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فروشگاه کتاب های الکترونیکی ایبوکو، با هدف فراهم کردن دسترسی آسان و دائمی به کتاب های الکترونیکی در خدمت شماست. در صورت نیاز به کتابی خاص که در وبسایت ایبوکو موجود نمی باشد، می توانید درخواست خود را به آدرس پست الکترونیکی search@ebooko.ir ارسال کنید تا در صورت امکان، در سریعترین زمان به سایت اضافه شود. علاوه بر این، در صورتی که تمایل دارید تا نسخه پرینت و صحافی شده یکی از کتاب های ایبوکو را از طریق پست دریافت کنید، می توانید درخواست خود را به آدرس print@ebooko.ir ارسال کنید.

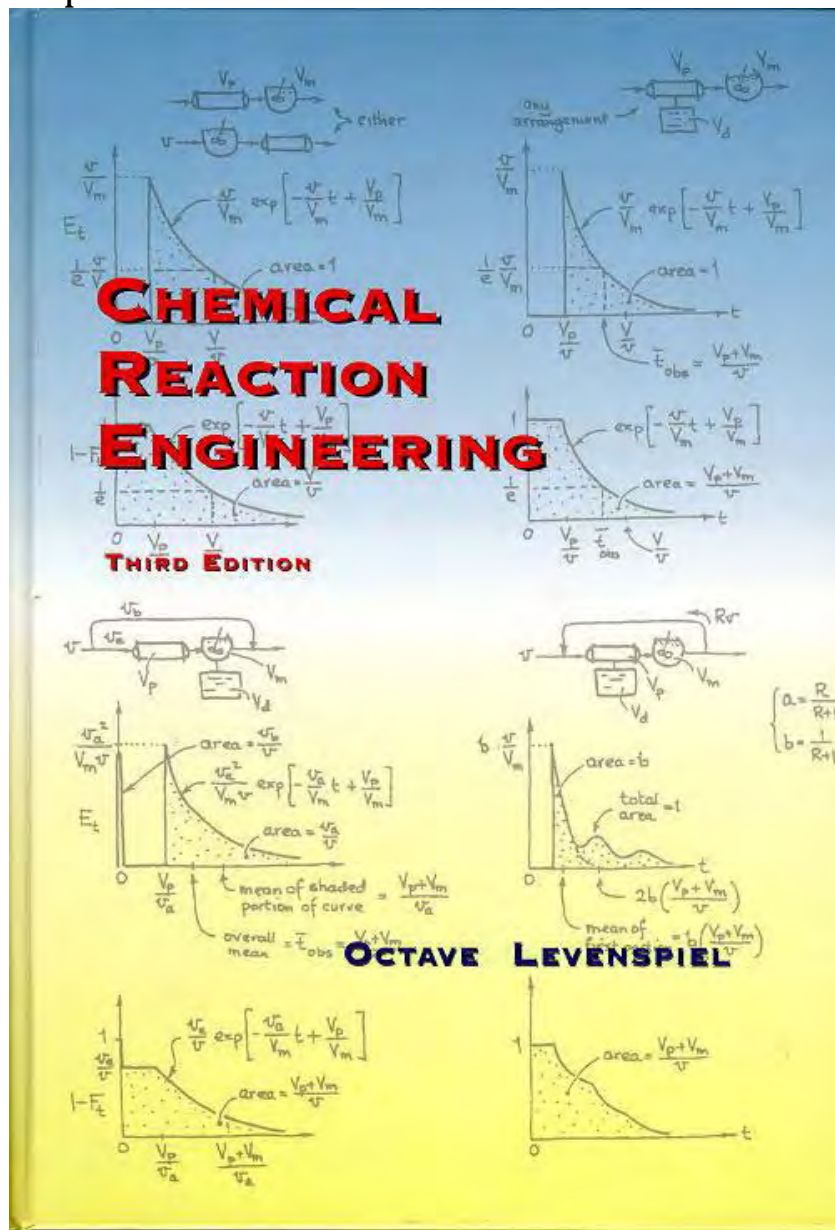
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Solutions Manuals

CHEMICAL REACTION ENGINEERING

3RD EDITION

Octave Levenspiel



SOLUTIONS MANUAL

to accompany

CHEMICAL REACTION ENGINEERING

THIRD EDITION

Includes Solutions to All 228 Odd-Numbered Problems

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1.1 Find the rate of reaction defined as

$$r_{O_2} = \frac{\text{mol } O_2 \text{ used}}{\text{sec} \cdot \text{m}^3 \text{ of tank}}$$

Evaluate terms

$$\bar{t} = \frac{V}{v} \text{ or } V = \bar{t} v$$

or (Volume of treatment tanks) = $\left(\frac{1}{3} \text{ day}\right) \left(32000 \frac{\text{m}^3}{\text{day}}\right) = 10667 \text{ m}^3$

O_2 used

$$\left(200 \frac{\text{mg}}{\text{lit}}\right) \left(\frac{1 \text{ gm}}{1000 \text{ mg}}\right) \left(\frac{\text{mol}}{32 \text{ gm}}\right) \left(\frac{1000 \text{ lit}}{\text{m}^3}\right) \left(\frac{32000 \text{ m}^3}{\text{day}}\right) = 2 \times 10^5 \frac{\text{mol } O_2}{\text{day}}$$

Thus the rate of reaction

$$\left. \begin{aligned} \frac{2.0 \times 10^5 \text{ mol } O_2 / \text{day}}{10667 \text{ m}^3} &= 18.75 \text{ mol/m}^3 \cdot \text{day} \\ &= 2.17 \times 10^4 \text{ mol/m}^3 \cdot \text{s} \end{aligned} \right\} \leftarrow$$

1.3 Find $-r'_{C_{20}H_{42}}$ and $-r'''_{C_{20}H_{42}}$ --- evaluate terms

$$V_{\text{cat}} = \frac{50000 \text{ kg}}{800 \text{ kg/m}^3} = 62.5 \text{ m}^3 \text{ of catalyst}$$

$$W_{\text{cat}} = 50000 \text{ kg}$$

$$\text{MW}_{C_{20}H_{42}} = [20(12) + 42(1)] \frac{1}{1000} = 0.282 \text{ kg/mol}$$

$$F_{\text{feed}} = (6000 \text{ m}^3/\text{day})(900 \text{ kg/m}^3) = 5400000 \text{ kg/day}$$

So $-\frac{dN_{C_{20}H_{42}}}{dt} = \left(\frac{5400000 \text{ kg/day}}{0.282 \text{ kg/day}}\right) \left(\frac{\text{day}}{24(3600) \text{ s}}\right) (0.6) = 133 \text{ mol reacted/s}$

Thus the rate of disappearance of $C_{20}H_{42}$

$$-r' = \frac{1}{W_{\text{cat}}} \frac{dN}{dt} = \frac{1}{50000} (133) = 0.0027 \text{ mol/kg cat} \cdot \text{s}$$

$$-r''' = \frac{1}{V_{\text{cat}}} \frac{dN}{dt} = \frac{1}{62.5} (133) = 2.13 \text{ mol/m}^3 \text{ cat} \cdot \text{s}$$

2.1 Without experimental data we cannot answer this question. The order of reaction need not match the stoichiometry, and often doesn't

2.3 Why should the way you write the stoichiometry affect the rate of reaction? The rate expression remains unchanged.

2.5
$$r_R = -2r_A = -\frac{2}{3}r_B, \text{ or } -r_A = -\frac{1}{3}r_B = \frac{1}{2}r_R$$

2.7 a) We are given $-\frac{dp_A}{dt} = k_p p_A^2$
 $\begin{matrix} \nearrow & \nearrow & \nearrow \\ \text{atm/hr} & 3.66 & (\text{atm})^2 \end{matrix}$
 Balancing dimensions we find $k_p = 3.66 (\text{atm})^{-1} (\text{hr})^{-1}$ ← a)

b) For an ideal gas $p_A V = n_A RT$ or $p_A = C_A RT$

thus $-\frac{dp_A}{dt} = 3.66 p_A^2$... becomes ... $-\frac{d(C_A RT)}{dt} = 3.66 (C_A RT)^2$

or $-\frac{dC_A}{dt} = \underbrace{[3.66 (\text{atm})^{-1} \text{hr}^{-1}] RT}_{\text{new rate constant} = k'} C_A^2$

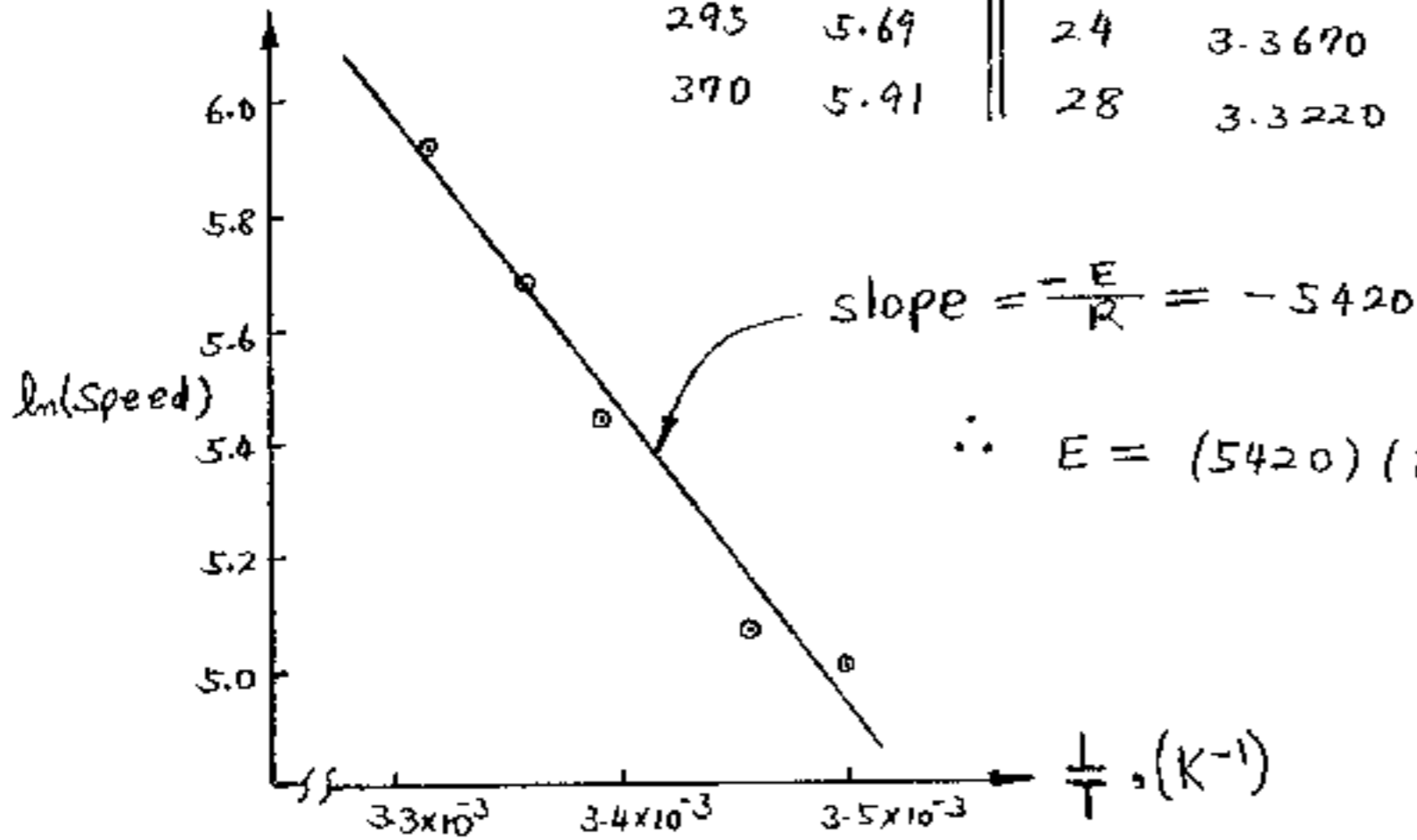
where $k' = 3.66 \frac{1}{\text{atm} \cdot \text{hr}} \cdot \frac{(1 \text{atm})(22.4 \text{L})}{(1 \text{mol})(273 \text{K})} \cdot (400 \text{K}) = 120 (\text{hr})^{-1} (\text{mol/L})^{-1}$ ← b)

2.9 From Eq. 35 we write

$$\begin{aligned} \frac{k_{650}}{k_{500}} &= e^{-\frac{E}{R} \left(\frac{1}{T_{650}} - \frac{1}{T_{500}} \right)} \\ &= e^{-\frac{300,000}{8.314} \left(\frac{1}{923} - \frac{1}{773} \right)} \\ &= 1971 \end{aligned}$$

2.11

| Speed | ln S | T | $(\frac{1}{T}) \times 10^3$ |
|-------|------|----|-----------------------------|
| 150 | 5.01 | 13 | 3.4965 |
| 160 | 5.07 | 16 | 3.4602 |
| 230 | 5.44 | 22 | 3.3898 |
| 295 | 5.69 | 24 | 3.3670 |
| 370 | 5.91 | 28 | 3.3220 |

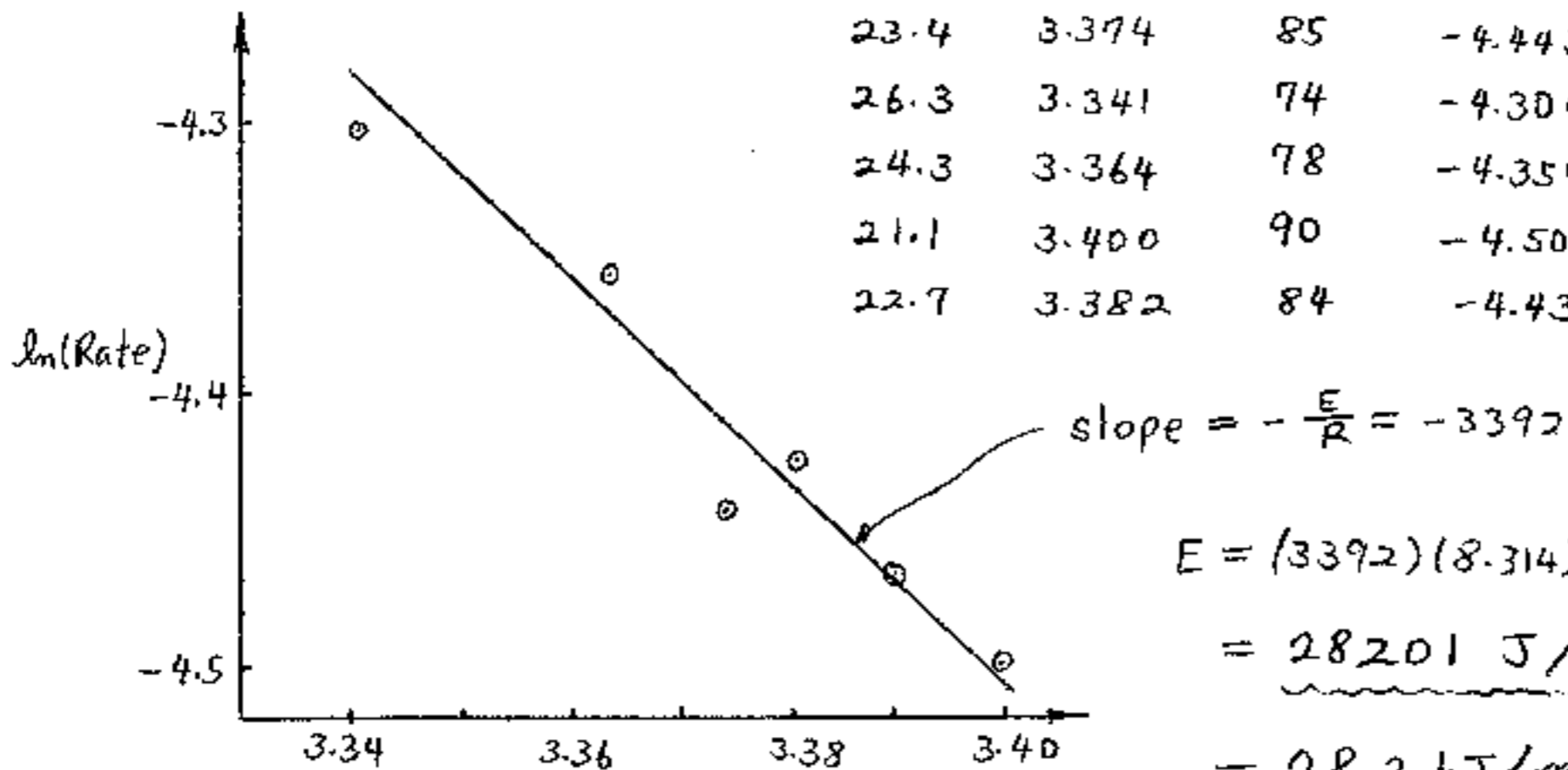


$$\therefore E = (5420)(8.314) = \underline{45062 \text{ J}}$$

$$\approx \underline{45 \text{ kJ}}$$

2.13

| T | $\frac{1}{T} \times 10^3$ | Days | $\ln(\text{Rate}) = \ln(\frac{1}{\text{days}})$ |
|------|---------------------------|------|---|
| 22.0 | 3.390 | 87 | -4.466 |
| 23.4 | 3.374 | 85 | -4.443 |
| 26.3 | 3.341 | 74 | -4.304 |
| 24.3 | 3.364 | 78 | -4.357 |
| 21.1 | 3.400 | 90 | -4.500 |
| 22.7 | 3.382 | 84 | -4.431 |



$$E = (3392)(8.314)$$

$$= \underline{28201 \text{ J/mol}}$$

$$= \underline{28.2 \text{ kJ/mol}}$$

2.15 $-r_A = kC_A^n$... $\frac{-r_2}{-r_1} = \frac{k(2C_A)^n}{kC_A^n} = 2^n$ $\therefore n = 1.585$ ←

↑
3

2.17 Guess that $-r_A = k C_A^a C_B^b$
 There are 3 unknowns: k , a and b
 But we have 3 equations

| C_A | C_B | $-r_A$ |
|-------|-------|--------|
| 2 | 125 | 50 |
| 2 | 64 | 32 |
| 3 | 64 | 48 |

$$50 = k(2)^a(125)^b \quad \dots (i)$$

$$32 = k(2)^a(64)^b \quad \dots (ii)$$

$$48 = k(3)^a(64)^b \quad \dots (iii)$$

Divide (iii) by (ii) gives $a=1$

Divide (i) by (ii) gives $b=2/3$

Replace a and b in (i) gives $k=1$

$$\therefore -r_A = C_A C_B^{2/3} \leftarrow$$

2.19 a) Consider the mechanism $2A \xrightleftharpoons[k_2]{k_1} A + A^*$ and let us find its rate expression.
 $A^* \xrightarrow{k_3} R + S$

For reactant A: $-r_A = k_1[A]^2 - k_2[A^*][A] \quad \dots (i)$

For intermediate: $-r_{A^*} = k_1[A]^2 - k_2[A^*][A] - k_3[A^*] = 0$

steady state approximation

from which $[A^*] = \frac{k_1[A]^2}{k_2[A] + k_3} \quad \dots (ii)$

Replacing (ii) in (i) so as to eliminate the unmeasurable A^* gives

$$-r_A = \frac{k_1 k_3 [A]^2}{k_2 [A] + k_3} \quad \dots (iii)$$

And when $k_2[A] \gg k_3$

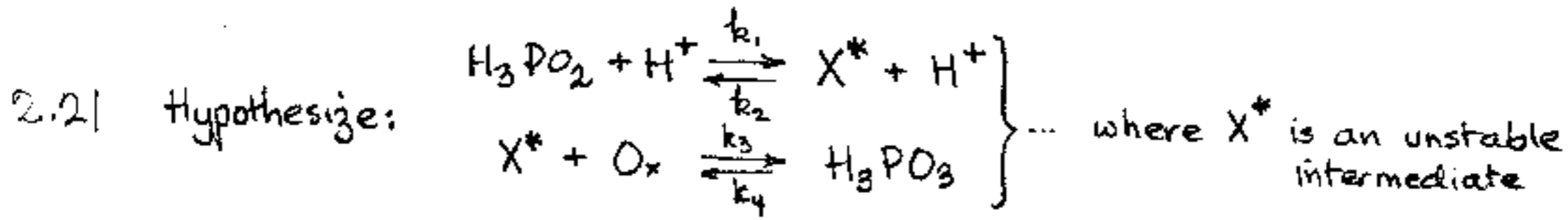
$$-r_A = \frac{k_1 k_3}{k_2} [A] \quad \dots \text{ or first order rx } \leftarrow a)$$

b) Now at low enough C_A we may reach conditions where $k_2[A] \ll k_3$. In such a situation Eq. (iii) will reduce to

$$-r_A = k_1 [A]^2 \quad \dots \text{ or } 2^{\text{nd}} \text{ order kinetics}$$

Hence lower C_A more and more. This mechanism predicts that a point will be reached where the reaction order will start rising from one, and will approach and eventually become two. \leftarrow

b)



Then as in the example, pg 19, we write

$$r_{\text{H}_3\text{PO}_3} = k_3[\text{X}^*][\text{O}_x] - k_4[\text{H}_3\text{PO}_3] \dots \dots \dots \text{(i)} \quad \text{steady state assumption}$$

$$r_{\text{X}^*} = k_1[\text{H}_3\text{PO}_2][\text{H}^+] - k_2[\text{X}^*][\text{H}^+] - k_3[\text{X}^*][\text{O}_x] + k_4[\text{H}_3\text{PO}_3] \stackrel{\leftarrow}{=} 0$$

Thus
$$[\text{X}^*] = \frac{k_1[\text{H}_3\text{PO}_2][\text{H}^+] + k_4[\text{H}_3\text{PO}_3]}{k_2[\text{H}^+] + k_3[\text{O}_x]} \dots \dots \dots \text{(ii)}$$

Assuming $k_4 = 0$ (and we are certainly free to do this since this is our model, our brainchild), replacing (ii) in (i) then gives

$$r_{\text{H}_3\text{PO}_3} = \frac{k_1 k_3 [\text{H}_3\text{PO}_2][\text{H}^+][\text{O}_x]}{k_2[\text{H}^+] + k_3[\text{O}_x]} \dots \dots \dots \text{(iii)}$$

Now when $k_3[\text{O}_x] \gg k_2[\text{H}^+]$... i.e. high oxidizer concentration, Eq.(iii) gives

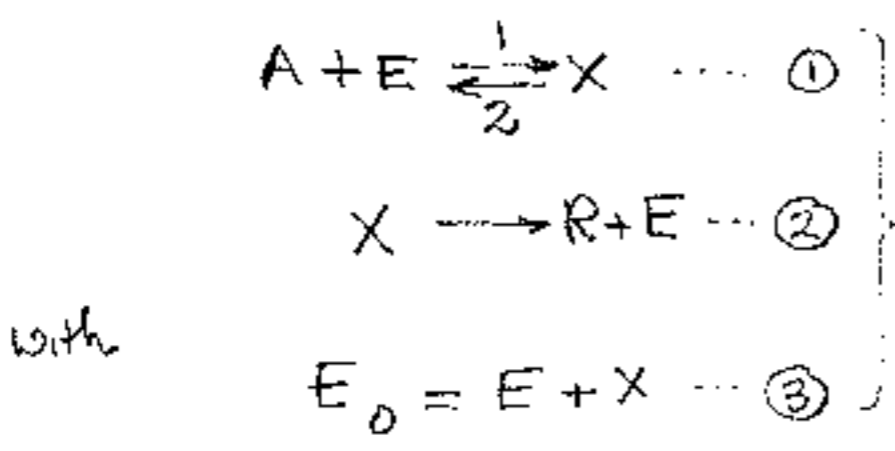
$$r_{\text{H}_3\text{PO}_3} = k_1[\text{H}_3\text{PO}_2][\text{H}^+] \dots \dots \dots \text{(iv)}$$

On the other hand when $k_2[\text{H}^+] \gg k_3[\text{O}_x]$... i.e. low oxidizer concentration Eq.(iii) gives

$$r_{\text{H}_3\text{PO}_3} = \frac{k_1 k_3}{k_2} [\text{H}_3\text{PO}_2][\text{O}_x] \dots \dots \dots \text{(v)}$$

Eqs (iv) & (v) fit the evidence hence the hypothesized model is accepted.

2.23



M-M assume that the reverse reactions of ① approach equilibrium quickly, or

$$K = \frac{[\text{X}]}{[\text{A}][\text{E}]} = \frac{k_1}{k_2} \dots \text{④}$$

R-H assume that quickly $\frac{d[\text{X}]}{dt} = 0 \dots \text{⑤}$

2.23
(continued)

For M-M

From (2)

$$r_R = k_3 X \quad \dots (6)$$

From (5)

$$X = \frac{k_1}{k_2} AE$$

Eliminate E with (2)

$$X = \frac{k_1}{k_2} A(E_0 - X)$$

or

$$X = \frac{\frac{k_1}{k_2} AE_0}{1 + \frac{k_1}{k_2} A} \quad \dots (7)$$

Eq (7) in (6) gives

$$r_R = \frac{k_3 AE_0}{\frac{k_2}{k_1} + A}$$

These equations give essentially the same result

For B-H

From (2)

$$r_R = k_3 X \quad \dots (8)$$

From (5)

$$\frac{dX}{dt} = 0 = k_1 AE - (k_2 + k_3) X$$

Eliminate E with (2)

$$k_1 A(E_0 - X) - (k_2 + k_3) X = 0$$

or

$$X = \frac{k_1 AE_0}{k_1 A + k_2 + k_3} \quad \dots (9)$$

Eq (9) in (8) gives

$$r_R = \frac{k_3 AE_0}{\frac{k_2 + k_3}{k_1} + A}$$

This is called the Michaelis constant, C_M

Note: By careful analysis of careful experiments Chance, in J. Biol. Chem. 151 553 (1943) favors the Briggs-Haldane mechanism, later evidence reinforces this choice. Thus we end up today with the so-called Michaelis-Menten equation which is in fact the B-H modification of the M-M equation

3.1 Since the reaction order, hence concentration dependency, is not known we are not given enough information to find the rate of reaction at the higher concentration ←

3.3 For the 2nd order disappearance of a single reactant Eq 16, pg 49 gives

$$kt = \frac{1}{C_{A0}} \left(\frac{X_A}{1-X_A} \right) \quad \dots \text{ or } \dots \quad t = \frac{1}{kC_{A0}} \left(\frac{X_A}{1-X_A} \right)$$

Now for 50% conversion: $t_{50} = \frac{1}{kC_{A0}} \left(\frac{1/2}{1-1/2} \right) = \frac{1}{kC_{A0}} = 5 \text{ min}$

For 75% conversion: $t_{75} = \frac{1}{kC_{A0}} \left(\frac{3/4}{1-3/4} \right) = \frac{3}{kC_{A0}} = 15 \text{ min}$

∴ the extra time needed is 10 minutes ←

3.5 Since the fractional disappearance is independent of initial concentration we have a first order rate, or

$$-\frac{dC}{dt} = kC \quad \dots \text{ or } \dots \quad \ln \frac{C_0}{C} = kt \quad \dots \text{ where } C = \text{monomer concentration}$$

We also can find the rate constant. Thus replacing values

$$\ln \frac{C_0}{0.8C_0} = k(34 \text{ min}) \quad \dots \text{ or } \quad k = \frac{-\ln 0.8}{34 \text{ min}} = 0.00657 \text{ min}^{-1}$$

Hence the rate of disappearance of monomer is given by

$$-r = -\frac{dC}{dt} = (0.00657 \text{ min}^{-1})C \quad \leftarrow$$

3.7 Mago's betting habits, and his losses, can be described by

$$-\frac{d\$}{dt} = k\$ \quad \dots \text{ or } \quad \ln \frac{\$}{\$_0} = -kt \quad \dots \text{ where } \$ = \text{money at hand}$$

Now at $t=0 \dots \$_0 = 180$
 $t=2 \text{ hrs } \dots \$ = 135$ } from which we can find his "paupacity" constant

$$k = \frac{1}{t} \ln \frac{\$_0}{\$} = \frac{1}{2} \ln \frac{180}{135} = 0.144 \text{ hr}^{-1}$$

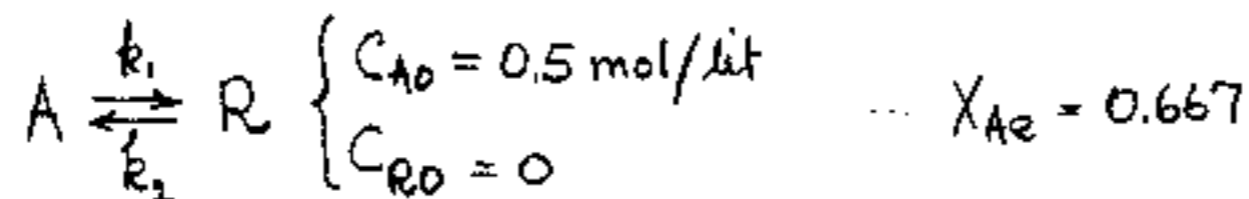
3.7 After his raise we have $t=0 \dots \$_0 = ?$
 (Continued) $t=3 \text{ hrs } \$ = 135$ } ... from this find $\$_0$

For Unchanged betting habits

$$\ln \frac{\$_0}{135} = (0.144)(3) \dots \text{ or } \$_0 = 208$$

Hence his raise is $208 - 180 \dots \text{ or } \$ 28$

3.9 For a first order reversible reaction



the integrated conversion equation in a batch reactor (constant volume because it is a liquid) is given by

$$-\ln \left(1 - \frac{X_A}{X_{Ae}} \right) = (k_1 + k_2)t$$

Replacing values we then find

$$-\ln \left(1 - \frac{1/3}{2/3} \right) = (k_1 + k_2) 8 \text{ min} \dots \therefore k_1 + k_2 = \frac{\ln 2}{8} = 0.086625 \text{ min}^{-1} \dots (i)$$

Now from thermodynamics we know that

$$K = \frac{C_{Re}}{C_{Ae}} = \frac{k_1}{k_2} = \frac{0.5 \times 2/3}{0.5 \times 1/3} = 2$$

equilibrium constant

Thus $k_1 = 2k_2$ (ii)

Solving (i) & (ii) gives $\begin{cases} k_2 = \frac{0.086625}{3} = 0.028875 \\ k_1 = 0.057750 \end{cases}$

Thus the rate expression for the disappearance of A.

$$-r_A = 0.05775 C_A - 0.028875 C_R$$

$\leftarrow \text{mol/lit} \cdot \text{min} \quad \leftarrow \text{min}^{-1} \quad \leftarrow \text{mol/lit} \quad \leftarrow \text{min}^{-1} \quad \leftarrow \text{mol/lit}$

3.11 From the table of data

$$\text{at } C_A = 500 \quad t = 100 \text{ min}$$

Thus

$$\text{at } t = 5 \text{ hrs} + 100 \text{ min} = 400 \text{ min}$$

$$C_A = 200 \frac{\text{mol}}{\text{m}^3} \quad \dots \text{ or } X_A = 0.6 \quad \leftarrow$$

3.13

Let A = galloping dominoes. Then by this game alone $-\left(\frac{d\$}{dt}\right)_A = k_A \$ \quad \dots \dots \dots (i)$

Let B = chuk-a-luck. Then by this game alone $-\left(\frac{d\$}{dt}\right)_B = k_B \$ \quad \dots \dots \dots (ii)$

Playing A & B simultaneously $-\frac{d\$}{dt} = -\left(\frac{d\$}{dt}\right)_A - \left(\frac{d\$}{dt}\right)_B = (k_A + k_B) \$ \quad \dots \dots \dots (iii)$

From the problem statement we can find k_A from (i), k_B from (ii). We then use these in (iii) to see how long he can play both games simultaneously. This is our strategy

Integrating (i) we get $\ln \frac{\$}{\$_0} = -k_A t \quad \dots \text{ or } \dots \quad k_A = \frac{1}{t} \ln \frac{\$}{\$_0}$
and with the data given $k_A = \frac{1}{4} \ln 2 \quad \dots \dots \dots (iv)$

Similarly with (ii) $k_B = \frac{1}{2} \ln 2 \quad \dots \dots \dots (v)$

Integrating (iii) gives $\ln \frac{\$}{\$_0} = -(k_A + k_B) t \quad \dots \text{ or } \dots \quad t = \frac{1}{k_A + k_B} \ln \frac{\$}{\$_0}$

and with (iv) & (v)

$$t = \frac{1}{\frac{3}{4} \ln 2} \ln \frac{1000}{10} = 8.87 \text{ hrs} \quad \leftarrow$$

Note: This is simply a case of two "1st order reactions" in parallel, see pg.49.

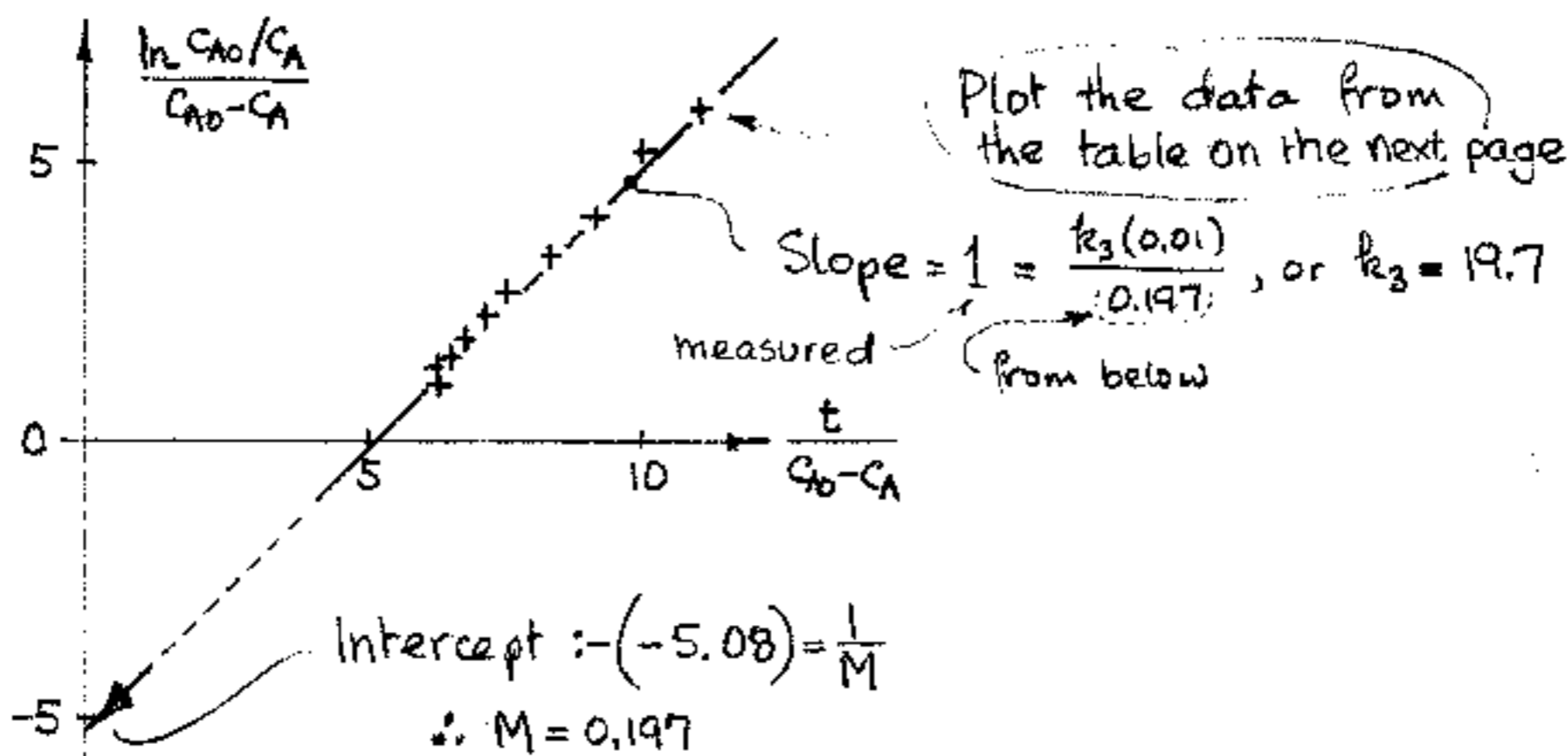
3.15 We can test the fit of the Michaelis-Menten type equation in many ways, integral or differential. We will sketch these different solutions in turn. But first let us transform the M-M equation into the following useful form

$$-r_A = \frac{k_3 C_{E0} C_A}{C_A + M} = \frac{k_4 C_A}{1 + k_5 C_A} \quad \dots \text{where } \begin{cases} k_4 = \frac{k_3 C_{E0}}{M} \\ k_5 = \frac{1}{M} \end{cases} \dots (i)$$

↙ use this form

Integral method Integrating (i) gives

$$\frac{\ln C_{A0}/C_A}{C_{A0} - C_A} = -k_5 + \frac{k_4 t}{C_{A0} - C_A} \quad \begin{cases} \text{slope: } k_4 = \frac{k_3 C_{E0}}{M} \\ \text{intercept: } -k_5 = \frac{1}{M} \end{cases} \dots (i)$$



From this figure the constants in Eq. (i) are

$$\left. \begin{array}{l} k_3 = 19.7 \text{ hr}^{-1} \\ M = 0.197 \frac{\text{mmol}}{\text{lit}} \end{array} \right\} \text{ thus } r_A = \frac{19.7 C_A C_{E0}}{0.197 + C_A}$$

3.15
(continued)

| t | C_A | $\frac{\ln C_{A0}/C_A}{C_{A0}-C_A}$ | $\frac{t}{C_{A0}-C_A}$ |
|----|--------|-------------------------------------|------------------------|
| 1 | 0.84 | 1.09 | 6.25 |
| 2 | 0.68 | 1.2 | 6.25 |
| 3 | 0.53 | 1.35 | 6.39 |
| 4 | 0.38 | 1.56 | 6.45 |
| 5 | 0.27 | 1.80 | 6.85 |
| 6 | 0.16 | 2.18 | 7.15 |
| 7 | 0.09 | 2.65 | 7.7 |
| 8 | 0.04 | 3.36 | 8.34 |
| 9 | 0.018 | 4.08 | 9.17 |
| 10 | 0.006 | 5.15 | 10.1 |
| 11 | 0.0025 | 6.01 | 11.0 |

↙ given
↘ for integral method, above

3.17 For first order processes

$$k = \frac{0.6931}{t_{1/2}} = \frac{0.6931}{76 \text{ min}} = 9.12 \times 10^{-3} \text{ min}^{-1}$$

After one day

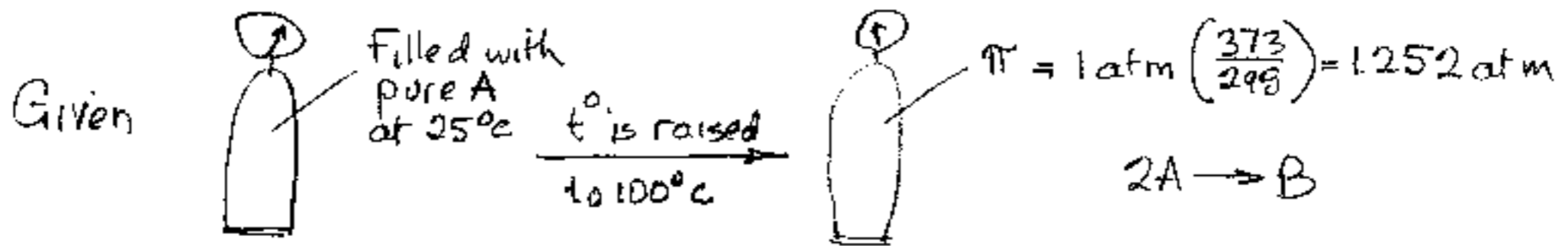
$$\frac{C_A}{C_{A0}} = e^{-kt} = e^{-(9.12 \times 10^{-3})(24 \times 60)} = 1.98 \times 10^{-6} \leftarrow$$

Thus the radioactivity drops to 2×10^{-6} of the original value.3.19 The time for complete conversion of an n^{th} order reaction from Eq. 29, is

$$t = \frac{C_{A0}^{1-n}}{(1-n)k} = \frac{(1)^{1-1/2}}{(1-1/2)3} = \frac{2}{3} \text{ hr}$$

Therefore after 1 hr $X_A = 1$, or $C_A = 0 \leftarrow$

E.21



Tabulate

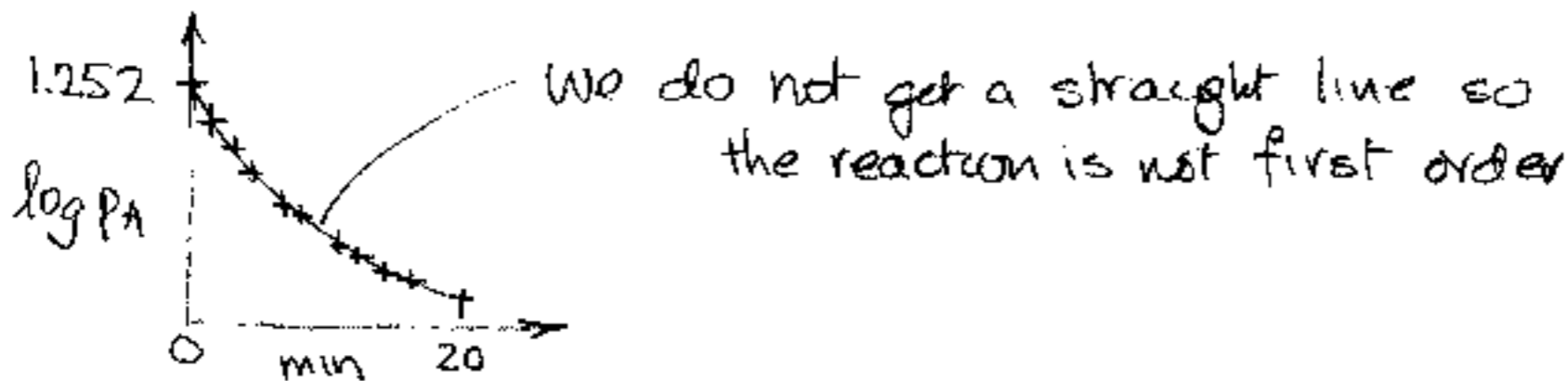
| ① time (min) | ② π (atm) | ③ p_A (atm) | ④ $1/p_A$ (atm ⁻¹) |
|-----------------|------------------|------------------|-----------------------------------|
| 0 | (1.252) | (1.252) | (0.800) |
| 1 | 1.14 | 1.028 | 0.975 |
| 2 | 1.04 | 0.828 | 1.208 |
| 3 | 0.982 | 0.712 | 1.404 |
| 4 | 0.940 | 0.628 | 1.592 |
| 5 | 0.905 | 0.558 | 1.792 |
| 6 | 0.870 | 0.488 | 2.049 |
| 7 | 0.850 | 0.448 | 2.232 |
| 8 | 0.832 | 0.412 | 2.427 |
| 9 | 0.815 | 0.378 | 2.646 |
| 10 | 0.800 | 0.348 | 2.873 |
| 15 | 0.754 | 0.256 | 3.90 |
| 20 | 0.728 | 0.204 | 4.90 |

← given → ← calc'd. →

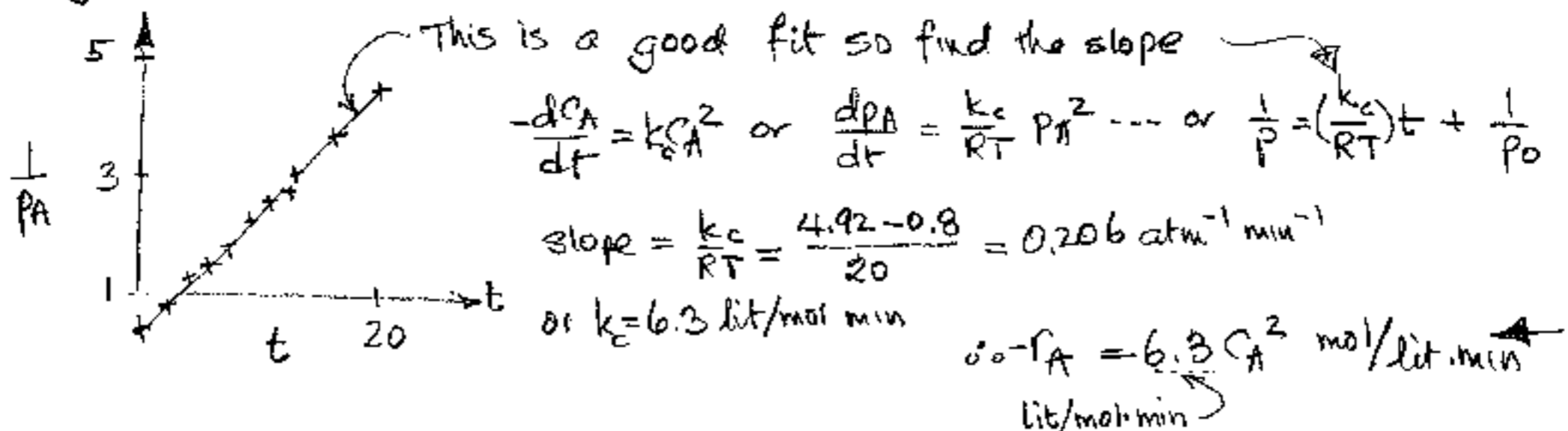
Column ③ is obtained from Eq 5, or

$$p_A = p_{A0} - \frac{a}{\Delta n} (\pi - \pi_0) = 1.252 - \frac{2}{(-1)} (\pi - 1.252) = 2p_A - 1.252$$

Try first order kinetics. For this plot as shown



Try second order kinetics. For this plot as shown



3.23 Let us try n^{th} order kinetics. Then from Eq 33a, taking ratios, we get

$$\frac{(n-1)kt_2}{(n-1)kt_1} = \frac{C_{A0} \left[\left(\frac{C_{A2}}{C_{A0}} \right)^{1-n} - 1 \right]}{C_{A0} \left[\left(\frac{C_{A1}}{C_{A0}} \right)^{1-n} - 1 \right]} \quad \dots (i)$$

Replacing values give,

$$2 = \frac{-1}{\left(\frac{1}{4} \right)^{1-n} - 1} \quad \dots \text{or } n = \frac{1}{2} \leftarrow \dots$$

Replacing in Eq 33a gives

$$\left(\frac{1}{2} - 1 \right) kt_2 = 1^{1-1/2} \left(\frac{\text{mol}}{\text{lit}} \right)^{1-1/2} [0-1]$$

or

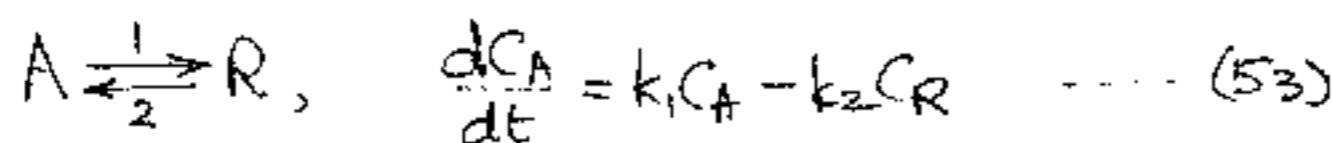
$$k = 1 \frac{(\text{mol})^{1/2}}{(\text{lit})^{1/2} \cdot \text{hr}}$$

$$\therefore -r_A = \left(1 \frac{\text{mol}^{1/2}}{\text{lit}^{1/2} \text{hr}} \right) C_A^{1/2}, \quad \frac{\text{mol}}{\text{lit} \cdot \text{hr}} \leftarrow$$

3.25 Here we are given p_A vs t data, so we have two possible approaches

- We could first transform our pressure readings into concentrations and then solve, or
- We could stay with pressure readings and then transform our final equation into concentration units

Let us stick with pressure units, and let us start by guessing first order reversible kinetics. Why reversible? Because at $t = \infty$ there is still some unreacted p_A . So the rate equation we will test is



On integration we get

$$\ln \left(1 - \frac{X_A}{X_{Ae}} \right) = \frac{k_1 t}{X_{Ae}} \quad \dots (54)$$

3.25
(continued)

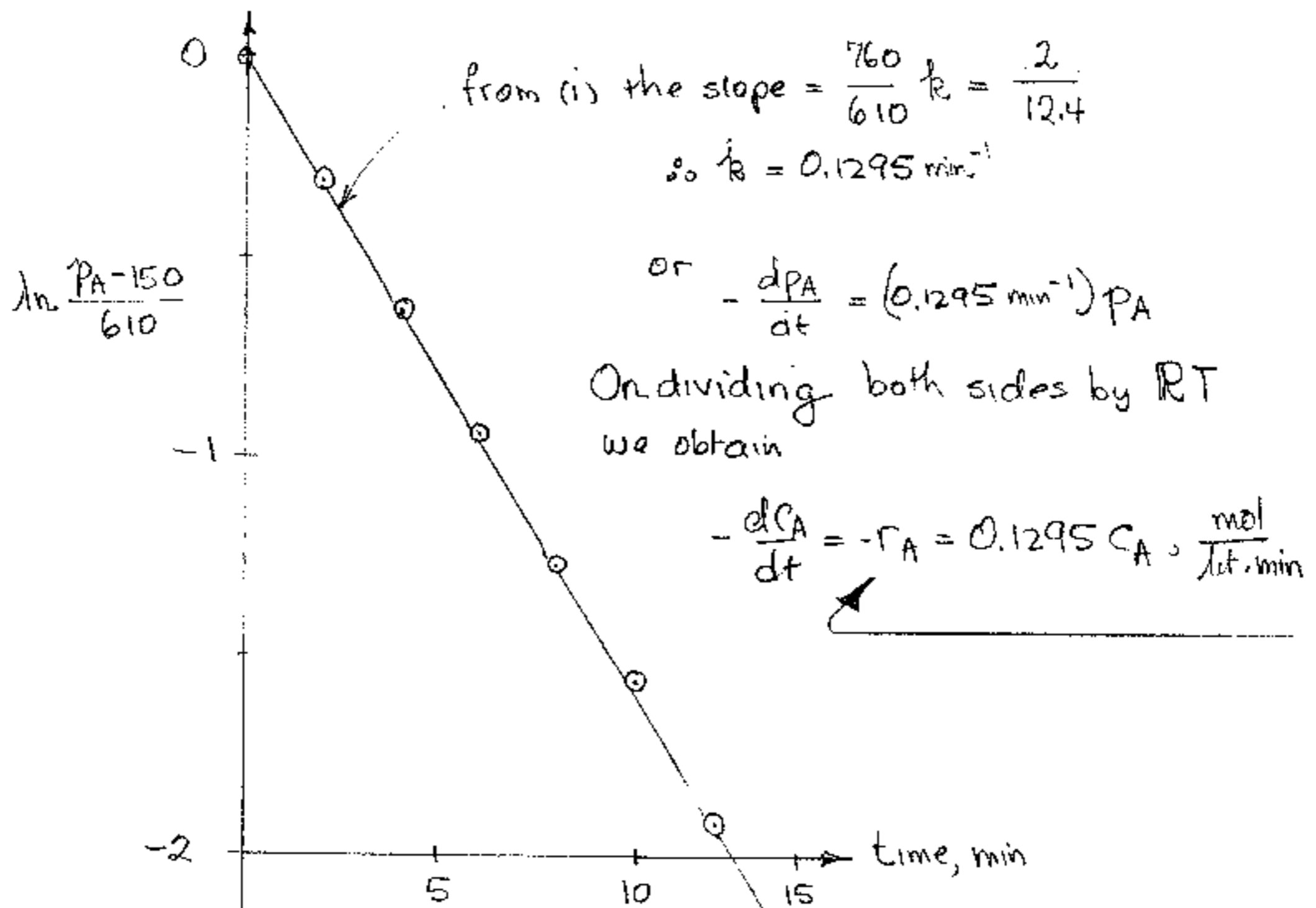
In pressure units this integrated expression becomes

$$\ln \frac{P_A - P_{Ae}}{P_{A0} - P_{Ae}} = \frac{k_c t}{(P_{A0} - P_{Ae})/P_{A0}} \quad \dots (i)$$

Let us see whether this equation fits the facts. So tabulate & plot

| t, min | P_A | $\frac{P_A - P_{Ae}}{P_{A0} - P_{Ae}}$ | $\ln \frac{P_A - P_{Ae}}{P_{A0} - P_{Ae}}$ |
|-----------------|-------|--|--|
| 0 | 760 | 1 | 0 |
| 2 | 600 | 450/610 | -0.3042 |
| 4 | 475 | 325/610 | -0.6296 |
| 6 | 390 | 240/610 | -0.9328 |
| 8 | 320 | 170/610 | -1.2777 |
| 10 | 275 | 125/610 | -1.5851 |
| 12 | 240 | 90/610 | -1.9196 |
| 14 | 215 | 65/610 | -2.2391 |
| ∞ | 150 | 0 | $-\infty$ |

Note: For 1st order rxn
 k_c and k_p have the
same value, time^{-1}



What this shows is that if we have isothermal 1st order kinetics we can use P_A or C_A without changing the rate constants

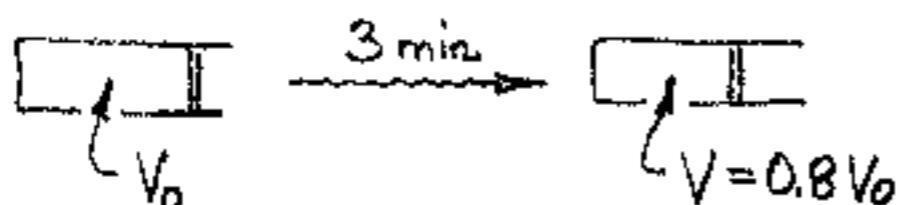
3.27 Since we are told that the reaction is elementary the stoichiometric equation shows that the reaction is 2nd order. So for a small relative concentration change we can write

$$-\frac{\Delta C_A}{\Delta t} = k \bar{C}_A^2$$

$$\text{or } k = -\frac{\Delta C_A}{\Delta t} \frac{1}{\bar{C}_A^2} = \frac{-0.2 \text{ mol/lit}}{7\frac{2}{3} \text{ hr}} \cdot \frac{1}{(19.9 \text{ mol/lit})^2} = 6.6 \times 10^{-5} \text{ lit}^2/\text{mol} \cdot \text{hr}$$

$$\therefore -r_{\text{NH}_2\text{-CO-NH}_2} = (6.6 \times 10^{-5}) C_{\text{NH}_2\text{-CO-NH}_2}^2 \text{ mol/lit} \cdot \text{hr} \leftarrow$$

3.29



| | | | | | | | |
|--------------------|---|-----|-----|-----|-----|-----|-----|
| | $2A \rightarrow B$ | | | | | | |
| Amount of A or B : | <table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="padding: 0 10px;">0.8</td> <td style="padding: 0 10px;">0.4</td> </tr> <tr> <td style="padding: 0 10px;">0.2</td> <td style="padding: 0 10px;">0.2</td> </tr> <tr> <td style="padding: 0 10px;">1.0</td> <td style="padding: 0 10px;">0.6</td> </tr> </table> | 0.8 | 0.4 | 0.2 | 0.2 | 1.0 | 0.6 |
| 0.8 | 0.4 | | | | | | |
| 0.2 | 0.2 | | | | | | |
| 1.0 | 0.6 | | | | | | |
| Amount of react : | | | | | | | |
| Total : | <table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="padding: 0 10px;">1.0</td> <td style="padding: 0 10px;">0.6</td> </tr> </table> | 1.0 | 0.6 | | | | |
| 1.0 | 0.6 | | | | | | |
| | $\therefore \epsilon_A = -0.4$ | | | | | | |

For a first order reaction in a variable volume set-up, we have from Eq. 79

$$-\ln\left(\frac{\epsilon_A + 1 - V/V_0}{\epsilon_A}\right) = kt \quad \dots \text{or} \dots \quad -\ln\left(\frac{-0.4 + 1 - 0.8}{-0.4}\right) = k \cdot 3 \text{ min}$$

$$\therefore k = \frac{\ln 2}{3} = 0.231 \text{ min}^{-1} \leftarrow$$

3.31 The units of the rate constant tells that this is a 2nd order reaction

$$-r_A = k C_A^2 = k_0 e^{-E/RT} C_A^2$$

Thus $k = k_0 e^{-E/RT}$

or $\ln k = \ln k_0 - \frac{E}{R} \left(\frac{1}{T}\right)$

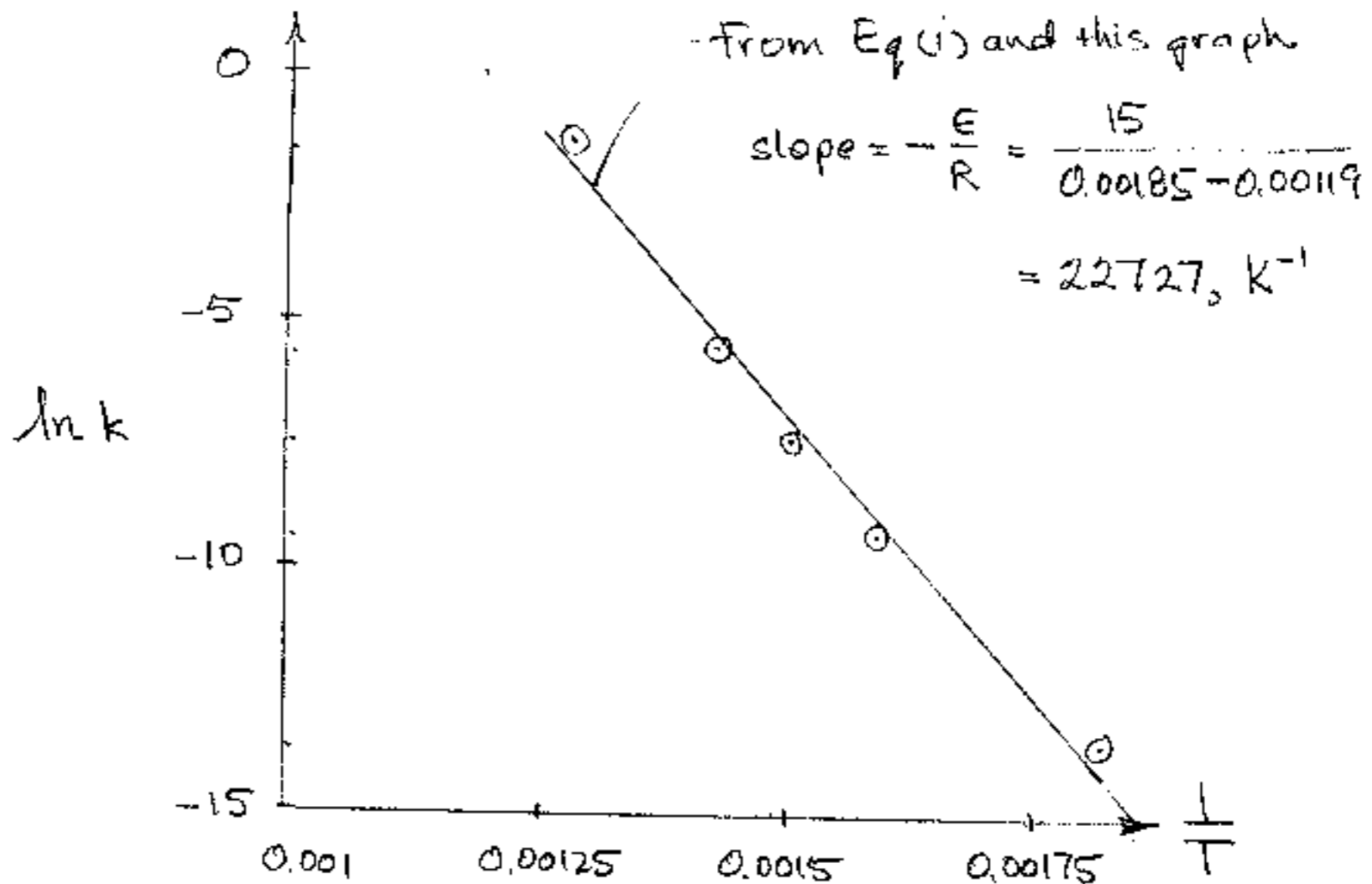
So to find the value of the rate constant, or k_0 and E/R , we must plot $\ln k$ vs $1/T$. The slope gives E/R and the intercept gives k_0 . Let us follow this procedure

