{13}X_2^2 - \frac{17}{13}X_2 + \frac{17}{26} = 0$$

$$X_2 = \frac{17}{13} \pm \frac{\sqrt{\frac{17^2}{13} - \frac{4.2}{13} \frac{17}{26}}}{\frac{2.2}{13}} = \frac{1.3077 \pm 1.1435}{0.3077}$$

$$= 0.534 \text{ or } 7.96 \quad \text{no}$$

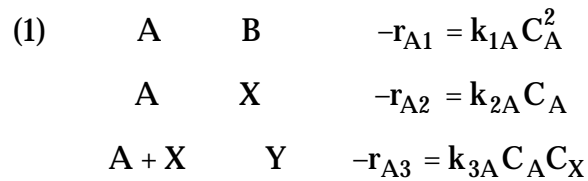
$$X_2 = 0.534$$

b) Want higher conversion

1) reduce pressure drop use larger pellets
 increase temperature larger k

2) Use CSTR followed by PFR.

(10 pts) 4) The following reactions were found to occur while trying to make a desired product B



Species X and Y are both foul pollutants

- What is the instantaneous selectivity of B with respect to the foul pollutants X and Y?
- How would you carry out this reaction to maximize the formation of B?

Additional Information

$$\begin{array}{l}
 k_{1A} = .5 e^{-10,000/T} \text{ min}^{-1}, T \text{ in degrees Kelvin} \\
 k_{2A} = 50 e^{-20,000/T} \text{ min}^{-1}, T \text{ in degrees Kelvin} \\
 k_{3A} = 100 e^{-5,000/T} \text{ min}^{-1}, T \text{ in degrees Kelvin}
 \end{array}$$

a)

$$r_B = -r_{A1}$$

$$r_x = -r_{A2} + r_{A3}$$

$$r_y = -r_{A3}$$

Selectivity of B with respect to x and y

$$\begin{aligned}
 S_{BXY} &= \frac{r_B}{r_x + r_y} = \frac{-r_{A1}}{-r_{A2}} = \frac{k_{1A}}{k_{2A}} C_A \\
 &= 0.01 \exp[10,000//T] C_A
 \end{aligned}$$

- In order to maximize the formation of B, S_{BXY} should be maximized.

High C_A use PFR

Low Temperature

(10 pts) 5) The catalytic reaction



to be carried out in a flow reaction system has the following rate law,

$$-r_A = \frac{kC_A}{(1 + K_A C_A)^2}$$

where

$$k = 1 \text{ min}^{-1}$$

$$K_A = 1 \text{ dm}^3/\text{mol}$$

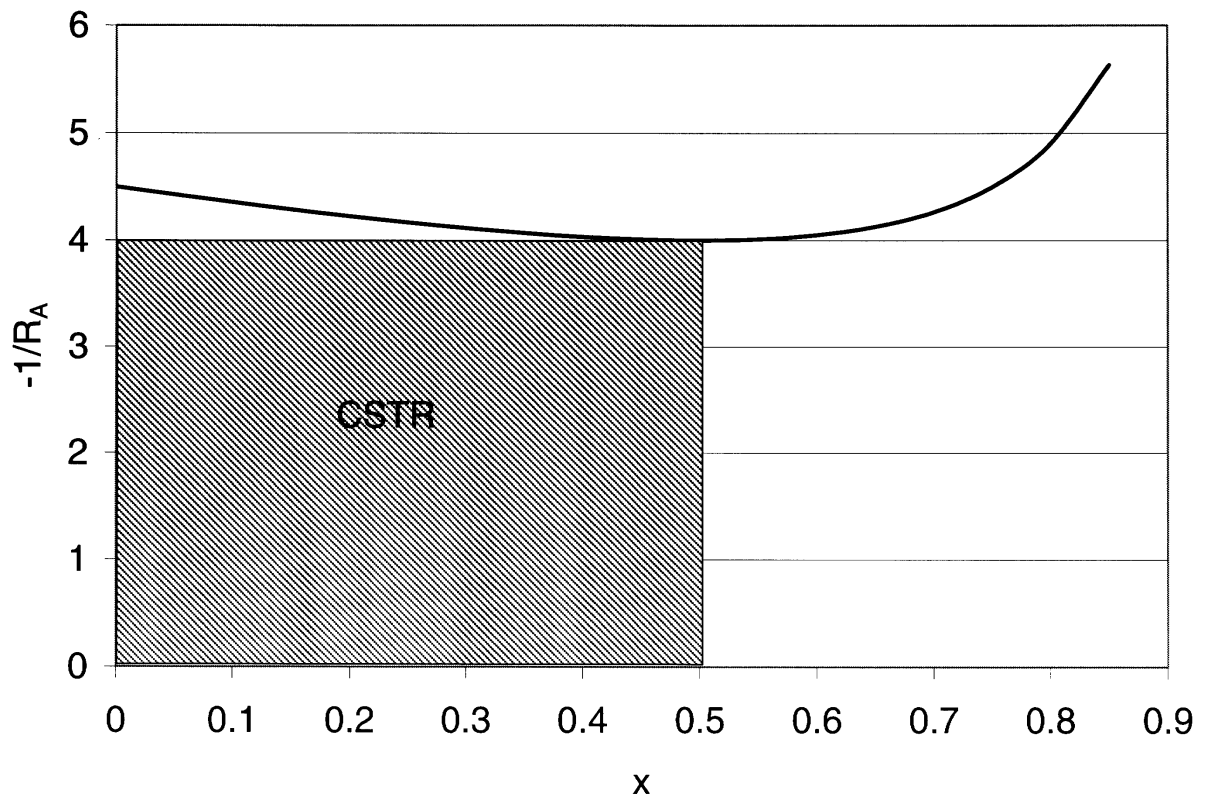
The entering concentration of A is $2 \text{ mol}/\text{dm}^3$. What type of reactor or combination of reactors would have the smallest volume to

- achieve 50% conversion?
- achieve 80% conversion?

$$C_A = C_{A0}(1 - X)$$

$$-\frac{1}{r_A} = \frac{(1 + K_A C_A)^2}{kC_A} = \frac{[1 + 2(1 - X)]^2}{2(1 - X)}$$

a) CSTR



b) CSTR followed by a PFR