3.31
(continued)

First let us tabulate

| $T, ^\circ\text{C}$ | T, K | $1/T, \text{K}^{-1}$ | k | $\ln k$ |
|---------------------|---------------|----------------------|------------------------|----------|
| 508 | 781 | 0.00128 | 0.1059 | -1.6974 |
| 427 | 700 | 0.00143 | 0.0031 | -5.7764 |
| 393 | 666 | 0.001502 | 0.000588 | -7.4388 |
| 356 | 629 | 0.001590 | 80.9×10^{-6} | -9.4223 |
| 273 | 546 | 0.001832 | 0.942×10^{-6} | -13.8753 |

Next plot as shown below



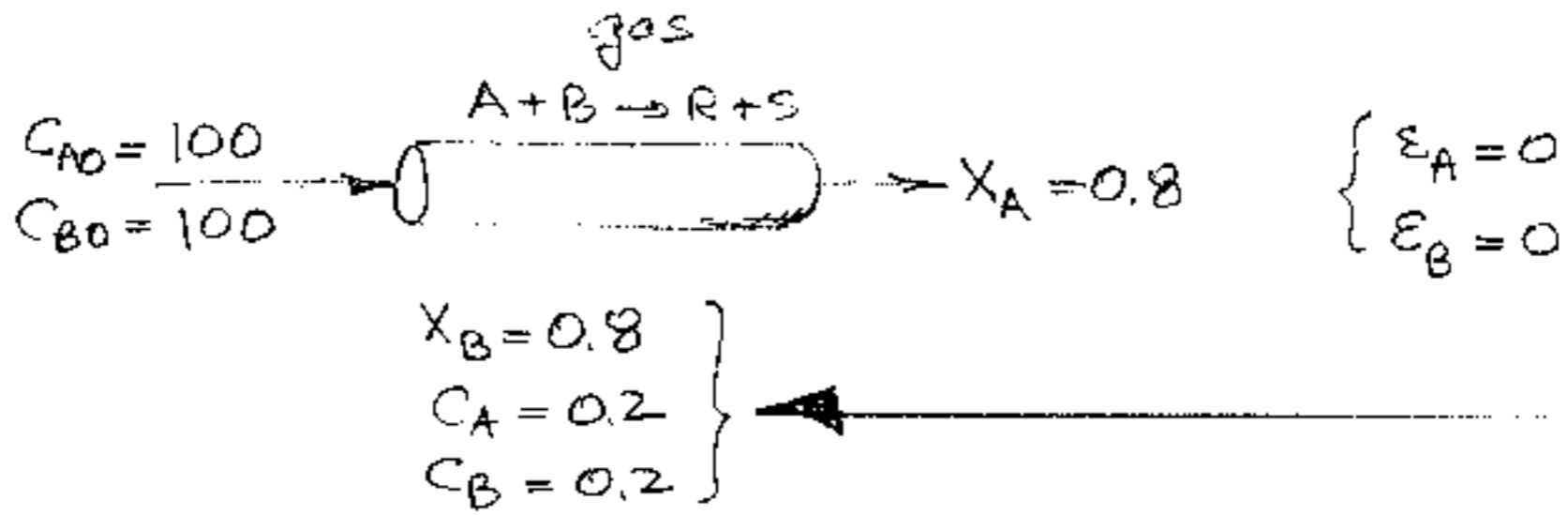
To find the value of k_0 take the second data point.
From Eq (i)

$$\begin{aligned} \ln k_0 &= \ln k - \frac{E}{R} \left(\frac{1}{T} \right) \\ &= 5.7764 - 22727 \left(\frac{1}{700} \right) = 38.2439 \\ \text{or } k_0 &= e^{38.2439} = 4.06 \times 10^{16} \end{aligned}$$

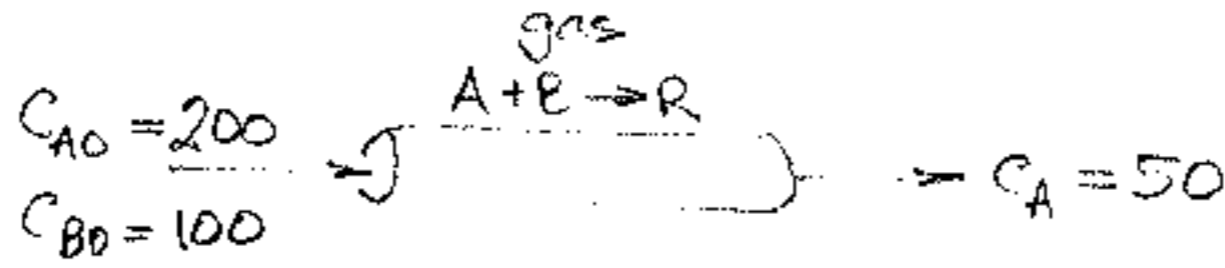
So for the temperature range covered in the reported data

$$-r_{\text{HI}} = 4.06 \times 10^{16} e^{-22727/T} C_A^2, \quad \frac{\text{mol}}{\text{cm}^3 \cdot \text{s}}$$

4.1



4.3



Take 300 moles of feed gas. Consider A

$$\left. \begin{array}{l} \text{At } X_A = 0 \quad V = 200A + 100B + 0R = 300 \\ \text{At } X_A = 1 \quad V = 0A - 100B + 200R = 100 \end{array} \right\} \epsilon_A = \frac{100 - 300}{300} = -\frac{2}{3}$$

Now consider B

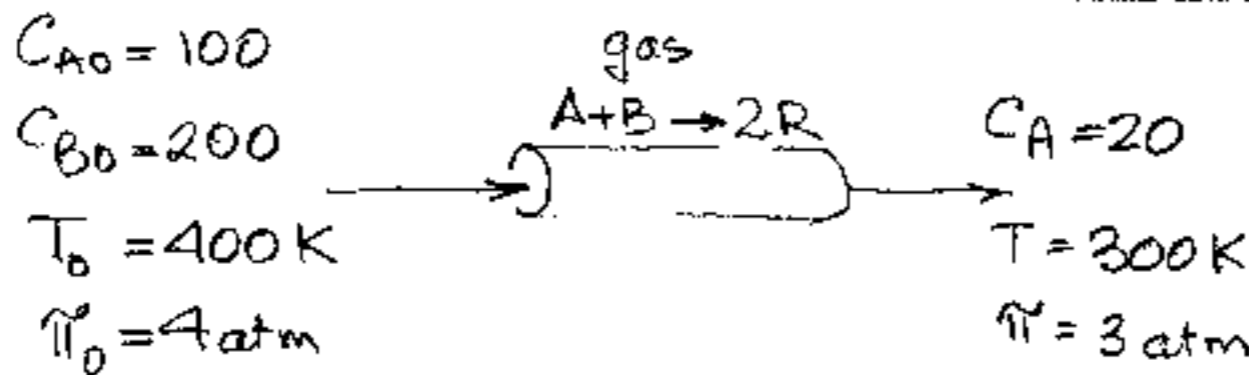
$$\left. \begin{array}{l} \text{At } X_B = 0 \quad V = 300 \\ \text{At } X_B = 1 \quad V = 100A + 0B + 100R = 200 \end{array} \right\} \epsilon_B = \frac{200 - 300}{200} = -\frac{1}{3}$$

∴ from Eq. 5

$$X_A = \frac{200 - 50}{200 - \left(\frac{2}{3}\right)50} = 0.9 \leftarrow$$

$$X_B = \frac{200 \times 0.9}{100} = 1.8 \dots \text{impossible} \leftarrow$$

4.5



Since the number of moles is unchanged $\epsilon_A = 0$ and $\epsilon_B = 0$

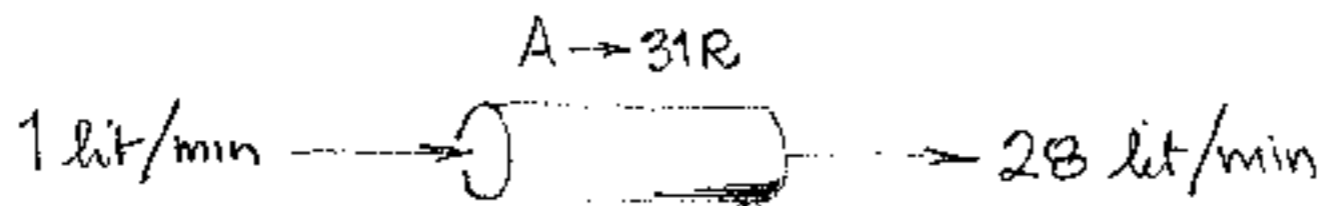
4.5
(continued)

$$X_A = \frac{1 - \frac{C_A}{C_{A0}} \left(\frac{T \pi_0}{T_0 \pi} \right)}{1 + E_A \frac{C_A}{C_{A0}} \left(\frac{T \pi_0}{T_0 \pi} \right)} = \frac{1 + \left(\frac{20}{100} \right) \left(\frac{300 \times 4}{400 \times 3} \right)}{1 + 0} = 0.8 \leftarrow$$

$$X_B = \frac{1}{b} \frac{C_{A0} X_A}{C_{B0}} = \frac{(1)(100)(0.8)}{200} = 0.4 \leftarrow$$

$$\therefore C_B = 200 - 80 = 120 \leftarrow$$

4.7



Let X be the fraction of popcorn popped, the conversion $1-X$ is then the fraction unpopped

$$\text{Outlet} = 31X + (1-X)1 = 28 \text{ lit/min}$$

$$\text{or } X = \frac{27}{30} = 0.9 \leftarrow$$

↑ the fraction popped.

5.1 By the definition of Eq 7 or 8 we have

$$\tau = \frac{1}{s} = \frac{1}{1 \text{ min}^{-1}} = 1 \text{ min} \leftarrow$$

From the discussion following Eq 24 \bar{t} is somewhat less than 1 min because the density decreases with conversion. Therefore $\bar{t} > 1 \text{ min} \leftarrow$

Discussion If we really needed it we could derive \bar{t} as follows, for a differential section of plug flow reactor

$$\left. \begin{aligned} dt &= \frac{dV}{v} \\ dV &= \frac{F_{A0} dX_A}{(-r_A)} \end{aligned} \right\} \begin{aligned} &\text{combining and integrating gives} \\ &\text{the expression for } \bar{t}, \text{ or with} \\ &(F_{A0}, \text{ mol/s}) = (C_{A0}, \text{ mol/m}^3)(v_0, \text{ m}^3/\text{s}) \end{aligned}$$

$$\bar{t} = C_{A0} \int_0^{X_{AF}} \frac{dX_A}{(-r_A) \frac{v}{v_0}} = C_{A0} \int_0^{X_{AF}} \frac{dX_A}{(-r_A) (1 - \epsilon_A X_A)} \quad \dots \quad (24)$$

changes with conversion \leftarrow for linear expansion

Note that knowing $\tau = \int \frac{dX_A}{-r_A}$ does not allow us to find \bar{t} unless $-r_A = f(C_A)$ is known. But anyway I don't see any need to find \bar{t} except in tracer studies.

5.3 For the mixed flow reactor

$$-r_A = \frac{C_{A0} - C_{AF}}{\tau} = \frac{C_{A0} - C_{AF}}{V/v} = \frac{1 - 0.01}{2/4} = 1.98 \frac{\text{mol}}{\text{lit} \cdot \text{min}} \leftarrow$$

and

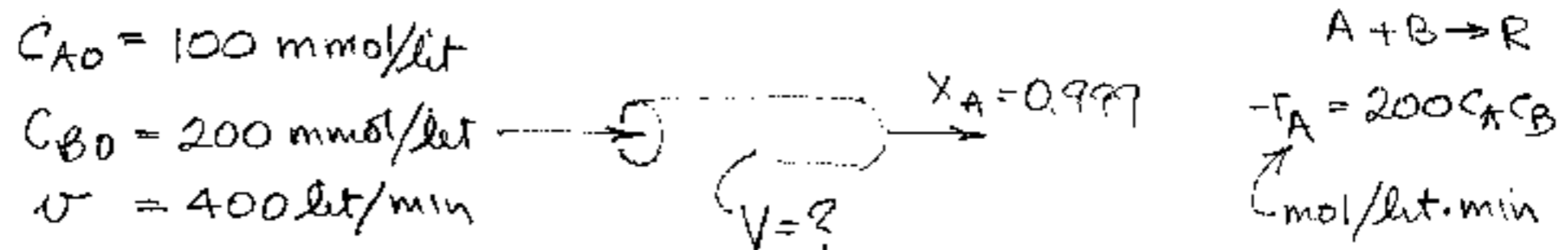
$$r_W = \frac{C_{WF} - C_{W0}}{\tau} = \frac{0.0002 - 0}{2/4} = 0.0004 \frac{\text{mol}}{\text{lit} \cdot \text{min}} \leftarrow$$

5.5

$$C_{A0} = 100 \text{ mmol/lit}$$

$$C_{B0} = 200 \text{ mmol/lit}$$

$$v = 400 \text{ lit/min}$$



For a 2nd order reaction, Eq 3.14 gives

$$k \tau C_{A0} (M-1) = \ln \left[\frac{M-X_A}{M(1-X_A)} \right] \quad \text{where } M = \frac{C_{B0}}{C_{A0}} \neq 1$$

Thus $M = \frac{200}{100} = 2$

Replacing all values

$$200(\tau)(0.1)(2-1) = \ln \left[\frac{2-0.999}{2(1-0.999)} \right] = 6.2156$$

or

$$\tau = 0.31 \text{ min}$$

Therefore

$$V = \tau v = (0.31)(400) = 124 \text{ lit} \leftarrow$$

5.7

First find the rate constant: $k = \frac{\ln 2}{t_{1/2}} = \frac{\ln 2}{5.2} = 0.1333 \text{ day}^{-1}$

Then for mixed flow, Eq 14a gives

$$\frac{a}{a_0} = \frac{1}{1+kE} = \frac{1}{1+(0.1333)30} = 0.2$$

$$\therefore \text{Fraction of activity removed} = 1 - 0.2 = 0.8 = 80\% \leftarrow$$

5.9

From Eq 3.58a, for this M-M type reaction,

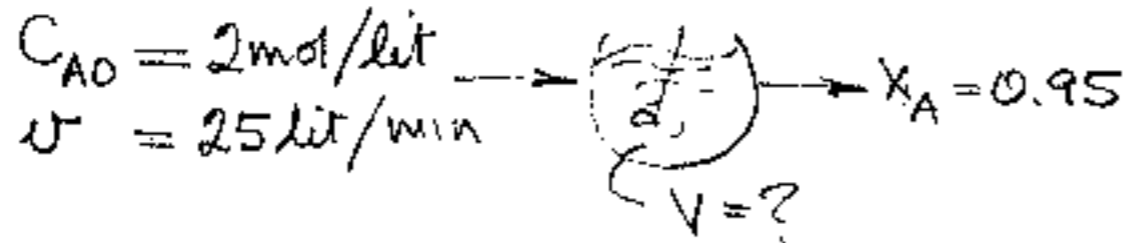
$$k_1 \frac{V}{v} = \ln \frac{C_{A0}}{C_A} + k_2 (C_{A0} - C_A)$$

Inserting $k_1 = 0.1$, $k_2 = 0.5$, $v = 25$, $C_{A0} = 2$ and $C_A = 0.1$ we get

$$V = \frac{25}{0.1} \left[\ln \frac{2}{0.1} + 0.5(2-0.1) \right]$$

$$= 986 \text{ lit} \approx 1 \text{ m}^3 \leftarrow$$

5.11



$$-r_A = \frac{0.1 C_A}{1 + 0.5 C_A}$$

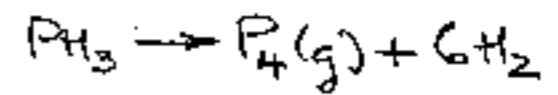
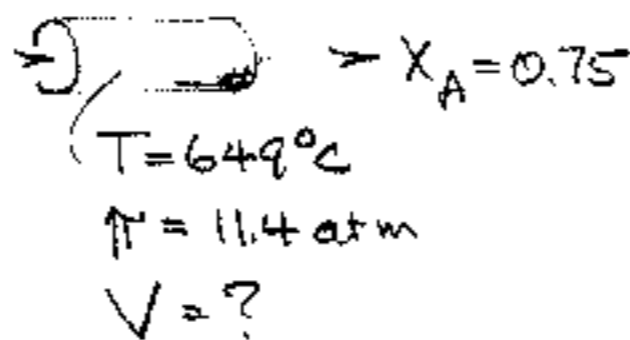
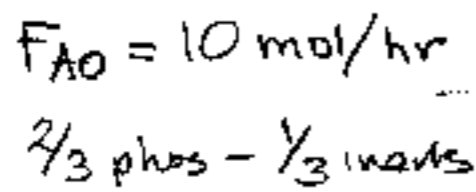
mol/lit·min

First of all $C_A = C_{A0}(1 - X_A) = 2(1 - 0.95) = 0.1$

Then for mixed flow

$$V = \frac{v(C_{A0} - C_A)}{-r_A} = \frac{25(2 - 0.1)}{\frac{(0.1)(0.1)}{1 + 0.5(0.1)}} = 4987.5 \text{ lit} \approx 5 \text{ m}^3 \leftarrow$$

5.13



$$-r_{\text{phos}} = (10 \text{ hr}^{-1}) C_{\text{phos}}$$

For a 1st order reaction.

$$k \frac{C_{A0} V}{F_{A0}} = (1 + \epsilon_A) \ln \frac{1}{1 - X_A} - \epsilon_A X_A \quad \dots \dots \dots (i)$$

Evaluate terms

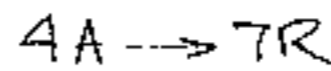
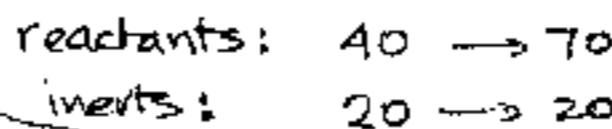
$$C_{A0} = \frac{P_{A0}}{RT} = \frac{11.4 \times \frac{2}{3}}{(0.08206)(649 + 273)} = 0.1 \frac{\text{mol}}{\text{lit}}$$

$$k = 10 \text{ hr}^{-1}$$

$$F_{A0} = 10 \text{ mol/hr}$$

$$\epsilon_A = 0.5$$

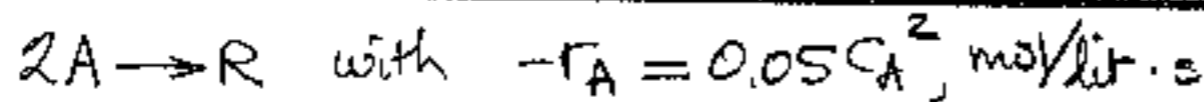
Replacing in (i) gives



$$\therefore \epsilon_A = \frac{90 - 60}{60} = \frac{1}{2}$$

$$V = \frac{10}{10(0.1)} \left[(1 + 0.5) \ln \frac{1}{0.25} - (0.5)(0.75) \right] = 17 \text{ lit} \leftarrow$$

5.15



Evaluate terms $\epsilon_A = \frac{1-2}{2} = -0.5$

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \epsilon_A C_A} = \frac{1 - 0.5}{1 + (-0.5)(0.5)} = \frac{2}{3}$$

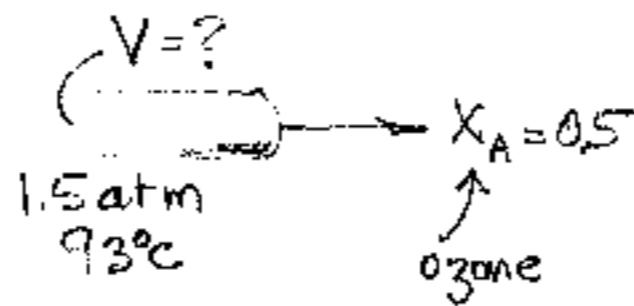
So for mixed flow

$$v = \frac{V(-r_A)}{C_{A0} X_A} = \frac{(2)(0.05 \times 0.5^2)}{1(2/3)} = 0.0375 \text{ lit/s} = 2.25 \text{ lit/min} \leftarrow$$

5.17

20% ozone (A)

80% air

 $v = 1 \text{ lit/s}$ 

$$-r_A = kC_A^2$$

$$k = 0.05 \text{ lit/mol}\cdot\text{s}$$

For a 2nd order reaction with expansion, Eq 23 gives

$$V = \frac{v}{C_{A0}k} \left[2\varepsilon_A(1+\varepsilon_A)\ln(1-X_A) + \varepsilon_A^2 X_A + (\varepsilon_A+1)^2 \frac{X_A}{1-X_A} \right] \dots (i)$$

Evaluate terms

$$C_{A0} = \frac{P_{A0}}{RT} = \frac{(1.5)(0.2)}{(0.08206)(366)} = 0.01 \frac{\text{mol}}{\text{lit}}$$

$$\varepsilon_A = \frac{11-10}{10} = 0.1$$

Replacing in (i) gives

$$V = \frac{1}{(0.01)(0.05)} \left[2(0.1)(1+0.1)\ln(1-0.5) + (0.1)^2(0.5) + (0.1+1)^2 \frac{0.5}{(1-0.5)} \right]$$

$$= 2125 \text{ lit} = 2.1 \text{ m}^3$$

5.19

 $C_{A0} = 120 \text{ mmol/lit}$

2 atm

30°C

various v_0 various C_A $A \rightarrow 3R$

Find a rate equation

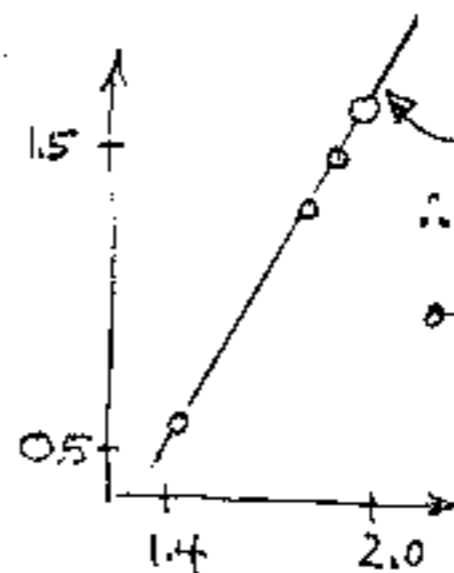
For each run

$$-r_A = \frac{C_{A0} X_A v_0}{V} = \frac{C_{A0} (C_{A0} - C_A) v_0}{(C_{A0} + \varepsilon_A C_A) V} = \frac{120(120 - C_A) v_0}{(120 + 2C_A)}$$

Now tabulate

| v_0 | C_A | $-r_A$ | $\log(-r_A)$ | $\log C_A$ |
|-------|-------|--------|--------------|------------|
| 0.06 | 30 | 3.6 | 0.5563 | 1.477 |
| 0.48 | 60 | 14.4 | 1.1584 | 1.778 |
| 1.5 | 80 | 25.7 | 1.41 | 1.903 |
| 8.1 | 105 | 44.2 | 1.6452 | 2.07 |

given data



Slope $n=2$

$$\therefore \log(-r_A) = \log k + 2 \log C_A$$

$$\text{or } 0.5563 = \log k + 2(1.477)$$

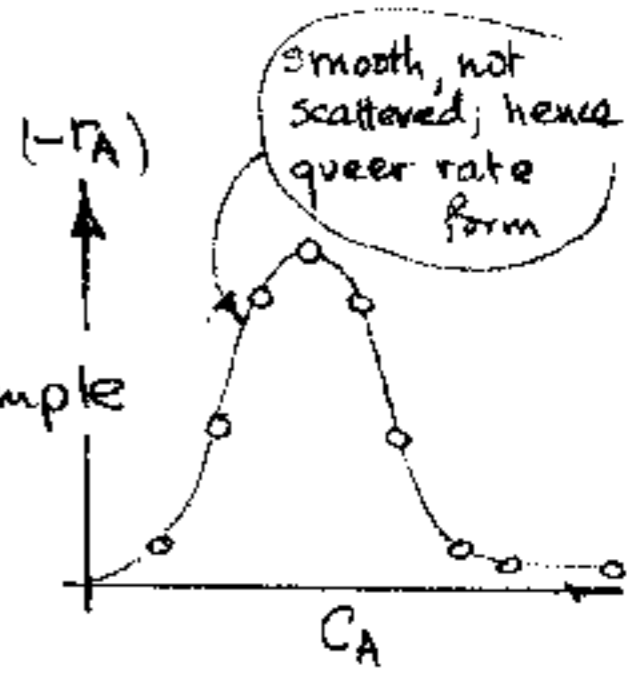
$$\therefore k = 0.004$$

$$\therefore -r_A = 0.004 C_A^2, \text{ mmol/lit}\cdot\text{min}$$

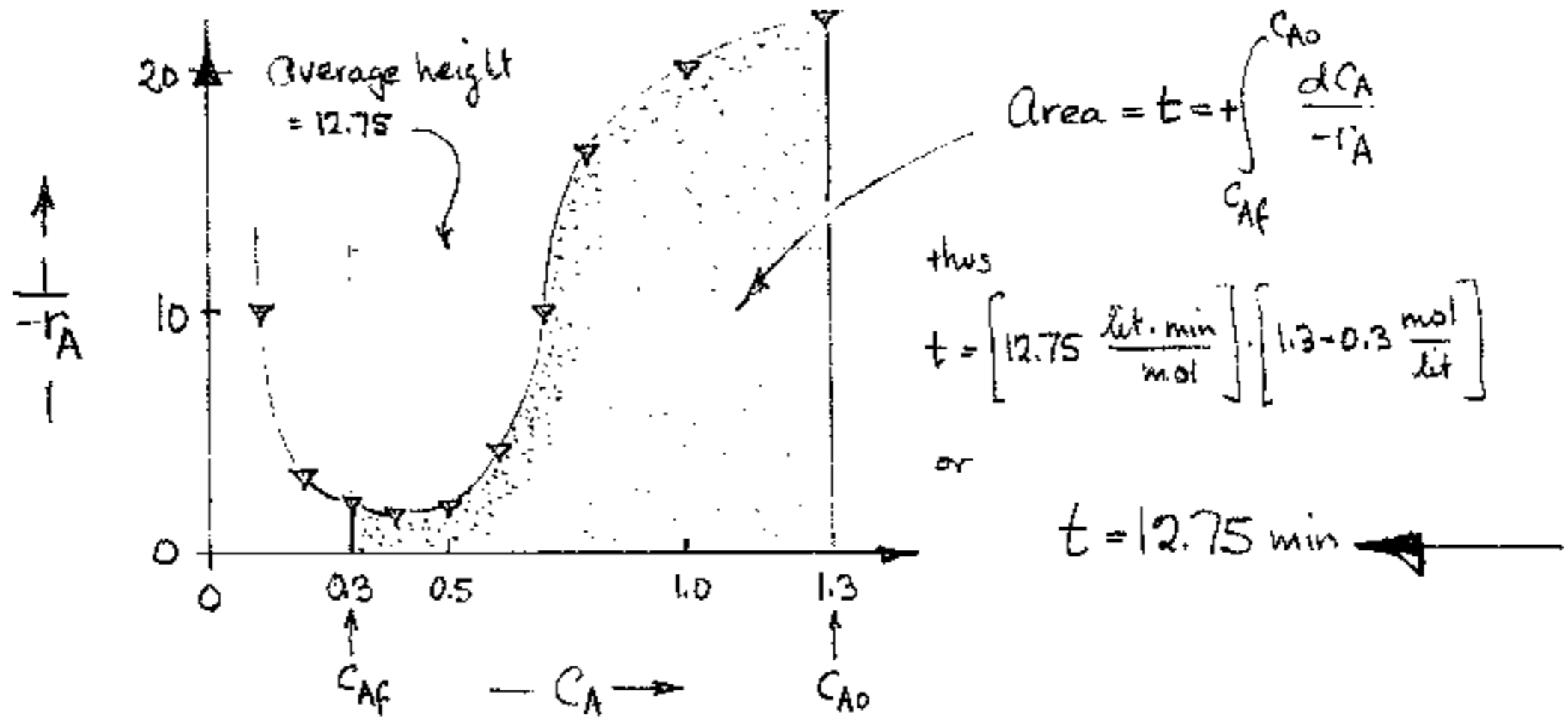
5.21 The approach which probably first comes to mind is to find a rate equation to represent the data, first order, second, etc., and then integrate it to give the time; thus

$$t = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} \quad \dots \text{Eq 4, since } \epsilon_A = 0$$

But a quick plot of the data shows that no simple rate form of chapter 3 will fit the data, so it looks like this approach won't work.



With a bit more thought we see that we were not asked to find a rate equation, we were just asked for t , and that this could be done by solving the general design equation, Eq 4 directly by graphical procedures. let us do this



This is the more general way of solving this problem since it does not require that we describe the rate by an equation.

5.23 a) Given

$$C_{A0} = 1.2 \text{ mol/lit}$$

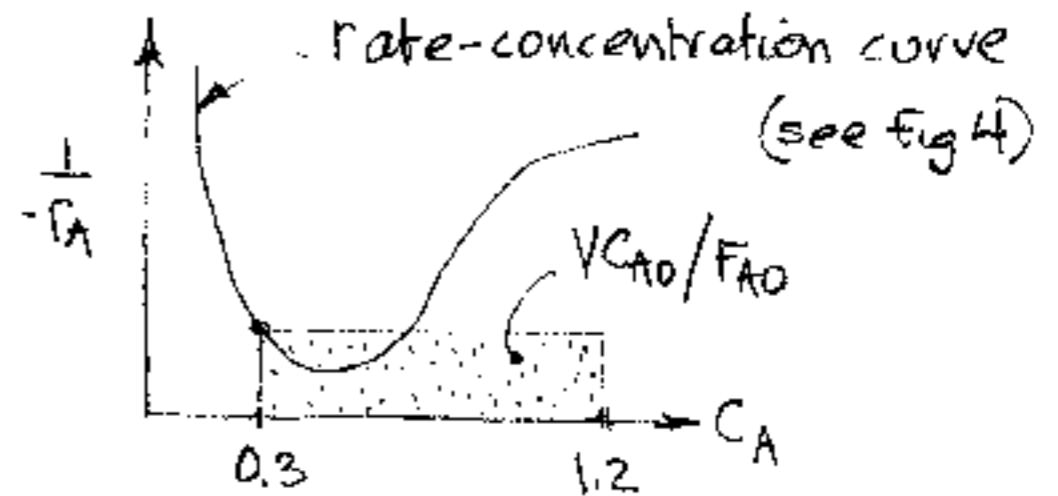
$$F_{A0} = 1000 \text{ mol/hr} \rightarrow \text{Reactor} \rightarrow X_A = 0.75$$

Since this is a liquid reaction $\epsilon_A = 0$, so $\frac{C_{AF}}{C_{A0}} = 1 - X_A$
 or $C_{AF} = C_{A0}(1 - X_{AF}) = 1.2(1 - 0.75) = 0.3 \text{ mol/lit}$

From the performance equation for mixed flow, Eq 13,

$$V = \frac{F_{A0} \cdot C_{A0} - C_{AF}}{C_{A0} \cdot -r_{AF}}$$

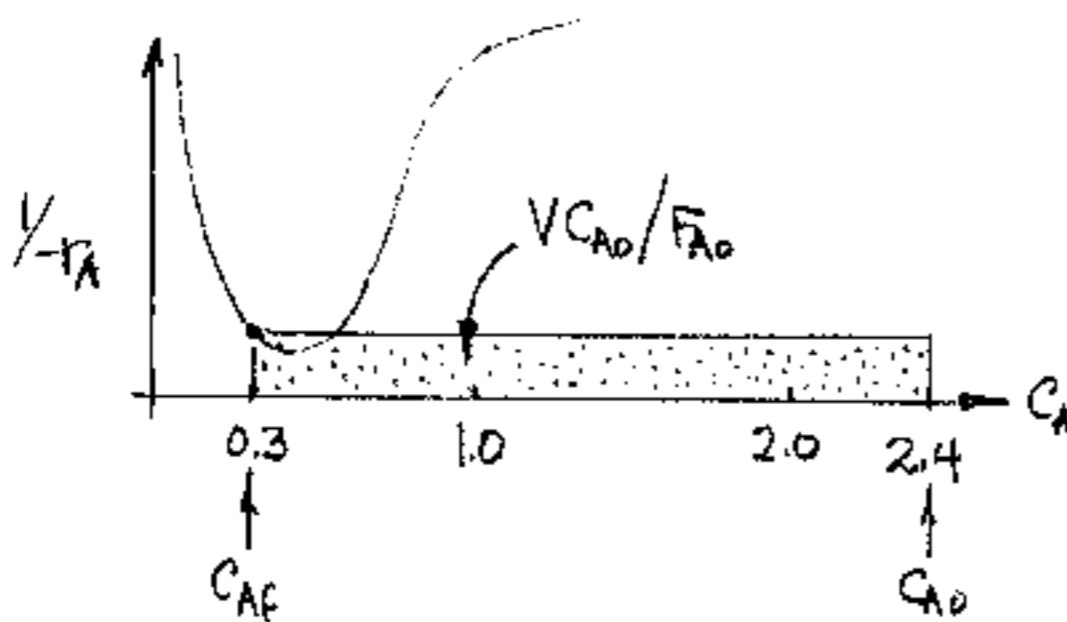
$$= \frac{1000 \frac{\text{mol}}{\text{hr}} \cdot (1.2 - 0.3 \frac{\text{mol}}{\text{lit}})}{1.2 \frac{\text{mol}}{\text{lit}} \cdot (0.5 \frac{\text{mol}}{\text{lit} \cdot \text{min}})} \cdot \frac{1 \text{ hr}}{60 \text{ min}} = 25 \text{ lit} \leftarrow \text{a)}$$



b) If F_{A0} is doubled while all else remained unchanged we see from

$$V = \frac{F_{A0} \cdot C_{A0} - C_{AF}}{C_{A0} \cdot -r_{AF}} \dots \text{that } V \text{ is doubled,}$$

$$\text{or } V = 50 \text{ lit.} \leftarrow \text{b)}$$



In doubling C_{A0} keeping all else the same, including F_{A0} , we get

$$V = \frac{F_{A0} \cdot C_{A0} - C_{AF}}{C_{A0} \cdot -r_{AF}}$$

$$= \frac{1000 \cdot (2.4 - 0.3) \cdot 1}{2.4 \cdot 0.5 \cdot 60}$$

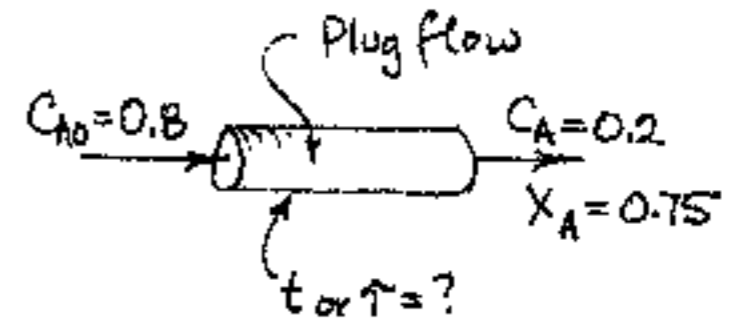
$$\text{or } V = 29.167 \text{ lit} \leftarrow \text{c)}$$

5.25 For a mixed flow reactor, with $\epsilon_A = 0$, we find the rate of reaction from Eq 13. Thus we tabulate as follows

| t, sec | C_{A0} | $C_{A, \text{out}}$ | $-\frac{1}{r_A} = \frac{t}{C_{A0} - C_{A, \text{out}}}$... at $C_{A, \text{out}}$ |
|-----------------|----------|---------------------|--|
| 300 | 2 | 0.65 | $300/(2-0.65) = 222$ |
| 240 | 2 | 0.92 | 222 |
| 250 | 2 | 1.00 | 250 |
| 110 | 1 | 0.56 | 250 |
| 360 | 1 | 0.37 | 572 |
| 24 | 0.48 | 0.42 | 400 |
| 200 | 0.48 | 0.28 | 1000 |
| 560 | 0.48 | 0.20 | 2,000 |

Holding time for plug flow.

We may solve this by using conversions as suggested in the text. However since $\epsilon_A = 0$ the use of concentrations poses no problems.

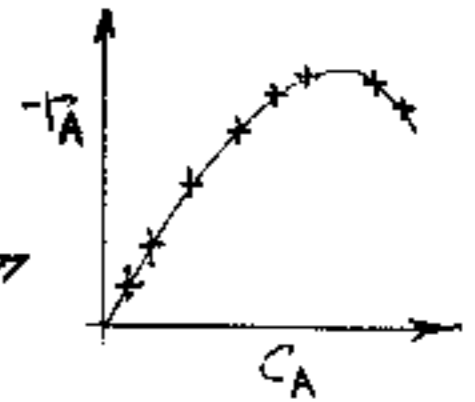


Let us use this. Then the performance expression is Eq. 19, or

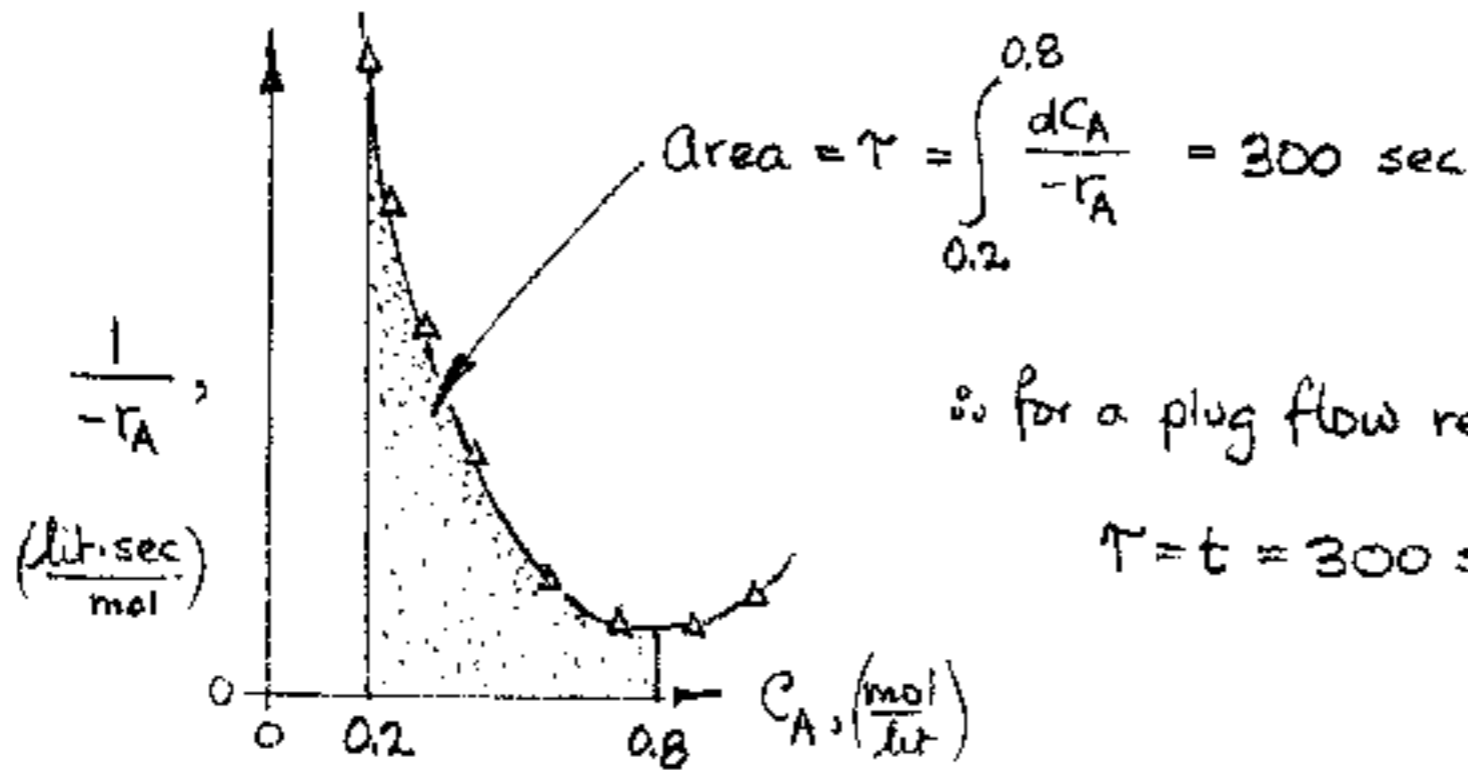
$$\tau = - \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

So tabulate $-r_A$ as shown in the table above.

Now a plot of C_A vs $-r_A$ gives a figure like this. This indicates that no simple rate expression, say n^{th} order, will fit the data, hence solve graphically.



This is done by plotting C_A vs $1/(-r_A)$ and integrating.



∴ for a plug flow reactor

$$\tau = t = 300 \text{ sec}$$

5.27a) Since the vat contains ~99% ethanol I guess that Imbibit fell-dead drunk - into the vat. This would decrease the volume available for fluid. Let's see if this could account for the decrease in conversion of googlix.

Secondly, since ethanol is in very large excess we can reasonably assume pseudo first order kinetics with respect to googlix (A). So for mixed flow Eq 13 gives, for before & after

$$k\tau_1 = \frac{X_{A1}}{1-X_{A1}} = \frac{0.8}{1-0.8} = 4$$

$$k\tau_2 = \frac{X_{A2}}{1-X_{A2}} = \frac{0.75}{1-0.75} = 3$$

Since $V_2/V_1 = \tau_2/\tau_1$ we have

$$V_2 = 100 \left(\frac{3}{4}\right) = 75 \text{ Imp gal}$$

So the decrease in volume is $\Delta V = 100 - 75 = 25 \text{ Imp. gal}$

$$\text{or } (25 \text{ Imp. gal}) \left(\frac{10 \# \text{H}_2\text{O}}{1 \text{ Imp. gal}} \right) \left(\frac{1 \text{ ft}^3}{62.4 \# \text{H}_2\text{O}} \right) = 4.01 \frac{\text{ft}^3}{\text{minute}}$$

Let us see if this is Imbibit's volume. With his density being $62.4 \#/\text{ft}^3$

$$\text{Imbibit's volume is } \frac{(18 \text{ stone})(14 \#/\text{stone})}{(62.4 \#/\text{ft}^3)} = 4.04 \frac{\text{ft}^3}{\text{minute}}$$

These volumes agree so Imbibit could well be in the vat. } ←

This hypothesis, or guess does fit the facts

b) Why did Watson never come up with this explanation?

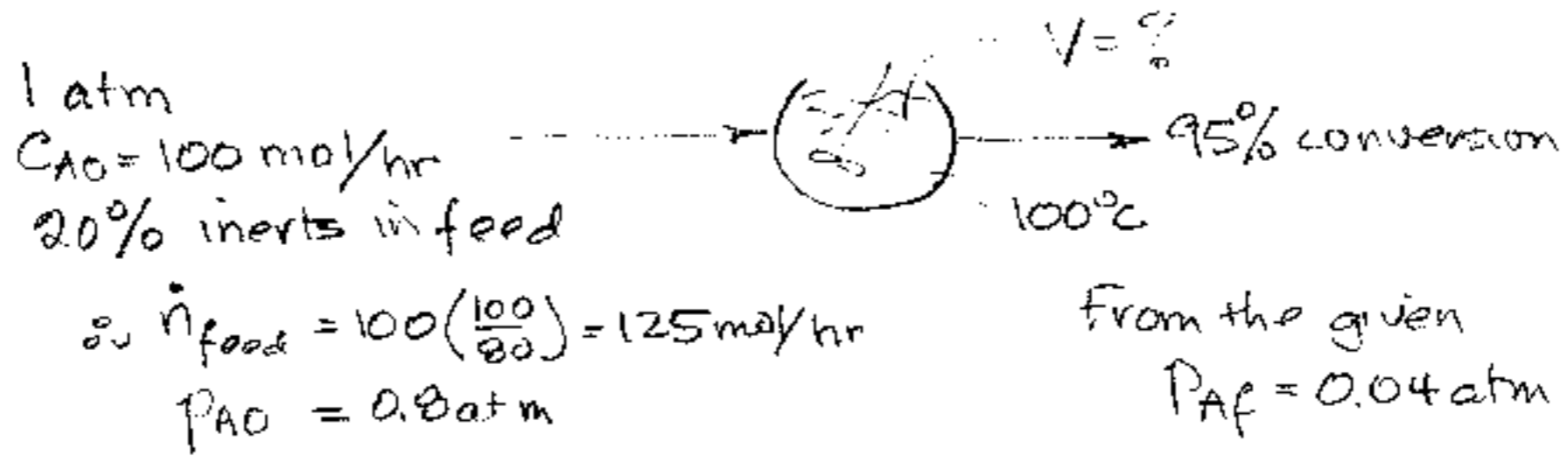
Because smoking near 99% alcohol was not really cool. ←

Note • Watson was not knowledgeable on pickling. You use dill for pickling in brine, not alcohol.

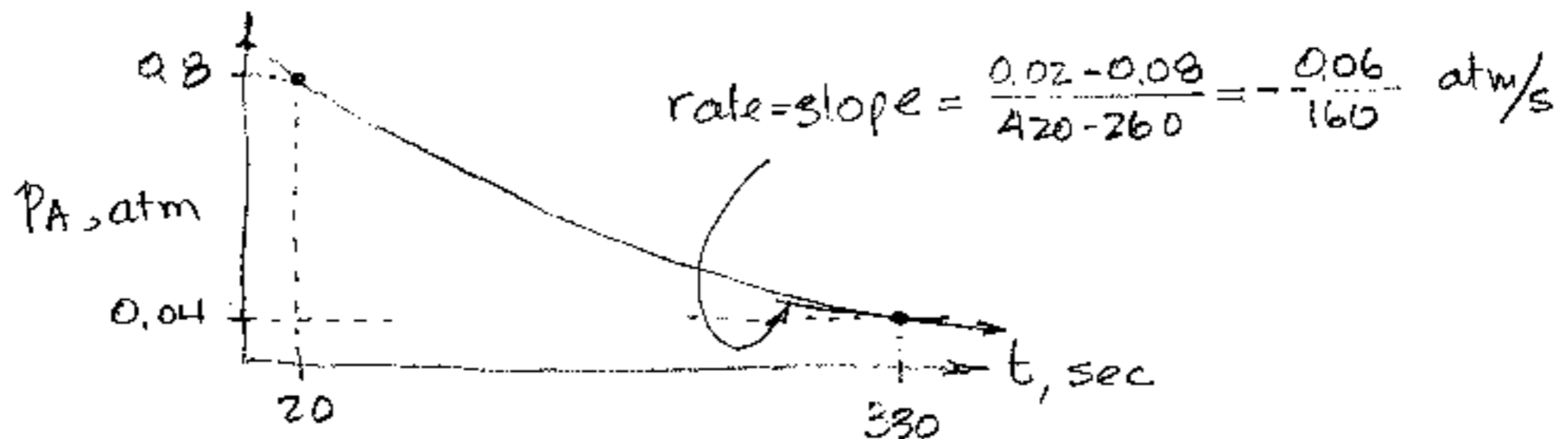
• Of course everyone knows that 1 Imp. gal is the volume of 10 # H₂O, and that 1 stone weighs 14 #.

5.29 (extension of problem 5.28)

Given a gas phase reaction $2A \rightarrow R + C$



For mixed flow we must find the rate at the exit conditions. Then we can proceed to finding the reactor size. So draw an accurate p_A vs t curve and find the slope (hence rate) at $p_A = 0.04 \text{ atm}$



The performance equation for mixed flow, Eq 13, in pressure units is

$$\tau = \frac{V}{v} = \frac{P_{A0} - P_A}{-r_A} = \frac{0.8 - 0.04}{(0.06/160)} = 2026.67 \text{ s}$$

But $\tau = \frac{V}{v}$ so evaluate v from $p v = n R T$. Thus

$$v = \frac{n R T}{p} = \frac{(125)(0.08206)(373)}{(1)} = 3826 \text{ lit/hr}$$

$$\therefore V = \tau v = (2026.67 \text{ s})(3826 \text{ lit/hr}) \left(\frac{1 \text{ hr}}{3600 \text{ s}} \right) = 2150 \text{ lit} = 2.15 \text{ m}^3 \quad \leftarrow$$

6.1 For a second order reaction: $kT = \frac{C_{A0} - C_A}{C_A^2}$, so for the two reactors

$$\frac{V_2}{V_1} = 2 = \frac{kT_2}{kT_1} = \frac{(C_{A1} - C_{A2})/C_{A2}^2}{(C_{A0} - C_{A1})/C_{A1}^2} = \frac{(0.5 - C_{A2})/C_{A2}^2}{(1 - 0.5)/0.5^2}$$

or

$$4C_{A2}^2 = 0.5 - C_{A2}$$

therefore

$$C_{A2} = 0.25 \text{ mol/lit.} \leftarrow$$

6.3 For the second order reaction

for the mixed flow reactor: $kT_m = \frac{C_{A0} - C_{A1}}{C_{A1}^2} = \frac{4 - 1}{1} = 3$

so for the plug flow reactor: $kT_p = 3kT_m = 9$

and $\frac{C_{A2}}{C_{A1}} = \frac{1}{1 + kT_p C_{A1}} = \frac{1}{1 + 9(1)} = 0.1$

$\therefore C_{A2} = 0.1 (C_{A1}) = 0.1 \text{ mol/lit} \leftarrow$

6.5

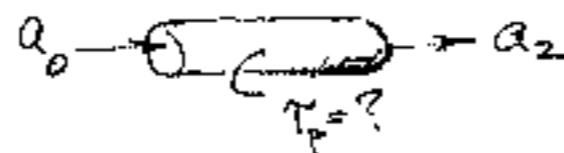


Radioactive decay follows first order kinetics, so here

$$k = \frac{\ln 2}{t_{1/2}} = \frac{0.6931}{14 \text{ min}} = 0.0495 \text{ min}^{-1}$$

so $\frac{a_2}{a_0} = \frac{a_2}{a_1} \cdot \frac{a_1}{a_0} = \frac{1}{(1 + k\bar{t}_i)} = \frac{1}{[1 + 0.0495(20160)]^2} = 1.0017 \times 10^{-6}$

For plug flow



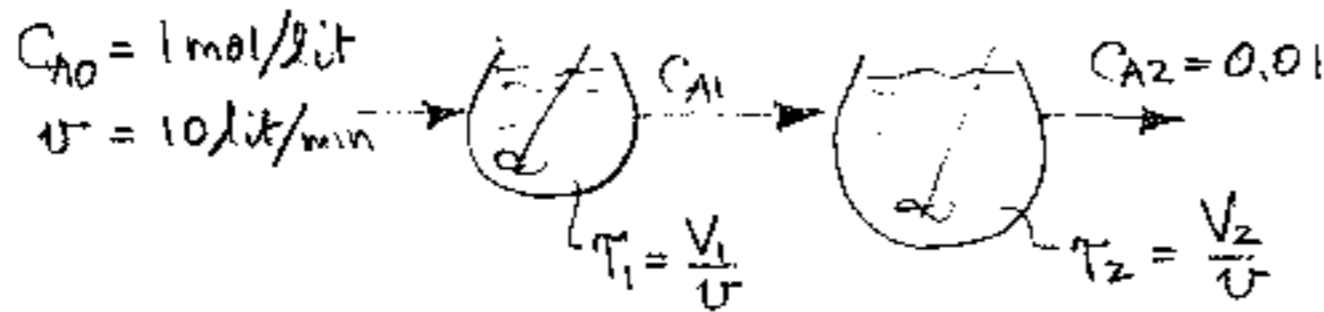
$$\frac{a_2}{a_0} = 1.0017 \times 10^{-6} = e^{-kT_p} = e^{-0.0495 T_p}$$

$$T_p = \frac{\ln(1.0017 \times 10^{-6})}{-0.0495}$$

$$= 279 \text{ min} = 4.65 \text{ hr} \leftarrow$$

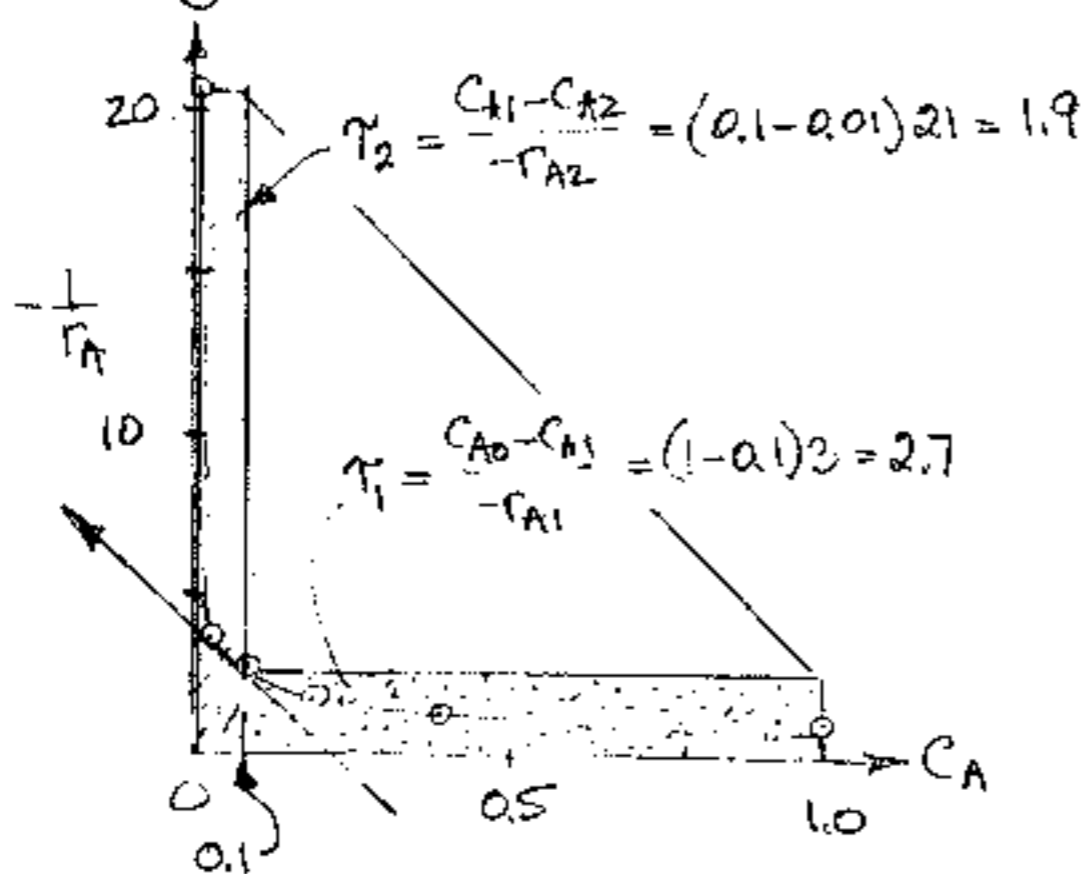
instead of 2 weeks for the MFR

6.7



$$-r_A = \frac{C_A}{0.2 + C_A} \frac{\text{mol}}{\text{lit} \cdot \text{min}}$$

It is best to solve this graphically. Thus by the method of maximization of rectangles



| C_A | $-\frac{1}{r_A} = \frac{0.2 + C_A}{C_A}$ |
|-------|--|
| 1 | 1.2 |
| 0.4 | 1.5 |
| 0.2 | 2 |
| 0.1 | 3 |
| 0.08 | 3.5 |
| 0.01 | 21 |

$$\therefore V_1 = \tau_1 v = 2.7(10) = 27 \text{ lit}$$

$$V_2 = \tau_2 v = 1.9(10) = 19 \text{ lit}$$

6.9 With recycle for a first order reaction we have

$$k\tau = (R+1) \ln \left[\frac{C_{A0} + RC_{Af}}{(R+1)C_{Af}} \right] = (2+1) \ln \left[\frac{10 + 2(1)}{(2+1)1} \right] = 3 \ln 4$$

Without recycle (plug flow)

$$k\tau = \ln \frac{C_{A0}}{C_{Af}} = \ln 10$$

Therefore

$$\frac{v_{\text{without}}}{v_{\text{with}}} = \frac{\tau_{\text{with}}}{\tau_{\text{without}}} = \frac{3 \ln 4}{\ln 10} = 1.8$$

no recycle is better

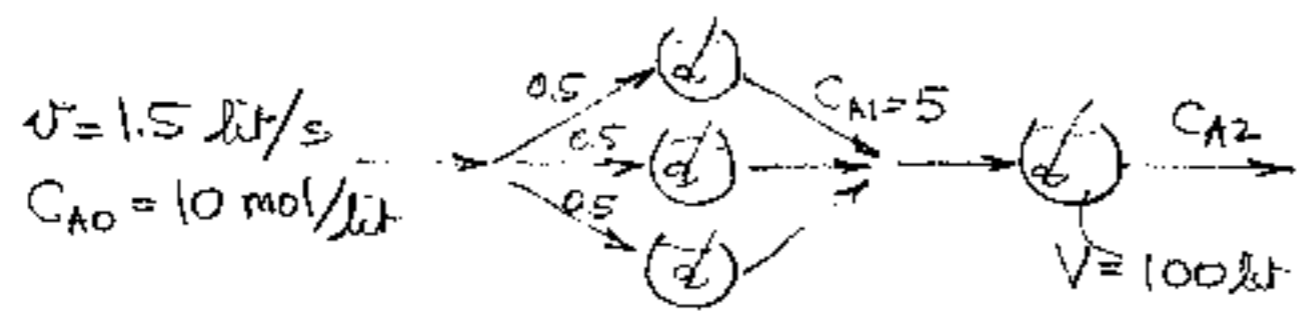
6.11 For this autocatalytic reaction, the maximum rate occurs where $C_A = C_R$. Thus operate at $C_A = 5$, if possible. Here

$$-r_A = 0.001 C_A C_R = 0.001 \times 5 \times 5 = 0.025$$

So for mixed flow

$$\tau = \frac{10-5}{0.025} = \frac{5}{0.025} = 200s = \frac{V}{v} = \frac{V}{1.5}$$

Thus $V = 300 \text{ lit}$, or 3 mfr side by side. Thus we should hook the 4 reactors as shown



For the fourth reactor $\tau = V/v = 100/1.5 = 66.7s$, so

$$66.7s \rightarrow \tau = \frac{5-C_{A2}}{k C_{A2} C_{R2}} = \frac{5-C_{A2}}{0.001 C_{A2} (10-C_{A2})}, \text{ or } C_{A2} = 3.496 \frac{\text{mol}}{\text{lit}}$$

6.13 From $\frac{1}{2}$ life data for radioactive decay (first order kinetics) we have

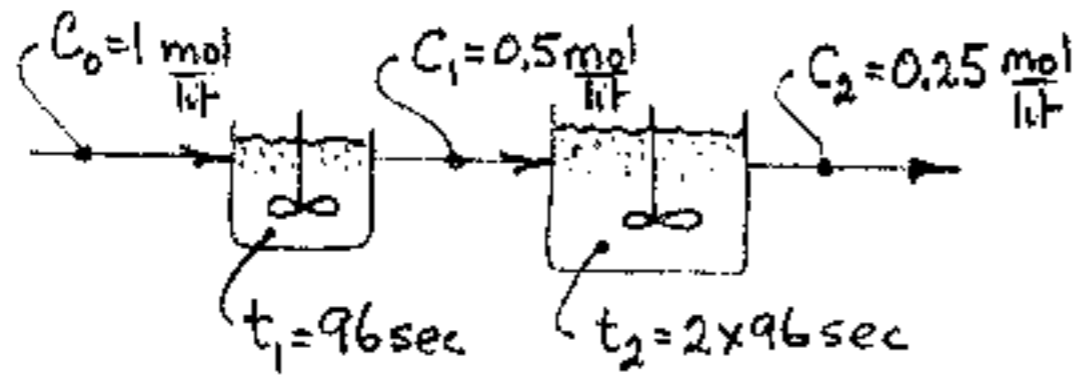
$$-\frac{dC}{dt} = kC \quad \text{or} \quad \ln \frac{C_0}{C} = kt \quad \text{or} \quad \ln 2 = k(20 \text{ hrs}) \quad \text{or} \quad k = \frac{\ln 2}{20 \text{ hr}}$$

and for 2 equal sized tanks in series Eq 6.6a gives

$$\frac{C_{out}}{C_0} = \frac{1}{(1+k\tau_i)^2} = \frac{1}{\left(1 + \frac{\ln 2}{20} (400)\right)^2} = \frac{1}{(1+20 \ln 2)^2} = 0.00453$$

∴ only 0.453% of the activity remains,
99.5% of the activity has disappeared

6.15



We have 2 pieces of kinetic information, what happens in the 2 reactors, thus we can fit a kinetic equation with 2 constants. So let us try an n^{th} order equation.

$$\left. \begin{array}{l} \text{For 1st reactor: } \tau_1 = \frac{C_0 - C_1}{k C_1^n} \\ \text{For 2nd reactor: } \tau_2 = \frac{C_1 - C_2}{k C_2^n} \end{array} \right\} \text{ combining ... } \frac{\tau_1}{\tau_2} = \frac{C_0 - C_1}{C_1 - C_2} \left(\frac{C_2}{C_1} \right)^n$$

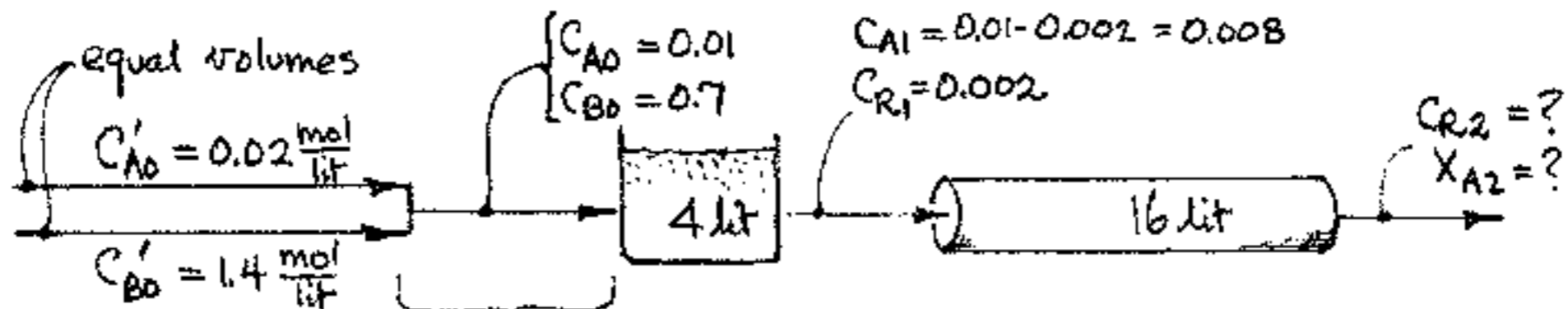
$$\therefore n = \frac{\log \frac{\tau_1}{\tau_2} + \log \frac{C_1 - C_2}{C_0 - C_1}}{\log \frac{C_2}{C_1}} = \frac{\log \frac{1}{2} + \log \frac{1}{2}}{\log \frac{1}{2}} = 2$$

and on replacing in the 1st equation $k = \frac{C_0 - C_1}{\tau_1 C_1^n} = \frac{0.5}{96 (0.5)^2} = \frac{1}{48} \frac{\text{lit}}{\text{mol} \cdot \text{s}}$

Hence the rate

$$-r_A = \left(\frac{1}{48} \frac{\text{lit}}{\text{mol} \cdot \text{sec}} \right) C_A^2 = \left(1.25 \frac{\text{lit}}{\text{mol} \cdot \text{min}} \right) C_A^2 \quad \leftarrow$$

6.17



imaginary section in which the 2 feed streams are mixed.

Simplification: Since $C_{A0} = 1/70 \cdot C_{B0}$ we may assume that $C_{B0} \approx \text{constant}$, and that the reaction is 1st order with respect to A.

$$\text{For the mixer: } k \tau_m = \frac{C_{A0} - C_{A1}}{C_{A1}} = \frac{0.010 - 0.008}{0.008} = \frac{1}{4}$$

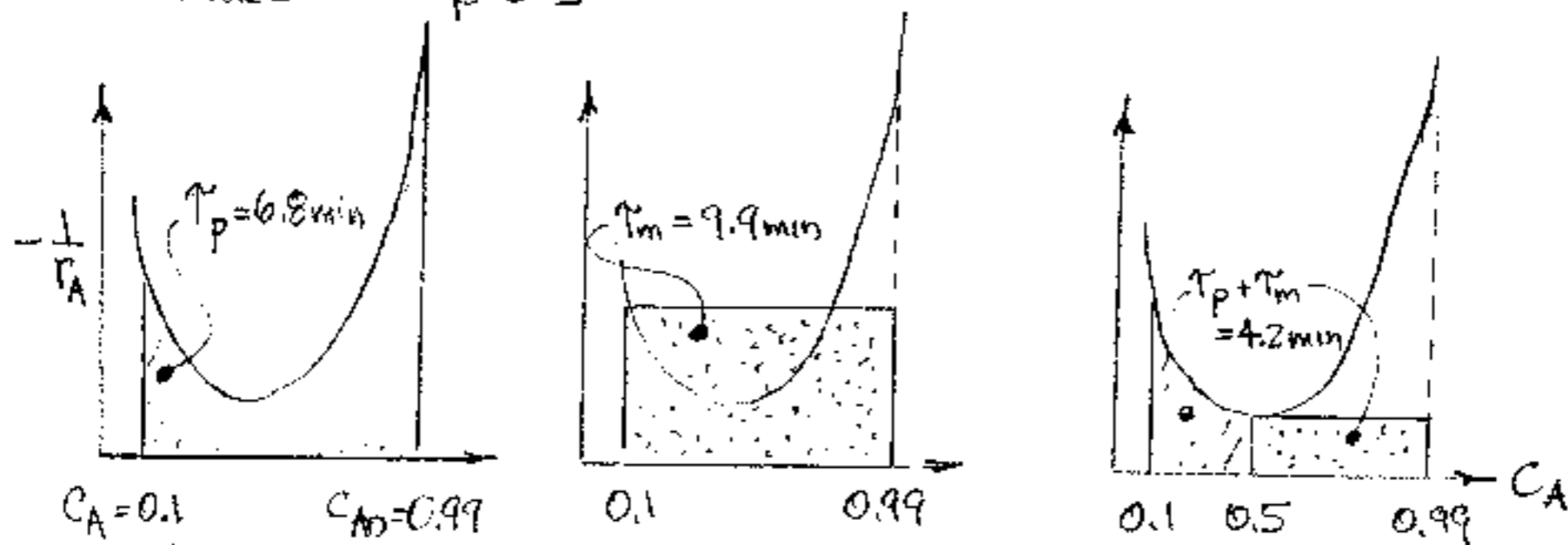
$$\text{For the reactor: } k \tau_p = 4 (k \tau_m) = 4 \left(\frac{1}{4} \right) = - \int_{0.008}^{C_{A2}} \frac{dC_A}{C_A} = \ln \frac{0.008}{C_{A2}} \quad \dots \text{ or } C_{A2} = 0.00293$$

$$\therefore X_A = 0.707 \quad \& \quad C_{R2} = 0.00793 \quad \leftarrow$$

6.19 Let us solve by using the graphical procedure, and let's use concentrations, not conversions. First prepare the $1/r_A$ vs C_A curves from the data of the table, below

| C_A | C_R | $-r_A = k C_A C_R$ | $\frac{1}{-r_A}$ |
|-------|-------|--------------------|------------------|
| 0.99 | 0.01 | 0.0099 | 101.01 |
| 0.95 | 0.05 | 0.0475 | 21.05 |
| 0.90 | 0.1 | 0.09 | 11.11 |
| 0.70 | 0.3 | 0.21 | 4.76 |
| 0.50 | 0.5 | 0.25 | 4.00 |
| 0.30 | 0.7 | 0.21 | 4.76 |
| 0.10 | 0.9 | 0.09 | 11.11 |

Now make the plots



So

$$T_p = 6.8 \text{ min} \quad \leftarrow \text{a)}$$

$$T_m = 9.9 \text{ min} \quad \leftarrow \text{b)}$$

$$T_{\text{best}} = T_m + T_p = 2 + 2.2 = 4.2 \text{ min} \quad \leftarrow \text{c)}$$

6.21 Originally we had plug flow, 1st order, $X_A = 0.9$

$$\frac{C_A}{C_{A0}} = e^{-kT}$$

$$C_{A0} = 10 \rightarrow \text{[]} \rightarrow C_{A1}$$

$$\text{or } kT = \ln \frac{C_{A0}}{C_A} = \ln 10 = 2.3 \quad \text{--- (i)}$$

With recycle

$$kT = (R+1) \ln \left[\frac{C_{A0} + R C_{AF}}{(R+1) C_{AF}} \right] = (2+1) \ln \left[\frac{10 + 2 C_{AF}}{(2+1) C_{AF}} \right] \quad \text{--- (ii)}$$

6.21
(continued)

Combining (i) & (ii) gives

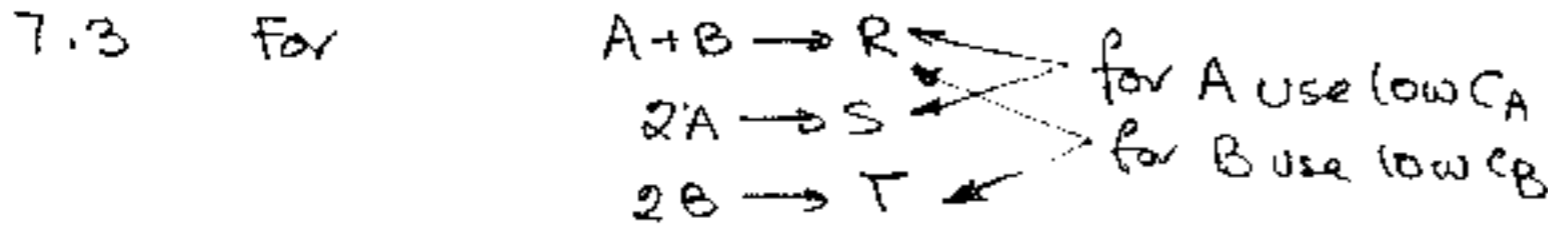
$$3 = (2+1) \ln \left[\frac{10+2C_{Af}}{(2+1)C_{Af}} \right]$$

Solving for C_{Af} gives

$$C_{Af} = 2.24, \text{ or } X_{Af} = 0.776 \leftarrow$$



- 7.1 a) Use a MFR with some particular concentration of A
 b) Use a PFR, with low X_A
 c) Use a MFR, with high X_A

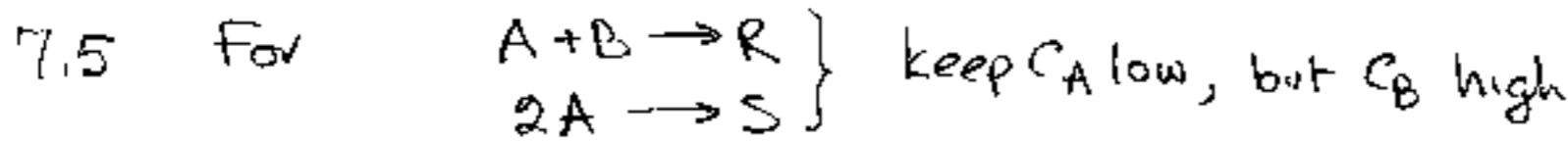


Thus

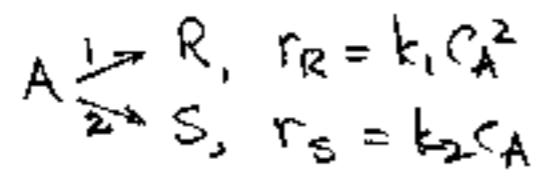


drip A and B in slowly
 keep X_A high
 keep X_B high

Don't have an excess of either A or B

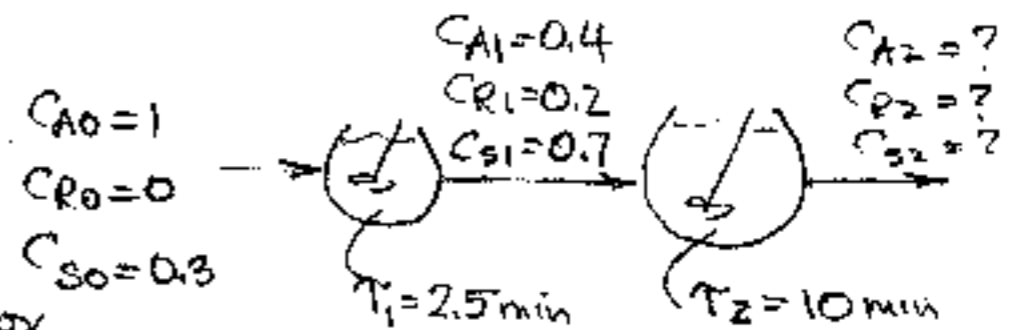


7.7 Given



and

$$\begin{array}{l} C_{A0} = 1 \\ C_{R0} = 0 \\ C_{S0} = 0.3 \end{array}$$



For mixed flow in the first reactor

$$\tau_1 = \frac{C_{R1} - C_{R0}}{k_1 C_A^2} \quad \therefore k_1 = \frac{0.2 - 0}{2.5 (0.4)^2} = 0.5$$

Also

$$\tau_1 = \frac{C_{S1} - C_{S0}}{k_2 C_A} \quad \therefore k_2 = \frac{0.7 - 0.3}{2.5 (0.4)} = 0.4$$

For the second reactor

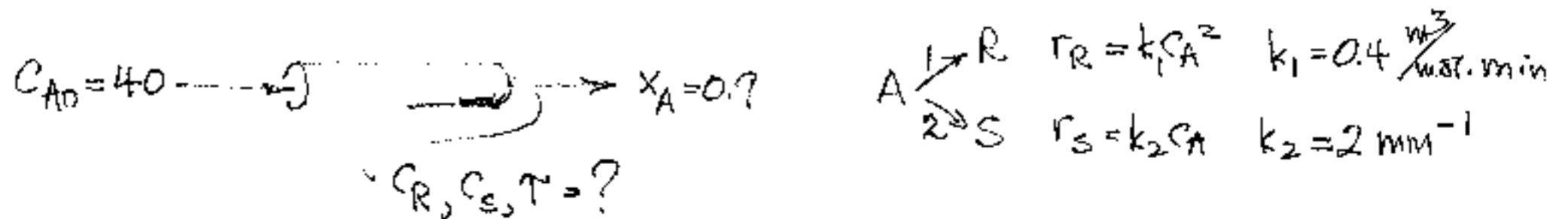
$$\tau_2 = \frac{C_{A1} - C_{A2}}{k_1 C_A^2 + k_2 C_A} = \frac{0.4 - C_{A2}}{0.5 C_{A2}^2 + 0.4 C_{A2}} = 10 \quad \therefore C_{A2} = 0.0745$$

Also

$$\tau_2 = \frac{C_{R2} - C_{R1}}{k_1 C_{A2}^2} \quad \therefore C_{R2} = 0.2 + 10 (0.5) (0.0745)^2 = 0.2278$$

$$\text{and } C_{S2} = 0.7 + 10 (0.4) (0.0745) = 0.998$$

7.9



First determine $Q(S/A)$.

$$Q(S/A) = \frac{r_S}{r_R + r_S} = \frac{2C_A}{0.4C_A^2 + 2C_A} = \frac{1}{1 + 0.2C_A}$$

$$C_S = \int_4^{40} Q(S/A) dC_A = \int_4^{40} \frac{dC_A}{1 + 0.2C_A} = \frac{1}{0.2} \ln(1 + 0.2C_A) \Big|_4^{40} = 5 \ln \frac{9}{1.8} = 8$$

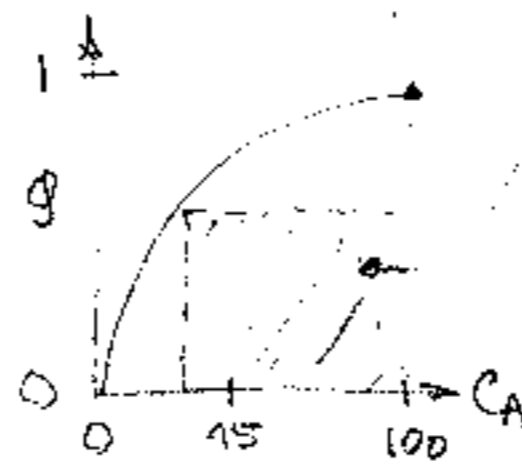
$$\therefore \begin{cases} C_A = 4 \\ C_S = 8 \\ C_R = 28 \end{cases}$$

$$\tau = \int \frac{dC_A}{-r_A} = \int \frac{dC_A}{2C_A + 0.4C_A^2} = \frac{1}{0.4} \int \frac{dC_A}{5C_A + C_A^2} = 2.5 \left[\frac{1}{5} \ln \frac{C_A}{C_A + 5} \right]_4^{40} = \frac{1}{2} \ln 2 = 0.347$$

7.11 To maximize C_R in a MFR first look at the $Q(R/A)$ vs C_A curve

| C_A | $Q(R/A)$ |
|-------|----------|
| 100 | 100/105 |
| 45 | 45/50 |
| 20 | 20/25 |
| 5 | 5/10 |
| 0 | 0 |

draw the curve



Solve by maximizing the area of the rectangle

$$Q(R/A) = \frac{0.4C_A^2}{0.4C_A^2 + 2C_A} = \frac{C_A}{C_A + 5}$$

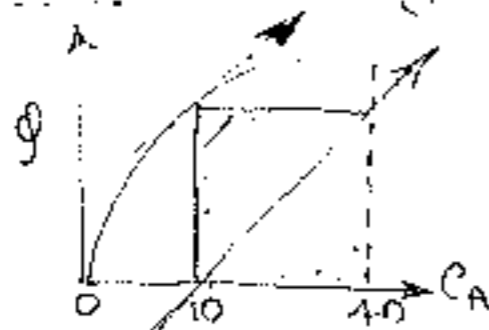
Method 1 Solve analytically

$$C_R = Q(-\Delta C_A) = \frac{C_A}{C_A + 5} (40 - C_A)$$

$$\frac{dC_R}{dC_A} = \frac{(40 - 2C_A)(C_A + 5) - (40C_A - C_A^2)}{(C_A + 5)^2} = 0 \quad \text{or } C_A = 10$$

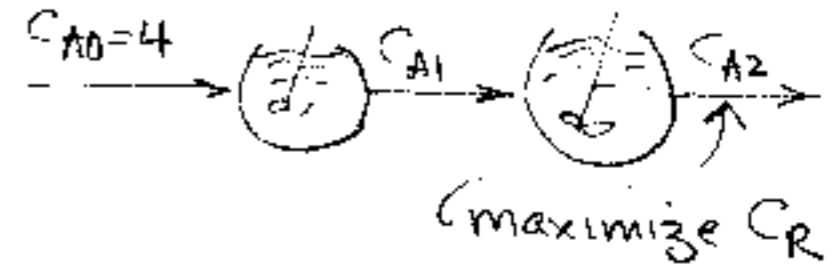
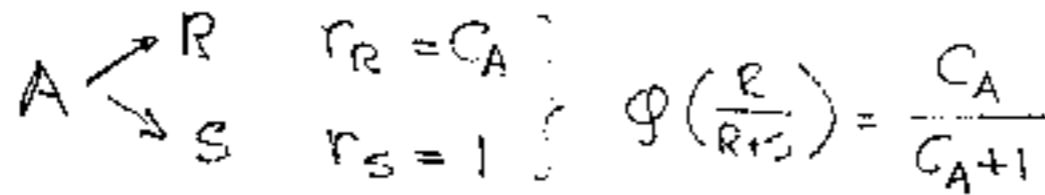
$$\begin{cases} C_R = 20 \\ C_S = 10 \end{cases}$$

Method 2 Solve graphically by maximizing the shaded rectangle

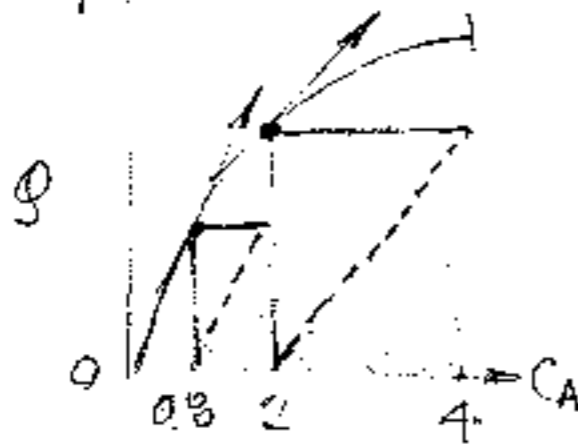


$$\text{For } \tau: \tau = \frac{C_{A0} - C_{Af}}{-r_A} = \frac{C_{A0} - C_{Af}}{0.4C_{Af}^2 + 2C_{Af}} = \frac{40 - 10}{0.4(10)^2 + 2(10)} = \frac{30}{60} = \frac{1}{2} \text{ min}$$

7.13



First plot ϕ vs C_A



The shaded areas of the two rectangles gives C_R . We maximize this by trial and error. This gives

$$C_{A1} = 2 \text{ and } C_{A2} = 0.8$$

P.S. I'm not sure that this is the best solution.

$$\begin{aligned} \tau_1 &= \frac{V_1}{v} = \frac{C_{A0} - C_{A1}}{-r_{A1}} = \frac{C_{A0} - C_{A1}}{1 + C_{A1}} = \frac{4 - 2}{1 + 2} = \frac{2}{3} \\ \text{and } \tau_2 &= \frac{V_2}{v} = \frac{C_{A1} - C_{A2}}{-r_{A2}} = \frac{2 - 0.8}{1 + 0.8} = \frac{2}{3} \end{aligned} \quad \left. \vphantom{\tau_1} \right\} \therefore \frac{V_1}{V_2} = 1$$

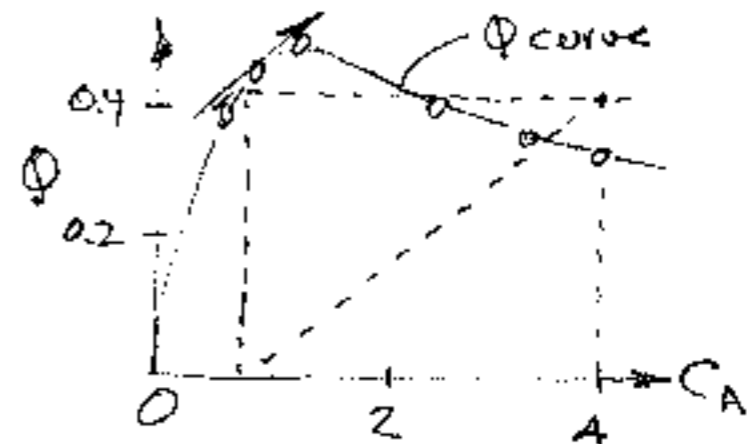
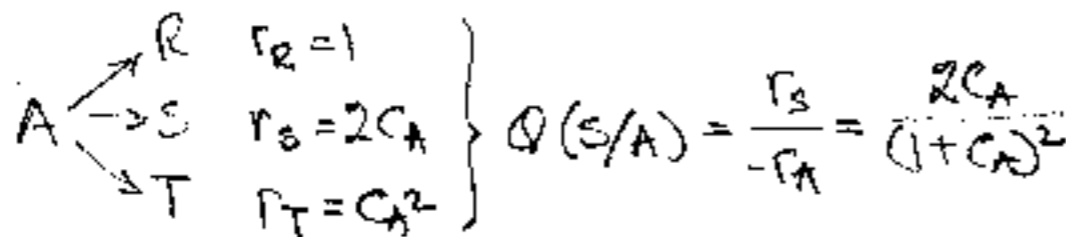
and

$$C_{R1} = \phi \cdot \Delta C_A = \frac{C_{A1}}{C_{A1}+1} (C_{A0} - C_{A1}) = \frac{2}{2+1} (4-2) = 1.33$$

$$C_{R2} = \frac{C_{A2}}{C_{A2}+1} (C_{A1} - C_{A2}) = \frac{0.8}{0.8+1} (2-0.8) = 0.533$$

$$\therefore C_{R_{\max}} = 1.86 \frac{\text{mol}}{\text{lit}} \leftarrow$$

7.15



a) For plug flow go to $C_{Af} = 0$ for maximum area

$$C_S = \int_0^A \frac{2C_A}{(1+C_A)^2} dC_A \approx (0.3984)A = 1.59$$

graphical integration

b) For mixed flow let's solve analytically. Note we could also solve graphically.

$$C_S = \phi(-\Delta C_A) = \frac{2C_A}{(1+C_A)^2} (4 - C_A)$$

differentiating & setting to zero gives

$$\frac{dC_S}{dC_A} = \frac{[2(4 - C_A) + 2C_A(-1)](1+C_A)^2 - 2C_A(4 - C_A)2(1+C_A)}{(1+C_A)^4} = 0$$

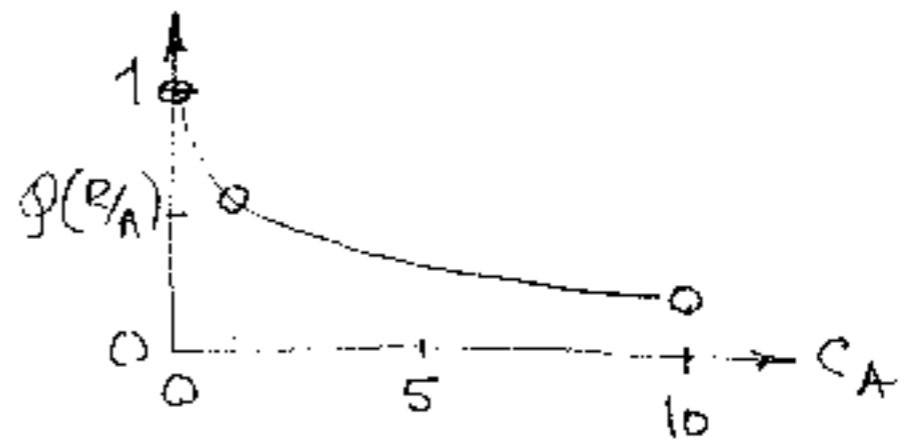
$$\therefore C_A \text{ (at } C_{S_{\text{opt}}}) = \frac{2}{3}$$

$$\phi \text{ (at } C_A = \frac{2}{3}) = \frac{2(\frac{2}{3})}{(1+\frac{2}{3})^2} = \frac{12}{25}$$

$$\therefore C_{S_{\max}} = \frac{12}{25} (4 - \frac{2}{3}) = 1.6 \leftarrow$$

7.17 For reactions in parallel first evaluate & draw the ϕ vs C_A curve

| C_A | $\phi(r_A) = \frac{16C_A^{1/2}}{16C_A^{1/2} + 12C_A + C_A^2}$ |
|-------|---|
| 10 | 0.185 |
| 1 | 0.55 |
| 0 | 1.0 |



The highest value for ϕ comes where $C_A = 0$ and where $\phi = 1$

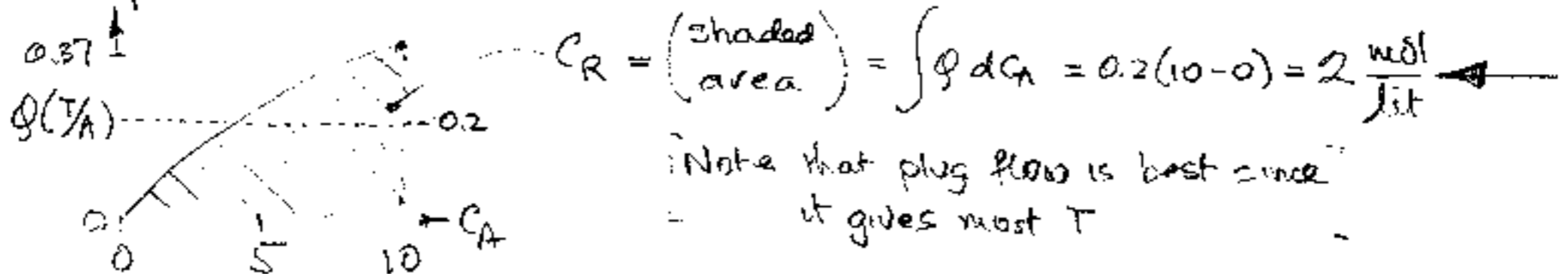
\therefore operate the mixed flow reactor at $X_A \rightarrow 1$, here



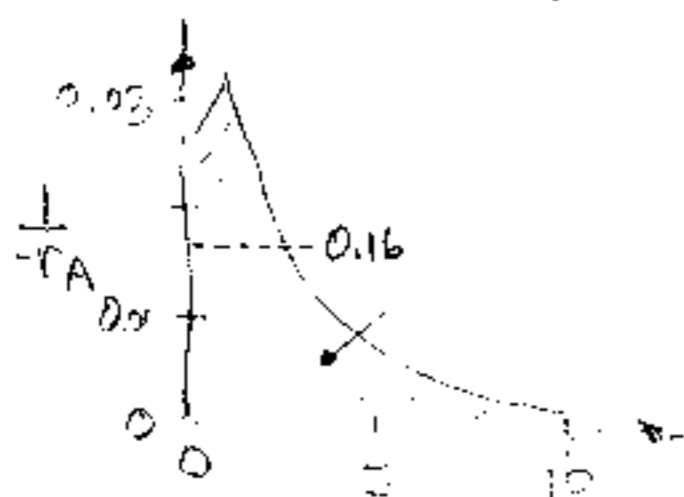
7.19 First find the ϕ vs C_A curve, then decide which reactor type to use

| C_A | $\phi(T/A) = \frac{C_A^2}{16C_A^{1/2} + 12C_A + C_A^2}$ | $\frac{1}{-r_A} = \frac{1}{16C_A^{1/2} + 12C_A + C_A^2}$ |
|-------|---|--|
| 10 | 0.37 | 0.0037 |
| 9 | 0.34 | 0.0042 |
| 4 | 0.167 | 0.0104 |
| 1 | 0.03 | 0.03 |
| 0.1 | | 0.16 |

Now plot



Next, to find τ plot $\frac{1}{-r_A}$ vs C_A

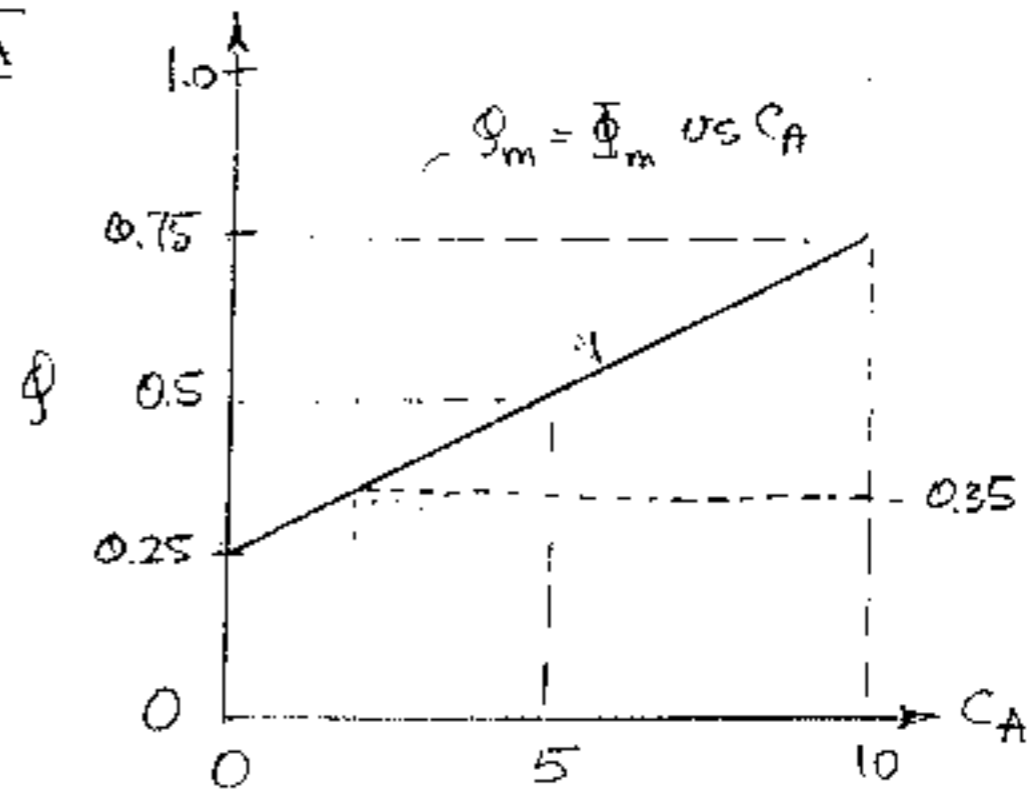


$$\tau = \int_0^{10} \frac{dC_A}{-r_A} = 0.016(10) = 0.16 \text{ min.}$$

$$\therefore V = \tau v = 0.16(1) = 0.16 \text{ m}^3 = 160 \text{ lit}$$

7.21 First let us calculate ϕ , the instantaneous fractional yield. This is obtained directly from the mixed flow run because $\phi_m = \bar{\Phi}_m$

| C_{A0} | C_A | C_R | $\phi = \bar{\Phi} = \frac{C_R}{C_{A0} - C_A}$ |
|----------|-------|-------|--|
| 100 | 90 | 7 | $7/10 = 0.7$ |
| 100 | 80 | 13 | 0.65 |
| 100 | 70 | 18 | 0.60 |
| 100 | 60 | 22 | 0.55 |
| 100 | 50 | 25 | 0.50 |
| 100 | 40 | 27 | 0.45 |
| 100 | 30 | 28 | 0.40 |
| 100 | 20 | 28 | 0.35 |
| 100 | 10 | 27 | 0.30 |
| 100 | 0 | 25 | $25/100 = 0.25$ |



So for mixed flow with $C_{A0} = 100$

$$C_{Rf} = \bar{\Phi} (-\Delta C_A) = \phi (-\Delta C_A) = 0.35 (100 - 20) = 28$$

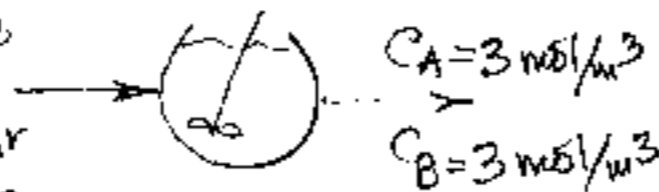
7.23

$$F_{A0} = 300 \text{ mol/hr}$$

$$C_{A0} = 30 \text{ mol/m}^3$$

$$F_{B0} = 300 \text{ mol/hr}$$

$$C_{B0} = 30 \text{ mol/m}^3$$



$$\phi(R/A) = \frac{50C_A}{50C_A + 100C_B} = \frac{1}{3}$$

$$\phi(S/A) = \frac{100C_B}{50C_A + 100C_B} = \frac{2}{3}$$

$$\therefore C_R = \phi(R/A) (-\Delta C_A) = \frac{1}{3} (30 - 3) = 9 \text{ mol/m}^3 \therefore R/S = \frac{1}{2}$$

$$V = \frac{F_{A0}}{C_{A0}} \cdot \frac{C_{A0} - C_A}{\frac{1}{20} C_A + \frac{1}{10} C_B} = \frac{300}{30} \cdot \frac{30 - 3}{\frac{3}{20} + \frac{3}{10}} = 600 \text{ lt}$$

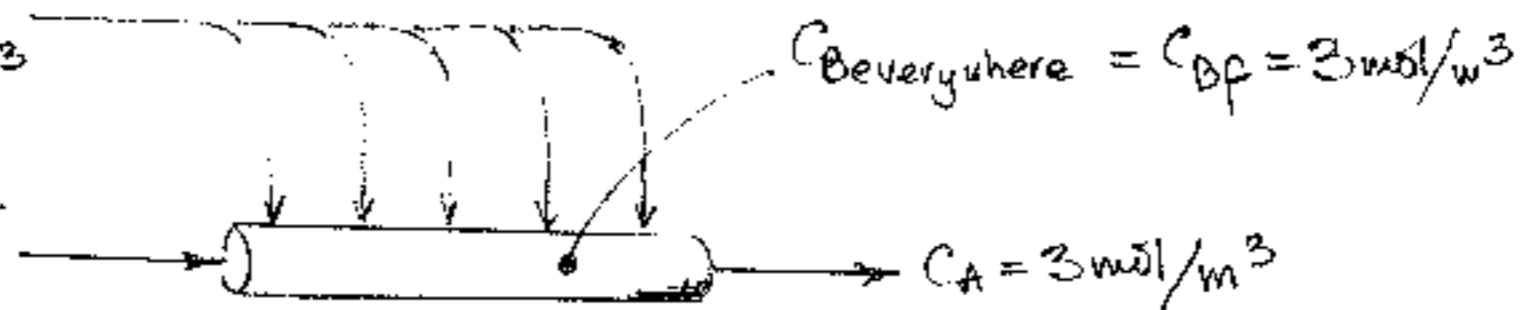
7.25

$$F_{B0} = 300 \text{ mol/hr}$$

$$C_{B0} = 30 \text{ mol/m}^3$$

$$F_{A0} = 300 \text{ mol/hr}$$

$$C_{A0} = 30 \text{ mol/m}^3$$



$$\text{Determine } \phi(R/A) = \frac{50C_A}{50C_A + 100C_B} = \frac{C_A}{C_A + 2C_B}$$

7.25
(continued)

$$\therefore C_{Rf} = \int_{C_{Af}}^{C_{A0}} q(R/A) dC_A = \int_3^{30} \frac{C_A}{C_A + 2C_B} dC_A = \left[C_A - 6 \ln(C_A + 6) \right]_3^{30} = 18.68$$

$$C_{Sf} = \int_{C_{Af}}^{C_{A0}} q(S/A) dC_A = \int_3^{30} \frac{2C_B}{C_A + 2C_B} dC_A = \left[6 \ln(C_A + 6) \right]_3^{30} = 8.32$$

$$\text{So } \frac{C_{Rf}}{C_{Sf}} = \frac{18.68}{8.32} \approx 2.25 \leftarrow$$

$$\text{Finally } V = \frac{F_{A0}}{C_{A0}} \int_{C_{Af}}^{C_{A0}} \frac{dC_A}{-r_A} = \frac{300}{30} \int_3^{300} \frac{dC_A}{50C_A + 100(3)} = \left[(10) \left(\frac{1}{50} \right) \ln(50C_A + 300) \right]_3^{300}$$

$$= 0.2773 \text{ m}^3 = 277.3 \text{ lit} \leftarrow$$

7.27 a) Villeneuve's question - What is the result of a single battle?

Let F = the number of French ships, and let B = the number of British ships. Then according to the problem statement

$$\left. \begin{aligned} -\frac{dF}{dt} &= k B \\ \frac{dB}{dt} &= k F \end{aligned} \right\} \begin{array}{l} \text{dividing one by the other} \\ \text{to eliminate the time} \\ \text{variable (as with multiple} \\ \text{reactions) we see} \end{array} \quad \frac{dF}{dB} = \frac{B}{F} \quad \dots (1)$$

Separating and integrating gives

$$\int_{F_0}^F F dF = \int_{B_0}^B B dB \quad \dots \text{ or } F_0^2 - F^2 = B_0^2 - B^2$$

If we start with $F_0 = 33$ & $B_0 = 27$, then at the end of the battle $B = 0$. Thus replacing in (1) gives

$$F^2 = 33^2 - 27^2 = 360 \quad \dots \text{ or } F = 19 - \epsilon \text{ ships} \leftarrow$$

7.27
(continued)Nelson's question - What is the result of 2 battles in succession?

Let the British fight f ships in the 1st battle, then $F_0 - f$ ships in the 2nd. Applying Eq (i) to the two battles we have

$$\text{For the 1st battle: } B_0^2 - B_1^2 = f^2 - 0$$

$$\text{For the 2nd battle: } B_1^2 - B_2^2 = (F_0 - f)^2 - 0$$

this means that the f ships are all destroyed

Combining gives

$$B_0^2 - B_2^2 = (F_0 - f)^2 + f^2 \quad \text{--- (ii)}$$

To maximize B_2 take $\frac{dB_2}{df} = 0$ from which we find $f = \frac{F_0}{2}$.

Thus the British should fight $\frac{1}{2}$ the French fleet in each battle.

So for $f = 16$ or 17 we find that the British are left with

$$B_2 = \sqrt{184}, \text{ or } 13 \text{ to } 14 \text{ ships} \leftarrow$$

The difference in the two answers shows how math. affected European history.

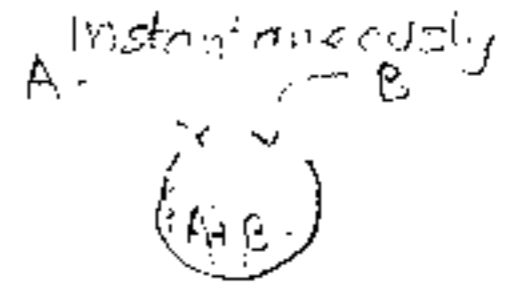
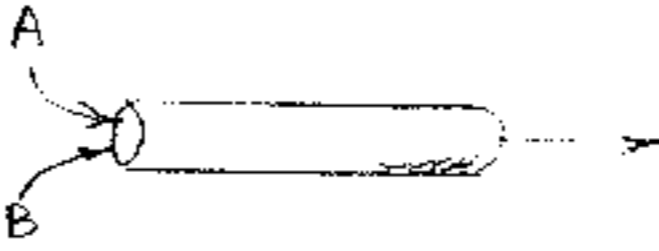
Comment Equation (i) represents the SQUARE FIREPOWER LAW. This says that the strength of a force is proportional to the square of its firepower, and it applies to battles with cooperative action. Thus 4 toughs working together as a team can take on 16 others --- one at a time.

The British war office had a couple of mathematicians on their staff who in essence did the above calculation. The French military probably were more "practical", and didn't spend money on "useless" activities.

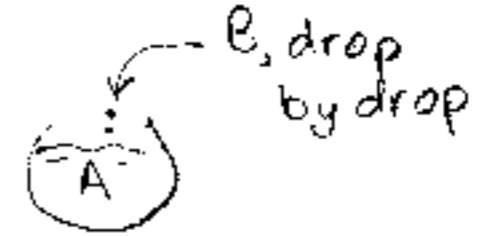
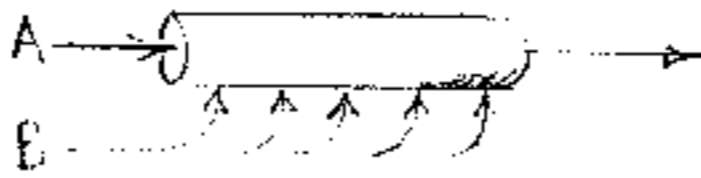
It would be interesting to consider historical battles (Thermopolae, Jutland, Coral sea, guerrilla warfare) from the standpoint of this law. For more on this subject see the section on Mathematics & Warfare in "World of Mathematics" by James Newman. This problem has many interesting extensions: suppose k values are unequal, suppose a 3rd party fights both (crazy solution), how to minimize the total killing but still achieve a decision, etc.

8.1

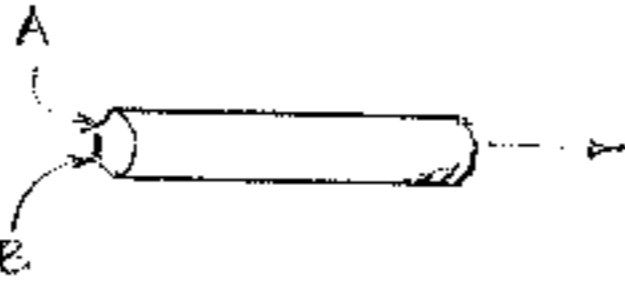
a) $r_1 = k_1 C_A C_B^2$
 $r_2 = k_2 C_R C_B$



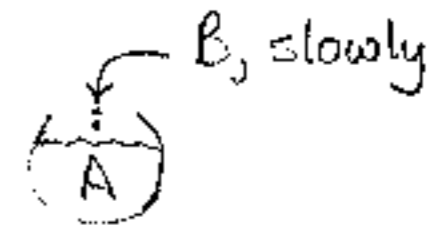
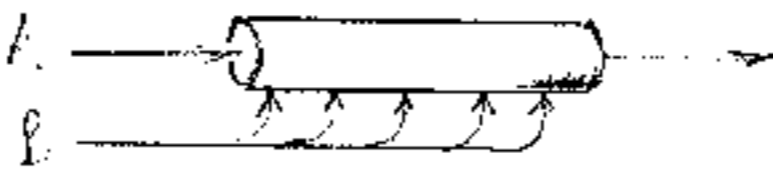
b) $r_1 = k_1 C_A C_B$
 $r_2 = k_2 C_R C_B^2$



c) $r_1 = k_1 C_A C_B$
 $r_2 = k_2 C_R^2 C_B$



d) $r_1 = k_1 C_A^2 C_B$
 $r_2 = k_2 C_R C_B$



8.3

Guess $A \rightarrow R \rightarrow S$. Now check Fig 14. This shows that the results don't fit these kinetics

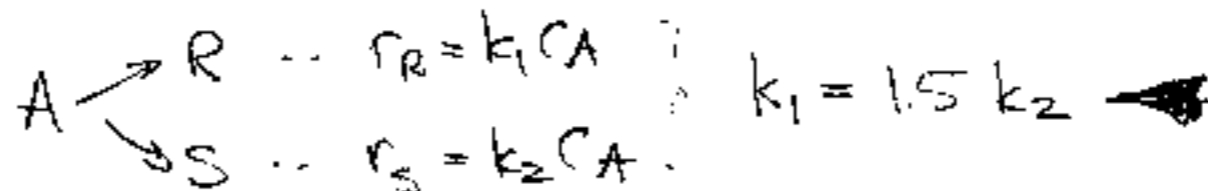
Next guess $A \rightarrow R \rightarrow S$ $\left. \begin{array}{l} r_R = k_1 C_A \\ r_S = k_2 C_A \end{array} \right\}$ Then for mixed flow

$$\tau = \frac{C_R - C_{R0}}{k_1 C_A}$$

$$\tau = \frac{C_S - C_{S0}}{k_2 C_A}$$

dividing gives $\frac{C_R}{C_S} = \frac{k_1}{k_2} = \text{constant}$

This agrees with the observed so we conclude that



8.5

Guess $A \rightarrow R \rightarrow S$. Then check Fig 14. This shows that our guess was correct and that

$$\frac{k_2}{k_1} = 0.25$$

Let us next evaluate the rate constants

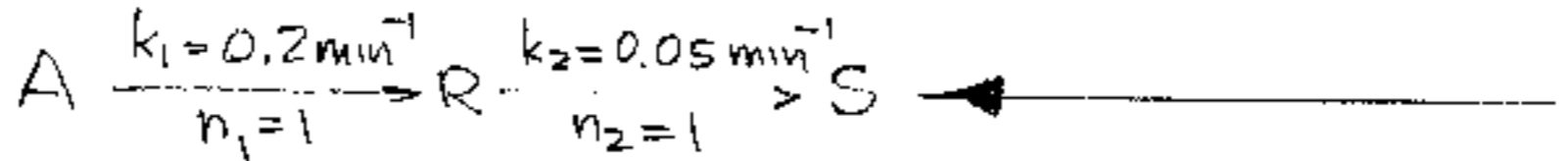
8.5
(continued)

For run 1 $\tau_1 = \frac{C_{A0} - C_A}{k_1 C_A} = \frac{100 - 50}{50 k_1} \Rightarrow k_1 = \frac{1}{\tau_1} = \frac{1}{5} = 0.2 \text{ min}^{-1}$

For run 2 $\tau_2 = \frac{100 - 20}{k_1 \cdot 20} = \frac{4}{k_1} \Rightarrow k_1 = \frac{4}{\tau_2} = \frac{4}{20} = 0.2 \text{ min}^{-1}$

these results are consistent

Therefore the kinetics are



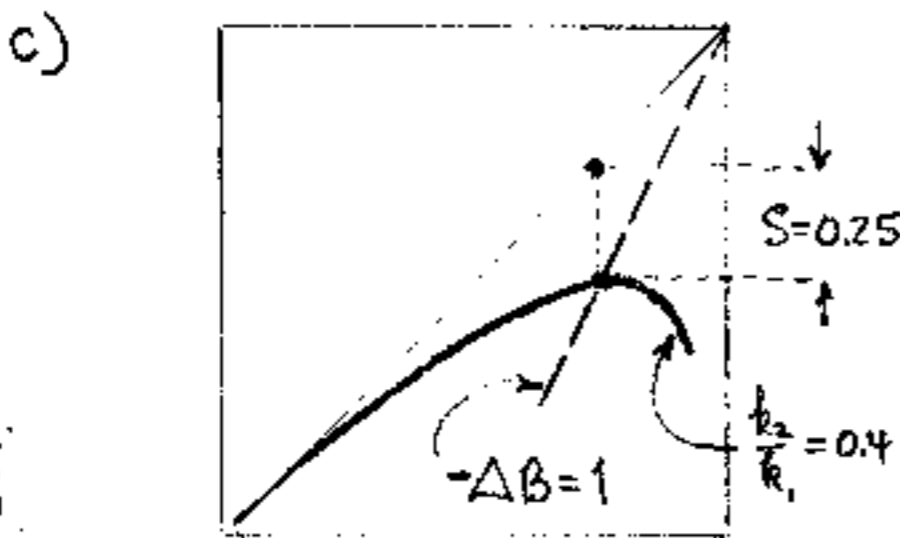
8.7 a) At the start $\begin{cases} A_0 = 1 \\ B_0 = 3 \end{cases}$
After some time $\begin{cases} B = 2.2 \\ S = 0.2 \end{cases}$

By material balance $-\Delta B = 0.8$, and using ΔB & S locates point X on Fig. 7.15.

At this point $k_2/k_1 = 0.85$

Following this k_2/k_1 line to $S = 0.6$ (point Y) gives $\begin{cases} A = 0.1 \\ R = 0.3 \\ S = 0.6 \\ B = 3 - 2(0.6) - 0.3 = 1.5 \end{cases}$ a)

b) Nothing b)

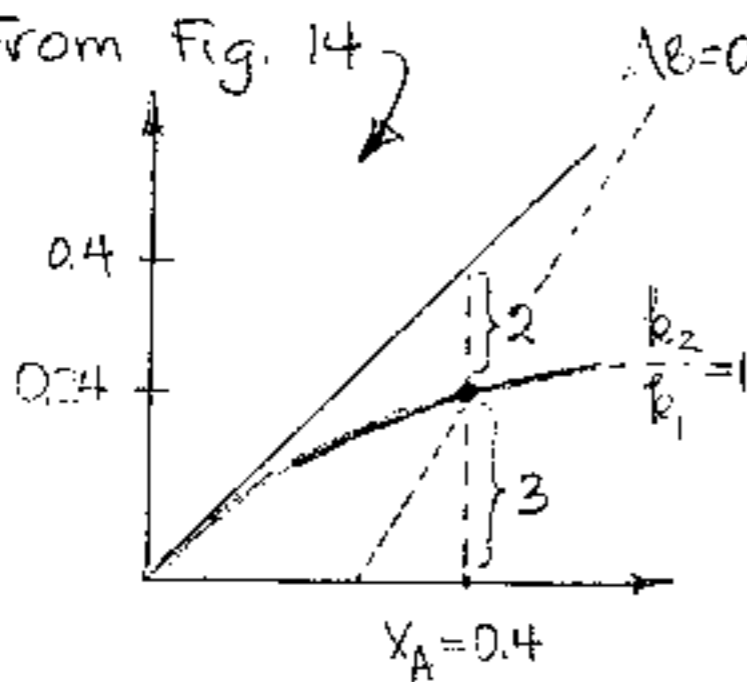


Since the reaction is rapid the R actually formed is probably less than what could be formed. Thus the observed k ratio, $k_2/k_1 = 0.4$ from Fig 7.15 is the upper bound to the true k ratio

$\therefore k_2/k_1 \leq 0.4$ c)

8.9

From Fig. 14



Thus

given $\rightarrow \frac{C_A}{C_{A0}} = 0.6$

$\frac{C_R}{C_{A0}} = 0.24$

$\frac{C_S}{C_{A0}} = 0.16$

$\frac{C_B}{C_{A0}} = 0.42$

$\frac{k_2}{k_1} = 1$

8.11 Evaluate k_1 and k_2 at various pH.

| pH | k_1 | k_2 |
|----|-------|-------|
| 2 | 3 | 11 |
| 4 | 5 | 7 |
| 6 | 7 | 11 |

From this table:

Operate at pH = 6 because it gives the highest k_1 and the highest k_2

8.13 Assume that $C_{A0} = 100$. Then

a) If you have produced lots of S & U, and if the second step reactions are relatively very slow, then the first step reactions are complete, so

$C_A = 0$ $C_R = 20$ $C_S = 20$ $C_T = 20$ and $C_U = 40$

b) The second step reactions are very fast, so any R formed has transformed into S and U. So $C_{R \text{ formed}} = 20 + 40 = 60$

Thus $C_T = \frac{1}{2} C_{R \text{ formed}} = 30$. So

$C_A = 10$ $C_R = 0$ $C_S = 20$ $C_T = 30$ and $C_U = 40$

8.17
(continued)

Integrating Eq (i) gives (see Eqs 18 and 19 in the text)

$$A = A_0 e^{-k_1 t} = 1440 e^{-t/240} \quad \dots (ii)$$

$$R = A_0 (1 - e^{-k_1 t}) - k_2 t = 1440 (1 - e^{-t/240}) - t \quad \dots (iii)$$

(a) 95% collected. From Eq (ii)

$$\frac{A}{A_0} = \frac{1}{20} = e^{-t/240}$$

or $t = 240 \ln 20 = 720 \text{ min} = 12 \text{ hr}$

∴ at 6pm 95% of the days garbage will have been collected } a)

(c) Time when bin is full. This will occur where $dR/dt = 0$. So from Eq (i)

$$\frac{dR}{dt} = 0 = k_1 A - k_2 \quad \dots \text{ or } A = \frac{k_2}{k_1} = \frac{1}{1/240} = 240 \text{ tons}$$

The time, from Eq (ii)

$$240 = 1440 e^{-t/240} \quad \dots \text{ or } t = 240 \ln 6 = 430 \text{ min}$$

(b) Max contents of the bin

or 1.20 pm } c)

$$R_{\max} = 1440 (1 - e^{-430/240}) - 430 \quad \dots \text{ or } R_{\max} = 430 \text{ tons } \leftarrow b)$$

(d) The bin empties when $R = 0$. Again look at Eq (iii)

$$R = 0 = 1440 (1 - e^{-t/240}) - t$$

or $e^{-t/240} + t = 1$

Solve by trial & error

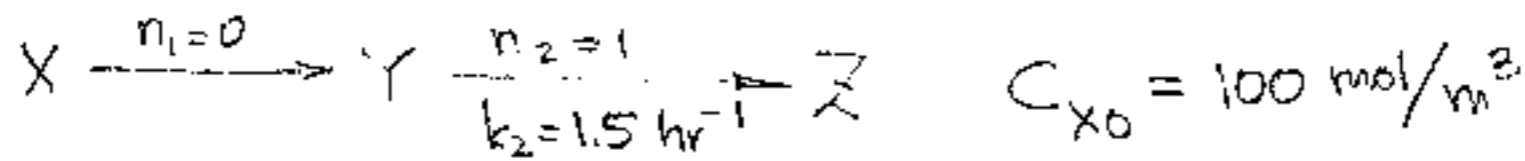
$$t = 1436 \text{ min} = 23 \text{ hr } 56 \text{ min}$$

∴ 5.56 am } d)

What this means that the incinerator works full time, the whole operation proceeds continuously

∴ It is well designed, but with nothing to spare

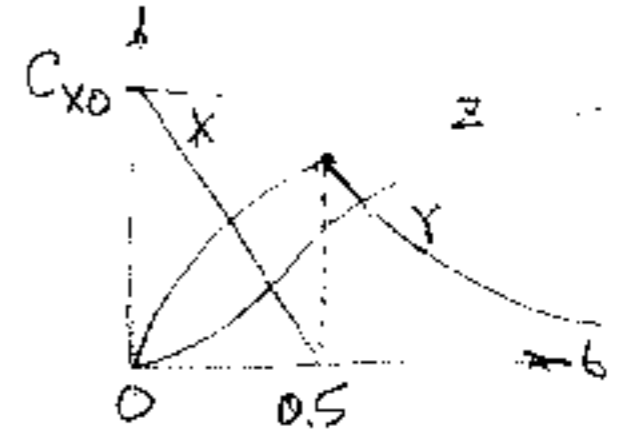
8.19 Let us follow the text. From Eq 22



We are given

$$k_1 = \frac{100 \text{ mol/m}^3}{1/2 \text{ hr}} = 200 \text{ mol/m}^3 \cdot \text{hr}$$

$$\therefore K = \frac{k_2 C_{X0}}{k_1} = \frac{(1.5)(100)}{200} = 0.75$$



(a) At half an hour one gets Y_{\max} (see Fig 8.8)

$$\frac{C_{Y_{\max}}}{C_{X0}} = \frac{1}{K} (1 - e^{-K}) = \frac{1}{0.75} (1 - e^{-0.75}) = 0.7035 \quad \leftarrow \text{a)}$$

(b) After one hour note that X is all gone and we only have Y & Z present

$$\begin{aligned} \frac{C_Y}{C_{X0}} &= \frac{1}{K} (e^{+K-k_2t} - e^{-k_2t}) \\ &= \frac{1}{0.75} (e^{-0.75-1.5} - e^{-1.5}) = 0.3323 \end{aligned}$$

$$\therefore \frac{C_Z}{C_{X0}} = 1 - 0.3323 = 0.6677 \quad \leftarrow \text{b)}$$

8.21 The reaction is $A \xrightarrow{6} R \begin{matrix} \xrightarrow{3} S \\ \xrightarrow{1} T \end{matrix}$ for which from Eq 49

$$\left(\frac{C_R}{C_{A0}}\right)_{\max} = \left(\frac{k_1}{k_{34}}\right)^{k_{34}/(k_{34}-k_1)} = \left(\frac{6}{4}\right)^{4/4-6} = 0.444$$

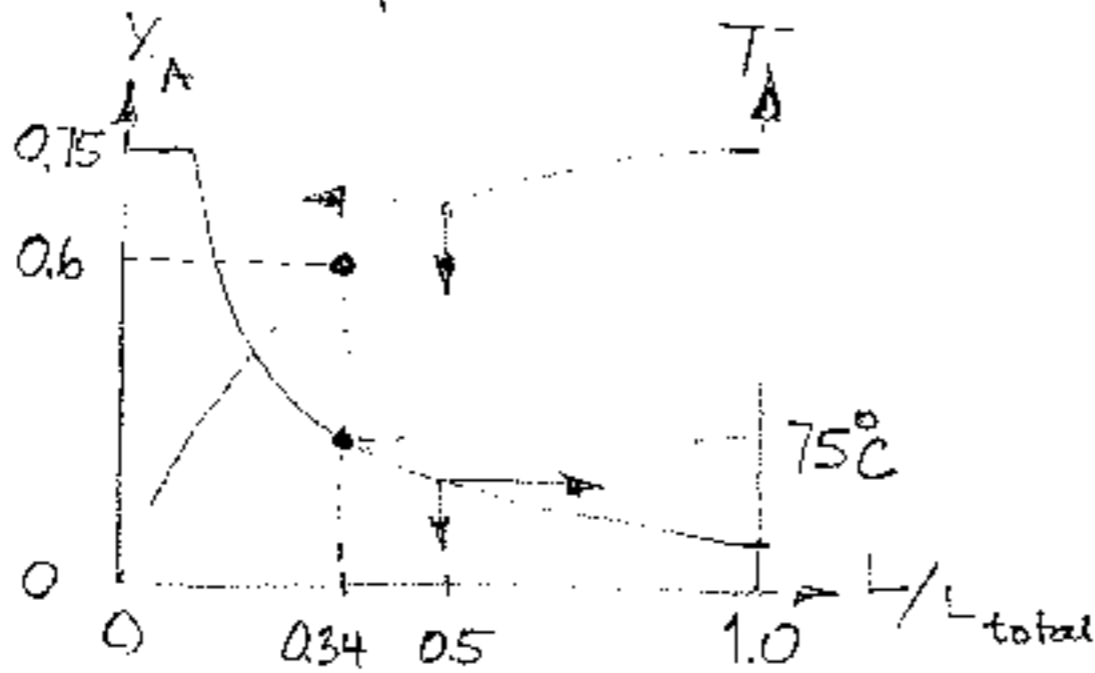
$$\text{or } C_{R_{\max}} = 0.444 \text{ mol/lit} \quad \leftarrow$$

From Eq. 50

$$t_{R_{\max}} = \frac{\ln(k_{34}/k_1)}{k_{34}-k_1} = \frac{\ln 4/6}{4-6} = 0.2027 \text{ h} = 12.2 \text{ min} \quad \leftarrow$$

Alternatively, from Fig. 13, for $\frac{k_{34}}{k_1} = \frac{2}{3}$... we find $\left(\frac{C_R}{C_{A0}}\right)_{\max} = 0.44 \quad \leftarrow$

9.1 Figure E4c presents the solution to this problem



From Fig. E4c we find $\tau_{X_A=0.6} = 0.34 \tau_{X_A=0.8}$

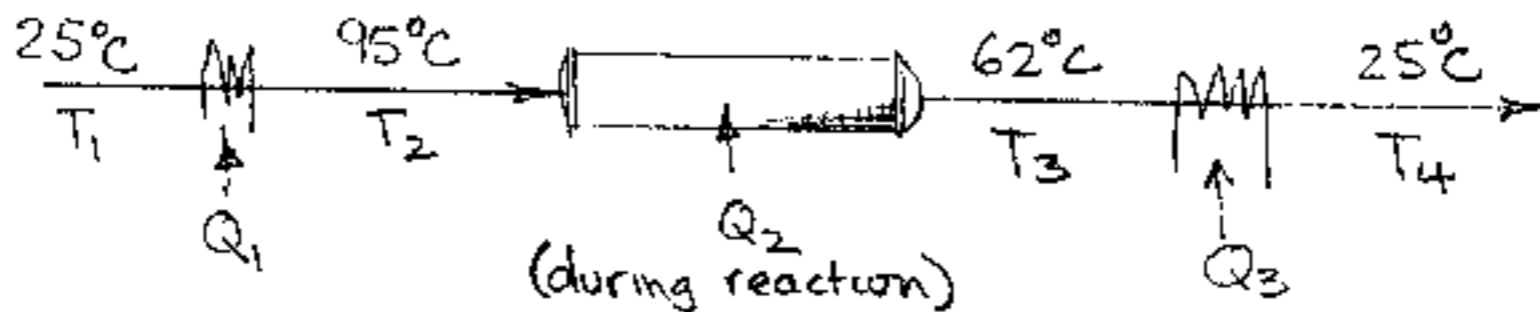
$$\therefore \tau_{X_A=0.6} = 0.34 (\tau_{X_A=0.8}) = 0.34 (1.62)$$

$$= 0.55 \text{ min} = 33 \text{ s}$$

Also

$$T_{\text{exit}} = 75^\circ \text{C}$$

9.3 From Fig E4a we find



For $C_{A0} = 4$ $C_{pA} = 1000 \text{ cal/4 mol A} \cdot \text{K} = 250 \text{ cal/mol A} \cdot \text{K}$

So the heat added to the flowing stream is

$$Q_1 = C_p (T_2 - T_1) = 250 (95 - 25) = +17500 \text{ heat} \quad \text{a)}$$

$$Q_2 = C_p (T_3 - T_2) + \Delta H_r (X_A) = 250 (62 - 95) + (-18000) 0.8$$

$$= -22650 \text{ cool} \quad \text{b)}$$

$$Q_3 = C_p (T_4 - T_3) = 250 (25 - 62) = +9250 \text{ cool} \quad \text{c)}$$

9.5 (a) Redo Example 4 with one change: $C_{A0} = 4 \rightarrow C_{A0} = 1 \text{ mol/lit.}$

Now for any first order reaction, reversible or irreversible, the X_A vs T curves are the same for all C_{A0} , except that the values of the rate curves are proportional to C_{A0} . So all the rate values in this problem are $1/4$ of those shown in Fig E4b. Thus the area under the $-1/r_A$ vs X_A curve is 4 times as great as that shown in Fig E4b, or

$$\text{area} = 4(0.405) = 1.62$$

Now for any reactor in plug flow

$$\frac{\tau}{C_{A0}} = \frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A} = \left(\text{area under the } \frac{1}{-r_A} \text{ vs } X_A \text{ curve.} \right) \quad \dots \quad (1)$$

$$\therefore \tau = C_{A0}(\text{area}) = 1(1.62) = 1.62 \text{ min}$$

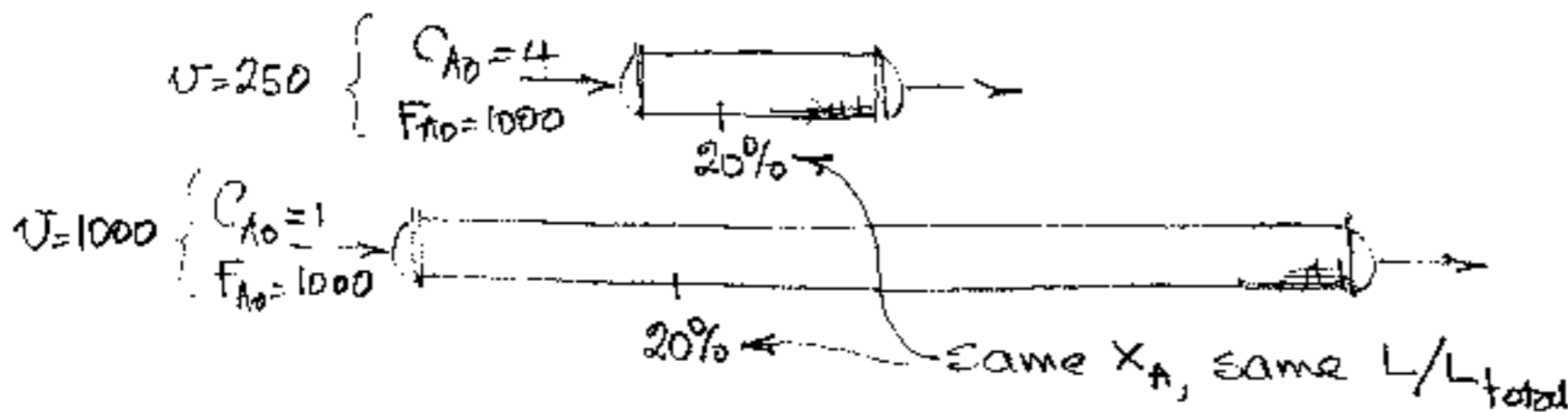
Also, from Eq (1),

$$V = F_{A0}(\text{area}) = 1000(1.62) = 1620 \text{ lit} \\ = 1.62 \text{ m}^3 \quad \left. \right\} \leftarrow \text{--- (2)}$$

This means that the reactor is 4 times as long as in Ex4.

(b) Since this is a first order reversible reaction the X_A vs T chart remains unchanged except that the values of the rate curves are one quarter of the values shown in Fig E4a.

\therefore the X_A vs L/L_{total} curves remain unchanged $\leftarrow \text{--- (b)}$



9.7 Redo Example 6 with one change: $C_{A0} = 4 \rightarrow C_{T0} =$

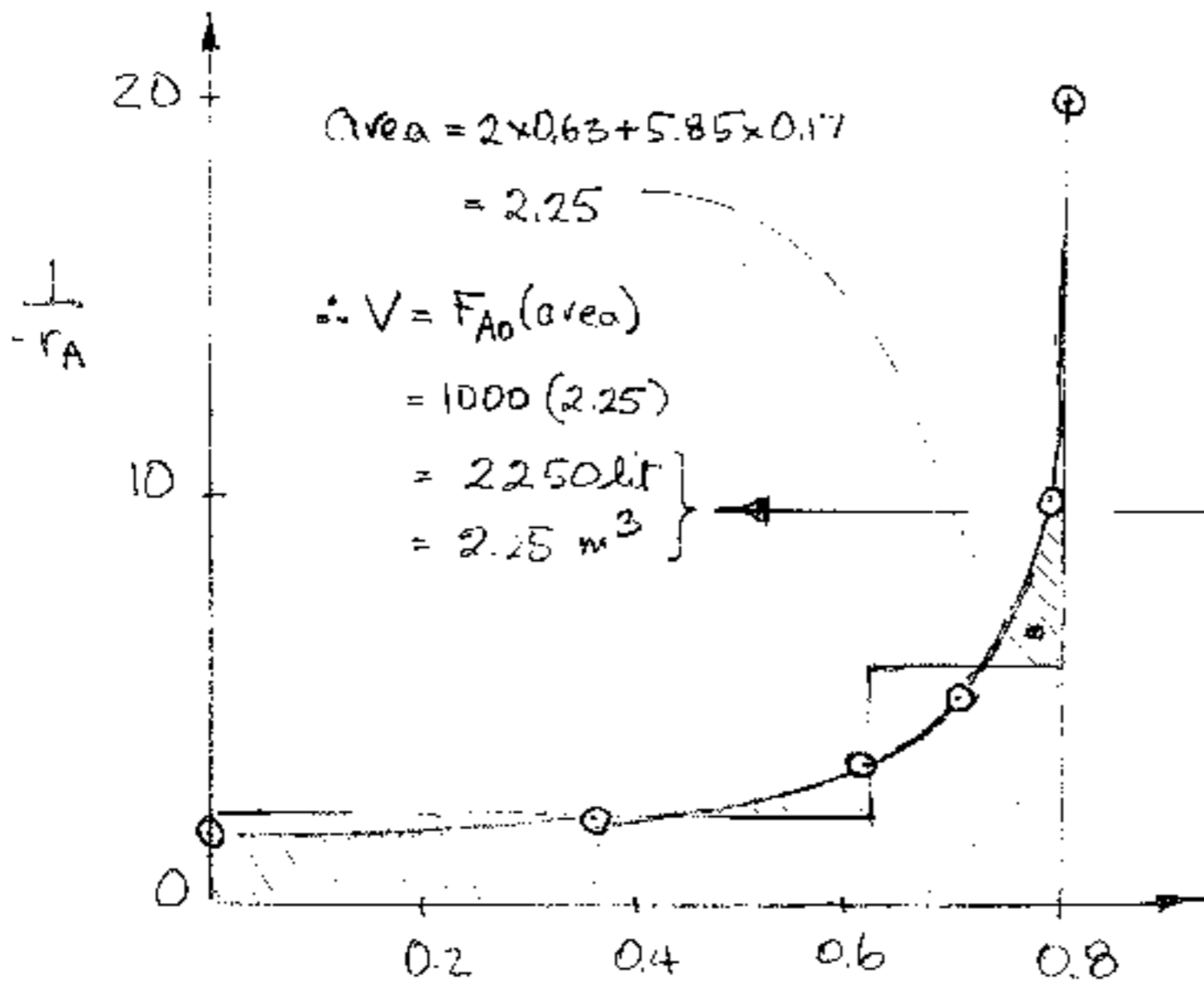
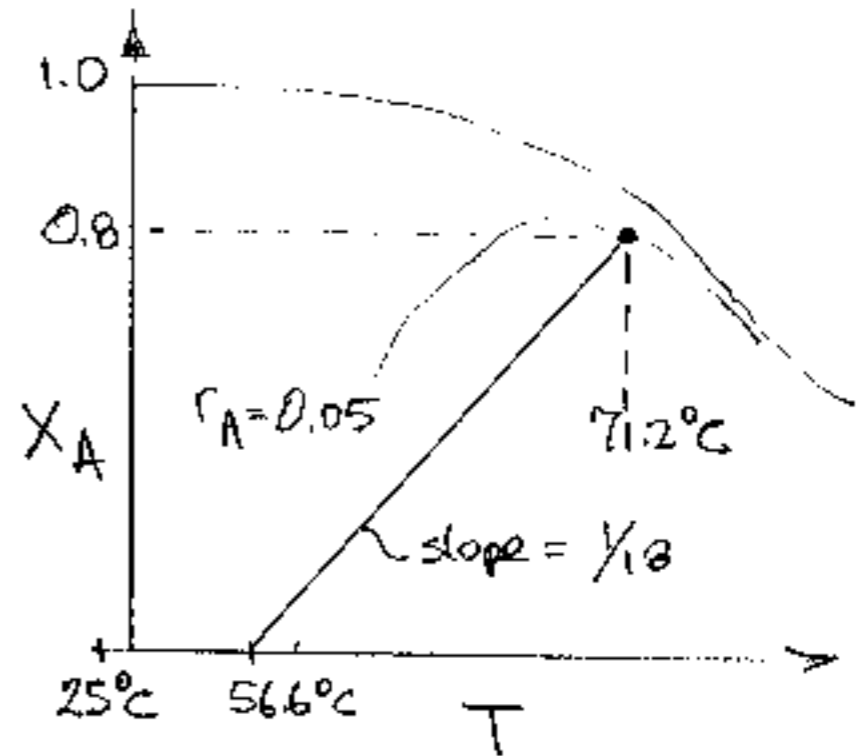
Here $C_p = 1000 \text{ cal/mol A}$

Therefore the slope of the adiabatic

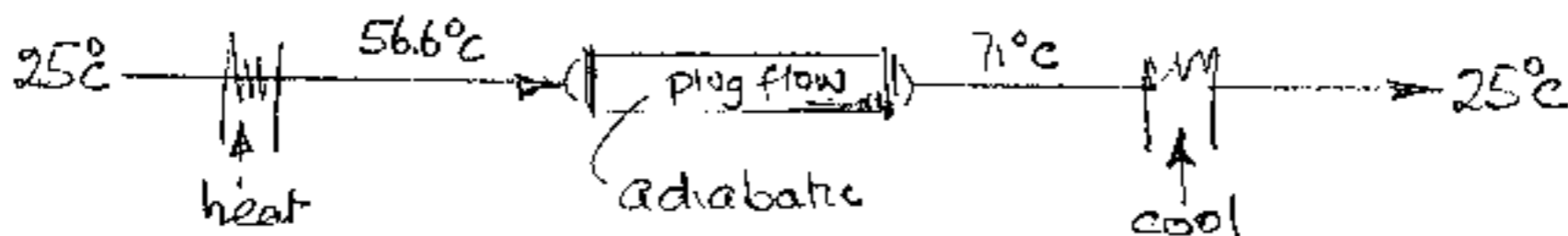
$$\text{slope} = \frac{C_p}{\Delta H_r} = \frac{1000}{-18000} = -\frac{1}{18}$$

Next, from Fig E3 directly we get

| X_A | $-r_A$ | $-Y r_A$ |
|-------|--------|----------|
| 0.9 | 0.05 | 20 |
| 0.785 | 0.1 | 10 |
| 0.705 | 0.2 | 5 |
| 0.62 | 0.3 | 3.3 |
| 0.36 | 0.5 | 2 |
| 0 | 0.6 | 1.66 |



Here the feed must be heated, not cooled



9.9 Look at Fig E3 which is drawn for $C_{A0} = 1 \text{ mol/lit}$.
 At $X_A = 0.95$ the highest reaction rate occurs at 45°C with a rate between 0.0075 and $0.008 \text{ mol/lit}\cdot\text{min}$.

So for $C_{A0} = 10$ we have $-r_A = 0.075 \sim 0.08$
 and for mixed flow

$$\tau = \frac{V}{v} = \frac{C_{A0} - C_{Af}}{-r_{Af}}$$

or

$$V = v \frac{(C_{A0} - C_{Af})}{-r_{Af}} = 100 \frac{(10 - 0.5)}{(0.075 \sim 0.08)} = 12667 \sim 11875 \text{ lit} \leftarrow$$

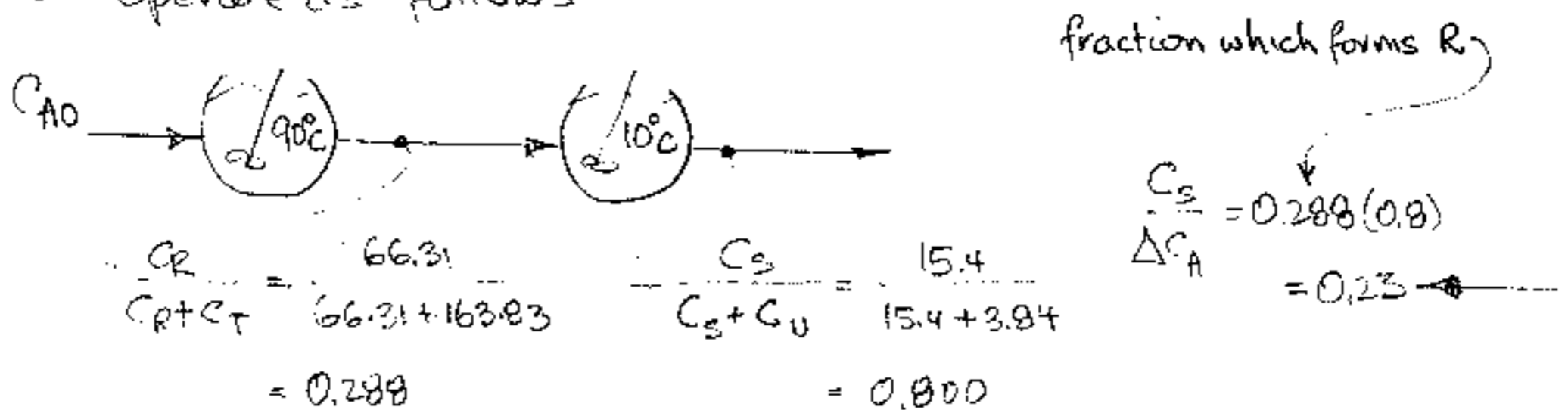
$$= 11.9 \sim 12.7 \text{ m}^3 \leftarrow$$

9.11 Because $E_1 > E_2$ and because $E_3 < E_4$ we want the first step to occur at high temperature, the second at low T. So let us evaluate the rate constants at these extremes.

| | $10^\circ\text{C} = 283\text{K}$ | $90^\circ\text{C} = 363\text{K}$ |
|-------|----------------------------------|----------------------------------|
| k_1 | 0.6199 | 66.21 |
| k_2 | 7.27 | 163.83 |
| k_3 | 15.4×10^{-7} | 0.0017 |
| k_4 | 3.84×10^{-7} | 0.0044 |

At the high temperature the rate constants of the first step are $\sim 10^4$ times larger than the rate constants for the 2nd step. So we can reasonably assume that the 2nd step does not go to any extent.

Then when all the A is gone we operate at low temperature. So operate as follows



10.1 For the 4 schemes: G, N, N, G ←

10.3 Here we have: N, N, N, G ←

10.5 a) We should operate at the maximum allowable temperature when

$$E_1 > E_2 \text{ and } E_1 > E_2 \quad \leftarrow \quad \text{a)}$$

b) We should have a falling temperature when

$$E_1 > E_3 \text{ and } E_1 < E_2 \quad \leftarrow \quad \text{b)}$$

10.7 From Example 1

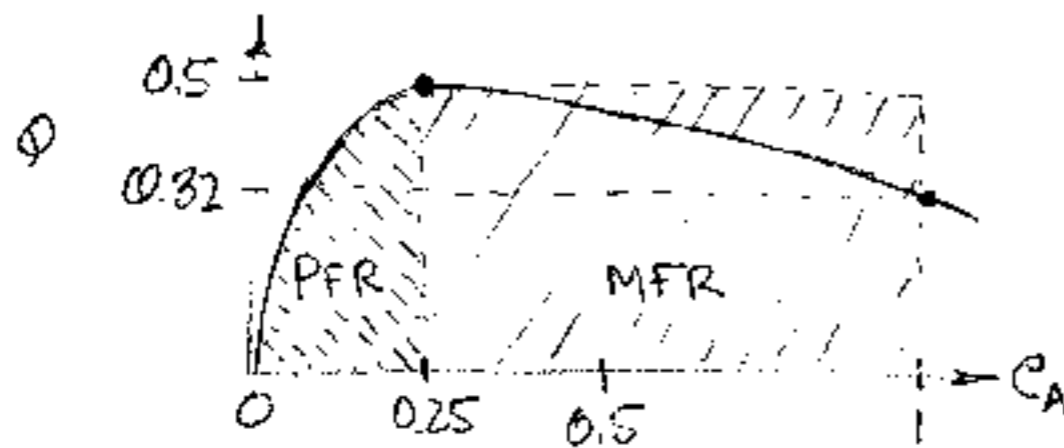
$$\phi(S/A) = \frac{0.2C_A}{0.025 + 0.2C_A + 0.4C_A^2}, \text{ and}$$

$$C_A = 0.25$$

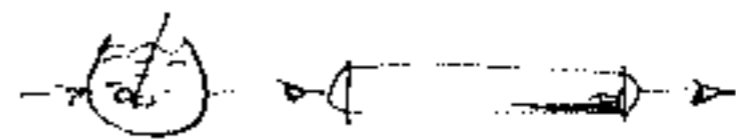
$$C_S = 0.375$$

$$\phi_{\max} = \frac{0.375}{1 - 0.25} = 0.5$$

The ϕ vs C_A curve is



so use MFR followed by PFR



For MFR: $C_{Sm} = \phi(C_{A0} - C_A) = 0.5(1 - 0.25) = 0.375$

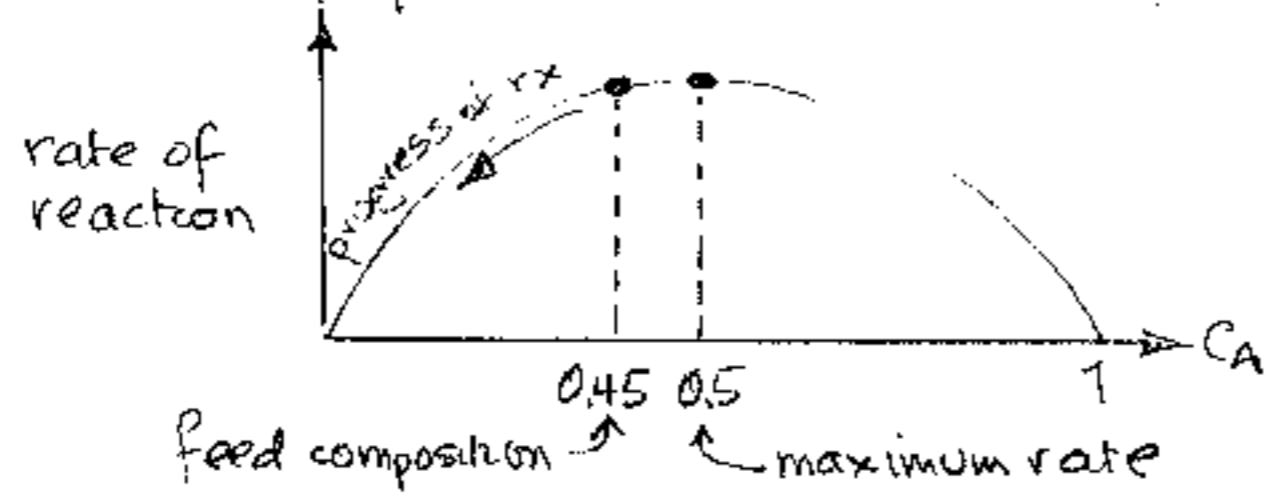
For PFR: $C_{Sp} = \int \phi dC_A = \int \frac{8C_A dC_A}{1 + 8C_A + 16C_A^2} = 8 \int_0^{0.25} \frac{C_A}{(1 + 4C_A)^2} dC_A$

But from a table of integrals: $\int \frac{x}{(a+bx)^2} dx = \frac{a}{b^2(a+bx)} + \frac{1}{b^2} \ln(a+bx) \Big|_0^2$

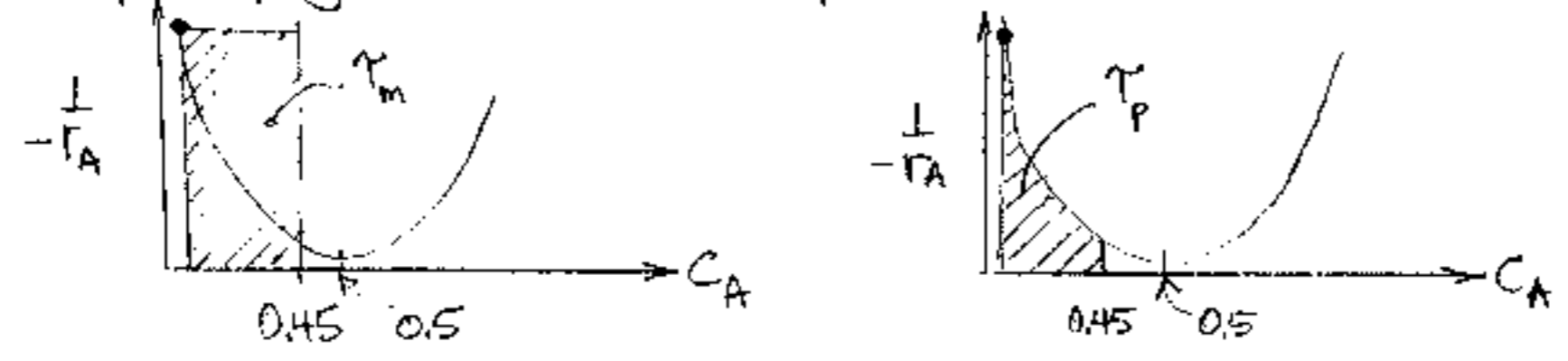
$$C_{Sp} = \left[\frac{1}{16} \frac{1}{1+4x} + \frac{1}{16} \ln(1+4x) \right]_0^{0.25} = \frac{1}{2} \left[\frac{1}{2} + \ln 2 - 1 \right] = 0.0966$$

$$\therefore C_{\text{total}} = C_{Sm} + C_{Sp} = 0.375 + 0.0966 = 0.4716 \quad \leftarrow$$

10.9 Since $C_A + C_B = 1$ for all C_A the maximum rate is at $C_A = C_B = 0.5$. Check this if you don't believe it. Thus

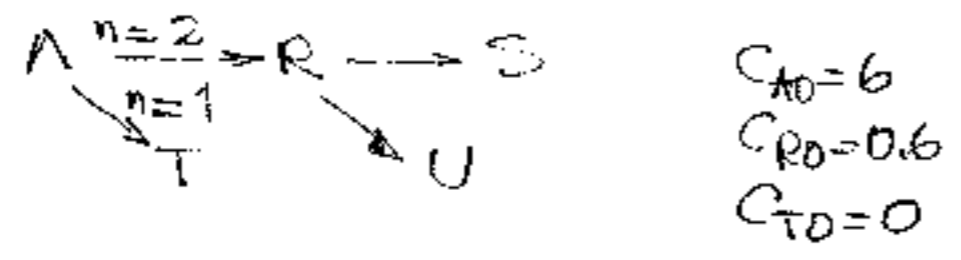


Compare plug with mixed flow performance



Plug flow is best. Do not use recycle as recommended in Fig P9

10.11



the feed has $C_R/C_T = \infty$.

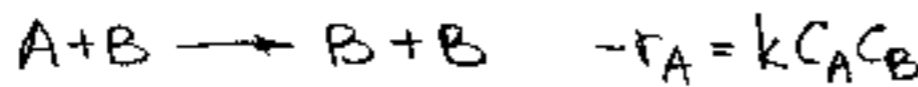
(a) So to maximize C_R/C_T do not react at all } ← a)
 The design of Fig P11 is no good }

(b) To minimize C_R/C_T run to completion. All the R will disappear. ← b)

Next reaction 1 is second order }
 reaction 2 is first order } keep C_A low

So use a large MFR, you will end up with most C_T ← b)

10.13

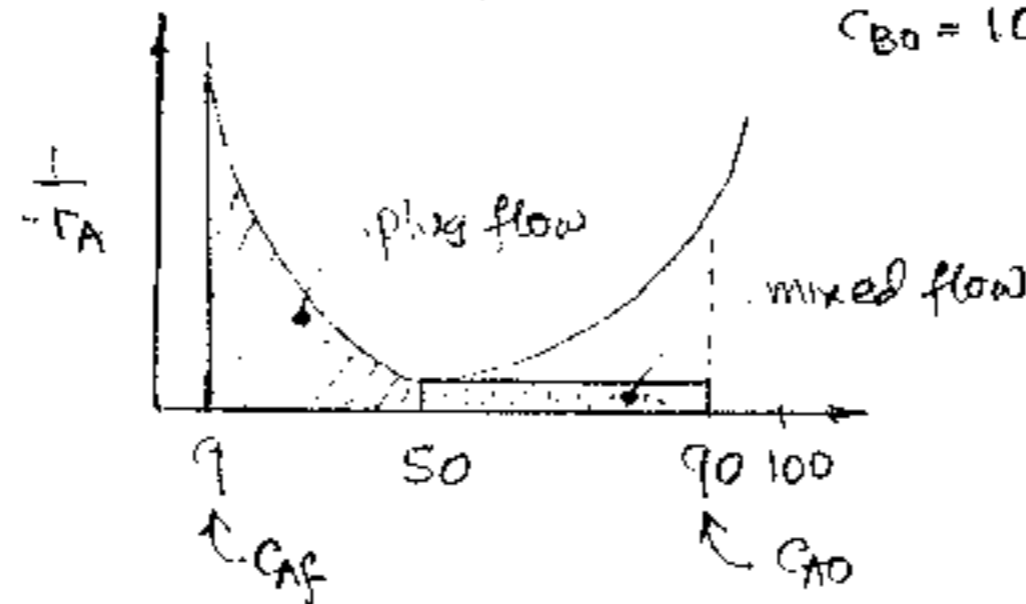


$$C_{A0} = 90$$

$$C_{B0} = 10$$

$$C_{Af} = 9$$

$$C_{Bf} = 91$$



Use a MFR followed by a PFR

10.15

Since $E_1 > E_2$ use a high temperature, or $T = 90^\circ\text{C}$

At $90^\circ\text{C} = 363\text{K}$ $k_1 = 30 e^{-20000/8.314(363)} = 0.0397 \text{ min}^{-1}$

$$k_2 = 1.9 e^{-15000/8.314(363)} = 0.0132 \text{ min}^{-1}$$

$$\therefore k_2/k_1 = 0.3322$$

From Fig 8.13 or Eqs 8.8 & 8.9 $\frac{C_{Rmax}}{C_{A0}} = 0.58$

$$t_{opt} = \frac{\ln(k_2/k_1)}{k_2 - k_1} = \frac{\ln 0.3322}{0.0132 - 0.0397} = 41.6 \text{ min}$$

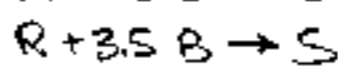
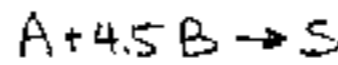
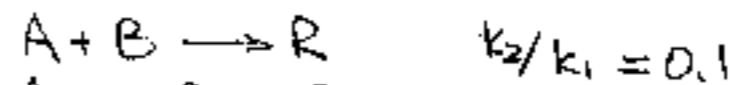
10.17

Let $A = C_3H_6$

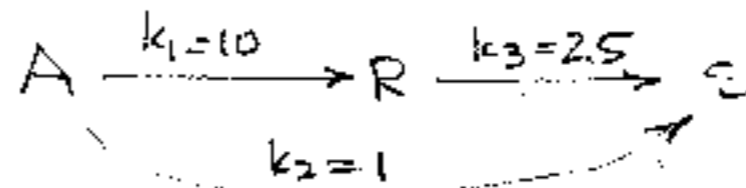
$B = O_2$

$R = C_3H_4O$ (desired)

then



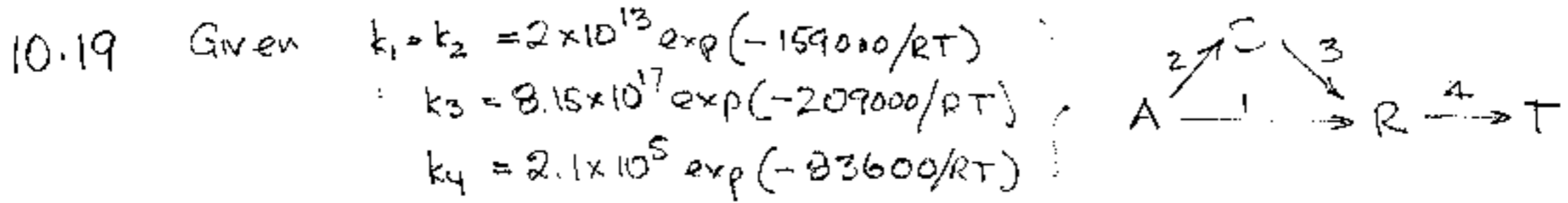
Rewrite the rates



From the Denbigh reaction set, eq 49 gives

$$\frac{C_{Rmax}}{C_{A0}} = \frac{k_1}{k_{12}} \left(\frac{k_{12}}{k_3} \right)^{k_3/(k_3-k_{12})} = \frac{10}{11} \left(\frac{11}{2.5} \right)^{2.5/(2.5-11)} = 0.588$$

Use plug flow



Since E_4 is much smaller than all the other E values use the highest allowable temperature, or 1200K.

At 1200K

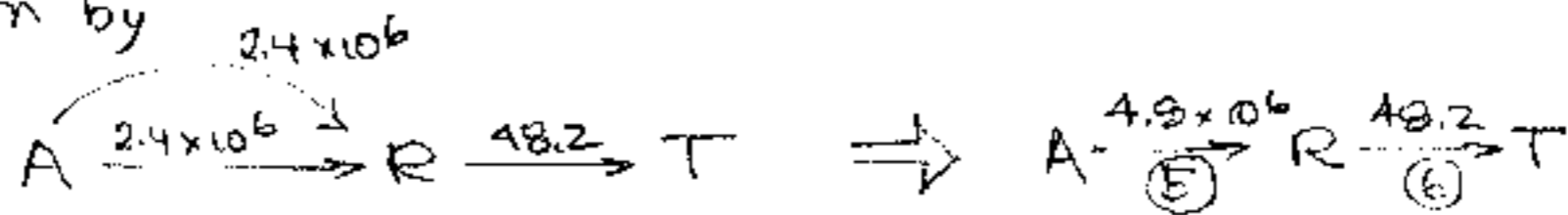
$$k_1 = 2.4 \times 10^6 \text{ hr}^{-1}$$

$$k_2 = 2.4 \times 10^6 \text{ hr}^{-1}$$

$$k_3 = 650 \times 10^6 \text{ hr}^{-1}$$

$$k_4 = 48.2 \text{ hr}^{-1}$$

Next since k_3 is much bigger than k_2 we can approximate the reaction by



Now find C_{Rmax} from Eq 8.8

$$\frac{C_{Rmax}}{C_{A0}} = \left(\frac{k_5}{k_6} \right)^{k_6/k_6 - k_5} = \left(\frac{4.8 \times 10^6}{48.2} \right)^{48.2/48.2 - 4.8 \times 10^6} = 0.99988$$

and

$$\bar{t}_{plug} = \frac{\ln(k_2/k_1)}{k_2 - k_1} = 2.4 \times 10^{-6} \text{ hr} = 0.0086 \text{ s}$$

With such a small time and such a high conversion practically any kind of reactor would be OK but in all cases straight plug flow is best

Do not recycle or bypass

Note: In the article mentioned in the problem statement the minimum residence time allowed was 1.8 s. For this, C_R is lower than C_{Rmax} . From Eq 8.7 we find, for this time

$$\frac{C_R}{C_{A0}} = \frac{k_5}{k_6 - k_5} \left[e^{-k_1 t} - e^{-k_2 t} \right] = (-1) \left[0 - 0.9762 \right] = 0.9762$$

11.1 a) Check to see if the results are consistent

By material balance: $\text{area} = \frac{M}{v} = \frac{1 \text{ mol}}{4 \text{ lit/min}} = 0.25 \text{ mol} \cdot \text{min/lit}$

From the graph: $\text{area} = (0.05 \text{ mol/lit})(5 \text{ min}) = 0.25 \text{ mol} \cdot \text{min/lit}$ } check

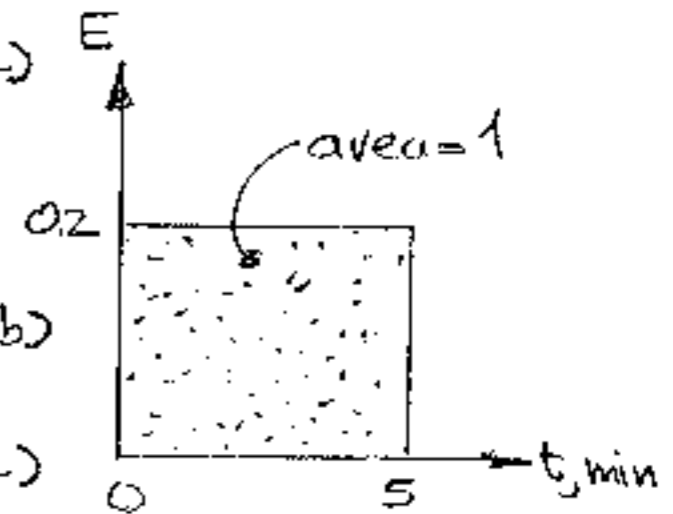
So the results are consistent ← a)

b) Mean $\bar{t} = V/v$ or $V = \bar{t}v = 2.5 \times 4 = 10 \text{ lit}$

by inspection ← b)

c) Find the E curve, from $t=0$ to 5

$E = \frac{C}{M/v} = \frac{C}{v/4} = 4C = 0.2$ ← c)



11.3 a) Check for consistency

By material balance: $\bar{t} = V/v = 60/4 = 15 \text{ sec}$

But from the experimental curve:

$\bar{t} = \frac{1}{2}(18 \times 1 + 21 \times 2) = 20 \text{ sec}$

compare

The tracer comes out too late. Thus the experiment was done incorrectly. Inconsistent ← something is wrong

11.5 a) From experiment

Mean of the curve: $\bar{t} = \frac{\sum tC}{\sum C} = \frac{30(15 \cdot \frac{h}{2}) + 65(90 \cdot \frac{h}{2})}{105 \cdot \frac{h}{2}} = 60 \text{ days}$

Area under the curve: $A = \frac{(120-20)}{2} \cdot 10^{-6} = 52.5 \frac{\text{unit} \cdot \text{days}}{\text{m}^3}$

From the material balance

$\text{Area} = \frac{M}{v}$

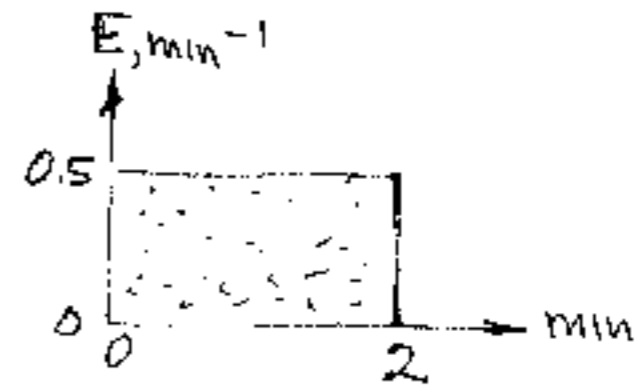
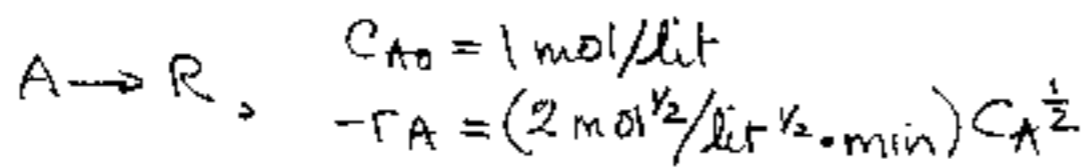
$\therefore M = (A)v = (52.5 \times 10^{-6} \frac{\text{unit} \cdot \text{day}}{\text{m}^3})(6000 \frac{\text{m}^3}{\text{s}})(\frac{3600 \times 24 \text{ s}}{\text{day}}) = 27216 \text{ units}$

b) Also because $\bar{t} = \frac{V}{v}$

$V = (\bar{t})v = 60 \text{ days}(6000 \frac{\text{m}^3}{\text{s}})(\frac{3600 \times 24 \text{ s}}{\text{day}}) =$

$= 3.11 \times 10^{10} \text{ m}^3$ ← b)

11.7 Calculate the conversion for



The performance equation is

$$\frac{C}{C_0} = \int_0^{\infty} \left(\frac{C}{C_0}\right)_{\text{batch}} E dt$$

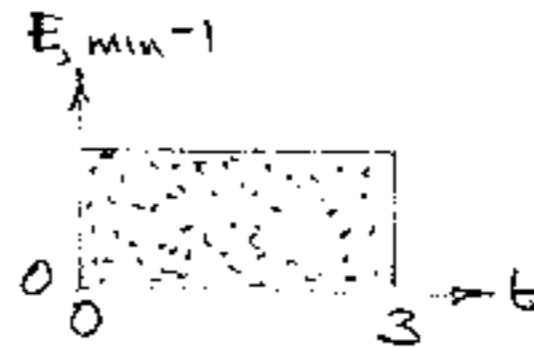
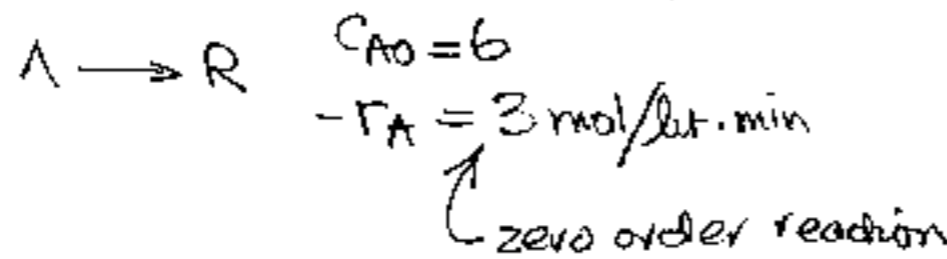
from Eq 3.29

$$\left. \begin{aligned} (n-1)k(C_{A0})^n t &= \left(\frac{C_A}{C_{A0}}\right)^{1-n} - 1 \\ \text{or } (-\frac{1}{2})(2)(1)t &= \left(\frac{C_A}{C_{A0}}\right)^{1/2} - 1 \\ \text{or } \frac{C_A}{C_{A0}} &= (1-t)^2 \end{aligned} \right\} \text{for a batch of material}$$

$$\therefore \frac{C}{C_0} = \int_0^2 (1-t)^2 \left(\frac{1}{2}\right) dt = \frac{0.5}{3} (1-t)^3 \Big|_0^2 = \frac{1}{6} (1+1) = \frac{1}{3}$$

$$\therefore X_A = \frac{2}{3} \leftarrow$$

11.9 Calculate the conversion for



The performance equation is $\frac{C_A}{C_{A0}} = \int_0^{\infty} \left(\frac{C_A}{C_{A0}}\right) E dt$

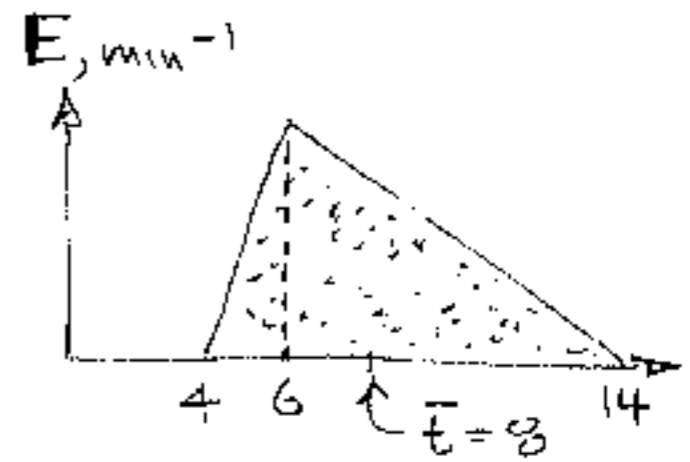
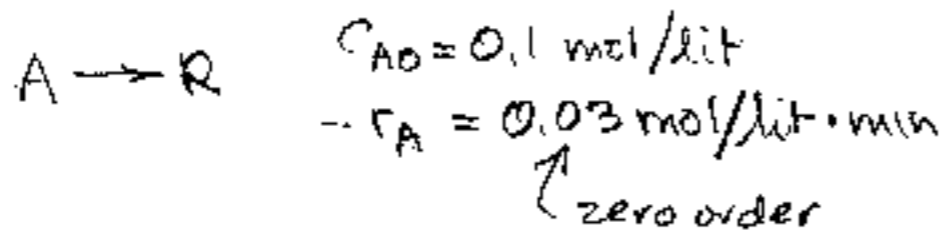
$$\left. \begin{aligned} \text{From Eq 3.31 } \dots \quad \frac{C_A}{C_{A0}} &= 1 - \frac{kt}{C_{A0}} \quad \text{for } t < \frac{C_{A0}}{k} = \frac{6}{3} = 2 \\ \frac{C_A}{C_{A0}} &= 0 \quad \text{for } t > 2 \end{aligned} \right\} \text{replace into above}$$

$$\frac{C_A}{C_{A0}} = \int_0^2 \left(1 - \frac{kt}{C_{A0}}\right) \frac{1}{3} dt = \int_0^2 \left(1 - \frac{3}{6}t\right) \frac{1}{3} dt = \frac{1}{6} \int_0^2 (2-t) dt$$

$$= \frac{1}{6} \left[\frac{(2-t)^2}{2} \right]_0^2 = \frac{1}{6} \left[\frac{2^2}{2} - 0 \right] = \frac{1}{3}$$

$$\therefore X_A = \frac{2}{3} \leftarrow$$

11.11 Calculate the conversion for



Performance equation

$$\frac{C_A}{C_{A0}} = \int \frac{C_A}{C_{A0}} E dt$$

From Eq 3.31 ... zero order

$$\frac{C_A}{C_{A0}} = 1 - \frac{kt}{C_{A0}} = 1 - \frac{0.03}{0.1} t \quad \dots \text{ for } t < \frac{C_{A0}}{k} = \frac{0.1}{0.03} = 3.33 \text{ min}$$

$$\frac{C_A}{C_{A0}} = 0 \quad \dots \text{ for } t > 3.33 \text{ min}$$

Here, nothing leaves the reactor before 4 min, so everything has reacted

$C_{Af} = 0, X_{Af} = 1$

11.13 For the solid particles

$$1 - X = \int (1 - X) E dt = \int_0^1 \left(1 - \frac{t}{1}\right)^3 \delta(t - t_0) dt$$

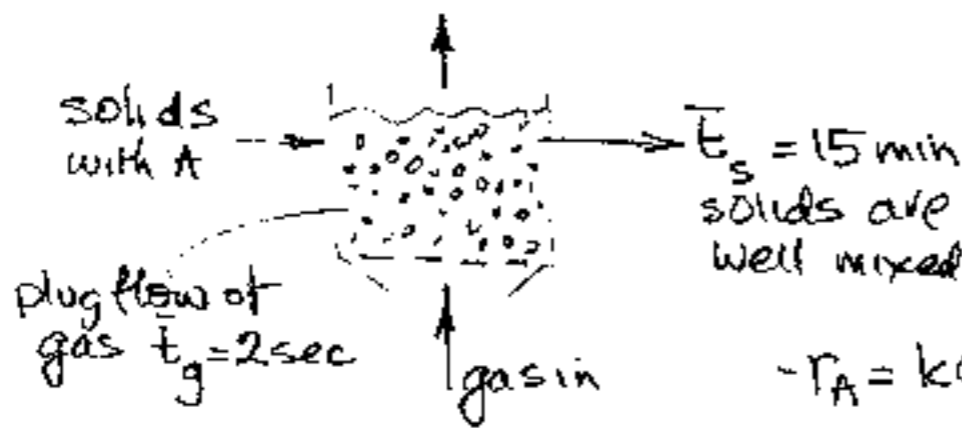
\uparrow
= 1 hr

$$= (1 - t)^3 \Big|_{\text{at } t = \frac{1}{2}} = \left(\frac{1}{2}\right)^3 = 0.125$$

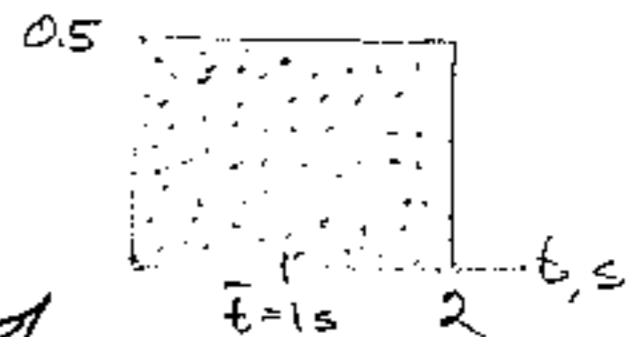


$\therefore X = 1 - 0.125 = 0.875$

11.15



E of A in the bed, A if unreacted



Conversion of A

A is released uniformly by solids, so

$$\frac{C_A}{C_{A0}} = \int \left(\frac{C_A}{C_{A0}}\right) E dt = \int_0^2 e^{-kt} \cdot 0.5 dt = 0.5 \int_0^2 e^{-t} dt = 0.5 e^{-t} \Big|_0^2 = 0.5 \left(1 - e^{-2}\right) = 0.4323$$

$\therefore X_A = 0.5677$

fraction of A decomposed.

12.1

This looks like two plug flow units side by side, from fig 1 with

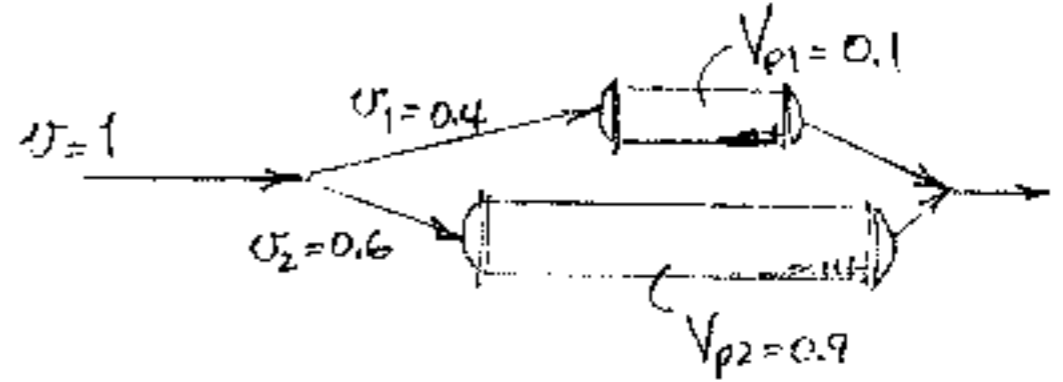
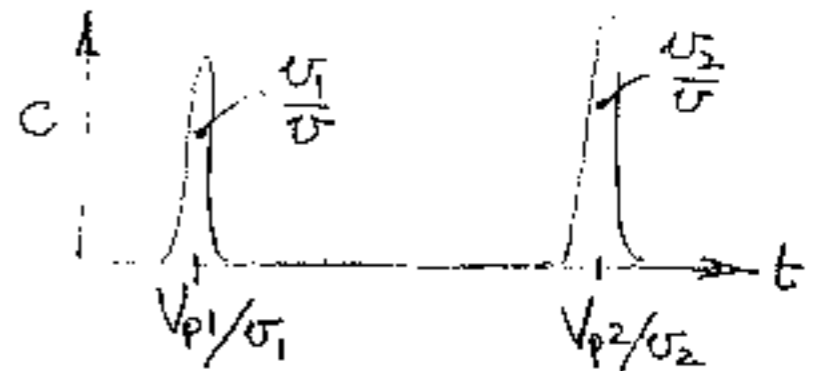
$V_{total} = 1 m^3$ and $U = 1 m^3/s$ we have

$$U_1 = \frac{16}{16+24} = 0.4 m^3/min$$

$$U_2 = \frac{24}{16+24} = 0.6 m^3/min$$

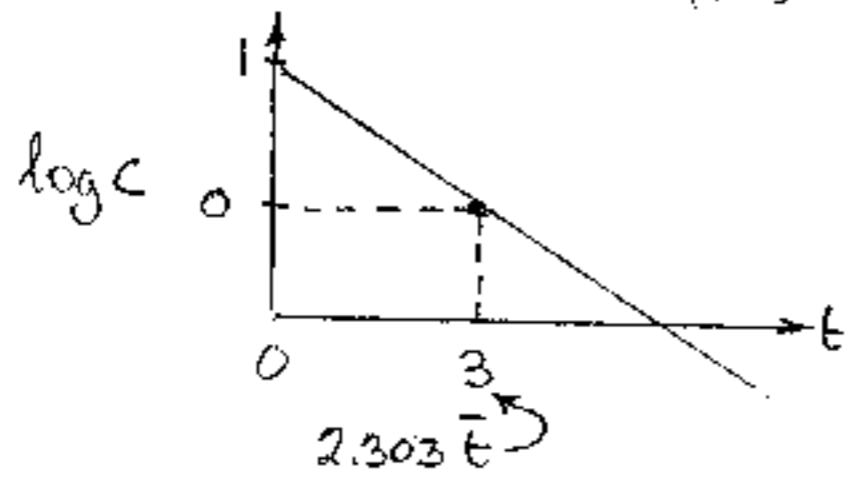
$$V_{p1} = \bar{t}_1 U_1 = (0.25)(0.4) = 0.1 m^3$$

$$V_{p2} = \bar{t}_2 U_2 = (1.5)(0.6) = 0.9 m^3$$



12.3

This looks like a mixed flow unit. Look at Fig. 2



Here $2.303 \bar{t} = 3$
 or $\bar{t} = 1.3 min$ } from experiment

But we know that

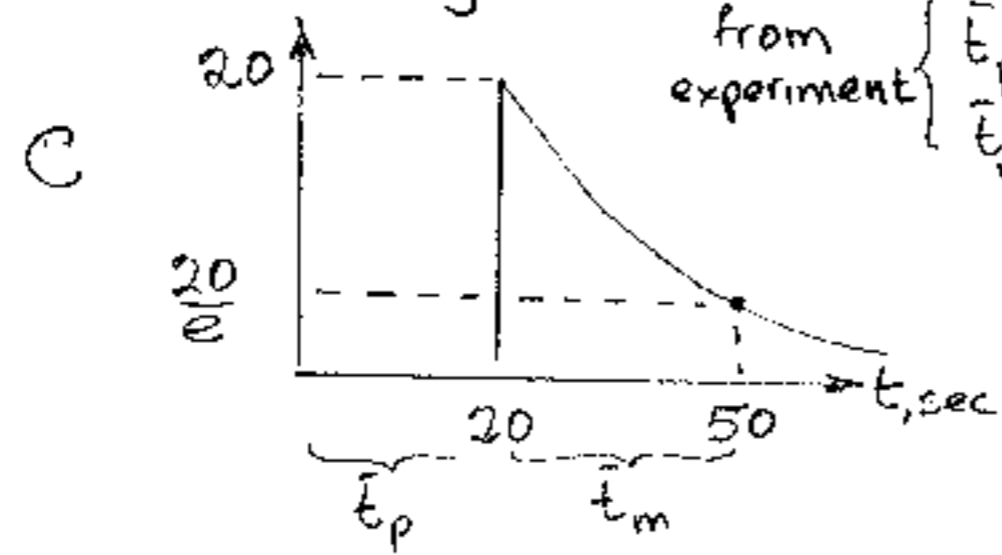
$$\bar{t} = \frac{V}{U} = \frac{1 m^3}{1 m^3/min} = 1 min$$

or less if there is dead space

What does this mean? Either the tracer used is not a proper tracer - denser than the fluid, adsorbs on the walls of the vessel, etc - or something else is wrong. Check the experiment

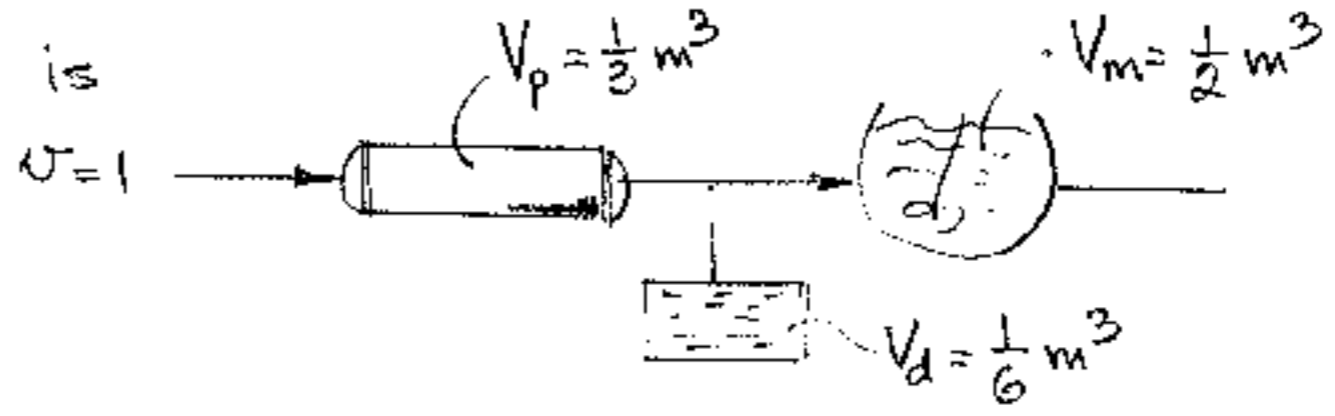
12.5

Again look at Fig 1



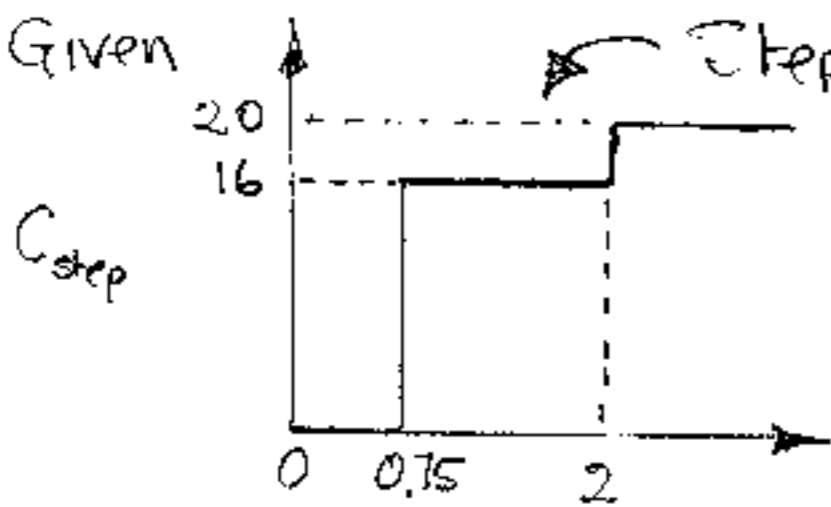
from experiment $\left\{ \begin{array}{l} \bar{t}_p = 20 \\ \bar{t}_m = 30 \end{array} \right\} \bar{t}_{active} = 50 s$
 $\bar{t}_{total} = \frac{V}{U} = 60 s$ } $\bar{t}_{dead} = 10 s$

Thus our model is

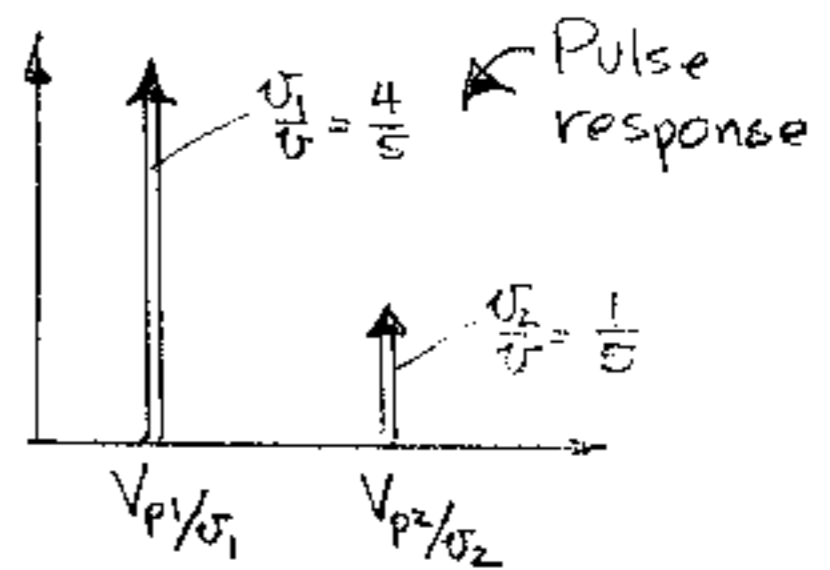


12.7

Given



$\Rightarrow C_{pulse}$



From the pulse response curve

$$U_1 = \frac{4}{5}\sigma = 0.8$$

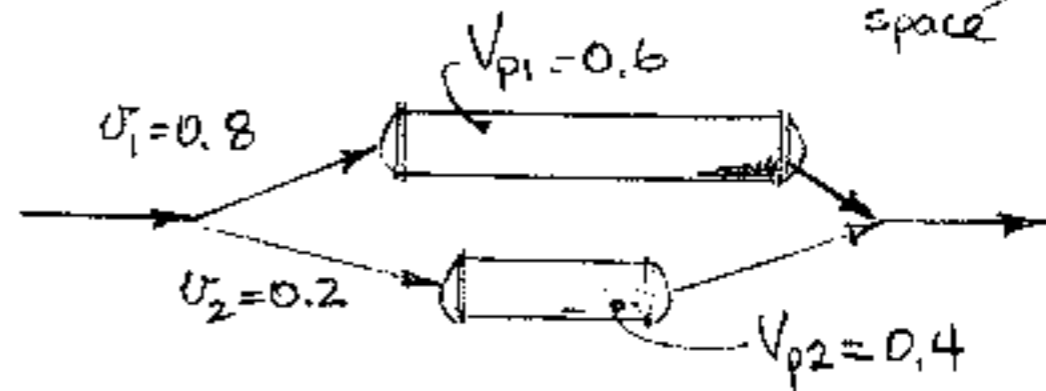
$$U_2 = \frac{1}{5}\sigma = 0.2$$

$$V_{p1} = U_1(0.75) = 0.8(0.75) = 0.6$$

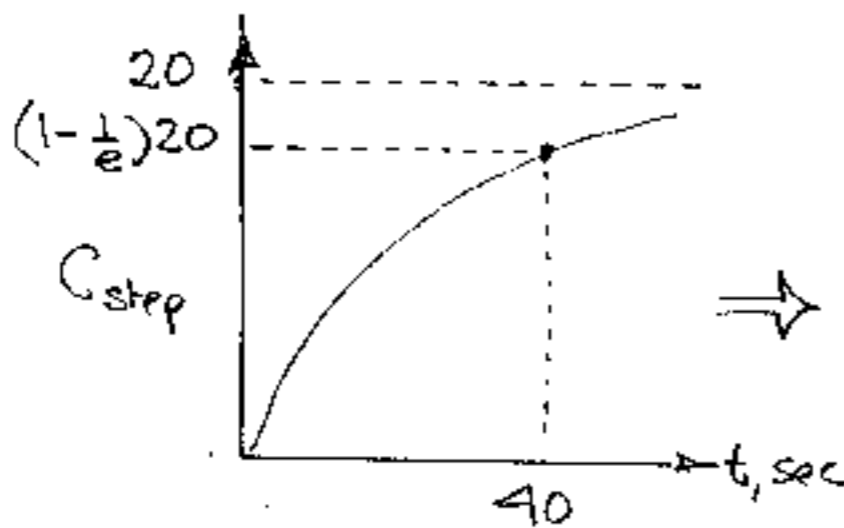
$$V_{p2} = U_2(2) = 0.2(2) = 0.4$$

note: no dead space

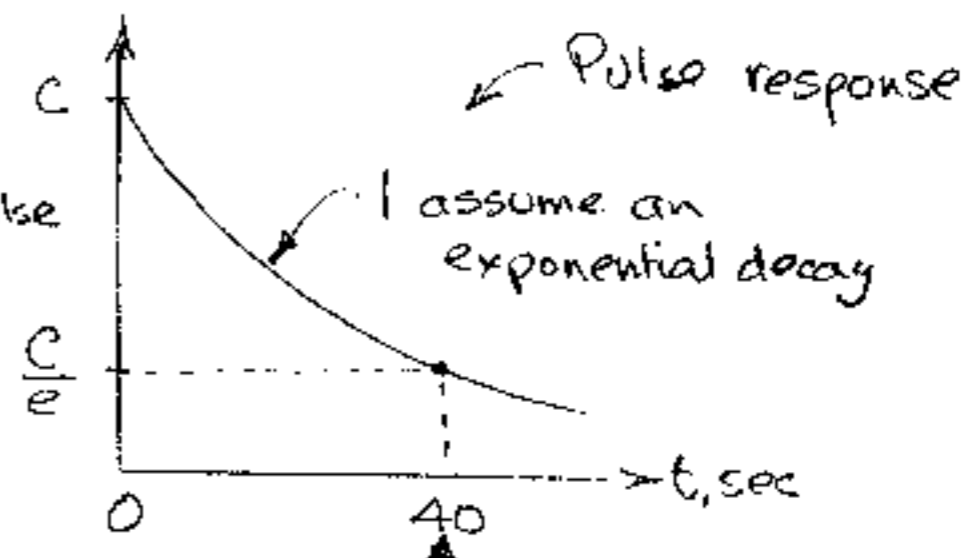
So the flow model is



12.9



$\Rightarrow C_{pulse}$

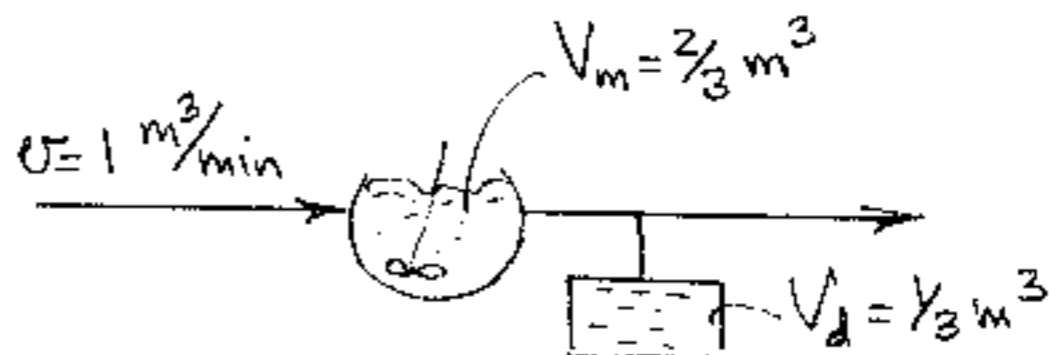


For mixed flow alone this should be 60sec. However, this curve comes out early, meaning dead spaces are present. This tracer curve shows that $\bar{t} = 40 sec$, thus

$$V_m = \frac{2}{3} m^3$$

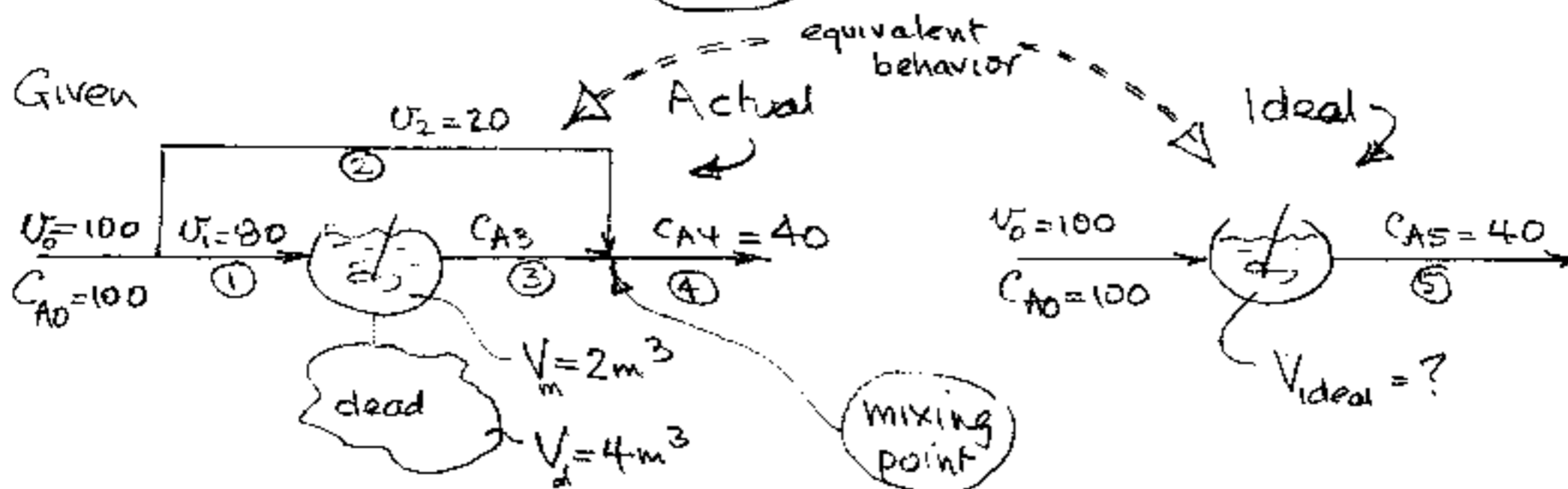
$$V_d = \frac{1}{3} m^3$$

and our flow model is



60

12.11 Given



First let $C_{A0} = 100$
 $u_0 = 100$ } It is not necessary to do this, but this assumption makes the calculations simpler.

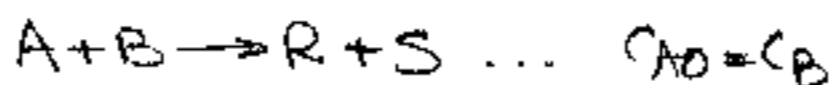
Now take a material balance about the mixing point

$$u_2 C_{A2} + u_3 C_{A3} = u_4 C_{A4}$$

or $20(100) + 80 C_{A3} = 100(40)$

or $C_{A3} = \frac{100(40) + 20(100)}{80} = 75$

Next evaluate the rate constant k from the actual 2m^3 MFR.
 For a 2nd order reaction



we have

$$\tau = \frac{V}{u} = \frac{C_{A0} - C_{A3}}{k C_{A3}^2}$$

or $k = \frac{C_{A0} - C_{A3}}{C_{A3}^2} \cdot \frac{u}{V} = \frac{100 - 75}{(75)^2} \cdot \frac{80}{2} = 14.222$

Finally, for the ideal reactor

$$\frac{V_{\text{ideal}}}{u} = \frac{C_{A0} - C_{A5}}{k C_{A5}^2}$$

or

$$V_{\text{ideal}} = \frac{C_{A0} - C_{A5}}{k C_{A5}^2} \cdot u = \frac{100 - 40}{14.22(40)^2} \cdot 100 = 0.2637 \text{ m}^3$$

This is so much smaller than 6m^3

(61)

13.1 Evaluate the intensity of dispersion for the middle section.

$$\bar{t}_2 = 1.66 \text{ s}$$

width at 61% = 0.70

∴ standard deviation, $\sigma_2 = 0.35$ (from Fig 4)

$$\sigma_2^2 = 0.1225$$

$$\Delta \bar{t} = 1.66 - 0.068 = 0.98 \text{ (from Fig P1)}$$

$$\Delta(\sigma^2) = 0.1225 - 0.0196 = 0.1029$$

$$\therefore \frac{D}{uL} = \frac{\Delta(\sigma^2)}{\Delta(\bar{t})^2} = \frac{0.1029}{2(0.98)^2} = 0.0536$$

$$\frac{D}{u d_p} = \frac{D}{uL} \left(\frac{L}{d_p} \right) = (0.0536) \left(\frac{10.37 - 5.08}{0.028} \right) = 10.1$$

From the blast furnace experiment

$$\frac{D}{u d_p} = 10.1$$

From the correlation for smaller solids, Fig 17:

$$\frac{D}{u d_p} = 0.5$$

Note: These results are very different. It could be because of the severe bypassing in the blast furnace, caused by the segregation of the solids and the severe channeling of the gas

13.3

| From | t, sec | \bar{t} , sec | C |
|-------------|--------|-----------------|-----|
| experiment: | 0-20 | 10 | 0 |
| | 20-25 | 22.5 | 60 |
| | 25-30 | 27.5 | 210 |
| | 30-35 | 32.5 | 170 |
| | 35-40 | 37.5 | 75 |
| | 40-45 | 42.5 | 35 |
| | 45-50 | 47.5 | 10 |
| | 50-55 | 52.5 | 5 |
| | 55-70 | 62.5 | 0 |

Calculate D/uL :

$$\sum C = 565$$

$$\sum tC = 17687.5$$

$$\sum t^2 C = 573781.25$$

$$\bar{t} = \frac{\sum tC}{\sum C} = 31.31 \text{ sec}$$

$$\sigma^2 = \frac{\sum t^2 C}{\sum C} - (\bar{t})^2 = 35.52 \text{ sec}^2$$

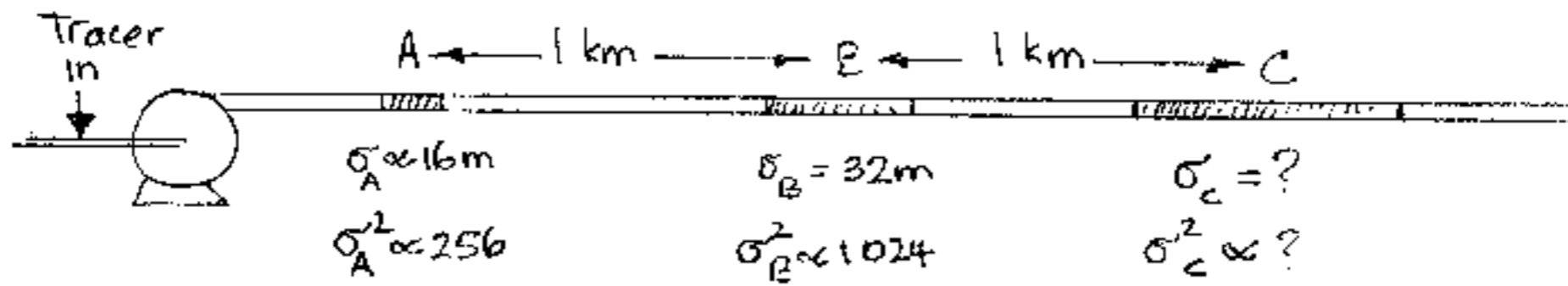
$$\frac{D}{uL} = \frac{\sigma^2}{2(\bar{t})^2} = 0.018$$

Now calculate the volume of the baffles

$$\left. \begin{aligned} \text{From mat. balance } V &= (1.21 \times 10^2)(\pi \times 1.75^2) = 1164 \text{ cm}^3 \\ v &= 1300 \text{ cm}^3/\text{min} = 21.67 \text{ cm}^3/\text{s} \end{aligned} \right\} \bar{t} = \frac{1164}{21.67} = 53.72 \text{ sec}$$

$$\therefore \text{Volume of baffles} = \frac{53.72 - 31.31}{53.72} (1164) = 486 \text{ cm}^3$$

13.5



Let us solve this with the dispersion model. We could also do this with the tanks-in-series model.

Then from Eq 8 $\sigma^2 = 2(DL/u^3)$

or $\sigma^2 \propto L$... or (spread)² $\propto L$

So $\sigma_C^2 - \sigma_B^2 = \sigma_B^2 - \sigma_A^2$

or $\sigma_C^2 - 1024 = 1024 - 256$

or $\sigma_C^2 = 1792$

or Width = $k \sigma_C = 42.3\text{m}$ ←

13.7

First find the σ^2 for this flow

$$Re = \frac{d u \rho}{\mu} = (0.255)(1.1) / 0.9 \times 10^{-6} = 3.12 \times 10^5$$

From Fig 15: $D/u d_t = 0.22$

From Eq 8: $\frac{D}{uL} = \left(\frac{D}{u d_t}\right) \left(\frac{d_t}{L}\right) = 0.22 \left(\frac{0.255}{1000000}\right) = 5.61 \times 10^{-8}$

$$\frac{\sigma^2}{t^2} = \sigma_{\theta}^2 = 2 \left(\frac{D}{uL}\right) = 2 (5.61 \times 10^{-8}) = 11.22 \times 10^{-8}$$

$\therefore \sigma = (11.22 \times 10^{-8})^{1/2} \frac{1000000}{1.1} = 304.5 \text{ sec}$

\therefore the width at $1\sigma = (304.5)(1.1) = 335 \text{ m}$

From 5/95 to 95/5 Fig 12 shows that this includes

$(1.655 \times 2) \sigma$ of width

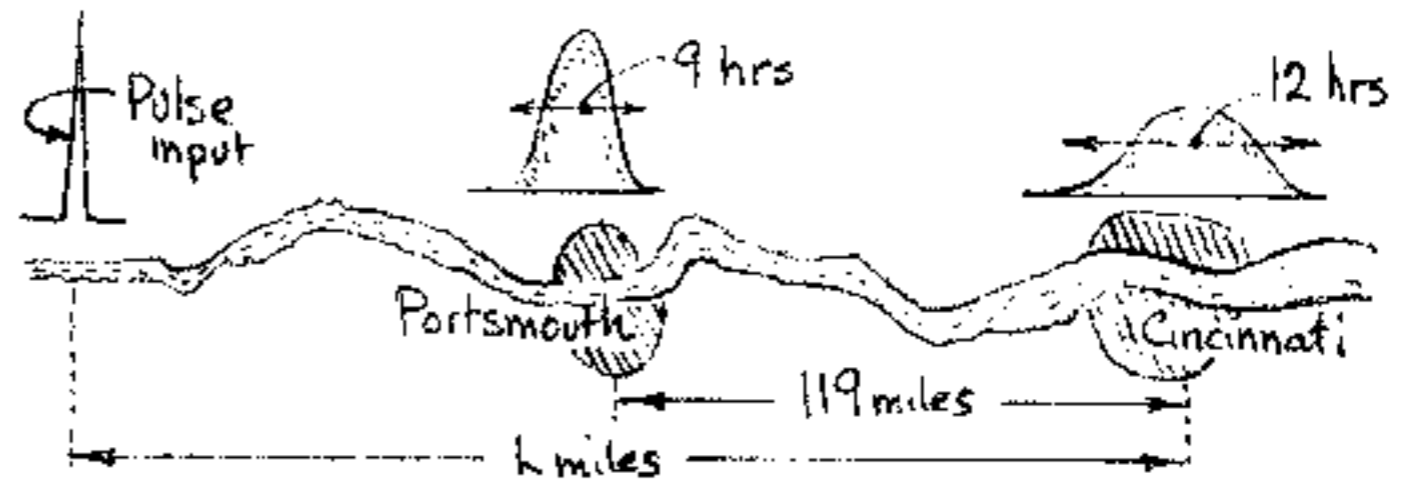
\therefore the 5/95 to 95/5% width is

$(335\text{m})(1.655 \times 2) = 1105 \text{ m}$ ←

↑
width of one σ^2

(62)

13.9 To start assume that a perfect pulse is injected. Then find how far upstream from Cincinnati this pulse was injected



According to any reasonable flow model (dispersion, tanks-in-series, or what have you)

$$\sigma_{\text{tracer curve}}^2 \propto (\text{distance from point of injection}) \quad \dots \text{or} \dots \quad (\text{spread of curve}) \propto \sqrt{\text{distance downstream from injection point}}$$

so from the Cincinnati reading ... $12 \text{ hrs} = k L^{1/2}$

and from the Portsmouth reading .. $9 \text{ hrs} = k (L - 119)^{1/2}$

Dividing one by the other & solving for L gives

$$L = 272 \text{ miles}$$

Since the dumping may not be instantaneous any location where $L \leq 272$ miles is suspect or

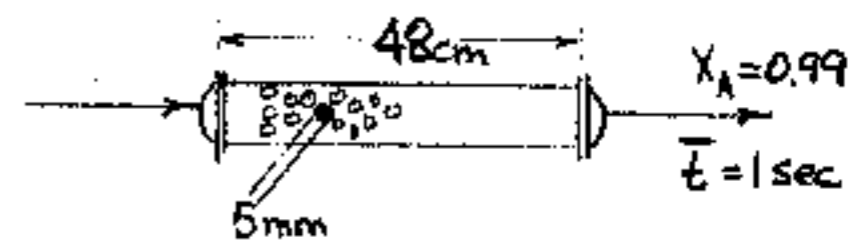
Ashland
Huntington
Pomeroy

Note: This solution assumes that different stretches of the Ohio river have the same flow & dispersion characteristics (a reasonable assumption), & that no suspect tributary joins the Ohio within 272 miles upstream from Cincinnati (a poor assumption - check a map for the location of Charleston W.Va. on the Kanawah.)

13.11 First calculate k assuming plug flow, then account for dispersion

a) Find k assuming plug flow

For a 1st order reaction, $E_A = 0$, we have



$$k\tau = \ln \frac{C_{A0}}{C_A} \quad \dots \quad k_{\text{plug}} = \frac{1}{\tau} \ln \frac{C_{A0}}{C_A} = \frac{1}{(1 \text{ sec})} (4.6) = 4.6 \text{ sec}^{-1} \quad \leftarrow \text{a)}$$

13.11 b) Find k accounting for deviation from plug flow according to the dispersion model
(continued)

From the curve of Fig 17 we find for $Re_p = 200$ & $\epsilon = 0.4$

$$\frac{D\epsilon}{u d_p} = 1 \quad \dots \text{thus} \quad \frac{D}{u d_p} = 2.5$$

The size ratio of real to plug flow reactor, or what is equivalent, the ratio of the corresponding rate constants is found either from Fig 19 or from Eq 22 if the k ratio or the L ratio is close to unity.

Use Eq. 22. Then

$$\begin{aligned} \frac{L}{L_p} = \frac{k_{true}}{k_{measured}} &= 1 + k_T \left(\frac{D}{uL} \right) = 1 + k_T \left(\frac{D}{u d_p} \right) \left(\frac{d_p}{L} \right) \\ &= 1 + 4.6 (2.5) \left(\frac{5 \text{ mm}}{480 \text{ mm}} \right) = 1.1198 \end{aligned}$$

$$\therefore k_{true} = (4.6 \text{ sec}^{-1})(1.1198) = 5.15 \text{ sec}^{-1} \quad \leftarrow \dots \dots \dots \text{b)}$$

Note: Direct use of Eq. 19 pg 314 (trial & error unfortunately) would give a more accurate answer.

Also, are you sure that $k_{true} > k_{plug}$? Convince yourself.

$$\text{c) Error in assuming plug flow} = \left(\frac{5.15 - 4.60}{5.15} \right) \times 100 = 11\% \text{ underestimate} \quad \leftarrow \dots \dots \dots \text{c)}$$

13.13 For plug flow with $X_A = 0.999$, or $C_A = 1.000$ and $C_{A0} = 1000$

$$\frac{C_A}{C_{A0}} = e^{-k\bar{t}} \quad \dots \text{or} \quad k\bar{t} = \ln \frac{1000}{1} = 6.9078 \quad \dots \text{or} \quad k = 0.69078$$

$$\text{From Fig P13} \quad \sigma^2 = \frac{4^2}{24} = \frac{2}{3}$$

So from Eq 21

$$\frac{C_A}{C_{A0}} = \exp \left[(-k\bar{t}) + \frac{k^2 \sigma^2}{2} \right] = \exp \left[-6.9078 + \frac{(0.69078)^2 \cdot \frac{2}{3}}{2} \right]$$

$$\text{or} \quad = 0.001172$$

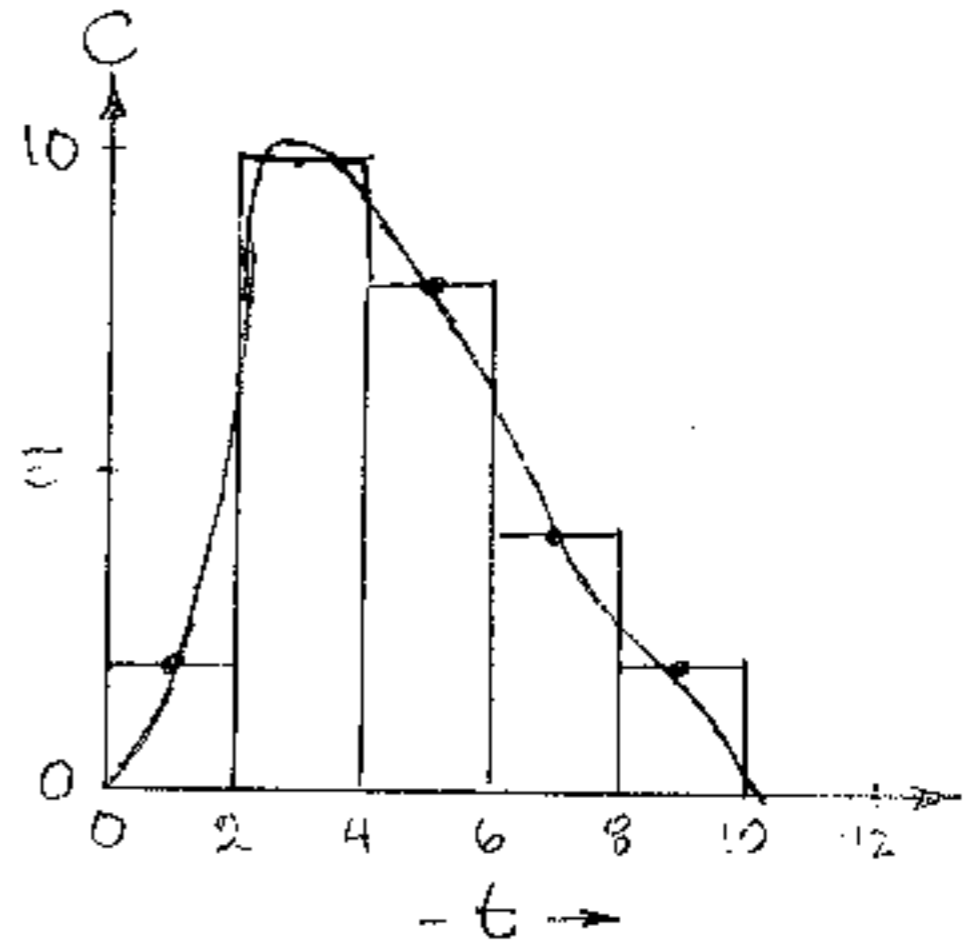
$$\therefore C_A = 1.17 \quad \leftarrow \dots \dots \dots$$

14.1 From experiment

| t | t _{mean} | C |
|-------|-------------------|----|
| 0-2 | 1 | 2 |
| 2-4 | 3 | 10 |
| 4-6 | 5 | 8 |
| 6-8 | 7 | 4 |
| 8-10 | 9 | 2 |
| 10-12 | 11 | 0 |

with linear interpolation

Find the variance & then N



From Eqs 13.1 and 13.3

$$\bar{t} = \frac{\sum tC}{\sum C} = \frac{1(2) + 3(10) + 5(8) + 7(4) + 9(2)}{2 + 10 + 8 + 4 + 2} = \frac{118}{26} = 4.538$$

$$\sigma^2 = \frac{\sum t^2 C}{\sum C} - \bar{t}^2 = \frac{1^2(2) + 3^2(10) + \dots}{2 + 10 + \dots} - (4.538)^2 = 4.4038$$

From Eq 3

$$\frac{1}{N} = \sigma_{\theta}^2 = \frac{\sigma^2}{\bar{t}^2} = \frac{4.4038}{(4.538)^2} = 0.2138$$

$$\therefore N = \frac{1}{0.2138} = 4.68 \text{ tanks} \leftarrow$$

14.3 The analogy with mixed flow should be evident. All we need to do is to identify the various quantities. Referring to the sketch

Introduction rate of fresh bills v



Removal rate of used bills

Number of bills in circulation

$$\left. \begin{aligned} v &= 10^9 \text{ bills/yr} \\ V &= 1.25 \times 10^9 \text{ bills} \end{aligned} \right\} \bar{t} = \frac{V}{v} = 1.25 \text{ yrs}$$

n = no. of bills

n_0 = total no. of bills.

$$E(t) = \frac{\text{fraction}}{\text{yr}} = \frac{n}{n_0}$$

14.3 a) How many new bills will be in circulation at any time t ?
(continued)

$$F(t) = 1 - e^{-t/\bar{t}} = 1 - e^{-t/1.25} \quad \left. \begin{array}{l} t=0 \quad F(t)=0 \\ t=\infty \quad F(t)=1 \end{array} \right\} \leftarrow$$

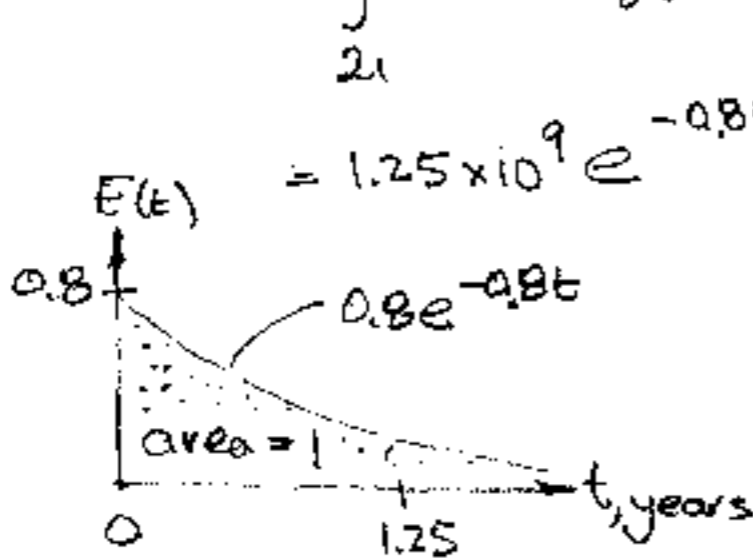
b) The number of bills in circulation which are over 21 yrs of age is given by the $E(t)$ function. Thus

$$n = \int_{21}^{\infty} n_0 E(t) dt \quad \text{--- where } n_0 = 1.25 \times 10^9$$

$$E(t) = \frac{1}{\bar{t}} e^{-t/\bar{t}} = 0.8 e^{-0.8t}$$

$$\therefore n = \int_{21}^{\infty} (1.25 \times 10^9) (0.8 e^{-0.8t})$$

$$= 1.25 \times 10^9 \left[-\frac{1}{0.8} e^{-0.8t} \right]_{21}^{\infty} = (-1.25 \times 10^9) \left[\frac{1}{e^{\infty}} - \frac{1}{e^{0.8(21)}} \right] = 63.2 \text{ bills}$$



We get this 20¢ because we assume a continuous distribution of ages when in fact this is not so

14.5 For plug flow

$$k\bar{t} = \ln \frac{C_{A0}}{C_A} = \ln \frac{1000}{1} = 6.9078$$

For small deviation from plug flow, by the tanks in series model first calculate σ^2 from the tracer curve. From Fig 13. P13

$$\sigma^2 = \frac{a^2}{24} = \frac{4^2}{24} = \frac{2}{3}$$

$$\bar{t} = 10$$

From Eq 3

$$\frac{1}{N} = \frac{\sigma^2}{\bar{t}^2} = \frac{2/3}{(10)^2} = 0.67 \times 10^{-2} \quad \dots \therefore N = 150 \text{ tanks}$$

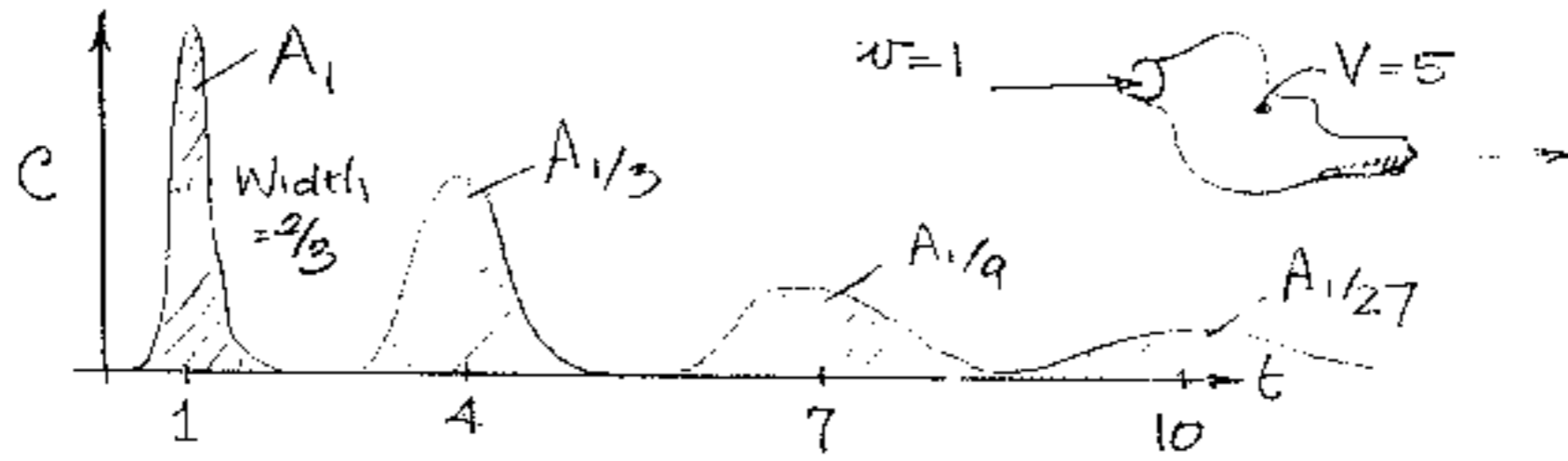
$$\therefore k\bar{t}_i = \frac{6.9078}{150} = 0.0461$$

For tanks in series

$$\frac{C_A}{C_{A0}} = \frac{1}{(1 + k\bar{t}_i)^N} = \frac{1}{(1 + 0.0461)^{150}} = \frac{1}{863} = 0.00116$$

$$\therefore C_A = 1.16 \leftarrow$$

14.7



First approximate each pulse by plug flow. Then from Fig 12.1

$$\frac{A_2}{A_1} = \frac{1}{3} = \frac{R}{R+1} \quad \therefore R = \frac{1}{2}$$

$$\frac{V_{p1}}{(R+1)v} = 1 = \frac{V_{p1}}{(\frac{1}{2}+1)v} \quad \therefore V_{p1} = \frac{3}{2}$$

$$\frac{V_{p1}}{(R+1)v} + \frac{V_{p2}}{Rv} = 3 = \frac{3/2}{(\frac{1}{2}+1)v} + \frac{V_{p2}}{(\frac{1}{2})v} \quad \therefore V_{p2} = 1$$

So $V_{active, total} = \frac{3}{2} + 1 = 2.5$

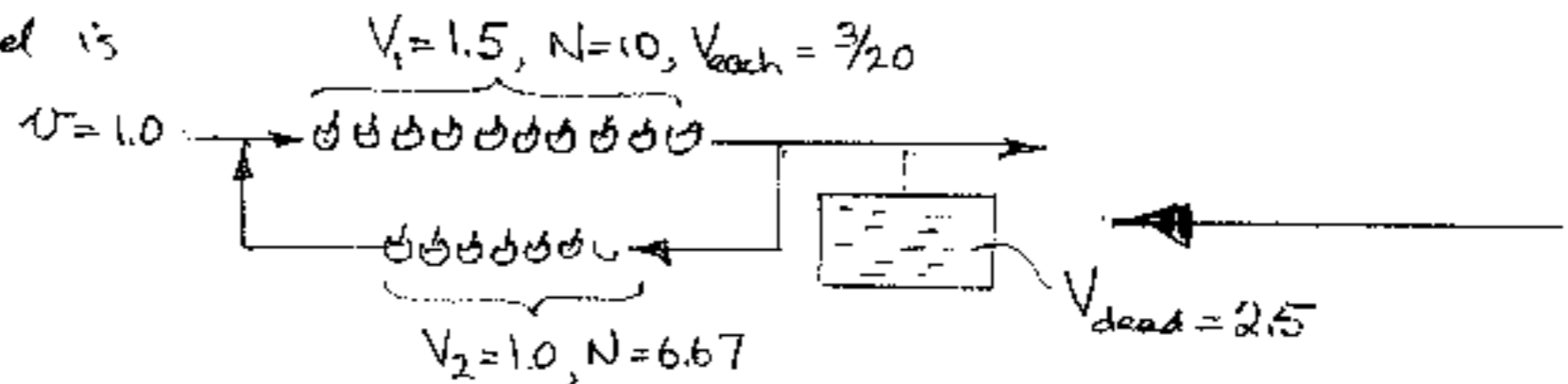
$\therefore V_{dead} = 5 - 2.5 = 2.5$

Now consider that the pulse output has width. Then from Fig 3

$$\frac{\Delta \theta}{\theta_{max}} = \frac{2/3}{1} = \frac{2}{\sqrt{N_1-1}} \quad \therefore N_1 = 10 \text{ tanks}$$

and $N_2 = \frac{2}{3} N_1 = \frac{2}{3}(10) = 6.67 \text{ tanks}$

Thus our model is



Verify

$$\bar{t} = \frac{\sum tC}{\sum C} = \frac{1(A_1) + 4(A_1/3) + 7(A_1/9) + 10(A_1/27) + 13(A_1/81) + 16(A_1/243) + \dots}{A_1 + A_1/3 + A_1/9 + A_1/27 + A_1/81 + A_1/243 + \dots}$$

$$= \frac{1 + \frac{4}{3} + \frac{7}{9} + \frac{10}{27} + \frac{13}{81} + \frac{16}{243} + \frac{19}{729} + \dots}{1 + \frac{1}{3} + \frac{1}{9} + \frac{1}{27} + \frac{1}{81} + \frac{1}{243} + \frac{1}{729} + \dots} = \frac{3.7339}{1.4993} = 2.49 \approx 2.5$$

This limit equals $\frac{V_1 + V_2}{v} = \frac{1.5 + 1.0}{1} = 2.5$

the limit \nearrow

14.9 For N tanks in series
Fig 25 pg 292 shows that ...

$$N = 1 + 4 \left(\frac{\theta_{\max}}{\Delta\theta} \right)^2$$

location of the maximum
width of the curve at 60% of its maximum height.

Using a ruler with mm scale and a keen eye we find from Fig P21

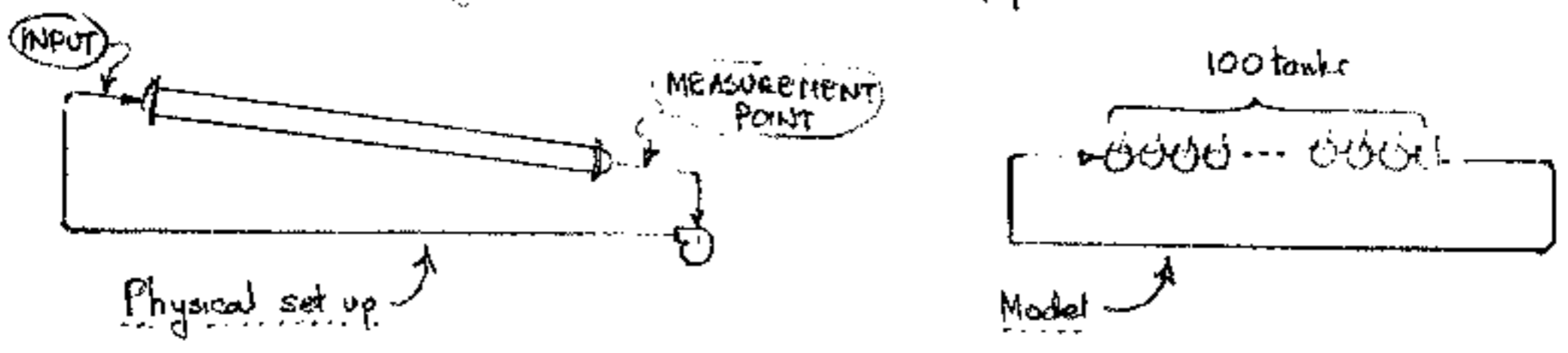
for 1st peak: $N_{1\text{ pass}} = 1 + 4 \left(\frac{16.2\text{ mm}}{3.2\text{ mm}} \right)^2 = 104$ tanks ... or $N = 104$ tanks/pass

for 2nd peak: $N_{2\text{ passes}} = 1 + 4 \left(\frac{22.6}{4.6} \right)^2 = 202$ tanks ... or $N = 101$ tanks/pass

for 3rd peak: $N_{3\text{ passes}} = 1 + 4 \left(\frac{48.7}{5.6} \right)^2 = 304$ tanks ... or $N = 101$ tanks/pass

for 4th peak: $N_{4\text{ passes}} = 1 + 4 \left(\frac{65}{6.6} \right)^2 = 389$ tanks ... or $N = 97$ tanks/pass

These values average to $N \approx 100$ tanks/pass



14.11 To find the non ideal characteristics of the experimental reactor determine the proper D/uL to use for the dispersion model, or the proper N value to use for the tanks-in-series model.

This is done in one of two ways — by matching the experimental tracer curve with the family of curves shown in Fig. 13.9 (for the dispersion model) or with Fig. 2 (for the tanks-in-series model), or by calculating σ_{θ}^2 and from that D/uL or N .

Let us use the latter procedure. So first calculate \bar{t} and σ^2 from the table of data with Eqs. 13.1 and 13.3. This gives

$$\begin{aligned} \sum C &= 213 & \bar{t} &= 2149/213 = 10.09 \text{ min} \\ \sum tC &= 2149 & \sigma^2 &= 37695/213 - (10.09)^2 = 75.1168 \\ \sum t^2C &= 37695 & \sigma_{\theta}^2 &= \frac{\sigma^2}{\bar{t}^2} = \frac{75.1168}{(10.09)^2} = 0.7378 \end{aligned}$$

Next determine the behavior in an ideal plug flow reactor

$$k = 0.456 \text{ min}^{-1} \quad k\bar{t} = (0.456)(10.09) = 4.6$$

$$\text{So for plug flow} \quad X_A = 1 - e^{-kt} = 1 - e^{-4.6} = 0.99$$

Now we are ready to proceed with our problem

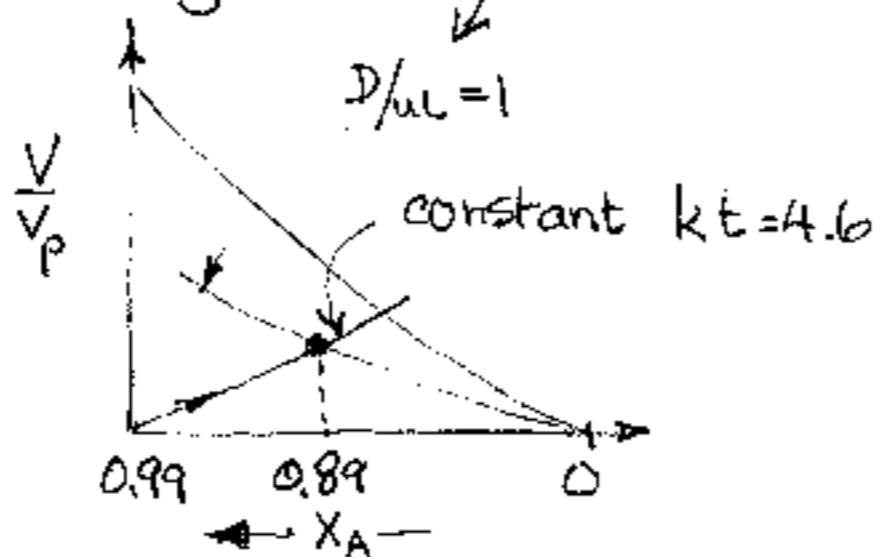
(a) Use the dispersion model

Here Eq. 13.15 relates σ_{θ}^2 with D/uL . So

$$\sigma_{\theta}^2 = 0.7378 = 2\left(\frac{D}{uL}\right) - 2\left(\frac{D}{uL}\right)^2 [1 - e^{-uL/D}]$$

Solve by trial and error. This gives $D/uL = 1$

Then from Fig. 13.19



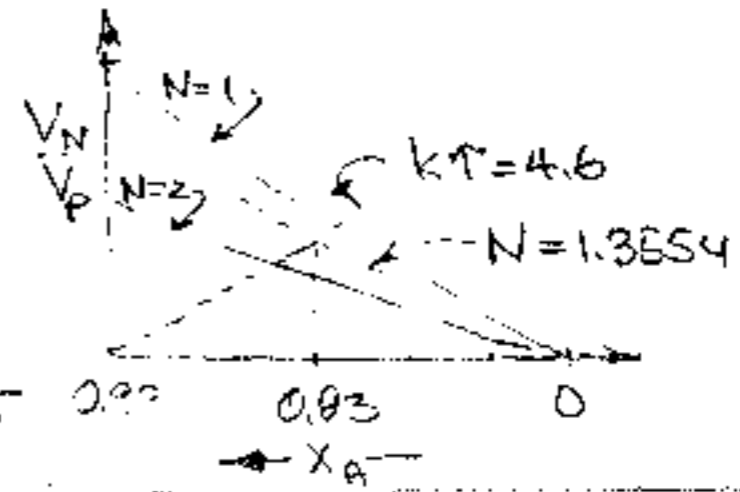
From this figure

$$X = 0.89 \quad \text{a)} \\ \text{disp.}$$

14.11 (b) Use the tanks-in-series model
(continued) from Eq. 3 we find

$$N = \frac{1}{\frac{\sigma^2}{\theta}} = \frac{1}{0.7388} = 1.3554 \text{ tanks}$$

So from Fig. 6.5 we find $X_{\text{tanks}} = 83\%$



(c) Use the tracer data directly.

From Eq 11.13 $\frac{C}{C_0} = \sum \left(\frac{C}{C_0} \right)_{\text{batch}} E \Delta t$

To find the E curve make the area under the C curve unity, or as shown in Example 11.1

$$E = \frac{C}{\text{area}} = \frac{C}{\sum C_i \Delta t} \quad \text{or} \quad E \Delta t = \frac{C}{\sum C}$$

| t, min | C | $e^{-0.456t_i} C_i / 213$ |
|-----------------|-----|---------------------------|
| 0 | 0 | 0 |
| 1 | 17 | 0.0506 |
| 3 | 38 | 0.0454 |
| 5 | 33 | 0.0158 |
| 7 | 26 | 0.0050 |
| 9 | 20 | 0.0015 |
| 11 | 16 | 0.0005 |
| 13 | 13 | 0.0002 |
| 15 | 10 | 0.0001 |
| 17 | 8 | 16×10^{-6} |
| 19 | 6 | 5×10^{-6} |
| 21 | 5 | 2×10^{-6} |
| 23 | 4 | $1 \times 10^{-6} = 0$ |
| 25-27 | 3 | - |
| 29-31 | 2 | - |
| 33-45 | 1 | - |

$\sum C = 213 \quad \sum = 0.1191$

Now follow the method of Example 11.4

$$\frac{C}{C_0} = \sum \left(\frac{C}{C_0} \right)_{\text{batch}} E \Delta t$$

$$= \sum e^{-kt} \frac{C}{\sum C}$$

$$= \frac{1}{\sum C} \sum e^{-0.456t_i} C_i$$

now to divide \uparrow

$$X_{\text{from curve}} = 0.88$$

(d) Which answer is most reliable

Naturally the direct use of the tracer curve gives the most reliable answer. In this problem the given RTD came from the dispersion model with $\beta/\alpha L = 1$. Thus we'd expect that the answers to parts a) and c) should agree. They do.

15.1 Given, a zero order reaction

For plug flow: $\frac{C_A}{C_{A0}} = 1 - X_A = 0.2 = 1 - \frac{kT}{C_{A0}} \dots$ or $\frac{kT}{C_{A0}} = 0.8$

For convective flow Eq 9 gives

$$\frac{C_A}{C_{A0}} = \left(1 - \frac{kT}{2C_{A0}}\right)^2 = \left(1 - \frac{0.8}{2}\right)^2 = 0.36 \therefore X_A = 0.64 \leftarrow$$

15.3 For second order and plug flow

$$\frac{C_A}{C_{A0}} = \frac{1}{1 + kC_{A0}T} \quad \text{or} \quad kC_{A0}T = \frac{C_{A0}}{C_A} - 1$$

and because $\frac{C_A}{C_{A0}} = 0.04 \quad kC_{A0}T = 25 - 1 = 24$

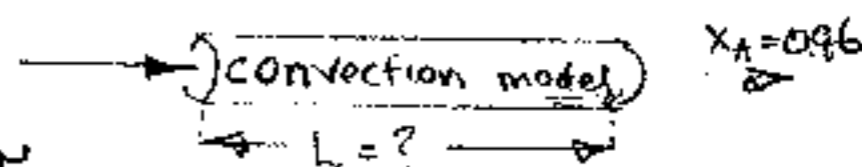
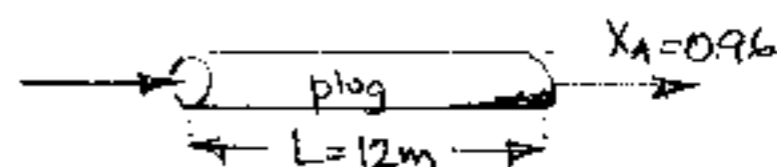
For the convection model let $y = kC_{A0}T$

then Eq 11 gives

$$X_A = 1 - \frac{C_A}{C_{A0}} = y \left[1 - \frac{y}{2} \ln\left(1 + \frac{2}{y}\right) \right] = 0.96$$

$$\therefore \frac{(kC_{A0}T)_{\text{conv}}}{(kC_{A0}T)_{\text{plug}}} = \frac{32}{24} = 1.33$$

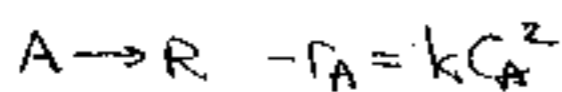
$$\therefore \frac{L_{\text{conv}}}{L_{\text{plug}}} = 1.33 \quad \text{or} \quad L_{\text{conv}} = 16 \text{ m} \leftarrow$$



| guess y | calculate X _A |
|---------|--------------------------|
| 24 | 0.9477 |
| 36 | 0.9644 |
| 30 | 0.9577 |
| 32 | 0.9602 |

solve by trial & error →

15.5



$\rho = 1000 \text{ kg/m}^3$

$\delta = 10^{-9} \text{ m}^2/\text{s}$

$k = 10^{-3} \text{ m}^3/\text{mol}\cdot\text{s}$

$C_{A0} = 50 \text{ mol/m}^3$

$-u = 10 \text{ mm/s} \rightarrow$

$X_A = ?$

$L = 20 \text{ m}$

$d_t = 10 \text{ mm}$

First find which regime applies (see Fig 2)

$$Re = \frac{d u \rho}{\mu} = \frac{0.01 (0.01) 1000}{10^{-3}} = 100$$

$$Bo = \frac{u d_t}{\delta} = \frac{0.01 (0.01)}{10^{-9}} = 10^5$$

$$\frac{L}{d_t} = \frac{20}{0.01} = 2000$$

Fig 2 shows that the reactor is in the intermediate regime between the convection and dispersion models.

So average the results.

15.5
(continued)

Dispersion model

$$D = \frac{u^2 d_t^2}{192 \theta} = \frac{(0.01)^2 (0.01)^2}{192 (10^{-9})} = 5.21 \times 10^{-2} \frac{\text{m}^2}{\text{s}}$$

$$\frac{D}{uL} = \frac{5.21 \times 10^{-2}}{(0.01)(20)} = 0.26$$

$$kC_{A0}\tau = (10^{-3})(50)(20/0.01) = 100$$

From Fig 13.20

$$\frac{C_A}{C_{A0}} = 0.022 \quad \dots \quad X_A = 0.978$$

Convection model

$$\frac{C_A}{C_{A0}} = 1 - kC_{A0}\tau \left[1 - \frac{kC_{A0}\tau}{2} \ln \left(1 + \frac{2}{kC_{A0}\tau} \right) \right] = 1 - 100 \left[1 - \frac{100}{2} \ln \left(1 + \frac{2}{100} \right) \right]$$

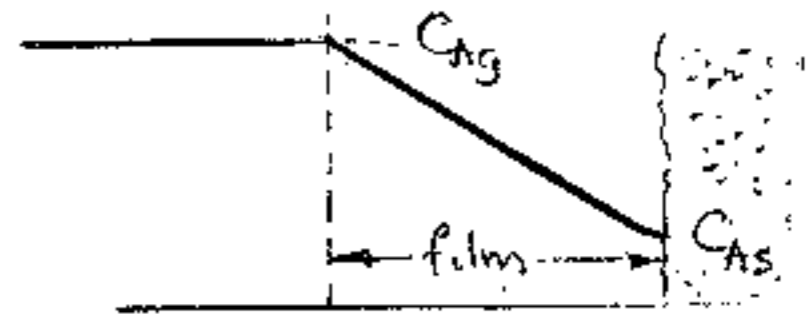
$$= 0.013$$

$$\therefore X_A = 0.987$$

Averaging gives $\bar{X}_A = \frac{0.978 + 0.987}{2} = 0.983$ ←

17.1 For the mass transfer step

$$-r_A'' = -\frac{1}{S} \frac{dN_A}{dt} = k_g (C_{Ag} - C_{As}) \quad \dots (i)$$



For the reversible reaction step

$$-r_A'' = k_s (C_{As} - C_{Ae}) \quad \dots (ii)$$

Combining (i) and (ii) to eliminate the unknown C_{As} gives

$$-r_A'' = \frac{1}{\frac{1}{k_g} + \frac{1}{k_s}} (C_{Ag} - C_{Ae})$$

17.3 For the interface between gas bubbles and liquid

$$(-r) = -\frac{1}{V} \frac{dN}{dt} = k_{AL} a_i (C_{Ai} - C_{AL}) \quad \dots (i)$$

gas-liquid mass transfer coefficient

area of gas-liquid interface per volume of reactor

For the interface between the solid catalyst particles & the surrounding liquid

$$(-r) = -\frac{1}{V} \frac{dN}{dt} = k'_{AL} a_s (C_{AL} - C_{As}) \quad \dots (ii)$$

liquid-solid mass transfer coefficient

area of liquid-solid interface per volume of reactor

For surface reaction

$$(-r) = -\frac{1}{V} \frac{dN}{dt} = k_1 C_{As} a_s \quad \dots (iii)$$

Combining (i) (ii) & (iii), eliminating the intermediate concentrations C_{AL} & C_{As} gives, on manipulation

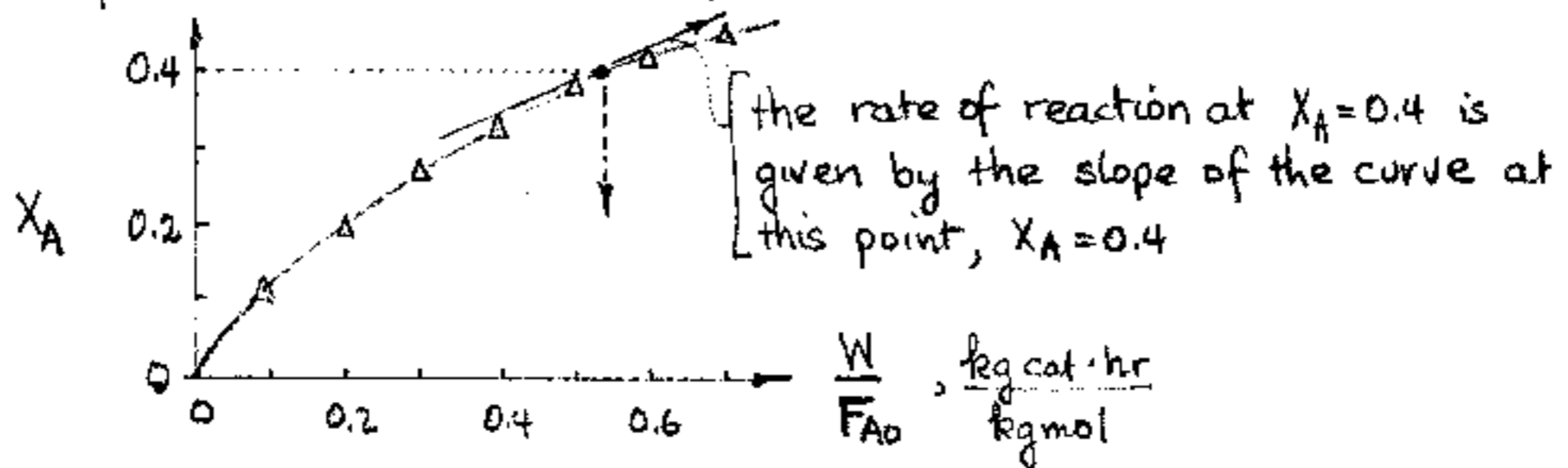
$$(-r) = -\frac{1}{V} \frac{dN}{dt} = \frac{1}{\frac{1}{k_{AL} a_i} + \frac{1}{k'_{AL} a_s} + \frac{1}{k_1}} C_{Ai}$$

rate based on unit volume of reactor

This expression is the special case of Eq 22.2 for slurry reactors.

18.1 We cannot tell. It isn't the depth of packing or the conversion level which counts, but the assumptions used when the data from the reactor are analysed. If you ASSUME a constant rate of reaction throughout the reactor then you are treating it as a differential reactor. If you ASSUME a changing rate of reaction with position then you have an integral reactor. It is simply a matter of how you are looking the rate.

18.3 a) First plot the data as shown



Since $\frac{W}{F_{A0}} = \int \frac{dX_A}{-r'_A}$... we have in differential form $\frac{dW}{F_{A0}} = \frac{dX_A}{-r'_A}$

hence the rate ... $-r'_A = \frac{dX_A}{d(W/F_{A0})}$... which is the slope of the curve.

So at 40% conversion

$$-r'_A = \frac{0.482 - 0.23}{0.8 - 0.1} = 0.36 \frac{\text{kmol converted}}{\text{kg cat} \cdot \text{hr}} \quad \leftarrow \text{a)}$$

b) For $F_{A0} = 400 \frac{\text{kmol}}{\text{hr}}$ in a packed bed to $X_A = 0.4$ $\frac{W}{F_{A0}} = 0.575$ from the figure

$$\therefore W = 0.575(400) = 230 \text{ kg cat} \quad \leftarrow \text{b)}$$

c) For completely mixed flow $\frac{W}{F_{A0}} = \frac{X_A}{-r'_{A, \text{at } 40\%}} = \frac{0.4}{0.36}$

$$\therefore W = 400 \left(\frac{0.4}{0.36} \right) = 444 \text{ kg cat} \quad \leftarrow \text{c)}$$

18.5 $A \rightarrow 3R$, $n=1 \dots 1^{st}$ order

$$\epsilon_A = \frac{1+3-(1+1)}{(1+1)} = 1$$

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \epsilon_A C_A} = \frac{2 - 0.5}{2 + 1(0.5)} = 0.6$$

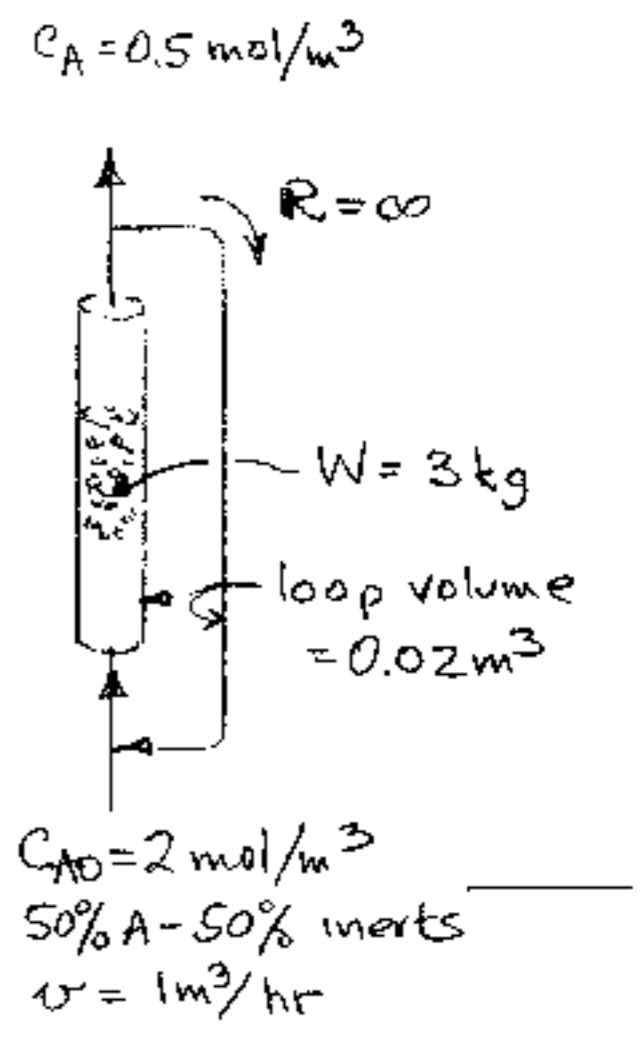
Mixed flow reactor

$$\frac{1}{k} = \frac{C_{A0} \sigma X_A}{W C_A} = \frac{2(1)(0.6)}{3(0.5)} = 0.8 \frac{m^3}{kg \cdot hr}$$

Thus

$$-r'_A = \left(0.8 \frac{m^3}{kg \cdot hr}\right) \left(C_A \frac{mol}{m^3}\right) \leftarrow$$

Note. The loop volume doesn't enter into the calculations.



18.7 Given $A \rightarrow R$,



$$\frac{W}{v} = \frac{C_{A0} X_A}{-r'_A}$$

$$\text{or } r'_A = \frac{C_{A0} X_A v}{W}$$

First find the rate at the 3 conditions

| v | X_A | C_A | $-r'_A = C_{A0} X_A v / W$ |
|-----|-------|-------|----------------------------|
| 3 | 0.2 | 8 | $10(0.2)(3)/4 = 1.5$ |
| 2 | 0.3 | 7 | $10(0.3)(2)/4 = 1.5$ |
| 1.2 | 0.5 | 5 | $10(0.5)(1.2)/4 = 1.5$ |

Therefore Zero order

$$-r'_A = 1.5 \text{ mol/kg} \cdot \text{hr} \leftarrow$$

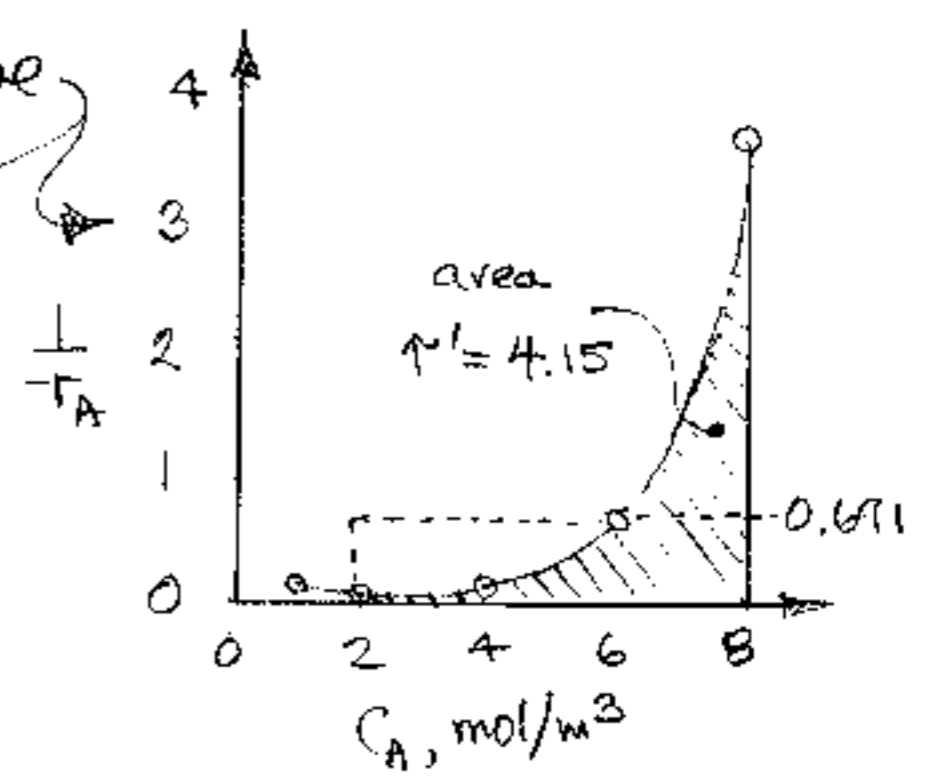
18.9 For the basket reactor (mixed flow) we have

| C_A | F_{A0} | X_A | $-r'_A = F_{A0} X_A / W$ | $1/-r'_A$ |
|-------|----------|-------|--------------------------|-----------|
| 8 | 0.14 | 0.2 | 0.28 | 3.57 |
| 6 | 0.42 | 0.4 | 1.68 | 0.595 |
| 4 | 1.67 | 0.6 | 10.02 | 0.1 |
| 2 | 2.5 | 0.8 | 20 | 0.05 |
| 1 | 1.25 | 0.9 | 11.25 | 0.089 |

For the packed bed

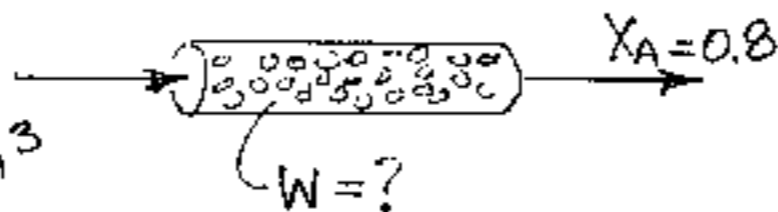
$$\tau = \frac{W C_{A0}}{F_{A0}} = \int_{C_A=2}^{C_{A0}=8} \frac{dC_A}{-r'_A} = \text{shaded area} = 4.15$$

$$\therefore W = 4.15 \frac{F_{A0}}{C_{A0}} = 4.15 \frac{1000}{8} = 519 \text{ kg} \leftarrow$$



18.11

$v = 1000 \text{ m}^3/\text{hr}$
 $C_{A0} = 100 \text{ mol/m}^3$



$$-r'_A = \frac{50C_A}{1+0.02C_A} \text{ mol/kg}\cdot\text{hr}$$

← this is the rate of Eq 3.57

For plug flow

$$\tau' = \frac{W}{v} = C_{A0} \int_0^{X_{AF}} \frac{dX_A}{-r'_A} = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r'_A} = \frac{1}{k'} \int_{20}^{100} \frac{1+0.02C_A}{50C_A} dC_A$$

Integration gives (see Eq 3.58a)

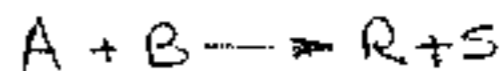
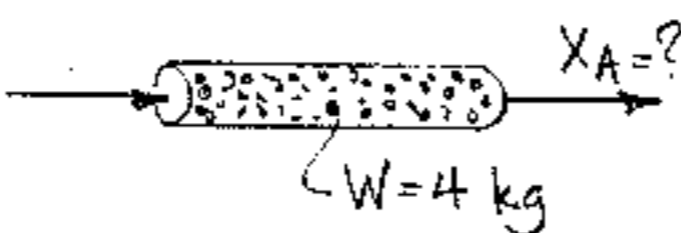
$$\frac{1}{k'} \tau' = \left[\ln \frac{C_{A0}}{C_A} + k(C_{A0} - C_A) \right]$$

or $W = \frac{v}{k'} \left[\ln \frac{C_{A0}}{C_A} + k_2(C_{A0} - C_A) \right]$

$$= \frac{1000 \text{ m}^3/\text{hr}}{50 \text{ m}^3/\text{kg}\cdot\text{s}} \left[\ln \frac{100}{20} + 0.02 \frac{\text{m}^3}{\text{mol}} (100 - 20) \right] = 64.19 \text{ kg cat} \leftarrow$$

18.13

$v_0 = 10 \text{ m}^3/\text{hr}$
 $C_{A0} = 0.1 \text{ mol/m}^3$
 $C_{B0} = 10 \text{ mol/m}^3$



$-r'_A = 0.6 C_A C_B \text{ mol/kg}\cdot\text{hr}$

For $C_{A0} = 0.01 C_{B0}$ we can assume that $C_B \approx \text{constant} = C_{B0} = 10 \text{ mol/m}^3$

$\therefore -r'_A = 0.6 C_A C_B = 0.6 C_A (10) = 6 C_A$

$\tau' = \frac{W}{v} = \frac{4}{10} = 0.4 \text{ kg}\cdot\text{hr}/\text{m}^3$

For a first order reaction

$$\frac{C_A}{C_{A0}} = e^{-k'\tau'} = e^{-6(0.4)} = 0.0907$$

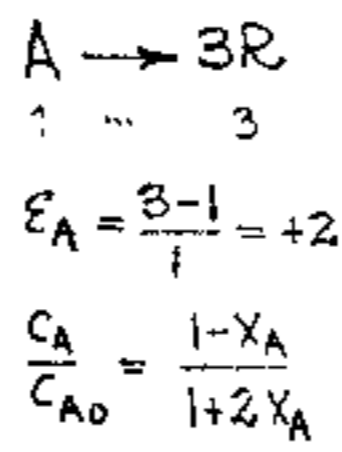
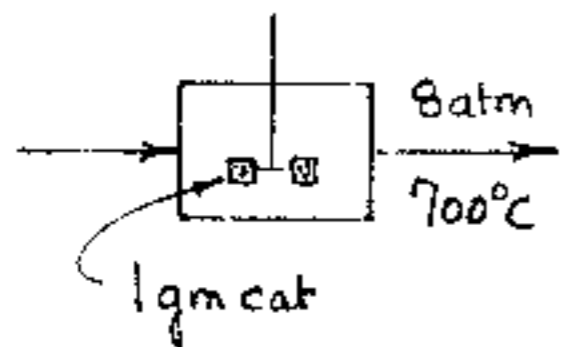
therefore

$X_A = 90.9\%$

$X_B = 0.909\%$



18.15 Sketch out what we know at the start:--



$$\frac{W}{F_{A0}} = \frac{X_A}{(-r'_A)} \quad \dots (i)$$

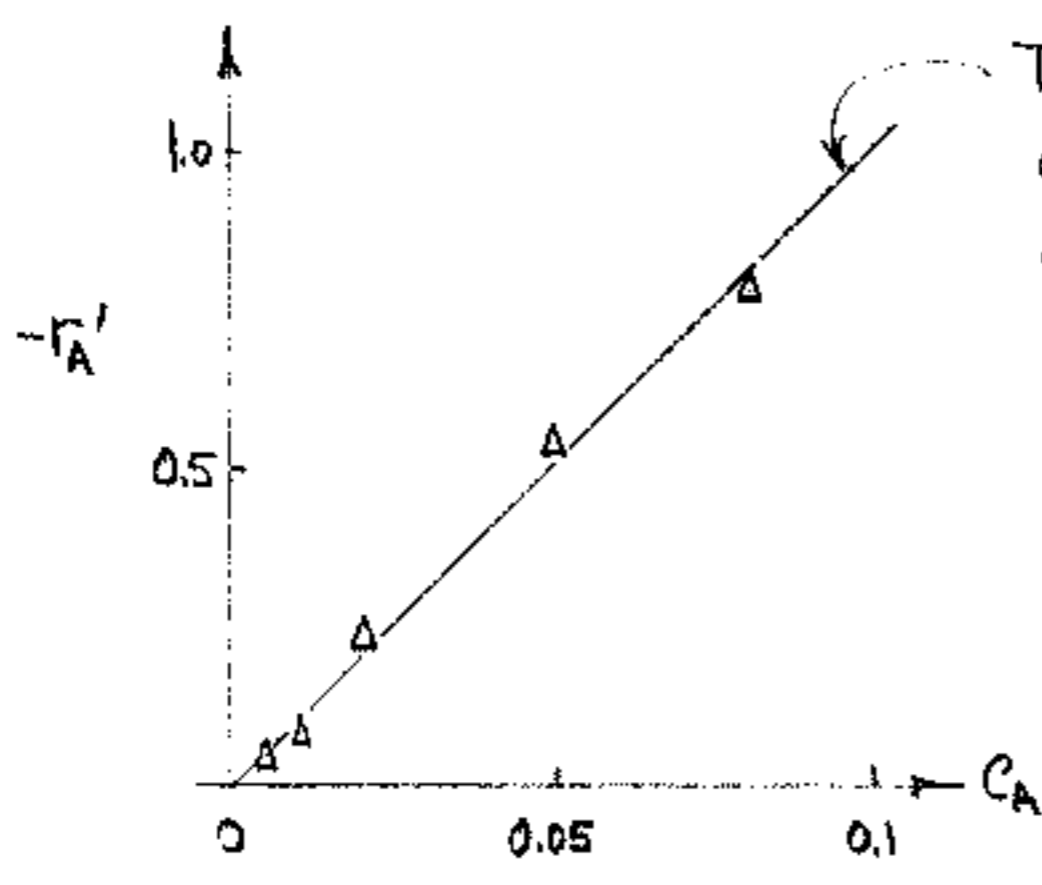
$\xrightarrow{\text{mol/hr}}$ $\xrightarrow{\text{mol/hr.gm cat}}$

$$C_A = \frac{P_A}{RT} = \frac{8}{(0.08206)(973)} = 0.1 \text{ mol/lit}$$

Now from the performance expression, (i), we can find $-r'_A$; the data give C_A . From these 2 quantities we should find a rate equation. So tabulate.

| C_A | $\frac{C_A}{C_{A0}} = \frac{P_A}{P_{A0}}$ | $X_A = \frac{1-C_A/C_{A0}}{1+2C_A/C_{A0}}$ | $F_{A0} = v C_{A0}$ | $-r'_A = \frac{X_A F_{A0}}{W}$ |
|-------|---|--|---------------------|--------------------------------|
| 0.08 | 0.8 | 0.2/2.6 | 10 | $(0.2/2.6) 10 = 0.769$ |
| 0.05 | 0.5 | 0.5/2 | 2.2 | 0.55 |
| 0.02 | 0.2 | 0.8/1.4 | 0.4 | 0.228 |
| 0.01 | 0.1 | 0.9/1.2 | 0.1 | 0.075 |
| 0.005 | 0.005 | 0.95/1.1 | 0.05 | 0.0432 |

Let us start by trying to fit a first order reaction, the simplest of rate forms. For this simply plot $-r'_A$ vs C_A , as shown below

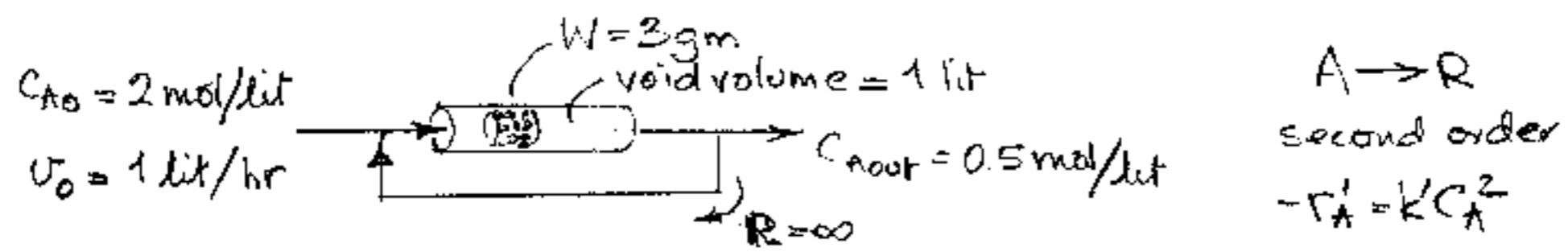


This gives a good straight-line fit of slope 10. thus our rate equation is

$$-r'_A = 10 C_A$$

$\xrightarrow{\text{mol/hr.gm cat}}$ $\xrightarrow{\text{mol/lit voids}}$
 $\text{lit voids/hr.gm cat}$

18.17



(a) Find the rate constant. First note that with $R = \infty$ we have mixed flow. The performance equation is then

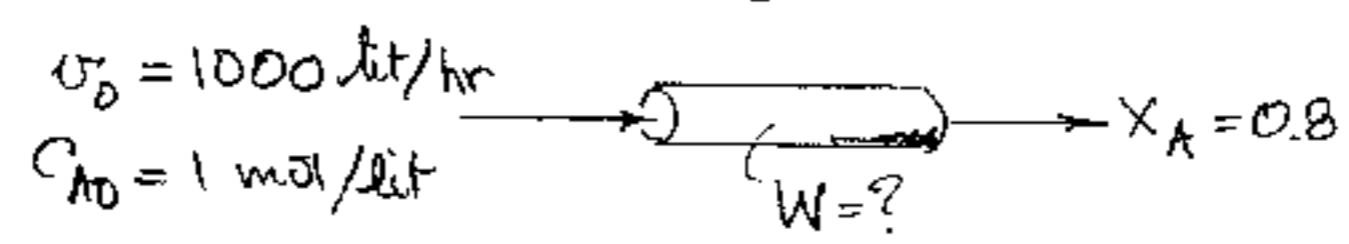
$$\tau' = \frac{WC_{A0}}{F_{A0}} = \frac{W}{v_0} = \frac{C_{A0} - C_A}{-r_A'} = \frac{C_{A0} - C_A}{k' C_A^2}$$

use these two terms

$$\therefore k' = \frac{v_0 \cdot (C_{A0} - C_A)}{W \cdot C_A^2}$$

$$= \frac{1 \text{ lit/hr} \cdot (2 - 0.5) \text{ mol/lit}}{3 \text{ gm} \cdot (0.5)^2 \text{ mol}^2/\text{lit}^2} = 2 \frac{\text{lit}^2}{\text{mol} \cdot \text{gm cat} \cdot \text{hr}} \quad \leftarrow \text{a)}$$

(b) For a packed bed (assume plug flow)



For plug flow

$$\tau' = \frac{W}{v_0} = \int \frac{dC_A}{k' C_A^2} = \frac{1}{k'} \left[\frac{1}{C_A} - \frac{1}{C_{A0}} \right]$$

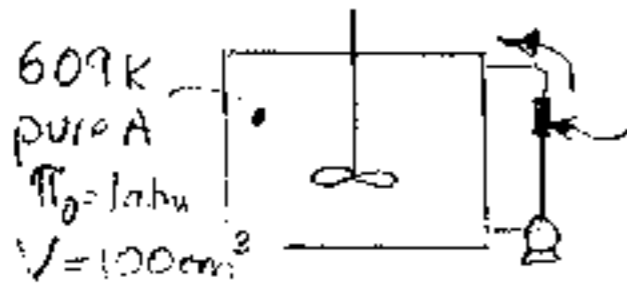
$$\therefore W = \frac{1000 \text{ lit/hr}}{2 \text{ lit}^2/\text{mol} \cdot \text{gm cat} \cdot \text{hr}} \left[\frac{1}{0.2 \text{ mol/lit}} - \frac{1}{1 \text{ mol/lit}} \right] = 2000 \text{ gm} = 2 \text{ kg} \quad \leftarrow \text{b)}$$

(c) Add inert solids

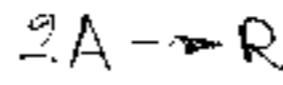
This does not change the rate equation $\dots -r_A' = k' C_A^2$
 or the performance equation $\dots \tau' = \int dC_A / -r_A'$

Therefore adding inerts makes the reactor bigger }
 but does not change the weight of catalyst needed for the process }

18.19



This batch circulation system is a constant volume system, so $\epsilon_A = 0$



First change p_A to C_A

$$C_{A0} = \frac{p_{A0}}{RT} = \frac{101325}{8.314 (609)} = 20 \text{ mol/m}^3$$

and from Eq 3.5

$$p_A = p_{A0} + \frac{a}{\Delta n} (\pi_0 - \pi)$$

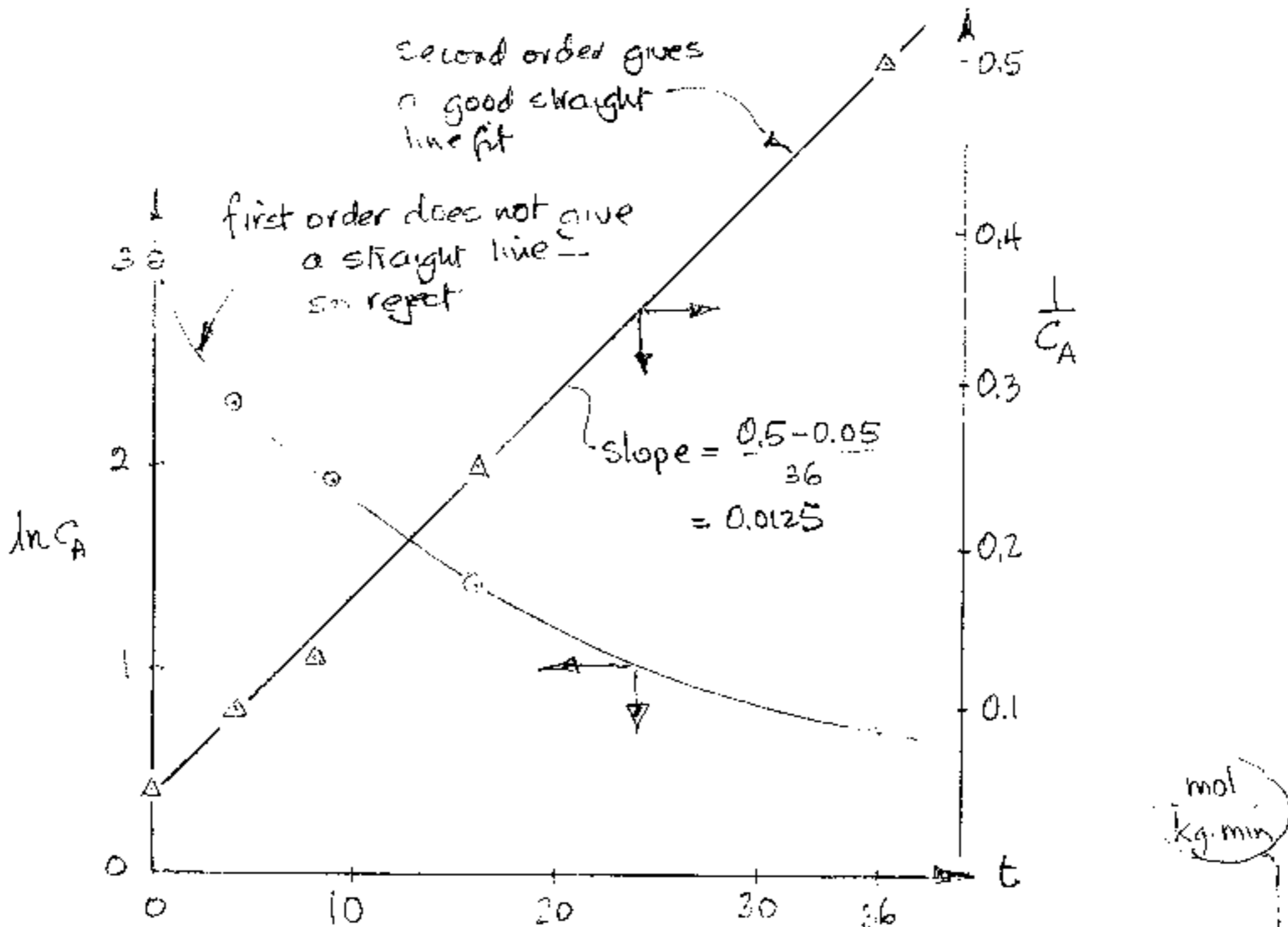
$$= 1 + \frac{2}{(-1)} (1 - \pi)$$

$$= 2\pi - 1 \quad (1)$$

Tabulate the data

| t | π | p_A | C_A | $\ln C_A$ | $1/C_A$ |
|----|-------|-------|-------|-----------|---------|
| 0 | 1.00 | 1 | 20 | 3 | 0.05 |
| 4 | 0.75 | 0.5 | 10 | 2.3 | 0.1 |
| 8 | 0.67 | 0.33 | 6.67 | 1.9 | 0.133 |
| 16 | 0.60 | 0.2 | 4 | 1.38 | 0.25 |
| 36 | 0.55 | 0.1 | 2 | 0.693 | 0.5 |

from Eq (1) first order test
second order test



Therefore the rate equation is: $r_A = 0.0125 C_A^2 \text{ mol/m}^3 \cdot \text{min}$

$$\text{or } r_A' = \frac{V}{W} r_A = \frac{100 \text{ cm}^3 (1000 \text{ gm})}{2 \text{ gm} (1 \text{ kg})} \left(\frac{\text{m}^3}{10^6 \text{ cm}^3} \right) (0.0125 C_A^2) = 6.25 \times 10^{-4} C_A^2$$

18.21

Given $A \rightarrow R$, $-r_A''' = 0.1 C_A^2$, mol/m³.s

$d_p = 6$ mm
 $D_{eff} = 10^{-6}$ m²/m.s
 $C_{A0} = 100$ mol/m³

Find the effectiveness factor & the amount slowed by diffusion

For n^{th} order rx: $M_T = \frac{d_p}{6} \sqrt{\frac{n+1}{2} \frac{k''' C_A^{n-1}}{D_{eff}}}$

$$= \frac{6 \times 10^{-3}}{6} \sqrt{\frac{2+1}{2} \frac{(0.1)(100)^{2-1}}{10^{-6}}} = 3.973$$

∴ from the chart of Fig 5 or 6: $\epsilon = 0.23$ ←

Note If we mistakenly assume 1st order kinetics

$M_T = L \sqrt{\frac{k'''}{D}} = \frac{6 \times 10^{-3}}{6} \sqrt{\frac{0.1}{10^{-6}}} = 0.3162$ or $\epsilon = 1$ ↙ quite wrong

18.23

| Run | d_p | W | C_{A0} | v | X_A | C_A | $k' = (C_{A0} - C_A)v / C_A W$ |
|-----|-------|-----|----------|-----|-------|-------|--------------------------------|
| 1 | 3 | 1 | 100 | 9 | 0.4 | 60 | 6 |
| 2 | 12 | 4 | 300 | 8 | 0.6 | 120 | 3 |

for mixed flow
 $k' = \frac{W}{v} = \frac{C_{A0} - C_A}{k' C_A}$

For no diffusion resistance $k_2'/k_1' = 1$

For strong resistance

$k_2'/k_1' = d_{p1}/d_{p2} = 1/4$

but from the data $k_2'/k_1' = 1/2$

∴ we are in the intermediate regime between strong & no pore diffusion resistance ←

18.25

| d_p | W | C_{A0} | v | X_A | C_A | $-r_A' = X_A v / W = k' C_A$ | k' |
|-------|-----|----------|-----|-------|-------|------------------------------|--------|
| 2 | 4 | 75 | 10 | 0.2 | 60 | $0.2(10)/4 = 0.5 = k'(60)$ | 0.0083 |
| 1 | 6 | 100 | 5 | 0.7 | 30 | $0.6(5)/6 = 0.5 = k'(30)$ | 0.0167 |

given

for mixed flow

$W/v = \frac{X_A}{-r_A'}$

Since $k_2'/k_1' = 2 = d_{p1}/d_{p2}$ this run was made in the regime of

strong pore diffusion resistance ←

18.27 All these runs were made at the same W/F_{A0} . We are also told that the recycle rate is high enough to have mixed flow throughout. Thus changing the recycle rate from run 1 to 2, or from run 3 to 4 with no change in rate shows that film resistance does not influence the rate.

Next, if the particles were non-porous then the smaller size (runs 1 & 2) should have double the rate of the larger size (runs 3 & 4). This is not what is measured hence the results are not consistent with the guess of non-porous particles.

Alright, let us see if the results are consistent with the assumption of porous particles

- if in the regime of no pore diffusion resistance the rates should be the same for large & small pellets
- if in the regime of strong pore diffusion the rate should halve from 4 to 2 in going to the larger particles

Our results are $1/2$ way between these two extremes, hence we must be operating under conditions where pore diffusion is just beginning to influence the rate

Thus we conclude:

Porous particles, no film resistance, pore resistance just beginning to intrude & affect the rate } ←

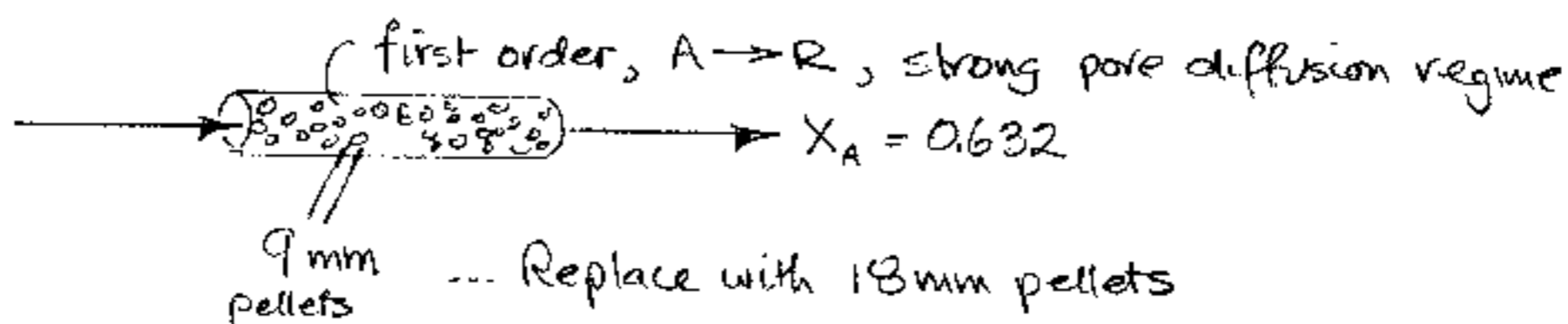
18.29 For mixed flow the reactor performance equation is: $\frac{W}{F_{A0}} = \frac{X_A}{(-r'_A)}$
and since the data show that the rate is
inversely proportional to pellet size Eq 25 pg 388 shows that
pore diffusion controls in both runs. So Table 2 pg 405 shows:

$$\frac{R_2}{R_1} = 0.25 \dots \text{and by eliminating pore diffusion} \\ \text{in backmix flow we can get} \dots \frac{C_R}{C_{A0}} = 0.44$$

$$\dots \text{and by eliminating pore diffusion \&} \\ \text{using plug flow we can get} \dots \frac{C_R}{C_{A0}} = 0.63$$

So use smaller pellets in a packed & we
should be able to achieve as high as $\dots \frac{C_R}{C_{A0}} = 0.63 \leftarrow$

18.31



Note that in the regime of strong pore diffusion resistance
doubling the pellet size halves the rate constant.

For 9mm pellets, plug flow, $\varepsilon_A = 0$

$$\ln \frac{1}{1-X_A} = (k'_{obs} \tau)'_1 \dots \text{or } X_A = 1 - e^{-k'_{obs,1} \tau_1}$$

$$\therefore k'_{obs,1} \tau_1 = \ln \frac{1}{1-0.632} = 1$$

For the 18mm pellets

$$(k'_{obs} \tau)'_2 = 2$$

$$\therefore X_{A2} = 1 - e^{-(k'_{obs} \tau)'_2} = 1 - e^{-\frac{1}{2}}$$

$$\text{or } X_{A2} = 0.393 \leftarrow$$

18.33

From experiment

pure A

$$v = 4 \text{ cm}^3/\text{s}$$

1 atm

325°C

10 gm of $d_p = 1.2 \text{ mm}$

$$X_A = 0.8$$

 $R = \infty$ (for catalyst $\rho = 2000 \text{ kg}/\text{m}^3$)

$$D_e = 10^{-6} \text{ m}^2/\text{mcat} \cdot \text{s}$$

Design a commercial unit for $X_A = 0.8$, either• a fluidized bed (mixed flow) using $d_p = 1 \text{ mm}$ particles• a packed bed (plug flow) using $d_p = 15 \text{ mm}$ particles

Which design needs less catalyst?

For the experimental run

$$\tau' = \frac{C_{A0} X_A}{-r'_{A,obs}} \quad \text{or} \quad -r'_{A,obs} = \frac{C_{A0} X_A}{W/v}$$

$$C_{A0} = \frac{P_{A0}}{RT} = \frac{101325}{(8.314)(325+273)} = 20 \text{ mol}/\text{m}^3$$

$$-r'_{A,obs} = \frac{20(0.8)}{0.01/4 \times 10^{-6}} = 0.0064 \text{ mol}/\text{kg} \cdot \text{s} \quad \dots \quad -r''_{A,obs} = -r'_{A,obs} \left(\frac{W}{v} \right) = 12.8 \text{ mol}/\text{m}^3 \cdot \text{s}$$

$$\therefore M_W = \frac{-r''_{A,obs} L^2}{D_e C_{A0}} = \frac{12.8 (1.2 \times 10^{-3})^2}{10^{-6} (20)(1-0.8)} = 0.128 \quad \dots \quad \epsilon_{\text{expt}} = 1$$

For the packed bed

$$L = 2.5 \times 10^{-3} \text{ m}$$

$$M_T = 2.5 \times 10^{-3} \sqrt{32/10^{-6}} = 4.472 \quad \dots \quad \epsilon = \frac{1}{M_T} = 0.2236$$

$$\text{and} \quad \frac{W}{v} = \frac{1}{k' \epsilon} \ln \frac{C_{A0}}{C_A} = \frac{1}{0.016(0.2236)} \ln \frac{20}{4} = 4500 \text{ kg}/\text{m}^3 \cdot \text{s}$$

For the fluidized bed

$$L = 1.67 \times 10^{-4} \text{ m}$$

$$M_T = 1.67 \times 10^{-4} \sqrt{32/10^{-6}} = 0.2987 \quad \dots \quad \epsilon = 1$$

$$\text{and} \quad \frac{W}{v} = \frac{1}{k' \epsilon} \frac{C_{A0} X_A}{C_{A0}(1-X_A)} = \frac{1}{0.0016(1)} \cdot \frac{0.8}{1-0.8} = 2500 \text{ kg}/\text{m}^3 \cdot \text{s}$$

Conclusion: The fluidized bed is better because it needs only 56% of the packed bed catalyst. \leftarrow

18.35 Check for pore diffusion resistance. If it is important it will affect the observed rate constant

$$k''' = \left(2 \frac{\text{m}^3}{\text{m}^3 \text{bed} \cdot \text{s}}\right) \left(\frac{2 \text{m}^2 \text{bed}}{1 \text{m}^2 \text{catalyst}}\right) = 4 \frac{\text{m}^3}{\text{m}^3 \text{cat} \cdot \text{s}}$$

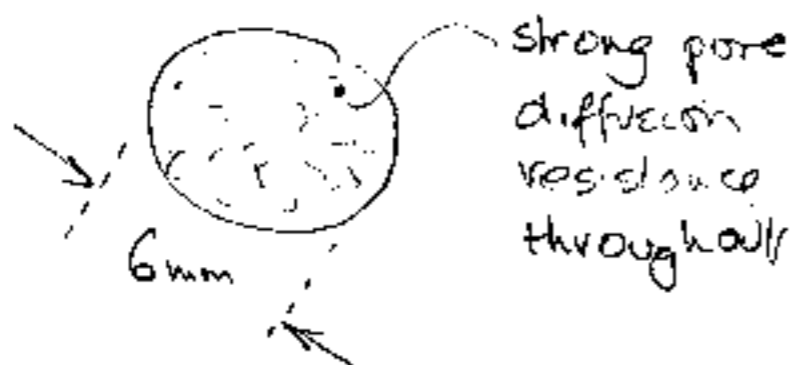
$$M_T = L \sqrt{\frac{k'''}{D}} = \frac{6 \times 10^{-3}}{6} \sqrt{\frac{4}{4 \times 10^{-8}}} = 10 \dots \% \text{ strong pore diffusion, and } \epsilon = 0.1$$

$$\therefore \eta''' = \frac{C_{A0} V_{\text{cat}}}{F_{A0}} = \int \frac{dC_A}{k''' \epsilon C_A} = \frac{1}{k''' \epsilon} \ln \frac{C_{A0}}{C_A}$$

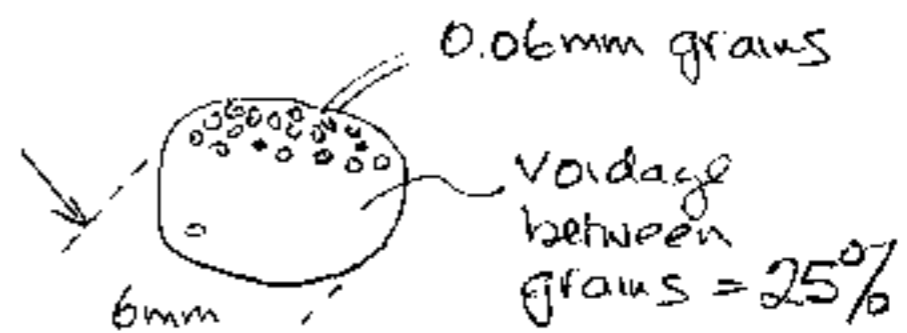
$$\text{or } V_{\text{cat}} = \frac{F_{A0}}{C_{A0} k''' \epsilon} \ln \frac{C_{A0}}{C_A} = \frac{10^4 / 3600}{10^3 (4) (0.1)} \ln \frac{10}{1} = 0.016$$

$$\therefore W = V_{\text{cat}} \rho_{\text{cat}} = V_{\text{cat}} \left(\frac{\rho_{\text{bulk}}}{\text{voidage}}\right) = 0.016 \left(\frac{2000}{0.5}\right) = 64 \text{ kg} \leftarrow$$

18.37

Original pellet

strong pore diffusion regime

Proposed pellet

model by the micro-macro pellet
strong diffusion resistance in grains
no diffusion resistance between grains

$$\frac{M_{T, \text{new}}}{M_{T, \text{old}}} = \frac{L_{\text{new}} \sqrt{k''' / D_e}}{L_{\text{old}} \sqrt{k''' / D_e}} = \frac{10^{-5}}{10^{-3}} = 0.01$$

$$\therefore \frac{\epsilon_{\text{new}}}{\epsilon_{\text{old}}} = 100 \quad \text{or} \quad W_{\text{new}} = \frac{1}{100} W_{\text{old}}$$

Considering the void volume between grains

$$V_{\text{new}} = V_{\text{old}} \frac{1}{100} \cdot \frac{1}{1-0.25} = 0.0133 V_{\text{old}}$$

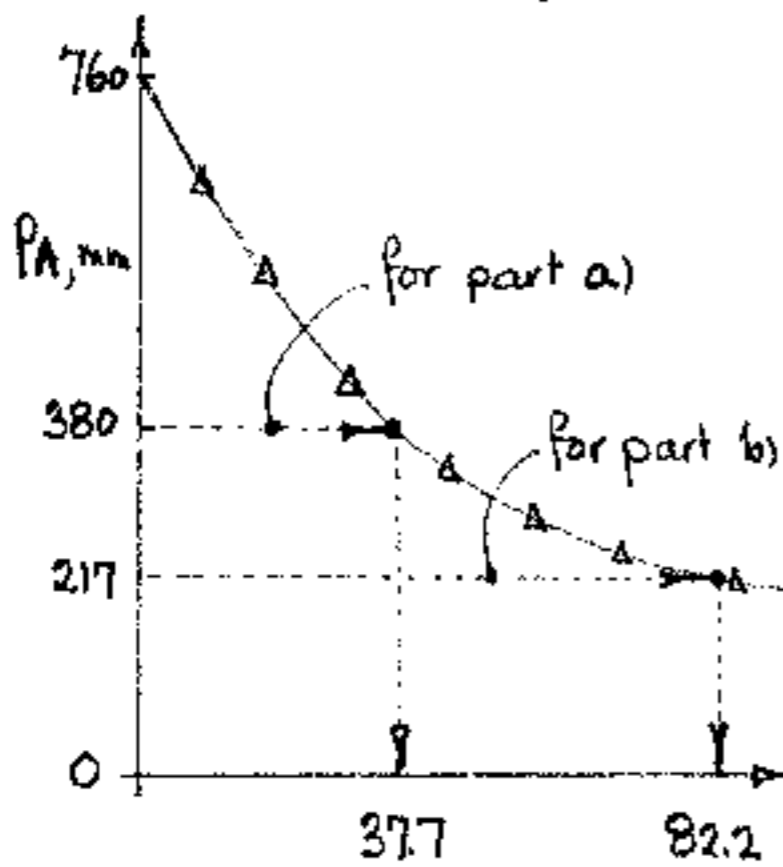
\therefore With this new catalyst we need

1% of weight of the original catalyst
or 1.33% the volume of the original reactor \leftarrow

18.39

The system given \uparrow should be equivalent to this \uparrow if we make the appropriate time correction. So what we are given is integral data in which we know X_A at various V_r/F_{A0} , see sketch.

Now $X_A = 0.5$ at $p_A = 380$ mm, & this occurs after 37.7 sections



$$\therefore \frac{V_r}{F_{A0}} = \frac{(37.7 \text{ cm}^3 \text{ cat})}{\left(10 \frac{\text{cm}^3 \text{ fluid}}{\text{sec}}\right) \left(\frac{1 \text{ mol}}{22400 \text{ cm}^3}\right)} = 84,400 \frac{\text{cm}^3 \text{ cat} \cdot \text{sec}}{\text{mol A}}$$

and for a feed $F_{A0} = 10^5 \text{ mol A/hr}$

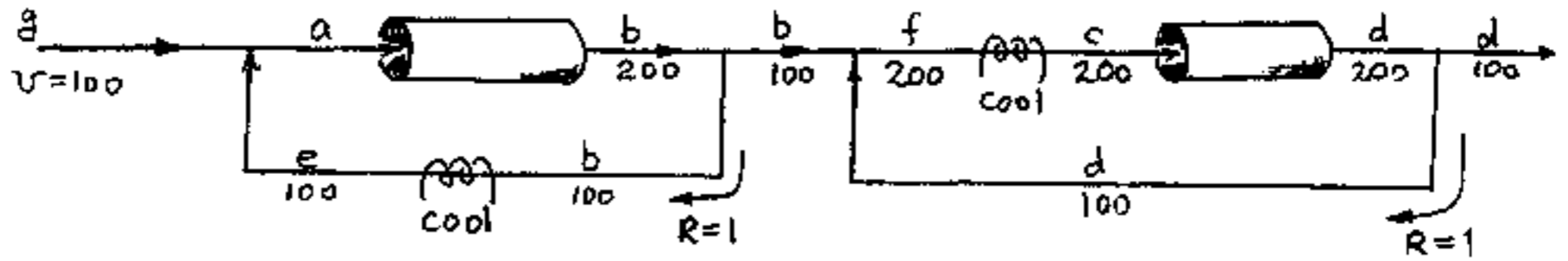
$$V_r = \left(84,400 \frac{\text{cm}^3 \text{ cat} \cdot \text{sec}}{\text{mol A}}\right) \left(\frac{10^5 \text{ mol A/hr}}{3600 \text{ sec/hr}}\right) = 2.34 \times 10^6 \text{ cm}^3 = 2.34 \text{ m}^3 \leftarrow \text{a)}$$

b) For $A \rightarrow 2.5R$ $\epsilon_A = 1.5$ & from $\frac{C_A}{C_{A0}} = \frac{1-X_A}{1+\epsilon_A X_A}$ we find $p_{A, \text{out}} = 760(0.2857)$ for $X_A = 0.5$.

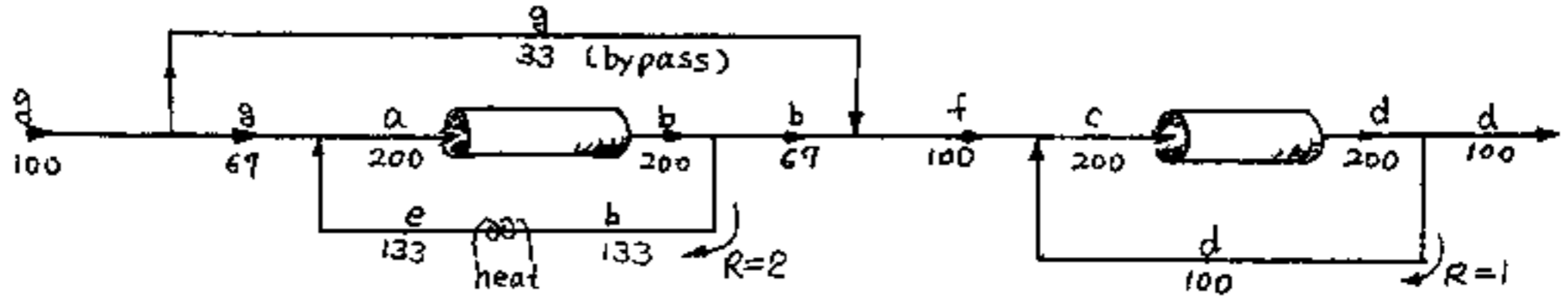
Thus the amount of catalyst needed is 82.2 m instead of 37.7 m. With all else unchanged

$$V_r = 2.34 \text{ m} \left(\frac{82.2}{37.7}\right) = 5.1 \text{ m}^3 \text{ of catalyst bed} \leftarrow \text{b)}$$

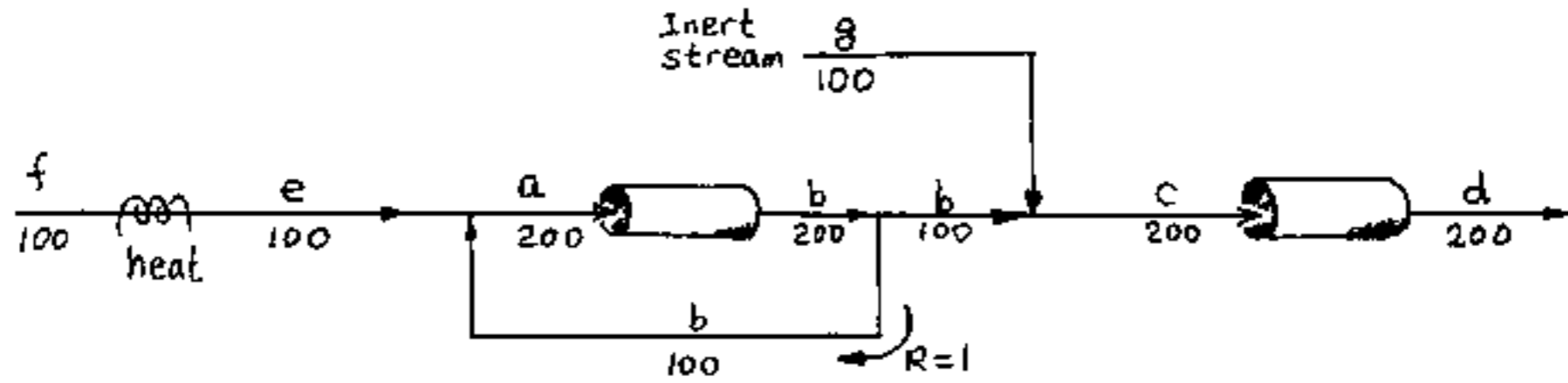
19.1



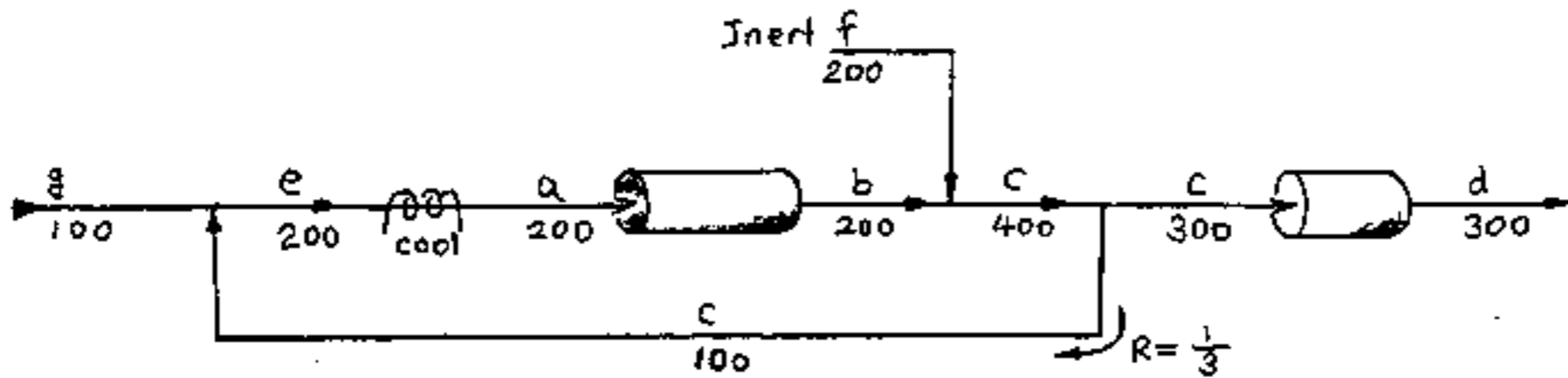
19.3



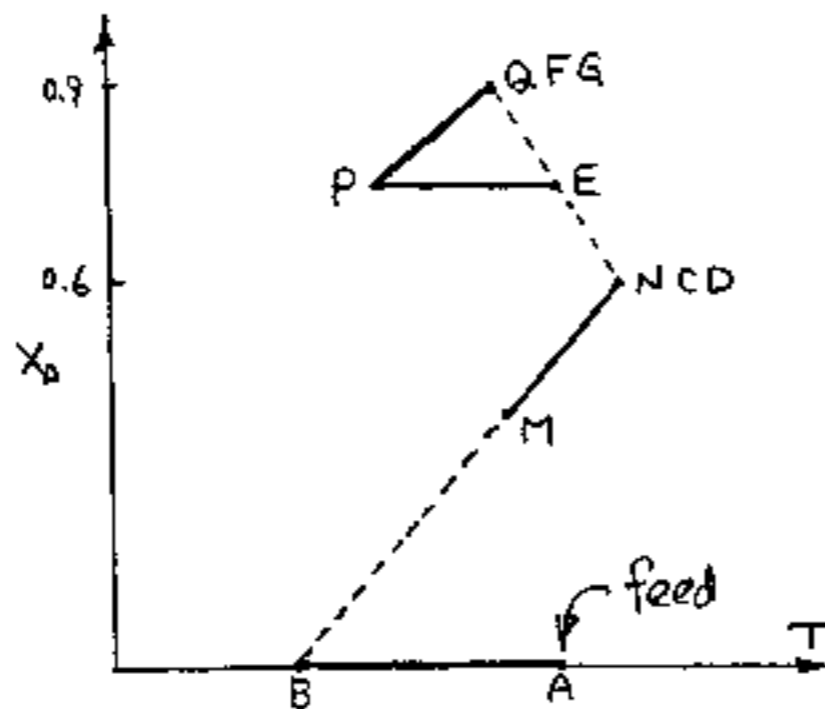
19.5



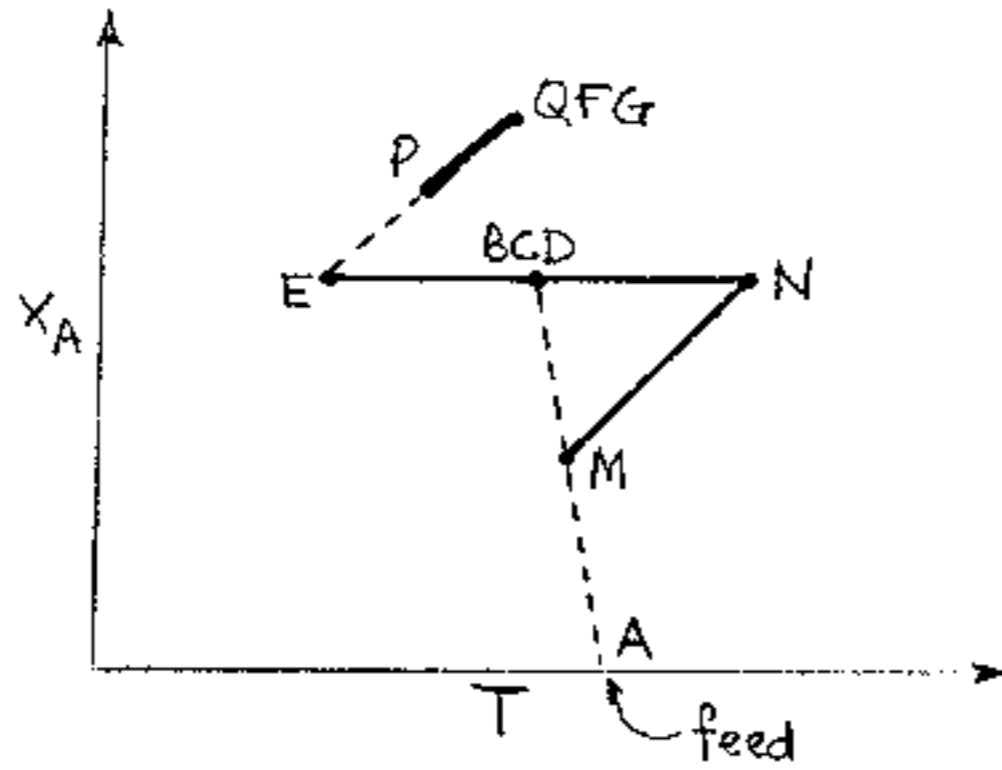
19.7



19.9

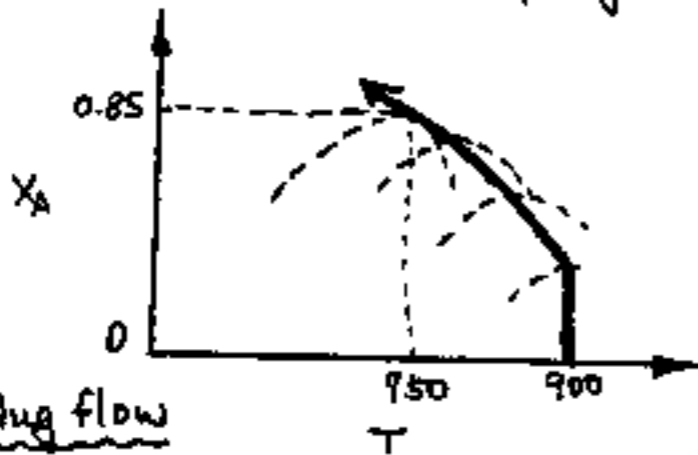


19.11



19.13

Optimal temperature progression



Plug flow

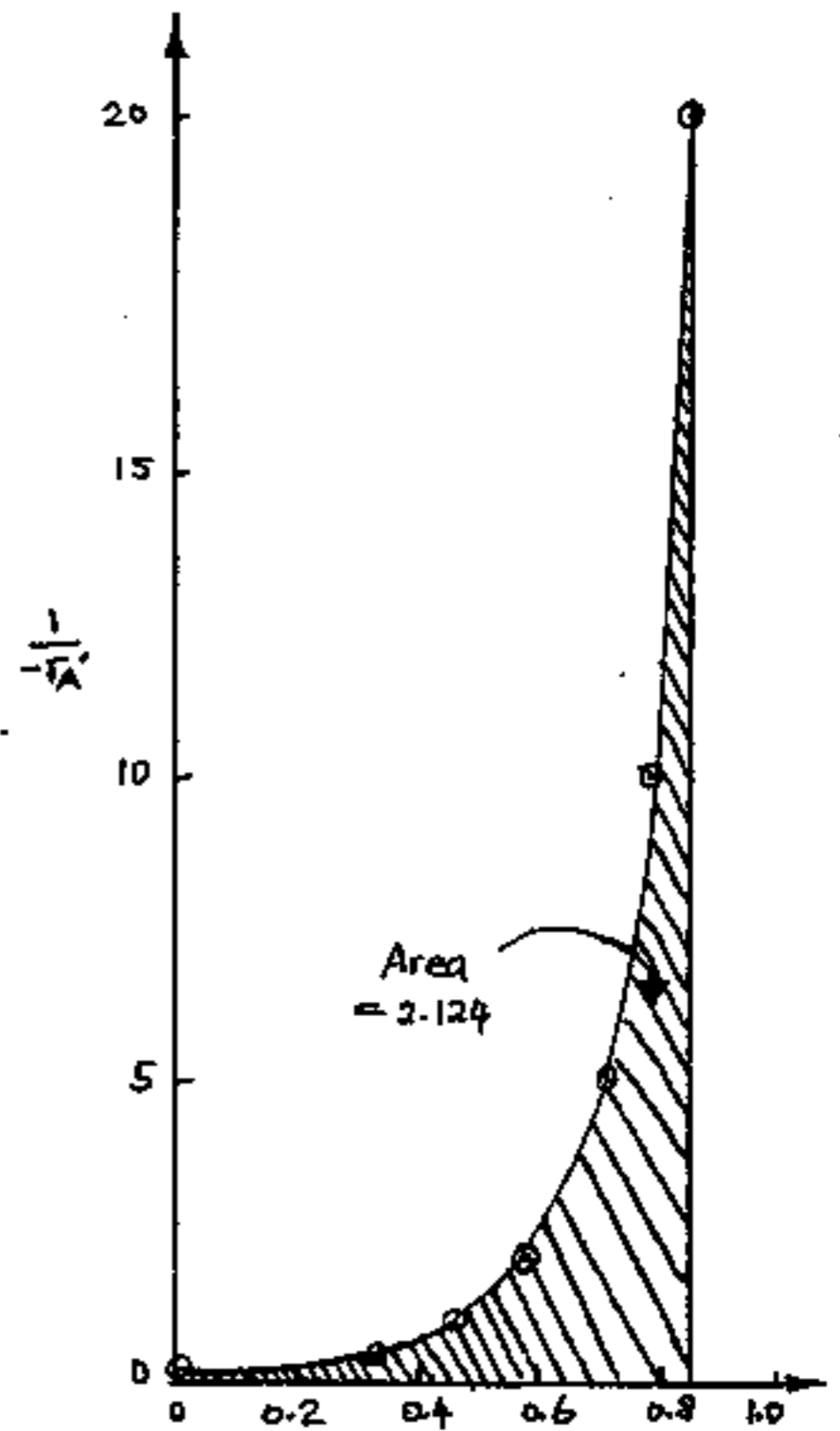
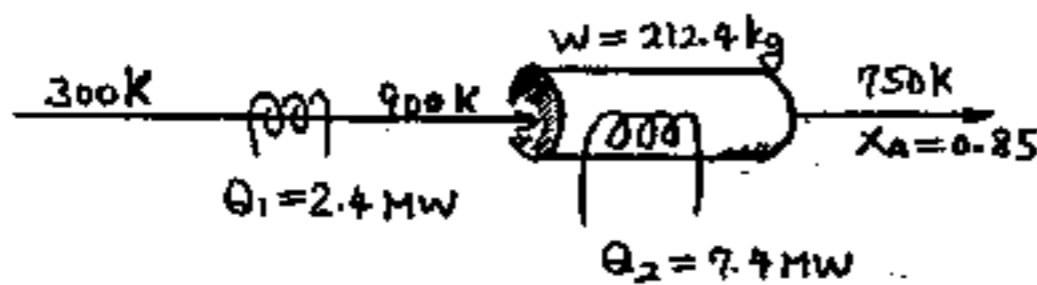
$$W = F_{A_0} \int_0^{0.85} \frac{dX_A}{-r_A'} = (100)(2.124) = 212.4 \text{ kg}$$

Heat added ahead of the reactor

$$Q_1 = F_{A_0} C_p \Delta T = (100)(40)(900-300) = 2.4 \times 10^6 \text{ J/s}$$

Heat removed from the reactor

$$\begin{aligned} Q_2 &= F_{A_0} X_A (-\Delta H_r) + F_{A_0} C_p (\Delta T) \\ &= (100)(0.85)(80000) + (100)(40)(900-750) \\ &= 7.4 \times 10^6 \text{ J/s} \end{aligned}$$



19.15 20% A - 80% inert, adiabatic reactor

$$\text{slope} = \frac{C_p}{-\Delta H_r} = \frac{40 \times 5}{80000} = \frac{1}{400}$$

Let us construct $\frac{1}{-r_A}$ vs X_A graph.

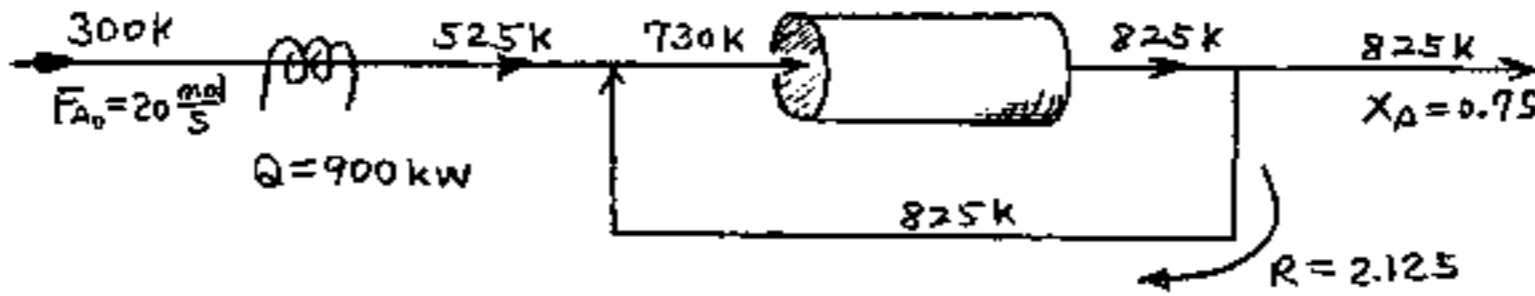
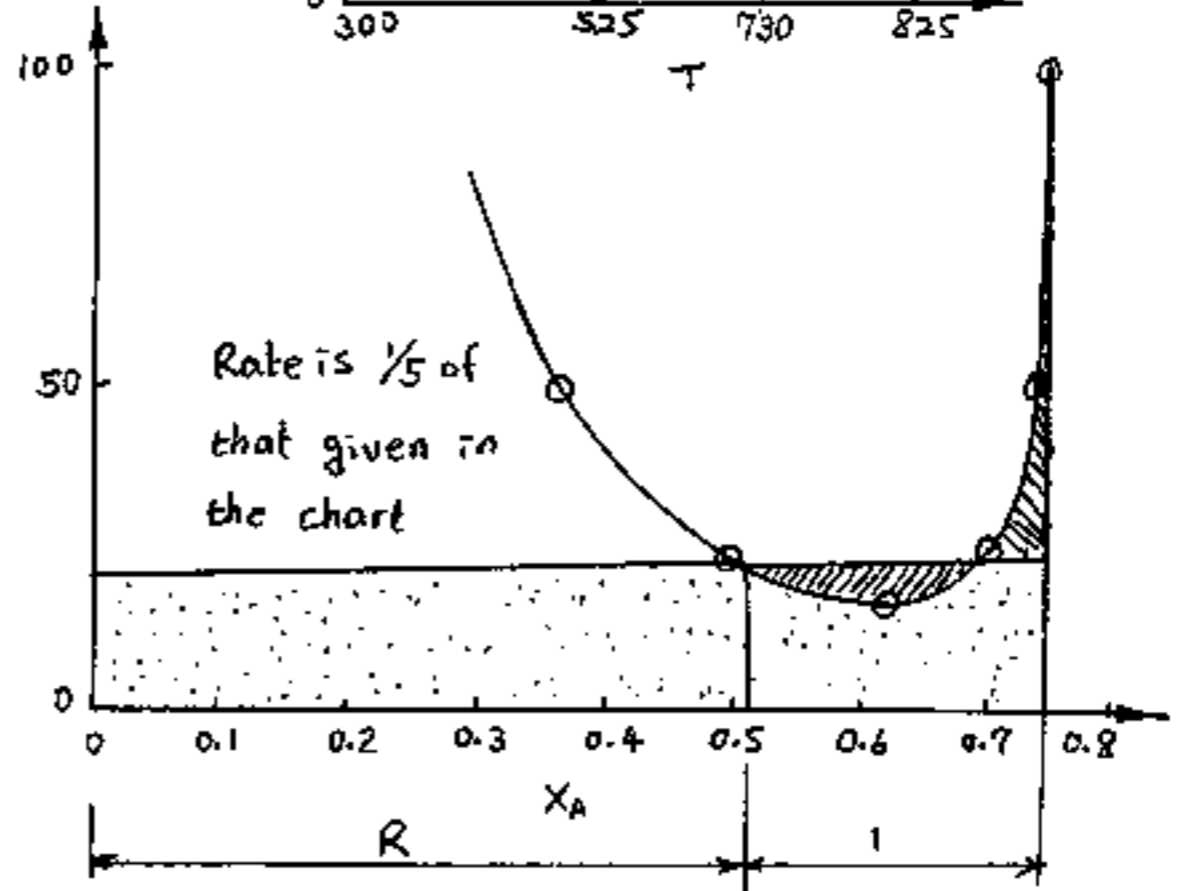
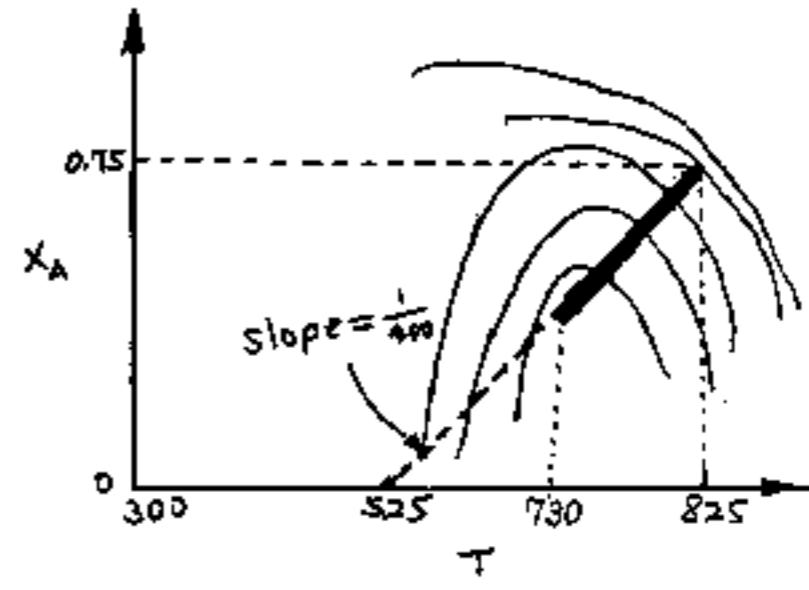
From this graph we can see that recycle flow is best and

$$R = \frac{0.51}{0.75 - 0.51} = 2.125$$

$$W = F_{A0} \frac{X_A}{-r_A} = (100 \times 0.2)(0.75)(22.8) = 342 \text{ kg}$$

Heat duty

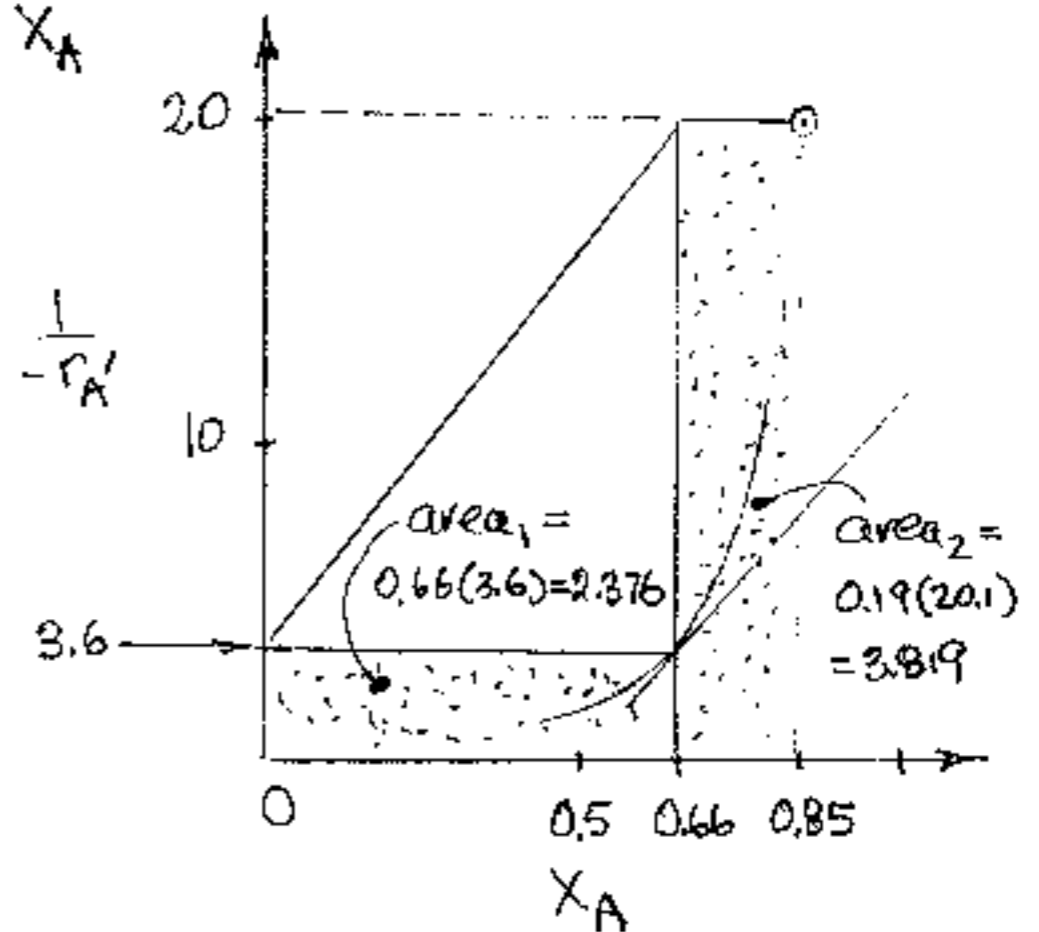
$$\begin{aligned} Q &= F_{\text{TOT}} \cdot C_p \Delta T - F_A X_A (-\Delta H_r) \\ &= (100)(40)(825 - 300) - (20)(0.75)(80000) \\ &= 9 \times 10^5 \text{ J/S (heating)} \end{aligned}$$



19.17 From Fig 11 plot the $\frac{1}{-r_A, \text{opt}}$ vs X_A curve. By the optimization of rectangles we find the minimum amount of catalyst needed

$$W_1 = F_{A0} (\text{area}_1) = 100(2.376) = 237.6 \text{ kg}$$

$$W_2 = F_{A0} (\text{area}_2) = 100(3.819) = 381.9 \text{ kg}$$



19.17
(continued)

Heat duty

$$Q_1 = [F_{A0}(C_p \Delta T) - X_A (-\Delta H_r)]$$

$$= 100 [40(815 - 300) - 0.66(+80000)]$$

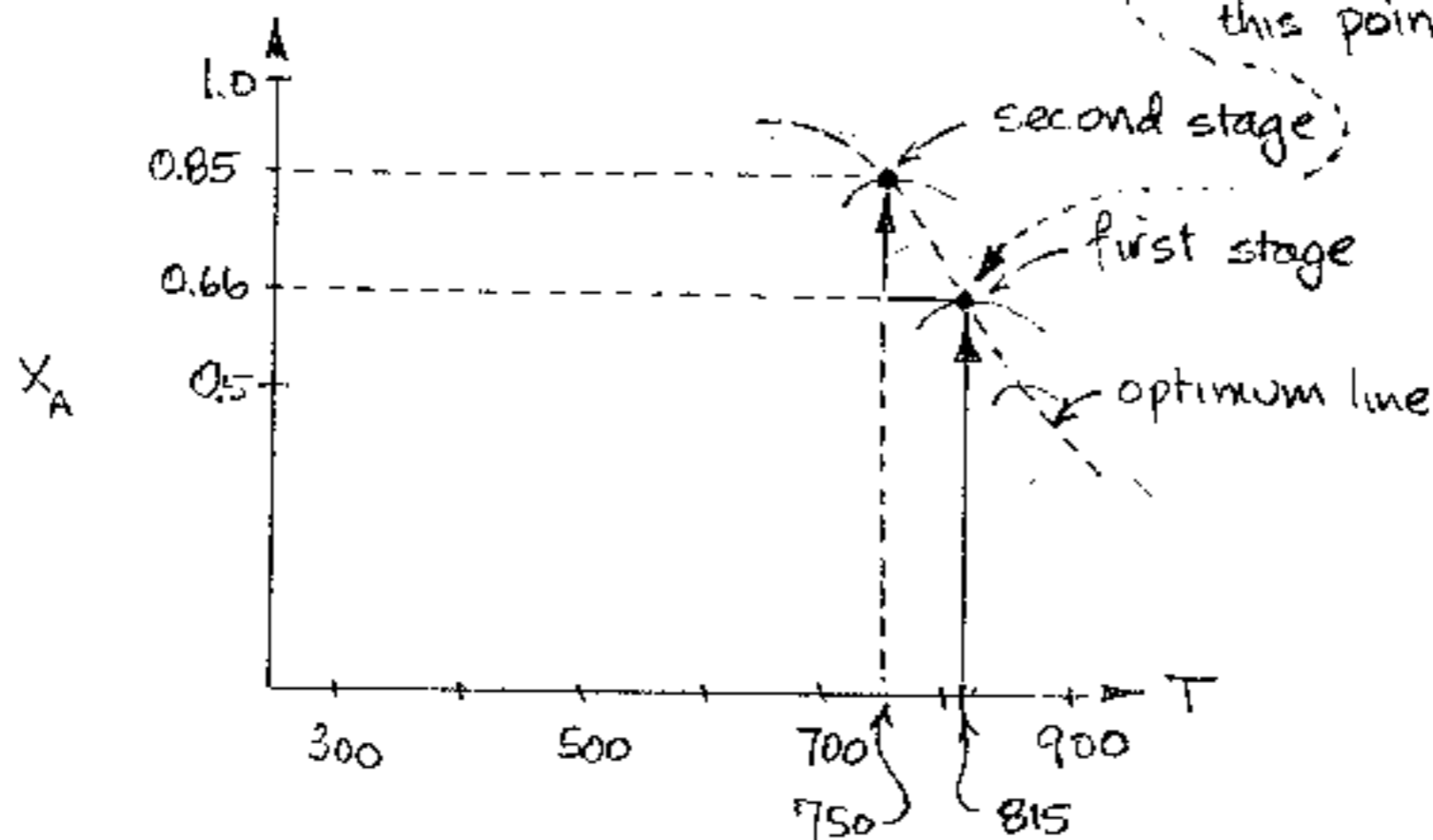
$$= -3.2 \text{ MW (remove)}$$

$$Q_2 = [F_{A0}(C_p \Delta T) - X_A (-\Delta H_r)]$$

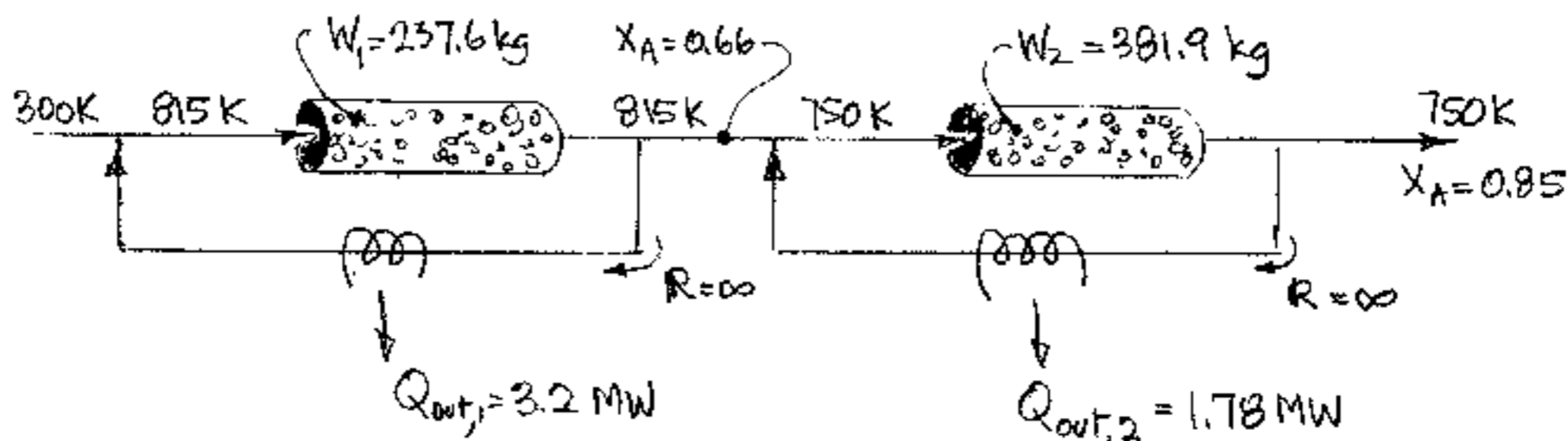
$$= 100 [40(750 - 815) - 0.19(+80000)]$$

$$= -1.78 \text{ MW}$$

The T vs X_A diagram (Fig 11) is then



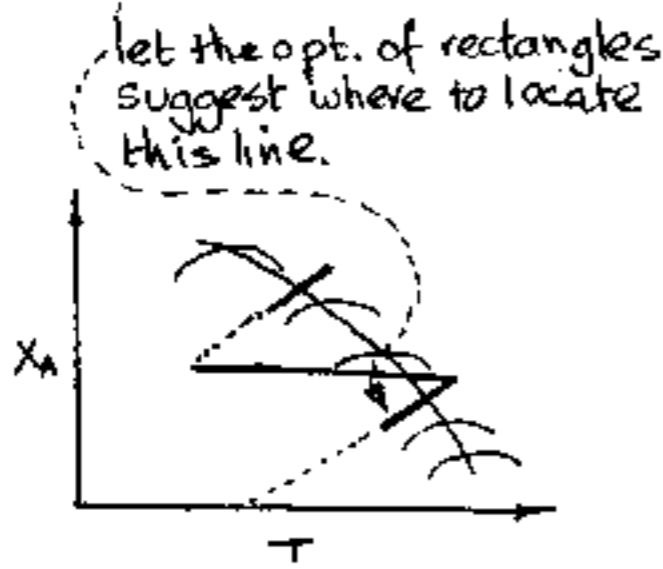
Final design.



19.19 20% A - 80% B, $X_A = 0.85$

$$\text{slope} = \frac{C_p}{-4Hr} = \frac{40 \times 5}{80000} = \frac{1}{400}$$

Plug flow with recycle is best.



$$W_1 = F_{A_0} \cdot \text{area 1} = (20)(4.64) = 92.8 \text{ kg}$$

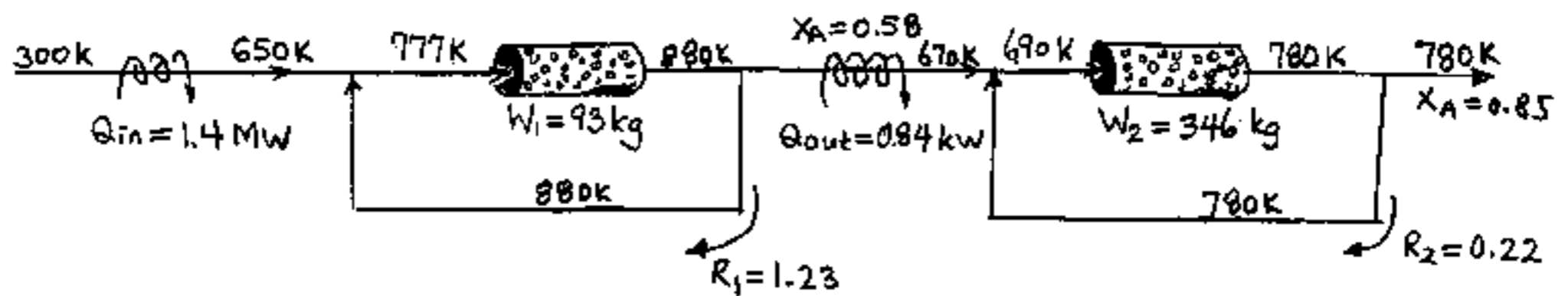
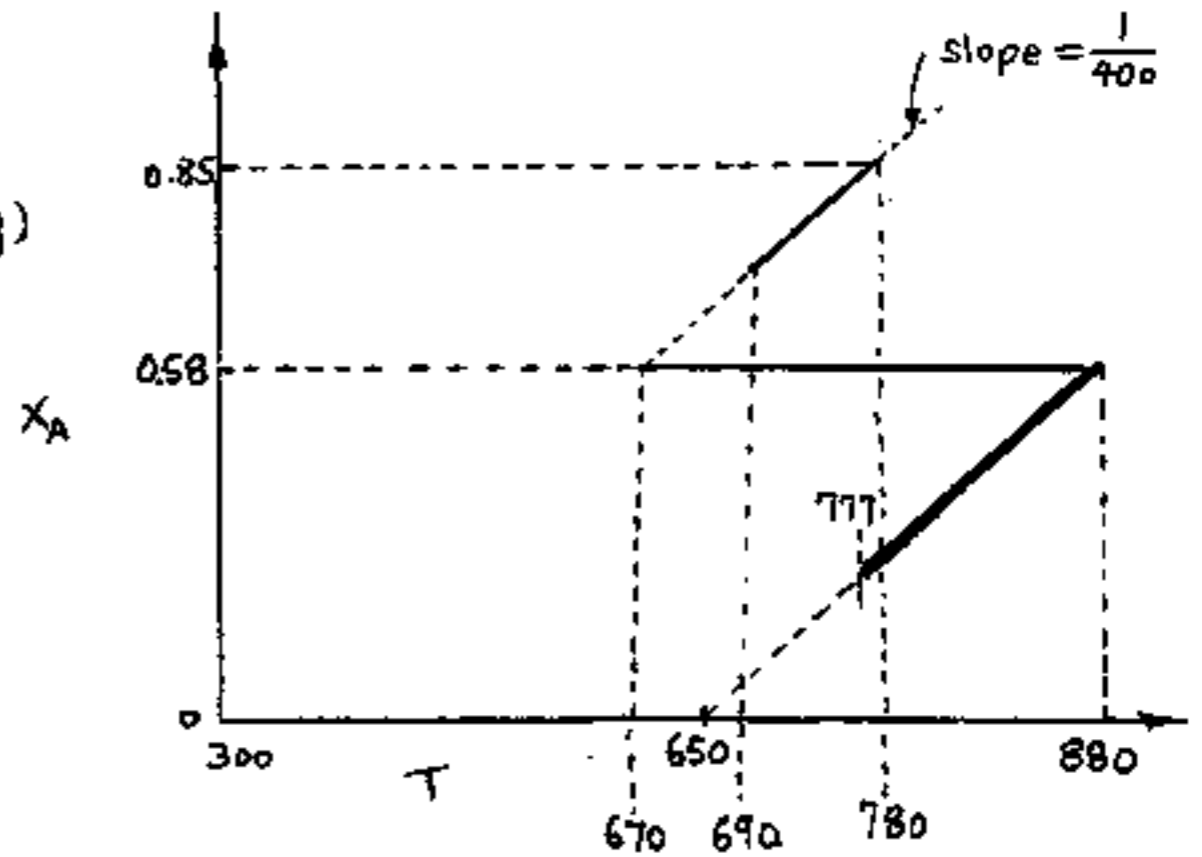
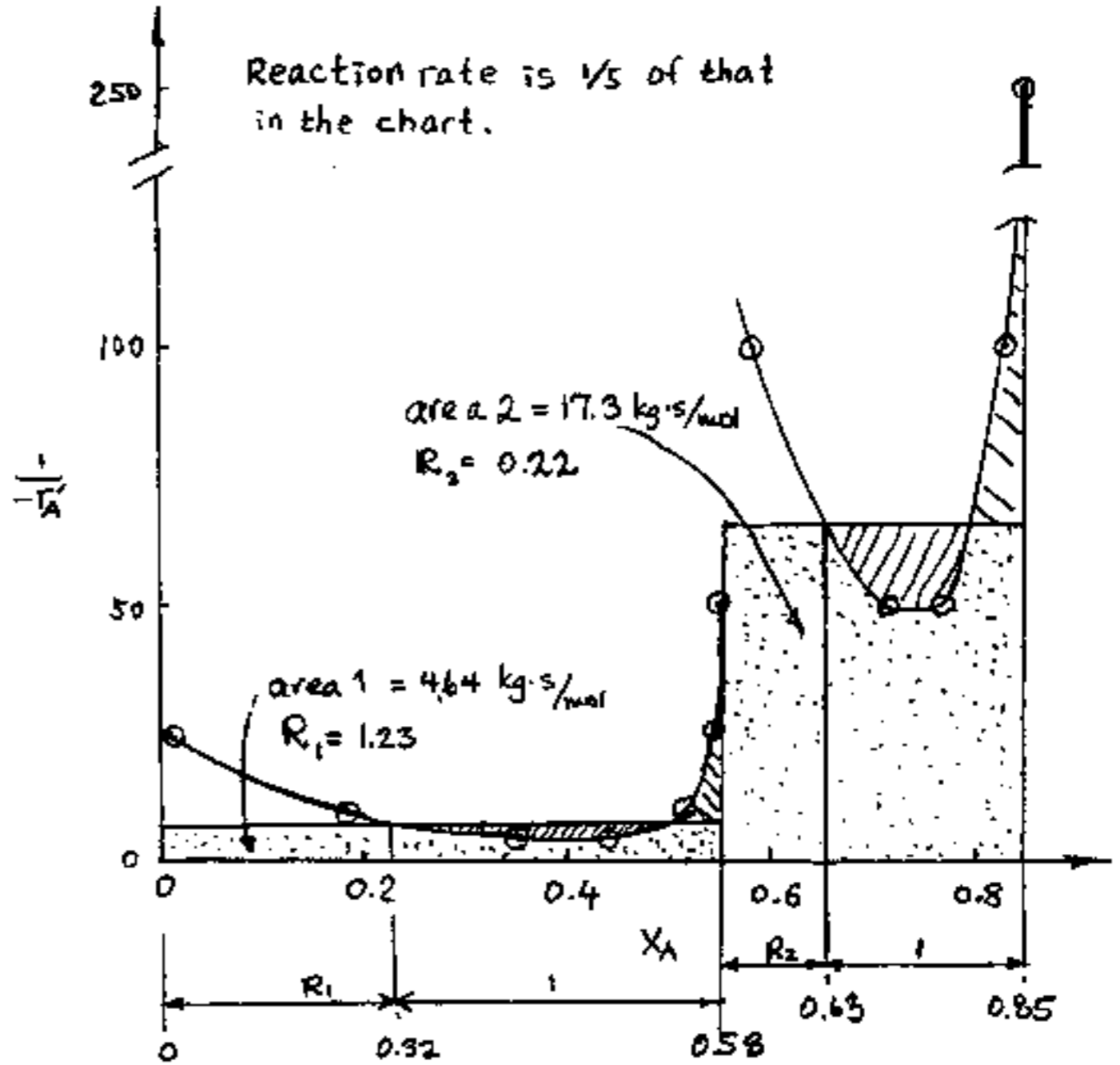
$$W_2 = F_{A_0} \cdot \text{area 2} = (20)(17.3) = 346 \text{ kg}$$

Heat duty

$$Q_1 = F_{A_0} C_p (\Delta T) = (20)(200)(650 - 300) = 1.4 \times 10^6 \text{ J/s (heating)}$$

$$Q_2 = F_{A_0} C_p (\Delta T) = (20)(200)(880 - 670) = -0.84 \times 10^6 \text{ J/s (cooling)}$$

Note that this solution was obtained after a few trials.



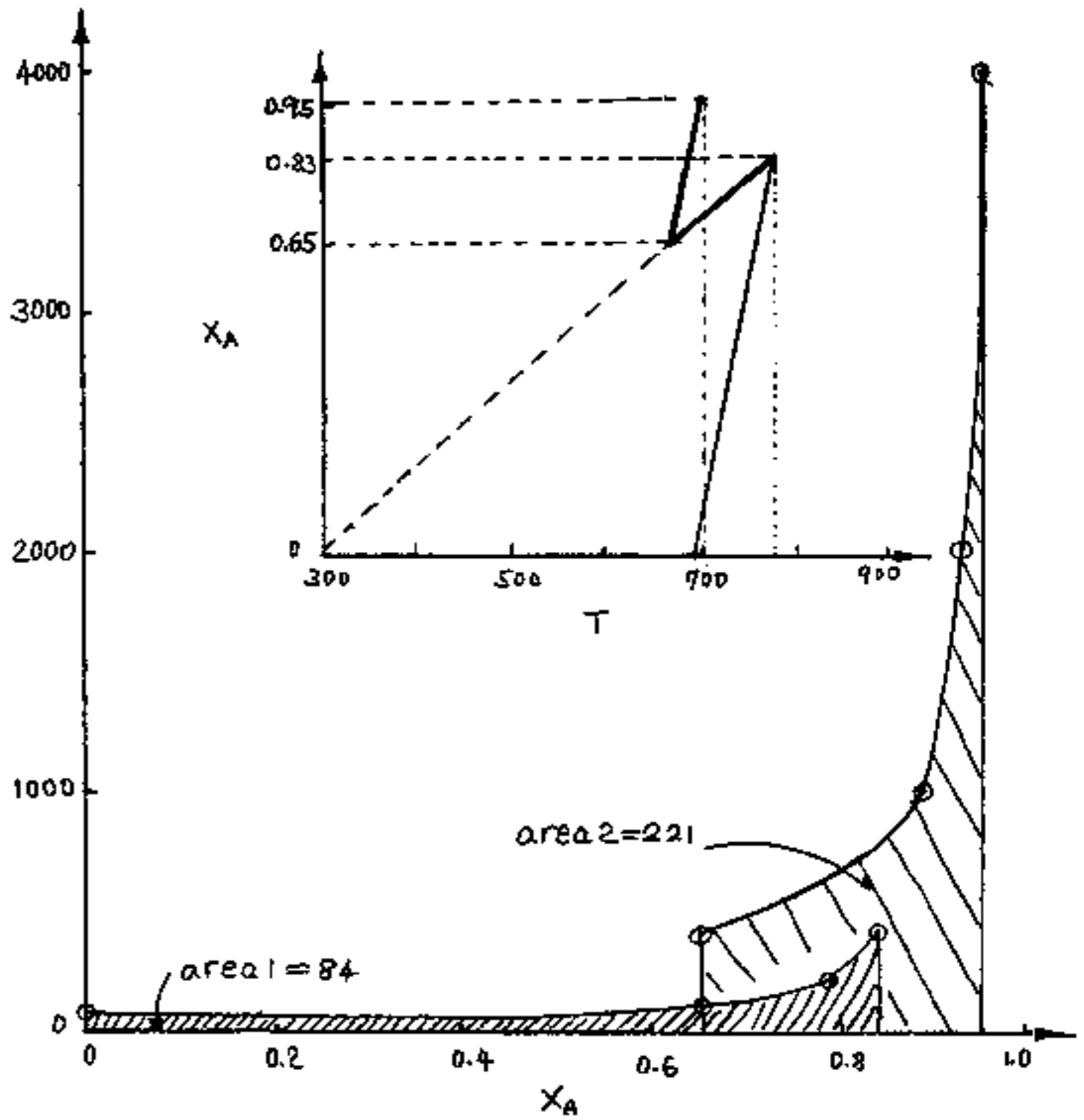
19.21 Injection of cold feed

$$\text{slope} = \frac{40 \times 20}{80000} = \frac{1}{100}$$

$$\frac{1}{-r_A'}$$

Fraction of feed A that goes to the first reactor

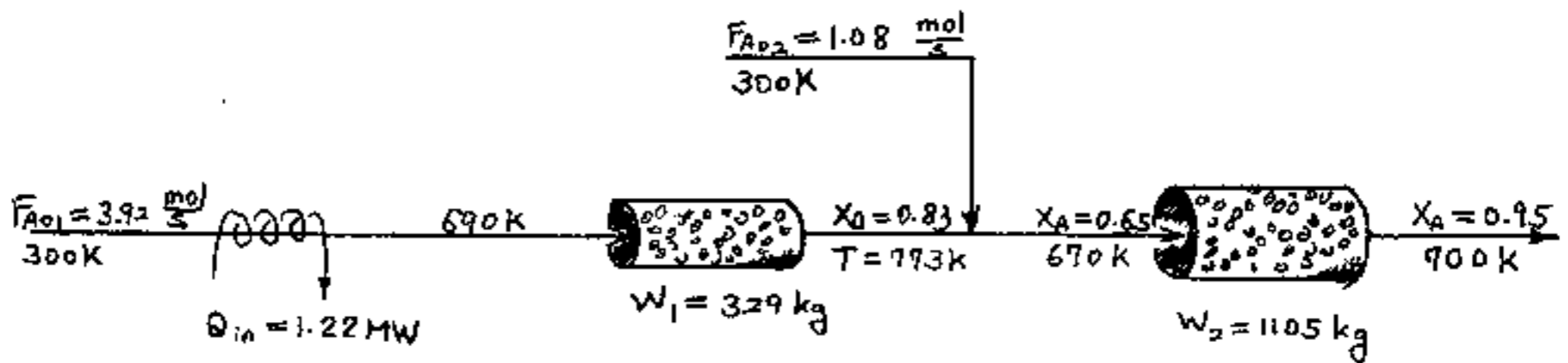
$$\frac{0.65}{0.83} = 0.7831$$



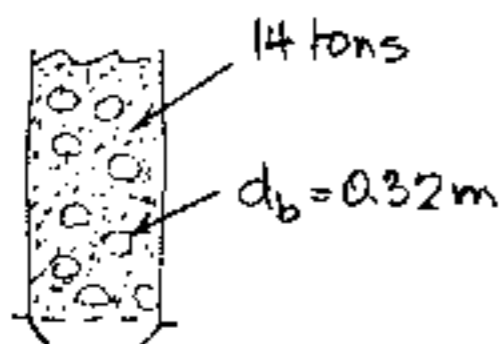
$$\begin{aligned} W_1 &= F_{A01} \cdot \text{area 1} = (5 \times 0.7831)(84) = 329 \text{ kg} \\ W_2 &= F_{A0} \cdot \text{area 2} = (5)(221) = 1105 \text{ kg} \end{aligned} \quad \left. \vphantom{\begin{aligned} W_1 \\ W_2 \end{aligned}} \right\} W_{\text{total}} = 1434 \text{ kg}$$

$$Q = F_{A01} \cdot C_p (\Delta T) = (5 \times 0.7831)(800)(670 - 300) = 1.22 \times 10^6 \text{ J/s (heating)}$$

Note: only one heat exchanger is needed in this design.



20.1



Refer to Example 1, from which we have

$$\left. \begin{aligned} \delta &= 0.196 & f_b &= 0.001 \\ \epsilon_f &= 0.6 & f_c &= 0.047 \\ K_{bc} &= 0.614 \text{ s}^{-1} & f_e &= 0.352 \end{aligned} \right\} f = 0.4$$

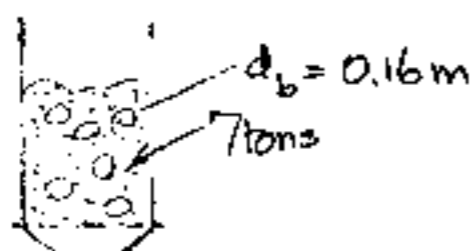
$$K_{ce} = 0.133 \text{ s}^{-1} \quad H_{BFB} = 2(2.875) = 5.57 \text{ m}$$

The performance expression becomes

$$\ln \frac{C_{A0}}{C_A} = \left[\frac{\dots}{0.4} \right] \cdot \frac{5.57(0.4)}{0.3} = 0.0415 (18.568) = 0.77$$

$$\frac{C_A}{C_{A0}} = 0.463 \quad \dots \text{ or } \dots \quad X_A = 53.7\% \quad \leftarrow \text{see Fig 10}$$

20.3



Solve the material balances

$$u_{br} = 0.711 (g d_b)^{1/2} = 0.711 (9.8 \times 0.16)^{1/2} = 0.8904 \text{ m/s}$$

$$u_b = 0.30 - 0.03 + 0.8904 = 1.16 \text{ m/s}$$

$$\delta = (0.3 - 0.03) / 1.16 = 0.2327$$

$$\epsilon_f = 1 - (1 - 0.5)(1 - 0.2327) = 0.6164$$

$$K_{bc} = 4.5 \left(\frac{0.03}{0.16} \right) + 5.85 \left[\frac{(20 \times 10^{-6})^{1/2} (9.8)^{1/4}}{(0.16)^{5/4}} \right] = 1.301 \text{ s}^{-1}$$

$$K_{ce} = 6.77 \left[\frac{0.5 (2 \times 10^{-5}) 1.16}{(0.16)^3} \right]^{1/2} = 0.3609 \text{ s}^{-1}$$

$$f_b = 0.001$$

$$f_c = 0.2327 (0.5) \left[\frac{3 \times 0.03 / 0.5}{0.89 - 0.03 / 0.5} + 0.33 \right] = 0.0636 \quad \left. \begin{aligned} & \\ & \end{aligned} \right\} f = 0.3836$$

$$f_e = (1 - 0.6164) - 0.0636 - 0.001 = 0.3190$$

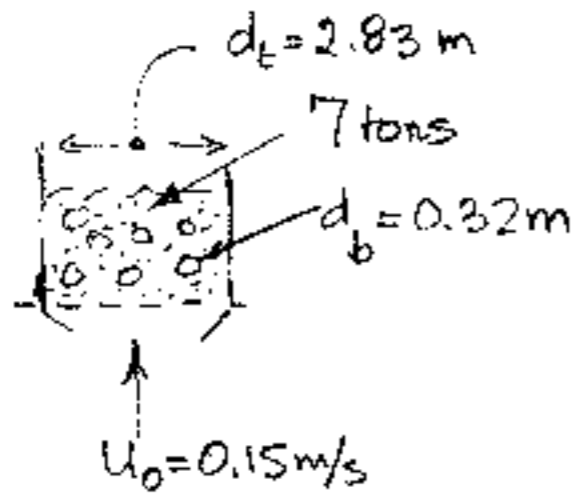
$$H_{BFB} = \frac{W}{\rho A (1 - \epsilon_f)} = \frac{7000}{2000 \pi (1 - 0.6164)} = 2.904 \text{ m}$$

$$\ln \frac{C_{A0}}{C_A} = \left[\frac{0.001(0.8) + \frac{1}{\frac{0.2327(1.301)}{0.3} + \frac{1}{\frac{0.2327(0.3609)}{0.3} + \frac{1}{0.3190(0.8)}}}}{0.3} \right] \cdot \frac{2.904}{0.3}$$

$$= [0.0837] 9.68 = 0.8102$$

$$\therefore \frac{C_A}{C_{A0}} = 0.445 \quad \dots \text{ or } \dots \quad X_A = 55.5\% \quad \leftarrow$$

20.5



Solve the material balance

$$u_{br} = 0.711 (9.8 \times 0.32)^{1/2} = 1.2592 \text{ m/s}$$

$$u_b = 0.15 - 0.03 + 1.2592 = 1.3792 \text{ m/s}$$

$$\delta = (0.15 - 0.03) / 1.3792 = 0.087$$

$$\epsilon_f = 1 - (1 - 0.5)(1 - 0.087) = 0.5435$$

$$K_{bc} = 4.5 \left(\frac{0.03}{0.32} \right) + 5.85 \left[\frac{(2 \times 10^{-5})^{1/2} (9.8)^{1/4}}{(0.32)^{5/4}} \right] = 0.6140 \text{ s}^{-1}$$

$$K_{ce} = 6.77 \left[\frac{0.5 (2 \times 10^{-5})^{1/2} (9.8)^{1/4}}{(0.32)^{5/4}} \right] = 0.1327 \text{ s}^{-1}$$

$$f_b = 0.001$$

$$f_c = 0.087 (0.5) \left[\frac{3(0.03)/0.5}{1.25 - 0.03/0.5} + 0.33 \right] = 0.0209 \quad \left. \vphantom{f_c} \right\} f = 0.4565$$

$$f_e = (1 - 0.5435) - 0.0209 - 0.001 = 0.4346$$

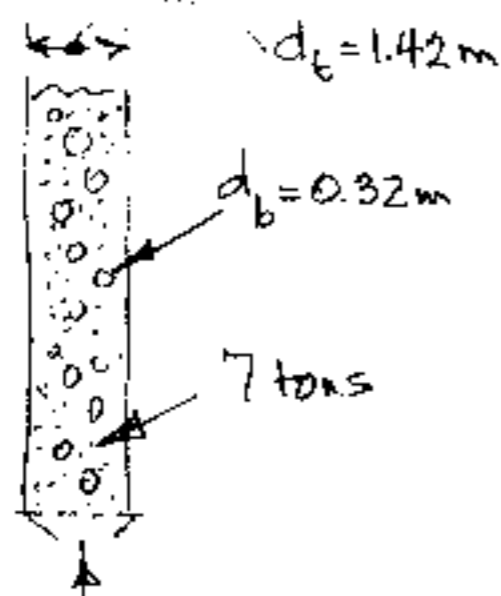
$$H_{trB} = W / \rho A (1 - \epsilon_f) = 7000 / (2000 (2\pi) (1 - 0.5435)) = 1.22 \text{ m}$$

$$\ln \frac{C_{A0}}{C_A} = \left[0.001(0.8) + \frac{1}{0.087(0.614) + \frac{1}{0.0209(0.8) + \frac{1}{0.087(0.1327) + \frac{1}{0.4346(0.8)}}} \right] \frac{1.22}{0.15}$$

$$= [0.0263] 8.133 = 0.2139$$

$$\therefore \frac{C_{AF}}{C_{A0}} = 0.8074 \quad \text{or} \quad X_A = 19\%$$

20.7



Again solve

$$u_{br} = 1.26 \text{ m/s}$$

$$u_b = 0.6 - 0.03 + 1.26 = 1.83 \text{ m/s}$$

$$\delta = \frac{0.6 - 0.03}{1.83} = 0.3115$$

$$\epsilon_f = 1 - (1 - 0.5)(1 - 0.3115) = 0.6558$$

$$\left. \begin{aligned} K_{bc} &= 0.614 \text{ s}^{-1} \\ K_{ce} &= 0.133 \text{ s}^{-1} \end{aligned} \right\} \text{from Example 1}$$

$$K_{ce} = 6.78$$

20.7
continued

$$f_b = 0.001$$

$$f_c = 0.3115(1-0.5) \left[\frac{3 \times 0.03/0.5}{1.26 - 0.03/0.5} + 0.33 \right] = 0.0748 \quad \left. \vphantom{f_c} \right\} f = 0.3442$$

$$f_e = (1 - 0.6558) - 0.0748 - 0.001 = 0.2684$$

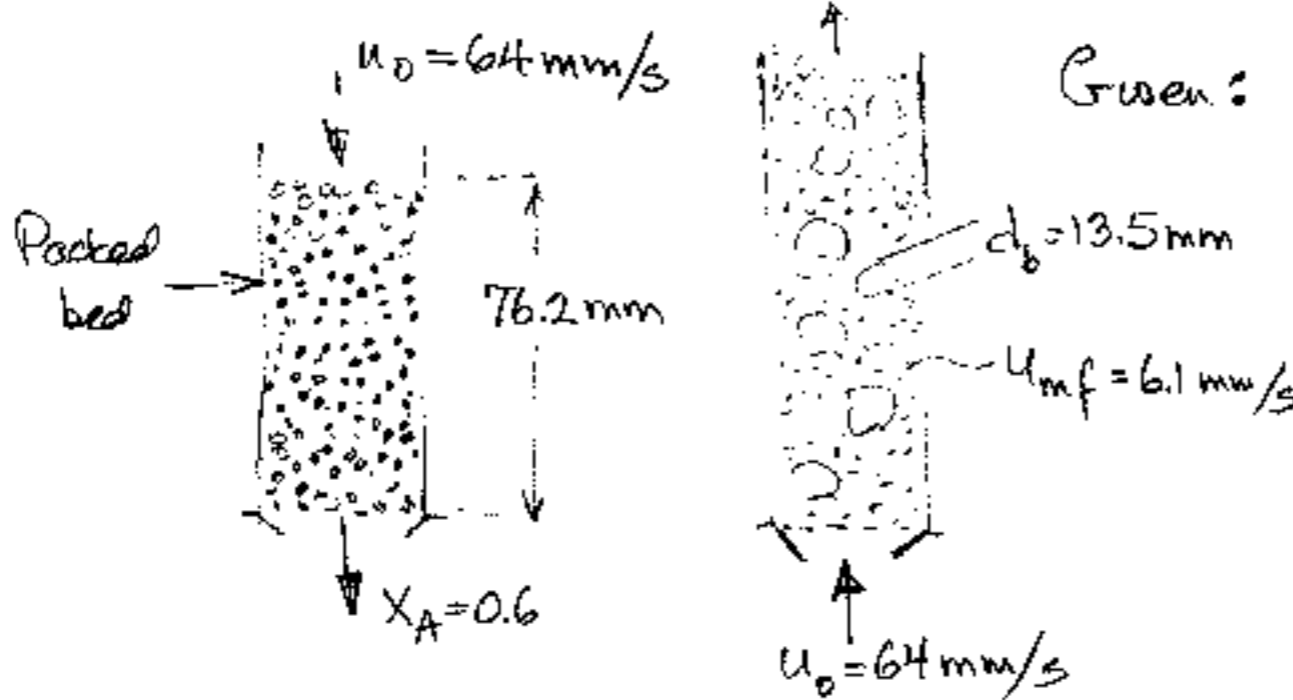
$$H_{BFB} = W/\rho A(1-\epsilon_f) = 7000/2000(\pi/2)(1-0.6558) = 6.4735 \text{ m}$$

$$\ln \frac{C_{A0}}{C_A} = \left[\frac{0.001(0.8) + \frac{1}{0.3115(0.614)} + \frac{1}{0.0748(0.8)} + \frac{1}{\frac{1}{0.3115(0.133)} + \frac{1}{0.2684(0.8)}} \right] \frac{6.4735}{0.6}$$

$$= [0.0641] 10.7892 = 0.6914$$

$$\therefore \frac{C_A}{C_{A0}} = 0.5009 \quad \dots \quad \text{or } X_A = 50\%$$

20.9



Given: First order reversible rx

$$X_{Ae} = 0.94$$

$$u_{mf} = 6.1 \text{ mm/s}$$

$$\epsilon_m = 0.4$$

$$\epsilon_{mf} = 0.5$$

$$\alpha = 0.33$$

$$D = 2 \times 10^{-5} \text{ m}^2/\text{s}$$

Find $X_{Ae2} = ?$

For a reversible first order reaction Eq 3.54 or Eq 5.22 gives

$$\text{For plug flow: } X_{Ae} \ln \frac{X_{Ae}}{X_{Ae} - X_{Ap}} = k''' \tau \quad \dots \quad (i)$$

$$\text{or } k''' = \frac{u}{V} X_{Ae} \ln \frac{X_{Ae}}{X_{Ae} - X_A} = \frac{u_0 A}{H_p A (1 - \epsilon_m)} X_{Ae} \ln \frac{X_{Ae}}{X_{Ae} - X_A}$$

$$= \frac{64}{76.2(1-0.4)} (0.94) \ln \frac{0.94}{0.94-0.60} = 1.3381 \frac{\text{m}^3}{\text{m}^3 \text{cat} \cdot \text{s}}$$

For the fluidized bed the performance equation (compare with eq (i)) is

$$X_{Ae} \ln \frac{X_{Ae}}{X_{Ae} - X_A} = \left[\frac{f_b k'''}{f_{\text{total}}} + \dots \right] \frac{H_{BFB} f_{\text{total}}}{u_0} \quad \dots \quad (ii)$$

20.9
continued

Evaluate terms in units of meters, not millimeters

$$u_{br} = 0.711(9.8 \times 0.0135)^{1/2} = 0.2586 \text{ m/s}$$

$$u_b = 0.064 - 0.0061 + 0.2586 = 0.3165 \text{ m/s}$$

Is this reactor in the BFB regime? Let's see

$$\frac{u_b}{u_e} = \frac{0.316}{0.006/0.5} = 26.3 \dots \text{yes it is a vigorously fluidized bed}$$

$$\delta = (0.064 - 0.0061) / 0.3165 = 0.1829$$

$$\varepsilon_p = 1 - (1 - 0.5)(1 - 0.1829) = 0.5915$$

$$K_{bc} = 4.5 \left(\frac{0.0061}{0.0135} \right) + 5.85 \left[\frac{(2 \times 10^{-5})^{1/2} (9.8)^{1/4}}{(0.0135)^{5/4}} \right] = 2.0333 + 10.0589 = 12.0922 \text{ s}^{-1}$$

$$K_{ce} = 6.77 \left[\frac{0.5 (2 \times 10^{-5}) 0.3165}{(0.0135)^3} \right]^{1/2} = 7.6785 \text{ s}^{-1}$$

$$f_b = 0.001$$

$$f_c = 0.1829(1 - 0.5) \left[\frac{2(0.0061)/0.5}{0.2568 - 3(0.0061)/0.5} + 0.33 \right] = 0.2393 \quad f = 0.4085$$

$$f_e = (1 - 0.5915) - 0.2393 - 0.001 = 0.1682$$

$$H_{BFB} = H_{fixed} \left(\frac{1 - \varepsilon_m}{1 - \varepsilon_{mf}} \right) \frac{1}{1 - \delta} = (0.0762) \left(\frac{1 - 0.4}{1 - 0.5} \right) \frac{1}{1 - 0.1829} = 0.1119 \text{ m}$$

Now replace values into Eq (ii)

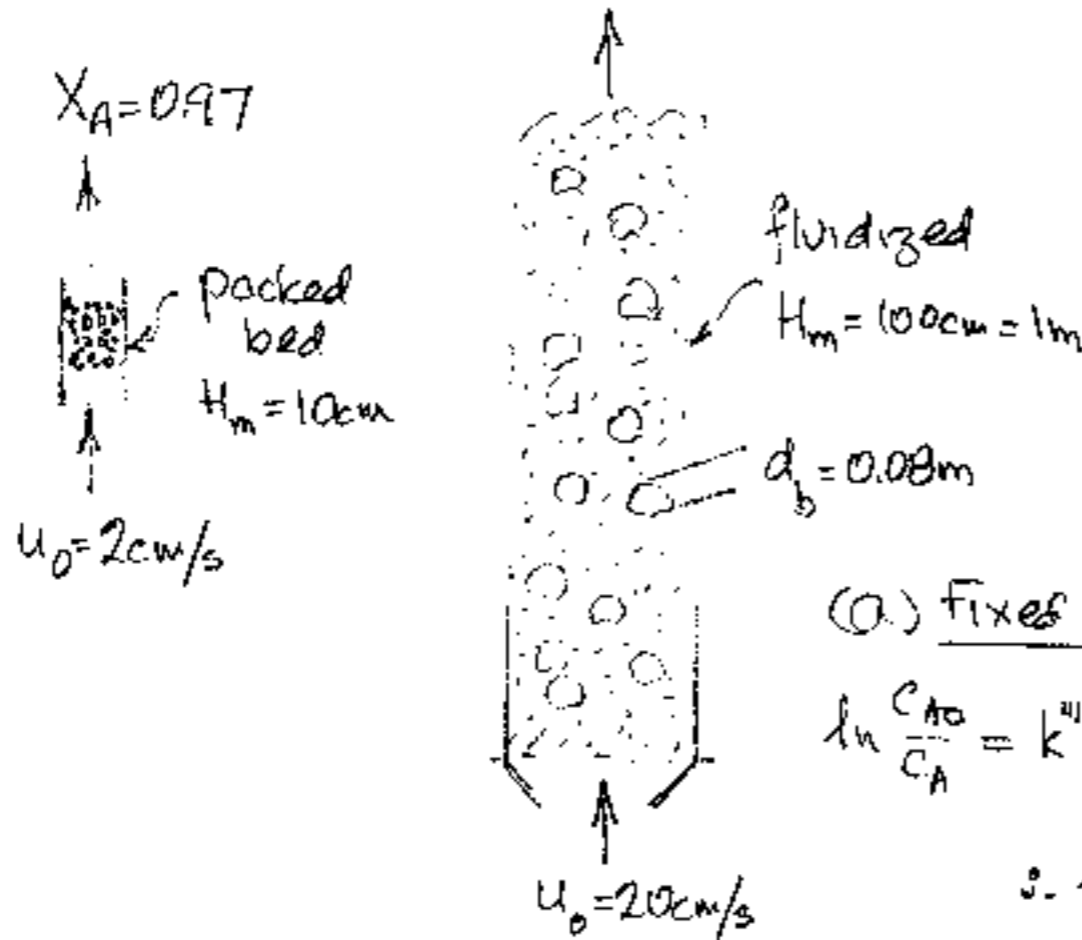
$$X_{Ae} \ln \frac{X_{Ae}}{X_{Ae} - X_A} = \left[\frac{0.001(1.3383) + \frac{1}{0.1829(12.0922)} + \frac{1}{0.2393(1.3381)} + \frac{1}{0.1829(7.6785)} + \frac{1}{0.1682(1.3381)} \right] \frac{0.1119}{0.064}$$

$$\ln \frac{0.94}{0.94 - X_A} = [0.4185] 1.7484 \left(\frac{1}{0.94} \right) = 0.7784$$

$$\therefore \frac{X_{Ae}}{X_{Ae} - X_A} = 2.1780 \quad \text{or } X_A = 0.5084$$

Note. Compare this calculated X_A value with that found experimentally, as shown in Fig 3, pg 520 of Mathis & Watson's paper.

20.11



$$\begin{aligned} \epsilon_m = \epsilon_{mf} &= 0.5 \\ D &= 3 \times 10^{-5} \text{ m}^2/\text{s} \\ u_{mf} &= 0.032 \text{ m/s} \\ \alpha &= 0.34 \end{aligned}$$

(a) Fixed bed experiment

$$\ln \frac{C_{A0}}{C_A} = k''' \frac{V_s}{v} = k''' \frac{H_m A (1 - \epsilon_m)}{u_0 A} = k''' \frac{0.1 (1 - 0.5)}{0.02}$$

$$\therefore k''' = \frac{0.02}{0.1 (1 - 0.5)} \ln \frac{100}{3} = 1.4026 \text{ m}^3/\text{m}^3 \text{ cat} \cdot \text{s}$$

(b) Fluidized bed

$$u_{br} = 0.711 (9.8 \times 0.08)^{1/2} = 0.6295 \text{ m/s}$$

$$u_b = 0.2 - 0.032 + 0.6295 = 0.7975 \text{ m/s}$$

$$\delta = (0.2 - 0.032) / 0.7975 = 0.2107$$

$$\epsilon_f = 1 - (1 - 0.5)(1 - 0.2107) = 0.6053$$

$$k_{bc} = 4.5 \left(\frac{0.032}{0.08} \right) + 5.85 \left[\frac{(3 \times 10^{-5})^{1/2} (9.8)^{1/4}}{(0.08)^{5/4}} \right] = 3.1325 \text{ s}^{-1}$$

$$k_{ce} = 6.77 \left[\frac{0.5 (3 \times 10^{-5}) 0.6295}{(0.08)^3} \right]^{1/2} = 0.9194 \text{ s}^{-1}$$

$$f_b = 0.001$$

$$f_c = 0.2107 (1 - 0.5) \left[\frac{e(0.032)/0.5}{0.7975 - 0.032/0.5} + 0.34 \right] = 0.0634 \quad \left. \vphantom{f_c} \right\} f = 0.3947$$

$$f_e = (1 - 0.6053) - 0.0634 - 0.001 = 0.3303$$

$$H_{BFB} = \frac{H_m (1 - \epsilon_m)}{1 - \epsilon_f} = \frac{1.0 (0.5)}{1 - 0.6053} = 1.2668 \text{ m}$$

$$\ln \frac{C_{A0}}{C_A} = \left[\frac{0.001 (1.4026) + \frac{1}{0.2107 (3.1325)} + \frac{1}{0.0634 (1.4026)} + \frac{1}{0.9194 (0.2107)} + \frac{1}{0.3303 (1.4026)} \right] \frac{1.27}{0.2}$$

$$= [0.1695] 6.334 = 1.0736$$

$$\therefore \frac{C_A}{C_{A0}} = 0.3418 \quad \dots \quad \text{or} \quad X_A = 34\% \quad \leftarrow \quad (b)$$

(c) Rig fixed bed

$$\frac{C_A}{C_{A0}} = e^{-k''' H_f f} = e^{-1.4026 (1.27) 0.3947} = 0.03 \quad \dots \quad \text{or} \quad X_A = 97\% \quad \leftarrow \quad (c)$$

21.1 Let us start by guessing the simplest rate form.

$$\left. \begin{aligned} -r_A' &= k' C_A a \\ -\frac{da}{dt} &= k_d a \end{aligned} \right\} \dots \text{if this doesn't fit the data then guess some other rate form}$$

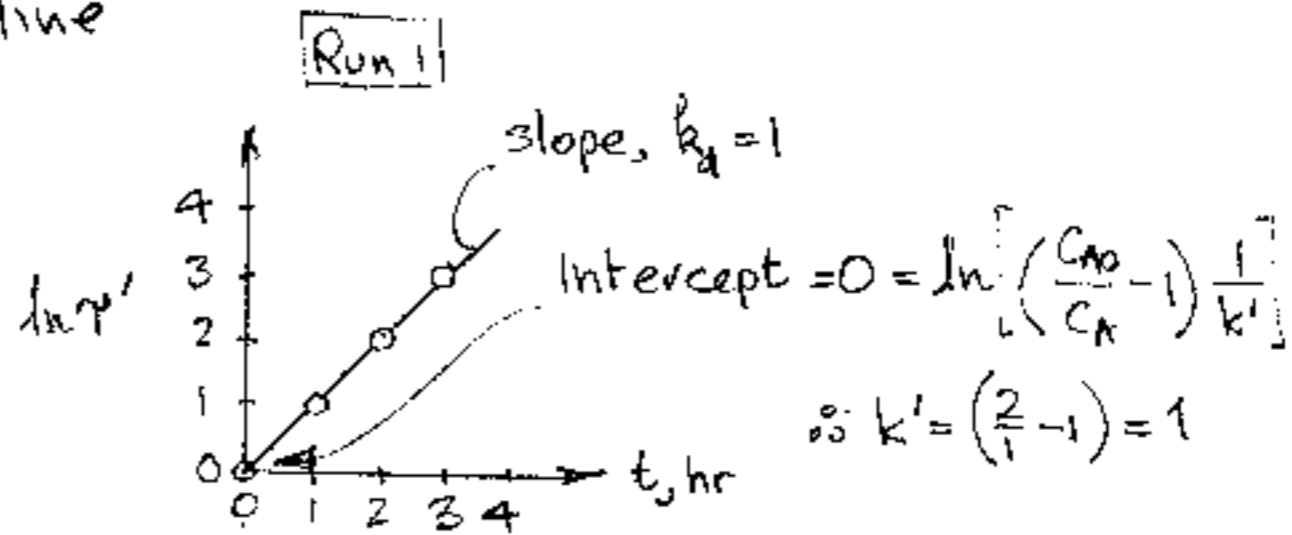
For mixed flow, constant $C_A = 0.5$ and changing τ' eq 27 gives

$$\left(\frac{C_{A0}}{C_A} - 1\right) = k' \tau' e^{-k_d \tau'}$$

$$\text{or } \underbrace{\ln \tau'}_y = \underbrace{\ln \left[\left(\frac{C_{A0}}{C_A} - 1\right) \frac{1}{k'} \right]}_a + \underbrace{k_d \tau'}_{bx}$$

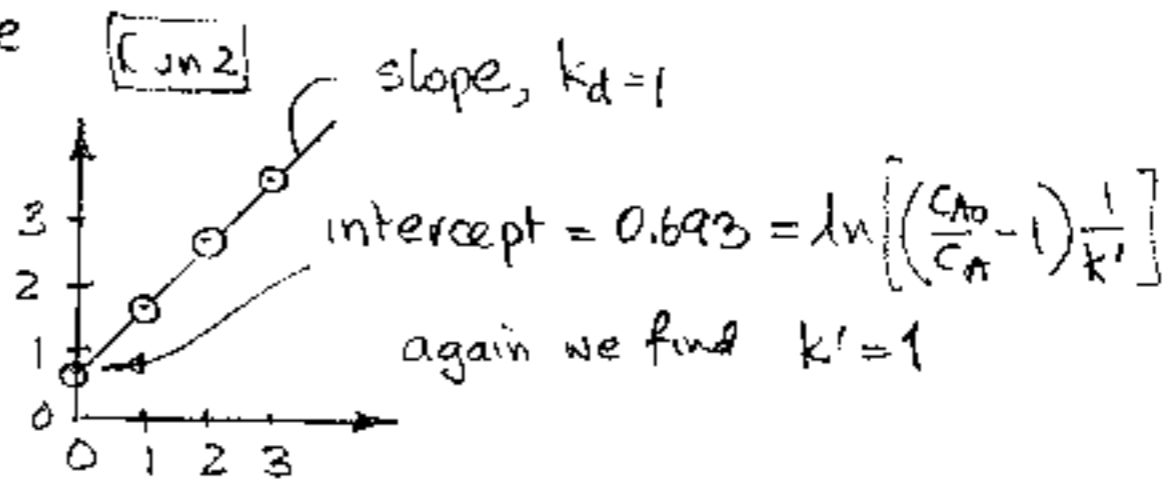
Let us test this expression, as shown in Fig 4, to see whether we get a straight line

| t | τ' | $\ln \tau'$ |
|---|----------------|-------------|
| 0 | 1 | 0 |
| 1 | e | 1 |
| 2 | e ² | 2 |
| 3 | e ³ | 3 |



Run #1 was made at one concentration, so it doesn't tell if we have a first order reaction. We need another run at a different C_A . We get this with run #2 which is at $C_A = 0.67$. Let's see if we will get the same k' value

| t | τ' | $\ln \tau'$ |
|---|-----------------|-------------|
| 0 | 2 | 0.693 |
| 1 | 2e | 1.693 |
| 2 | 2e ² | 2.693 |
| 3 | 2e ³ | 3.693 |



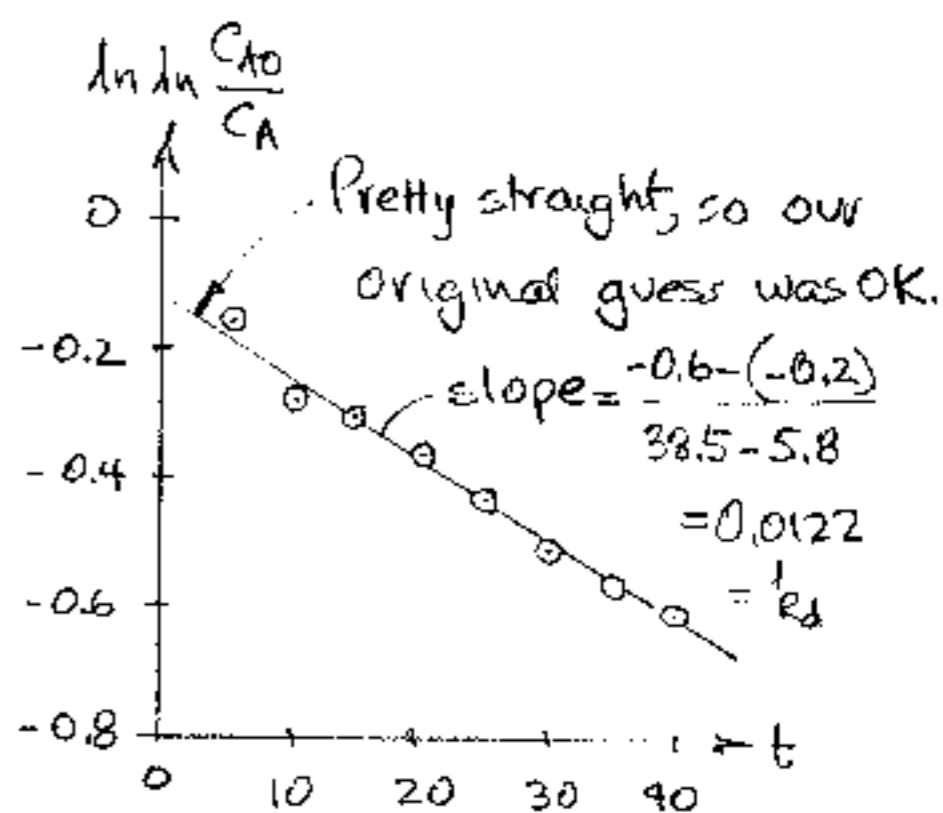
For both runs we find

$$\left. \begin{aligned} -r_A &= C_A a, \text{ mol/gm}\cdot\text{min} \\ -\frac{da}{dt} &= a, \text{ hr}^{-1} \end{aligned} \right\}$$

21.3 As we always should, we start by guessing the simplest of rate forms – first order reaction and first order deactivation. Then Eq 30 tests this rate form, as shown in Fig 5

$$\ln \ln \frac{C_{A0}}{C_A} = \ln(k'V') - k_d t$$

| t | X _A | $\frac{C_{A0}}{C_A} = \frac{1}{1-X_A}$ | $\ln \ln \frac{C_{A0}}{C_A}$ |
|----|----------------|--|------------------------------|
| 0 | - | - | - |
| 5 | 0.57 | 2.33 | -0.1696 |
| 10 | 0.53 | 2.13 | -0.2810 |
| 15 | 0.52 | 2.08 | -0.3092 |
| 20 | 0.50 | 2.00 | -0.3665 |
| 25 | 0.48 | 1.92 | -0.4248 |
| 30 | 0.45 | 1.82 | -0.5144 |
| 35 | 0.43 | 1.75 | -0.5760 |
| 40 | 0.41 | 1.69 | -0.6075 |



$$\therefore -\frac{da}{dt} = 0.0122 a, \text{ hr}^{-1}$$

21.5 The integrated rate forms for irreversible reactions with deactivation are derived in this chapter. The corresponding equations for reversible reactions in batch – batch reactions have not been developed by anyone anywhere. So let us do this here. Start by taking the simplest rate form, or first order throughout, or

$$-\frac{dC_A}{dt} = \frac{kW}{V} (C_A - C_{Ae}) a = k'' a (C_A - C_{Ae}) \quad \dots (i)$$

$$-\frac{da}{dt} = k_d a \quad \dots (ii)$$

Integrating (ii) and replacing in (i) gives

$$-\frac{dC_A}{dt} = k'' e^{-k_d t} (C_A - C_{Ae})$$

and on separation of variables and integrating again

$$\ln \frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}} = \frac{k''}{k_d} (1 - e^{-k_d t}) \quad \dots (iii)$$

21.5
continued

Now at $t = \infty$ this expression reduces to

$$\ln \frac{C_{A0} - C_{Ae}}{C_{A\infty} - C_{Ae}} = \frac{k''}{k_d} \quad \dots (iv)$$

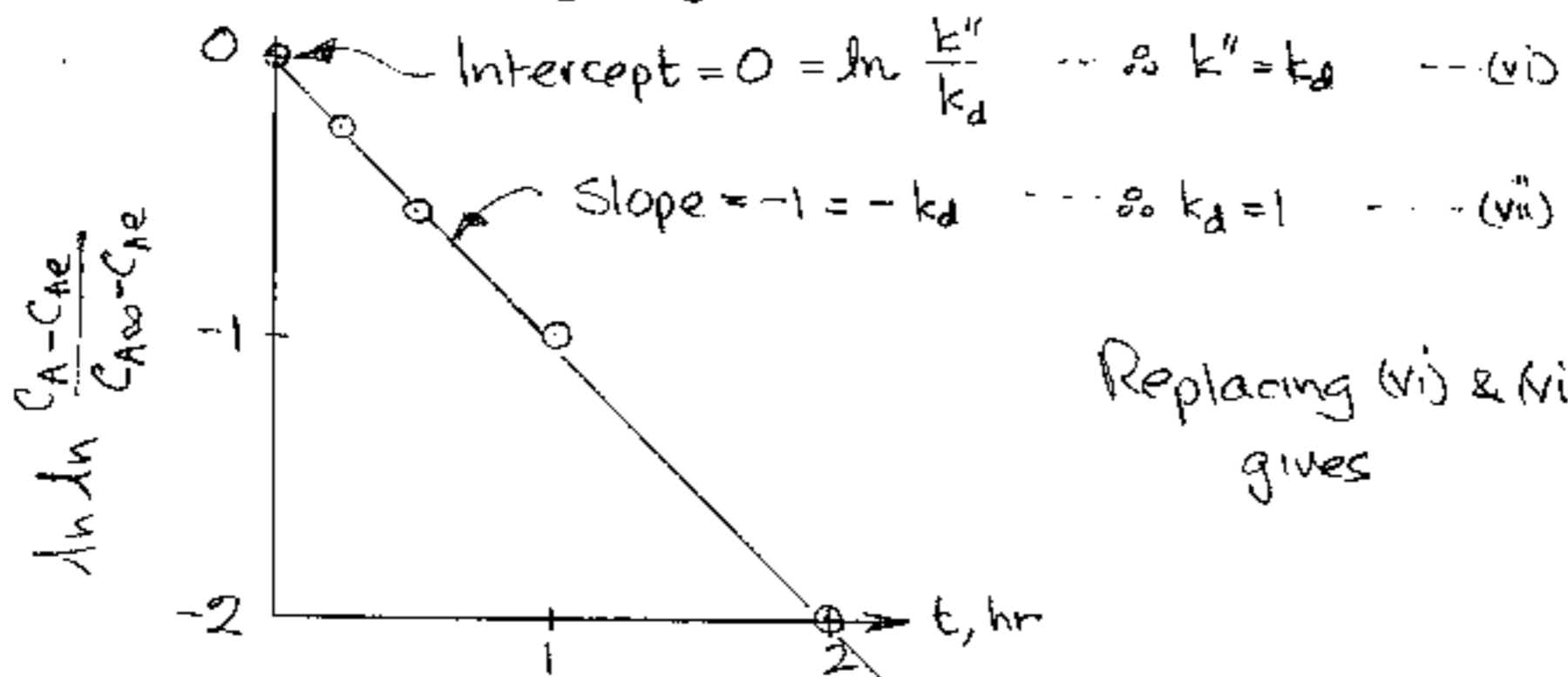
and on combining (iii) and (iv), rearranging and taking logs we obtain finally, for the batch-batch system

$$\ln \ln \frac{C_A - C_{Ae}}{C_{A\infty} - C_{Ae}} = \ln \frac{k''}{k_d} - k_d t \quad \dots (v)$$

This is the equation used to test the kinetics of Eqs (i) and (ii) in a batch-batch reactor. For this tabulate as shown below and then plot

| t | C | $\frac{C - C_e}{C_{\infty} - C_e}$ | $\ln \frac{C - C_e}{C_{\infty} - C_e}$ | $\ln \ln \frac{C - C_e}{C_{\infty} - C_e}$ |
|----------|----------------------|------------------------------------|--|--|
| 1 | 1 | $\frac{0.5}{0.684} = 0.731$ | 0.9995 | 0 |
| 1/4 | 0.901 | 2.18 | 0.789 | -0.237 |
| 1/2 | 0.830 | 1.794 | 0.584 | -0.538 |
| 1 | 0.766 | 1.446 | 0.369 | -1.000 |
| 2 | 0.711 | 1.147 | 0.1371 | -1.987 |
| ∞ | $C_{\infty} = 0.684$ | 1 | 0 | $-\infty$ |

Now plot and see if you get a straight line



$$\frac{dC_A}{dt} = 1 \cdot a (C_A - C_{Ae}) \quad \text{with} \quad -\frac{da}{dt} = a$$

$\left(\frac{\text{mol}}{\text{gm} \cdot \text{hr}} \right)$ $\left(\frac{\text{lit fluid}}{\text{gm cat}} \right)$ $\left(\text{hr}^{-1} \right)$

21.7 We are told that the reactor is being operated in the best possible way. What can we infer from this?

Since the reactor is being kept isothermal this means that all parts of the reactor - that bathed by high C_A , and that bathed by low C_A - deactivate at the same rate. Thus we conclude that deactivation is concentration independent, or

$$\frac{dC_A}{dt} = k_d C_A^0 a^d = k_d a^d$$

In addition, since we are at such high temperatures I think it reasonable to assume that we are dealing with a gas phase system, for which Eqs 48 & 50 apply.

Finally, we are not told whether diffusion resistance intrudes or not. So let us solve the problems both ways

In the absence of pore diffusion resistance Eq 48 gives

$$\frac{k'_1 a_1}{T_1^2} = \frac{k'_2 a_2}{T_2^2} = \text{constant, for all } T_1 \text{ \& } T_2$$

$$\begin{aligned} \text{or } \frac{a_2}{a_1} &= \frac{T_2^2}{T_1^2} \cdot \frac{k'_1}{k'_2} = \frac{T_2^2}{T_1^2} \frac{k'_0 \exp(-7200/T_1)}{k'_0 \exp(-7200/T_2)} \\ &= \left(\frac{800}{600}\right)^2 \exp\left[-7200\left(\frac{1}{600} - \frac{1}{800}\right)\right] = \left(\frac{800}{600}\right)^2 (0.0498) = 0.0885 \end{aligned}$$

So at the end of the run $a_2 = 8.85\%$ ←

In the presence of strong pore resistance Eq 50 gives

$$\frac{k'_1 a_1}{T_1^3} = \frac{k'_2 a_2}{T_2^3}$$

$$\text{or } \frac{a_2}{a_1} = \frac{T_2^3}{T_1^3} \exp\left[-7200\left(\frac{1}{600} - \frac{1}{800}\right)\right] = \left(\frac{800}{600}\right)^3 (0.0498) = 0.1180$$

So at the end of the run $a_2 = 11.8\%$ ←

21.9 For big particles, in the strong pore diffusion regime

$$X_A = 88\% \xrightarrow{t=250 \text{ days}} X_A = 64\%$$

For small particles, in the diffusion regime

$$X_A = 88\% \xrightarrow{t=?} X_A = 64\%$$

In the strong diffusion regime Eq 43 gives

$$\ln \frac{C_{A0}}{C_A} = \frac{k' r'}{M_T} \exp\left(-\frac{k_d t}{2}\right)$$

Taking logs

$$\ln \ln \frac{C_{A0}}{C_A} = \ln\left(\frac{k' r'}{M_T}\right) - \frac{k_d t}{2} \dots \dots \dots (i)$$

at t=0: $\ln \ln \frac{100}{12} = \ln\left(\frac{k' r'}{M_T}\right) - 0$

at t=250: $\ln \ln \frac{100}{36} = \ln\left(\frac{k' r'}{M_T}\right) - \frac{k_d}{2} (250)$ } combining gives $k_d = 0.004199$

In the diffusion resistance free regime Eq 42 gives

$$\ln \frac{C_{A0}}{C_A} = \frac{k' r'}{M_T} \exp(-k_d t)$$

Again taking logs gives

$$\ln \ln \frac{C_{A0}}{C_A} = \ln\left(\frac{k' r'}{M_T}\right) - k_d t \dots \dots \dots (ii)$$

Replacing values gives

at t=0: $\ln \ln \frac{100}{12} = \ln\left(\frac{k' r'}{M_T}\right) - 0$

at the end of the run when $X_A = 64\%$, but time is unknown

$$\ln \ln \frac{100}{36} = \ln\left(\frac{k' r'}{M_T}\right) - 0.004199 t$$

Combining equations gives

$$0.004199 t = \ln \ln \frac{100}{12} - \ln \ln \frac{100}{36}$$

the catalyst is killed more rapidly in the diffusion-free regime

$\therefore t = 125 \text{ days}$

21.11

Given: $v = 100 \text{ lit/min}$
 700°C
 8 atm

Run until $a = 0.1 a_{t=0}$

$W = 10 \text{ kg}$

$-r_A' = 0.030 C_A a \frac{\text{mol}}{\text{gm} \cdot \text{min}}$

$-\frac{da}{dt} = 3a^3, \text{ day}^{-1}$

Find (a) t , (b) \bar{X}_A

Focus on catalyst activity

For the decaying catalyst we have: $-\frac{da}{dt} = 3a^3$ day^{-1}

On integration: $\int_1^a \frac{da}{a^3} = 3 \int_0^t dt$

Thus the activity changes with run time by: $a = \frac{1}{\sqrt{1+6t}}$... (i)

So when $a = 0.1$ Eq (i) gives: $t = 16.5 \text{ days}$ \longleftarrow a)

b) Next focus on conversion. Using the pseudo steady-state assumption (activity changes slowly compared to the time of passage of reactant through the bed) we obtain

$$r' = - \int_{C_A}^{C_{A0}} \frac{dC_A}{k C_A a} = \frac{1}{k a} \ln \frac{C_{A0}}{C_A}$$

$$r' = \frac{W C_{A0}}{F_{A0}} = \frac{W}{v} = \frac{10 \text{ kg}}{100 \text{ lit/min}} = 100 \frac{\text{gm} \cdot \text{min}}{\text{lit}}$$

$0.03 \frac{\text{lit}}{\text{gm} \cdot \text{min}}$

hence the reactor output is related to catalyst activity by the expression: $\frac{C_A}{C_{A0}} = e^{-3a}$... (ii)

Now the mean conversion is the time average $C_{A,\text{out}}$ over the 16.5 days, or

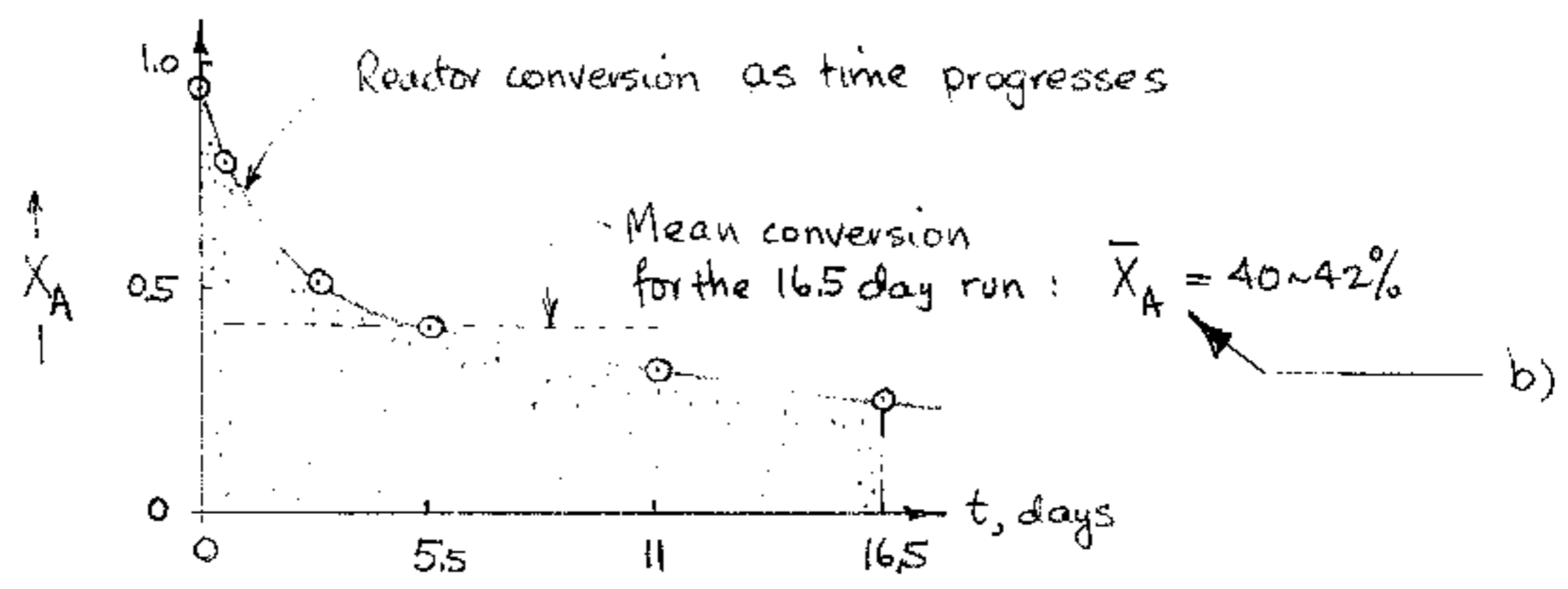
$$\bar{\frac{C_A}{C_{A0}}} = \frac{\int_{\text{beginning}}^{\text{end of run}} \left(\frac{C_A}{C_{A0}} \right)_{\text{anytime}} dt}{t_{\text{run}}}$$

21.11 continued Replacing (i) & (ii) in the above expression gives

$$\frac{\bar{C}_A}{C_{A0}} = \frac{1}{16.5} \int_0^{16.5 \text{ days}} e^{-3a} dt = \frac{1}{16.5} \int_0^{16.5} e^{-3\sqrt{1+6t}} dt \quad \dots (iii)$$

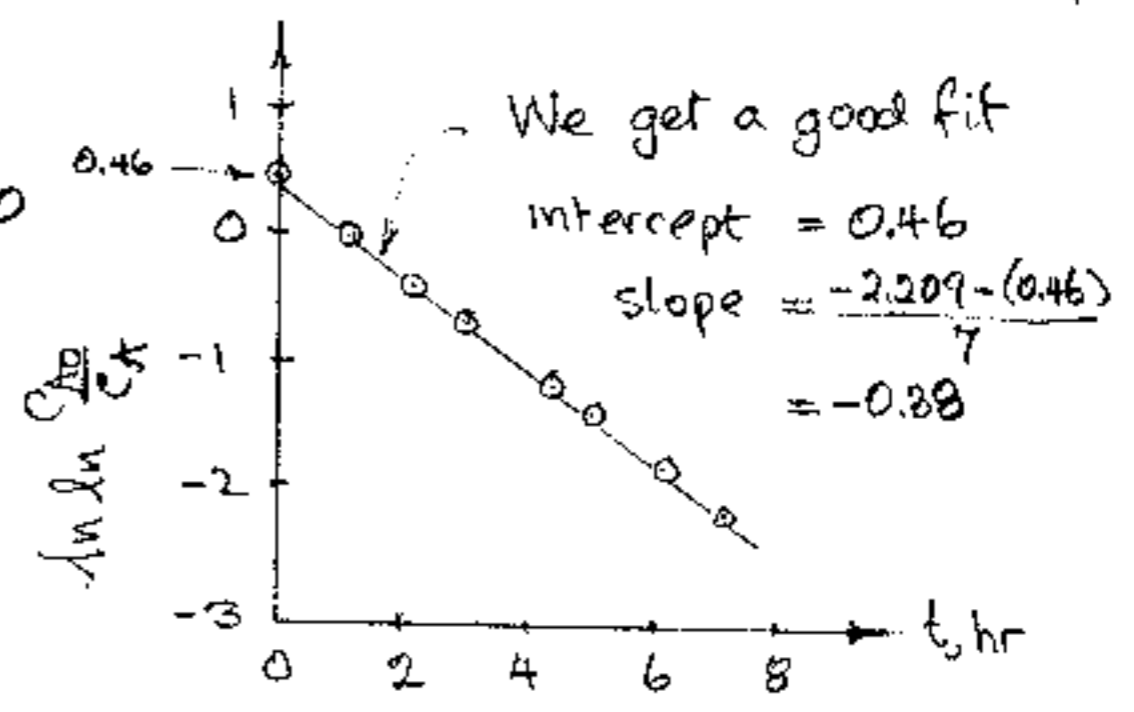
Evaluate this integral by tabulation & graphical integration Thus

| t | a | $e^{-3\sqrt{1+6t}}$ | $X_A = 1 - C_A/C_{A0}$ |
|------|-----|---------------------|------------------------|
| 0 | 1 | 0.05 | 0.95 |
| 0.5 | | 0.223 | 0.78 |
| 2.75 | | 0.488 | 0.51 |
| 5.5 | | 0.598 | 0.4 |
| 11 | | 0.693 | 0.31 |
| 16.5 | 0.1 | 0.74 | 0.26 |



21.13 Guess 1st order reaction & deactivation but with no diffusion resistance Then Eq 42 is the performance expression to be tested. So tabulate & plot

| t | X_A | C_{A0}/C_A | $\ln \ln \frac{C_{A0}}{C_A}$ |
|------|-------|--------------|--------------------------------|
| 0 | 0.795 | 4.878 | 0.46 |
| 1.25 | 0.635 | 2.740 | $7.8 \times 10^{-3} \approx 0$ |
| 2 | 0.510 | 2.041 | -0.338 |
| 3 | 0.397 | 1.658 | -0.6815 |
| 4.25 | 0.295 | 1.342 | -1.223 |
| 5 | 0.22 | 1.282 | -1.392 |
| 6 | 0.15 | 1.176 | -1.817 |
| 7 | 0.104 | 1.116 | -2.209 |



21.13 Equation 30 and Fig 5 give
continued

$$\ln \ln \frac{C_{A0}}{C_A} = \underbrace{\ln(k'r')}_{0.46} - \underbrace{k_d t}_{0.38}$$

Solving for k' :

$$k'r' = e^{-0.46} = 1.584 \quad \therefore k' = 3.86 \times 10^{-4} \text{ m}^3/\text{kg}\cdot\text{s}$$

\uparrow 4100 kg·s/m³

Since the text, in particular Ex 1, shows that this plot also fits the strong pore diffusion regime we should check this possibility. Let us do this at $t=0$

$$(M_{Td})_{t=0} = M_T = \frac{7.2 \times 10^{-5}}{6} \sqrt{\frac{(3.86 \times 10^{-4})(630)}{5 \times 10^{-10}}} = 0.264$$

with time a decreases so M_T gets smaller

Good, this verifies that we are in the diffusion-free regime

Hence the rate equation in the diffusion regime is given by

$$\left. \begin{aligned} -r'_A &= \left(3.86 \times 10^{-4} \frac{\text{m}^3}{\text{kg}\cdot\text{s}}\right) C_A a \\ -\frac{da}{dt} &= (0.38 \text{ hr}^{-1}) a \end{aligned} \right\} M_T < 0.4 \leftarrow$$

Note Suppose we would have assumed at the start that we were in the strong pore diffusion resistance regime. We'd get a straight on the graph, representing Eq 43.

$$\therefore \frac{k'r'}{M_T} = e^{0.46} = 1.584, \text{ or } \frac{k'r' \rho_s^{1/2}}{L(k' \rho_s)^{1/2}} = 1.584 \dots \text{ thus } k' = 2.7 \times 10^{-5}$$

Evaluate M_T

$$M_T = \frac{7.2 \times 10^{-5}}{6} \sqrt{\frac{(2.7 \times 10^{-5})(630)}{5 \times 10^{-10}}} = 7 \times 10^{-2}$$

— this value represents no resistance to diffusion. But this inconsistent with our original assumption of strong pore diffusion resistance

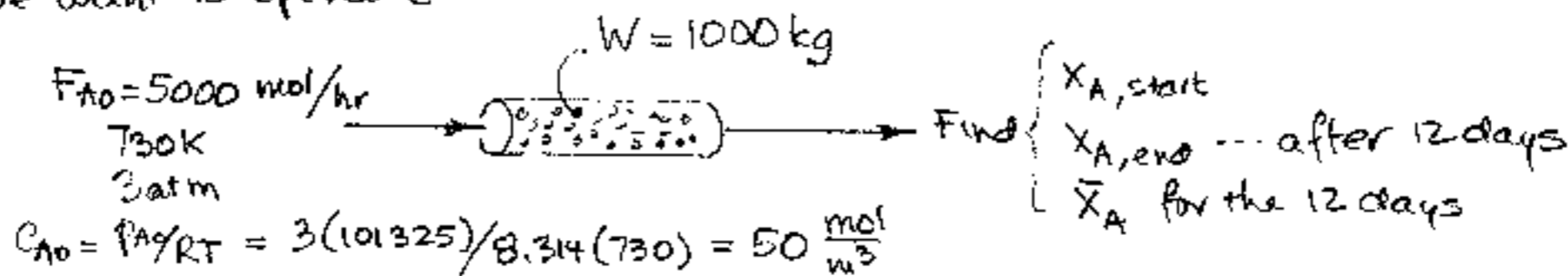
Whatever we assume we end up with the above answer which represents reaction free of diffusional resistance effects

21.15

Given $-\tau_A' = k' C_A^2 a = 0.2 C_A^2 a$, mol/hr.kg cat

$-\frac{da}{dt} = k_d (C_A + C_R) a = k_d C_{A0} a = 0.01 C_{A0} a$, day⁻¹ and $C_A = \left[\frac{\text{mol}}{\text{m}^3} \right]$

We want to operate



$$C_{A0} = P_A / RT = 3(101325) / 8.314(730) = 50 \frac{\text{mol}}{\text{m}^3}$$

a) $-\frac{da}{dt} = \left(0.01 \frac{\text{m}^3}{\text{mol}\cdot\text{day}} \right) \left(50 \frac{\text{mol}}{\text{m}^3} \right) a = 0.5 a$, day⁻¹ ← (a)

$\tau' = \frac{W C_{A0}}{F_{A0}} = \frac{(1000 \text{ kg})(50 \text{ mol/m}^3)}{5000 \text{ mol/hr}} = 10 \text{ kg/m}^3 \cdot \text{hr}$ ← (a)

At any time

$$\tau' = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} = \int_{C_A}^{C_{A0}} \frac{dC_A}{k' a C_A^2} = \frac{1}{k' a} \left[\frac{1}{C_A} - \frac{1}{C_{A0}} \right] = \frac{1}{k' a C_{A0}} \left[\frac{C_{A0}}{C_A} - 1 \right]$$

$\therefore k' a C_{A0} \tau' = \frac{C_{A0}}{C_A} - 1$... or $\frac{C_A}{C_{A0}} = \frac{1}{1 + 0.2 a (50) 10} = \frac{1}{1 + 100 a}$ ← (a)

(b) At the start

$$a = e^{-0.5t} = e^0 = 1$$

$\therefore \frac{C_A}{C_{A0}} = \frac{1}{1 + 100} \approx \frac{1}{100}$... or $X_{A,\text{start}} = 99\%$ ← (b)

(c) After 12 days

$$a = e^{-0.5(12)} = \frac{1}{400}$$

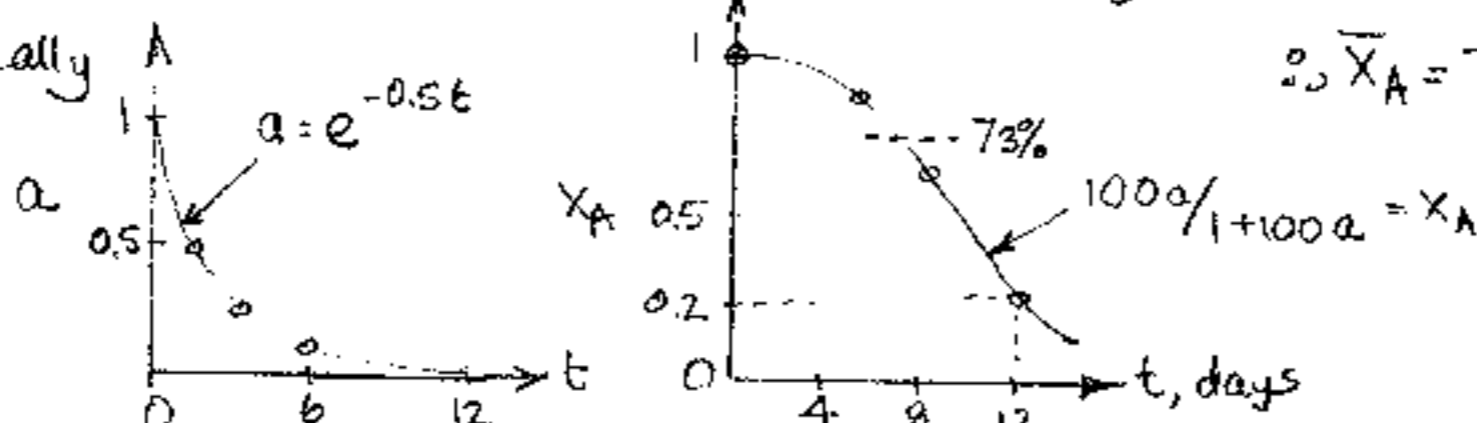
$\therefore \frac{C_A}{C_{A0}} = \frac{1}{1 + 100/400} = 0.8$... or $X_{A,\text{end}} = 20\%$ ← (c)

(d) Find \bar{X}_A :

$$\frac{\bar{C}_A}{C_{A0}} = \frac{1}{t_{\text{run}}} \int_0^{t_{\text{run}}} \frac{C_A}{C_{A0}} dt = \frac{1}{12} \int_0^{12} \frac{dt}{1 + 100 e^{-0.5t}}$$

$$= \frac{1}{12} \left[t + 2 \ln(1 + 100 e^{-0.5t}) \right]_0^{12} = 0.27$$

Graphically



$\therefore \bar{X}_A = 73\%$ ← (d)

22.1 First let us see if either extreme with its simplifications apply

$$C_A^* = \frac{p_A}{H_A} = \frac{1013250}{86000} = 11.78$$

constant throughout

At inlet $C_{B0} = 400 \text{ mol/m}^3$

guess $X_B \leq 90\%$ $C_B = 40 \text{ mol/m}^3$

Even up to $X_B = 0.9$ we have the extreme where $C_B \gg C_A$. Let us use the expressions for this extreme, but then check it at the end

Evaluate quantities needed to find the rate

$$a_c = \frac{6fs}{d_p} = \frac{6(0.58)}{5 \times 10^{-3}} = 696 \text{ m}^2/\text{m}^3$$

$$\therefore k_c a_c = (3.86 \times 10^{-5})(696) = 0.0269 \text{ s}^{-1}$$

$$M_T = L \sqrt{\frac{k' p_s}{\delta}} = \frac{5 \times 10^{-3}}{6} \sqrt{\frac{(1.77 \times 10^{-5})(1800)}{4.16 \times 10^{-10}}} = 7.3 \quad \therefore \epsilon = 0.13$$

Now to the rate equation

$$-r_A''' = \frac{1}{\frac{1}{86000(10^{-4})} + \frac{1}{0.02} + \frac{1}{0.0269} + \frac{1}{(1.77 \times 10^{-5})(1800)(0.13)(0.58)}} \cdot \frac{1013250}{86000}$$

$$= \frac{1}{0.116 + 50 + 37.17 + 416.3} \cdot \frac{1013250}{86000} = 0.0234$$

negligible main resistance

With constant p_A throughout the trickle bed and with the rate independent of C_B the material balance becomes very simple, as with a mixed flow reactor. Thus

$$F_{A0} X_A = F_{B0} X_B = (-r_A''') V_R$$

$$F_{B0} = v_L C_{B0} = (2 \times 10^{-4})(400) = 0.08 \text{ mol/s}$$

$$\therefore X_B = \frac{(-r_A''') V_R}{F_{B0}} = \frac{(0.0234)(5 \times 0.1)}{0.08} = 0.146 \approx 15\%$$

this is $< 90\%$, so it satisfies our assumption

22.3 This reaction is in mixed flow, so evaluate terms

$$a_c = \frac{6f_c}{d_p} = \frac{6(0.0056)}{10^{-5}} = 3360 \frac{\text{m}^2}{\text{m}^3}, \quad k_{Ac} a_c = 10^{-3}(3360) = 3.36 \text{ s}^{-1}$$

$$C_A = \frac{P_A}{H_A} = \frac{200(101325)}{2.776 \times 10^5} = 73 \frac{\text{mol}}{\text{m}^3} \quad \dots \text{stays constant}$$

$$C_B = 2000 \frac{\text{mol}}{\text{m}^3}$$

in any case
 $C_B \gg C_A$

So consider this to be a 1st order reaction with respect to A, or

$$-r_A = (5.96 \times 10^{-6} C_A^{-0.4} C_B^{0.4}) C_A$$

$$M_T = \frac{d_p}{6} \sqrt{\frac{n+1}{2} \cdot \frac{k' C_A^{-0.4} C_B^{0.4}}{\delta}} = \frac{10^{-5}}{6} \sqrt{\frac{1.6 (5.97 \times 10^{-6}) (73)^{-0.4} C_B^{0.4} \times 8900}{2 \times 10^{-9}}}$$

$$= 0.00325 \theta C_B^{1/2}, \text{ even at } C_B = 2000, M_T < 1 \therefore E_A = 1$$

Now to the rate

$$r_A''' = \frac{1}{\frac{1}{0.05} + \frac{1}{3.36} + \frac{1}{(5.96 \times 10^{-6}) 73^{-0.4} C_B^{0.4} (1)(0.0056) 8900}} \cdot \frac{101325 \times 200}{2.776 \times 10^5}$$

main resistance \rightarrow

$$= \frac{73}{20.2976 + 1872.6/C_B}$$

Now make a material balance $F_{A0} X_A = F_{B0} X_B = (-r_A''') V_{\text{reactor}}$
 not useful \rightarrow $\frac{1}{2} (C_{B0} - C_B) \dots$ useful.

$$\therefore 10^{-2} (2000 - C_B) = \frac{73}{(20.2976 + 1872.6/C_B)} \cdot 2 \quad \dots \text{ or } 2000 - C_B = \frac{14600}{(20.2976 + 1872.6/C_B)}$$

Solve for C_B by trial and error

| Guess C_B | LHS | RHS |
|-------------|-----|---------------------|
| 1700 | 300 | 466 |
| 1400 | 600 | 433 |
| 1560 | 440 | 452 |
| 1550 | 450 | 451 \leftarrow ok |

$$\therefore C_B = 1550 \text{ mol/m}^3$$

$$\text{and } X_B = 1 - \frac{1550}{2000} = 22.5\% \quad \leftarrow$$

Note We can use larger particles, or even less particles without lowering X_B significantly because the main resistance in the rate expression is in the mass transfer steps. To improve the conversion either increase the mass transfer steps, or better still increase the pressure.

22.5 First let us see if either extreme applies

$$C_A = \frac{p_A}{H_A} = \frac{101325}{28500} = 3.555 \text{ mol/m}^3 \quad \left. \begin{array}{l} \text{constant} \\ \text{At start: } C_{B0} = 1097 \text{ mol/m}^3 \\ \text{At end of run } C_B = 109.7 \text{ mol/m}^3 \end{array} \right\} \begin{array}{l} \text{Comparing we see that} \\ C_B \gg C_A \\ \text{throughout the run.} \end{array}$$

Use the equations for the $C_B \gg C_A$ extreme

$$a_c = \frac{6fs}{d_p} = \frac{6(0.25)}{2 \times 10^{-4}} = 5000 \frac{\text{m}^2}{\text{m}^3}$$

$$k_{Ac} a_c = 10^{-5} (5000) = 0.05 \text{ s}^{-1}$$

$$M_T = L \sqrt{\frac{k' p_s}{g_1}} = \frac{3 \times 10^{-4}}{6} \sqrt{\frac{0.05 (750)}{8.35 \times 10^{-10}}} = 10.6 \quad \therefore \varepsilon = \frac{1}{10.6} = 0.0944$$

We are now ready to write the rate expression

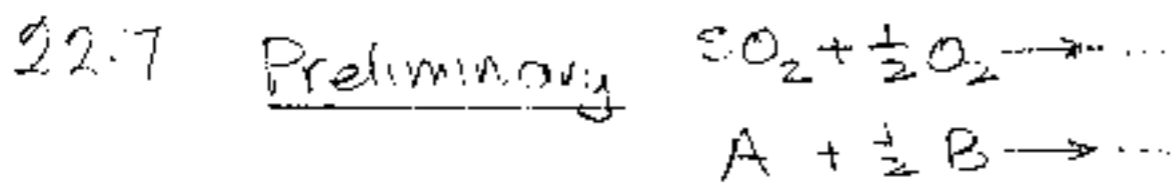
$$\begin{aligned} -r_A''' &= \frac{1}{\frac{1}{0.04} + \frac{1}{0.05} + \frac{1}{0.05(750)(0.0944)(0.25)}} \cdot \frac{101325}{28500} \\ &= \frac{1}{25 + 20 + 1.13} (3.555) = 0.0771 \text{ mol A/m}^3 \text{ reactor} \cdot \text{s} \end{aligned}$$

Finally go to the material balance. Writing it for A

$$F_{A0} X_A = \frac{V_r}{b} \left(-\frac{dC_B}{dt} \right) = (-r_A''') V_r$$

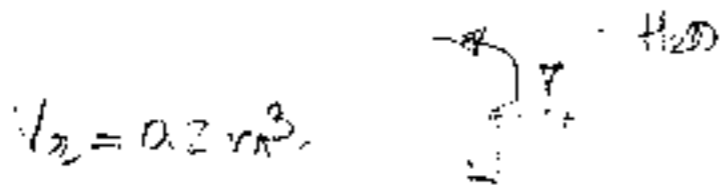
↑ useless
↑ use these terms to integrate

$$\begin{aligned} t &= \frac{V_r (C_{B0} - C_B)}{b V_r (-r_A''')} = \frac{0.65 (1097 - 109.7)}{\frac{2}{3} (1) (0.0771)} = \underline{\underline{12485 \text{ s}}} \\ &= \underline{\underline{3 \text{ hr } 28 \text{ min}}} \end{aligned}$$



$$-r'_A = 0.01553 C_B \text{ mol/kg}\cdot\text{s}$$

$$-r'_B = -\frac{1}{2} r'_A = 0.007765 C_B \text{ mol/kg}\cdot\text{s}$$



$$P_A = 0.002 (101325) \text{ Pa}$$

$$P_B = 0.21 (101325) \text{ Pa}$$

$$P = 1 \text{ atm}$$

$$D_0 = 0.01 \text{ m}^2/\text{s}$$

In terms of concentrations

$$C_{Ain} = \frac{P_A}{H_A} = \frac{0.002 (101325)}{380000} = 5.333 \times 10^{-4} \text{ mol/m}^3$$

$$C_{Bin} = \frac{P_B}{H_B} = \frac{0.21 (101325)}{73000} = 2446 \times 10^{-4} \text{ mol/m}^3$$

Note that $P_A \ll P_B$ & $C_A \ll C_B$

This is a puzzling problem because

- the chemical rate depends on B
- but A provides the mass transfer resistance

Let me guess that the overall rate is limited (or determined) by A, not B, thus is mass transfer controlled. If I am wrong then I will make the other assumption

Guess that the transfer of A controls the overall rate. Also, since $C_B \approx 500 C_A$ we can reasonably assume that C_B stays constant throughout the operation.

So write the chemical rate in terms of C_A . At inlet conditions

$$-r'_{A \text{ inlet}} = k' C_A^0 C_B^1 = k' \left(\frac{P_A}{H_A} \right) C_A = \left(k' \frac{P_B}{P_A} \frac{H_A}{H_B} \right)$$

$$= \left(0.01553 \cdot \frac{0.21}{0.2} \cdot \frac{380000}{73000} \right) C_A = 7.122 C_A \text{ mol/kg}\cdot\text{s}$$

$\text{m}^3/\text{kg}\cdot\text{s}$

Now the overall rate in the tower is

$$-r_A''' = \frac{1}{\frac{1}{(k'_0)_{lg}} + \frac{1}{k'_c} + \frac{1}{k' \left(\frac{P_B}{P_A} \frac{H_A}{H_B} \right)}} \cdot \frac{C_A}{H_A} \quad \dots (1)$$

Evaluate terms

2.7
continued

$$(k_c a_w)_{+g} = 0.01 \text{ s}^{-1}$$

$$a_c = \frac{6 \rho_s}{\rho_p} = \frac{6(0.6)}{0.005} = 720 \text{ m}^2/\text{m}^3$$

$$k_c = 4 \times 10^{-5} \text{ m/s}$$

$$M_T = \frac{d_p}{6} \cdot \frac{k' \rho_c}{D} = \frac{0.005}{6} \cdot \frac{7.122(850)}{5.75 \times 10^{-10}} = 2802$$

$$\epsilon = 257 \times 10^{-6} \dots \text{strong pore diffusion resistance}$$

Replace in (1)

$$-r_A''' = \frac{1}{\frac{1}{0.01} + \frac{1}{4 \times 10^{-5} (720)} + \frac{1}{7.122(850) (3574 \times 10^{-6})(0.6)}}$$

$C_A = 0.002 (10025)$
390000

\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow
 s^{-1} m/s m^3/m^3 $\text{m}^3/\text{kg}\cdot\text{s}$ kg/m^3 m^3/m^3

$$= \frac{1}{100 + 34.7 + 0.77} C_A$$

Note that the mass transfer resistance (100+34.7) is much greater than that of reaction (0.77), so our original guess is justified. Continue with the performance equation

For plug flow

$$\frac{V_2}{v_0} = \frac{0.2 \text{ m}^3}{0.01 \text{ m}^3/\text{s}} = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A'''} = \int_{C_A}^{C_{A0}} \frac{dC_A}{0.0074 C_A} = \frac{1}{0.0074} \ln \frac{C_{A0}}{C_A}$$

$$\therefore \frac{C_A}{C_{A0}} = e^{-V_2(0.0074)/v_0} = e^{-0.2(0.0074)/0.01} = 0.962$$

so the conversion of SO_2 $X_{\text{SO}_2} = X_A = 1 - 0.962$

23.1

$$M_H = \sqrt{\frac{D k C_B}{k_{A2}^2}} = \sqrt{\frac{10^{-6} (10) (10^2)}{1}} = 3.16 \times 10^{-2} \quad \therefore E = 1$$

$$-r_A^{III} = \frac{P_A}{\frac{1}{k_{AG} a} + \frac{H_A}{k_{AL} a E} + \frac{H_A}{k_C B E}} = \frac{10^2}{0.1 + \frac{10^2 (1)}{10^2 (1)} + \frac{10^2}{10 (10^2) (1)}} = 0.05 \frac{\text{mol}}{\text{hr.m}^3 \text{ reactor}}$$

↑ 50%
↑ 50%

(a) Reaction rate = 0.05 mol/hr.m³ reactor a)

(b) Resistance: 50% liquid film, 50% main body
 Reaction zone: main body of liquid b)
 Behavior in liquid film: physical transport

23.3

$$M_H = \sqrt{\frac{D k C_B}{k_{A2}^2}} = \sqrt{\frac{10^{-6} (10) (10^2)}{1}} = 3.16 \times 10^{-2} \quad \therefore E = 1$$

$$-r_A^{III} = \frac{P_A}{\frac{1}{k_{AG} a} + \frac{H_A}{k_{AL} a E} + \frac{H_A}{k_C B E}} = \frac{10^2}{0.1 + \frac{10^2 (1)}{10^2 (1)} + \frac{10^2}{10 (10^2) (10^{-1})}} = 3.33$$

↑ 33%
↑ 33%
↑ 33%

(a) Reaction rate = 3.33 mol/hr.m³ reactor a)

(b) Resistance: 1/3 in gas film, 1/3 in liquid film, 1/3 in main body
 Location of reaction zone: main body of liquid b)
 Behavior in liquid film: physical transport

23.5

$$M_H = \sqrt{\frac{D k C_B}{k_{A1}^2}} = \sqrt{\frac{10^{-6} (10^{-2}) (10^2)}{1}} = 10^{-2} \quad \therefore E = 1$$

$$-r_A^{III} = \frac{P_A}{\frac{1}{k_{AG} a} + \frac{H_A}{k_{AL} a E} + \frac{H_A}{k_C B E}} = \frac{10^2}{0.1 + \frac{10^2 (1)}{10^2 (1)} + \frac{10^2}{10^{-2} (10^2) (1)}} = 5$$

↑ 50%
↑ 50%

(a) Reaction rate = 5 mol/hr.m³ reactor a)

(b) Resistance: 50% in gas film, 50% in main body
 Reaction zone: main body of liquid b)
 Behavior of liquid film: physical transport

Q.7 Make one change in Example 1

$$C_B = 100 \Rightarrow \frac{1}{2} C_A = 1$$

First evaluate M_H and E_i and from this find Ξ

$$M_H = \frac{D k C_B}{k_A L} = \frac{(10^{-6} \cdot 10^6) \cdot 1}{1} = 1$$

$$E_i = 1 + \frac{1(1) 10^5}{2(5 \times 10^3)} = 1 + 50 = 51$$

Since $E_i > 5 M_H$ Fig 4 shows that we have a pseudo-1st order reaction in the film and

$$\Xi = M_H = 1$$

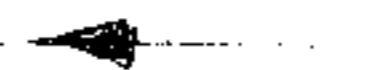
Now to the rate expression

$$-r_A''' = \frac{k_A C_A}{\frac{1}{k_f C_A} + \frac{k_A}{k_p E} + \frac{k_A}{k_p E^2}} = \frac{3 \times 10^5}{\frac{1}{201} + \frac{10^5}{20(1)} + \frac{10^5}{10^6(1^2)0.98}}$$

$$= \frac{5 \times 10^3}{100 + 5000 + 0.1} = \frac{5000}{5100} \approx 1 \text{ mol/hr} \cdot \text{m}^3 \text{ reactor}$$

↑
resistance is in the liquid film.

- (a) Main resistance is in liquid film
- (b) Reaction zone is in the liquid film
- (c) I can't tell
- (d) The rate is 1 mol/hr.m³ reactor



Q2.9 (a) Find $-r_A'''$ with reaction.

$$M_{tt} = \sqrt{\frac{3k_c E}{k_A}} = \infty \quad \text{--- because } k = \infty$$

$$E_i = 1 + \frac{D_B C_{B0} H_A}{D_A f_{A0}} = 1 + 0.64 \frac{250(10^{-4})}{2.02 \cdot 10^{-2}} = 1 + 800 = 801$$

... assume that all the resistance is in the gas phase. We'll see if this is true

$$\therefore E = 801$$

Next evaluate the rate equation

$$-r_A''' = \frac{P_A}{\frac{1}{k_{Ag} a} + \frac{H_A}{k_{L0} a E} + \frac{H_A}{k_c E f_{A0}}} = \frac{P_A}{\frac{1}{60} + \frac{10^{-4}}{0.02(801)} + 0} = \frac{0.02}{16.7 \times 10^{-3} + 4 \times 10^{-6}}$$

... 99.97% of the resistance. This verifies our assumption

$$-r_A''' = k_{Ag} a P_A = 60(0.02) = 1.2 \text{ mol/m}^3 \cdot \text{s}$$

Gas film controls

(b) Straight absorption

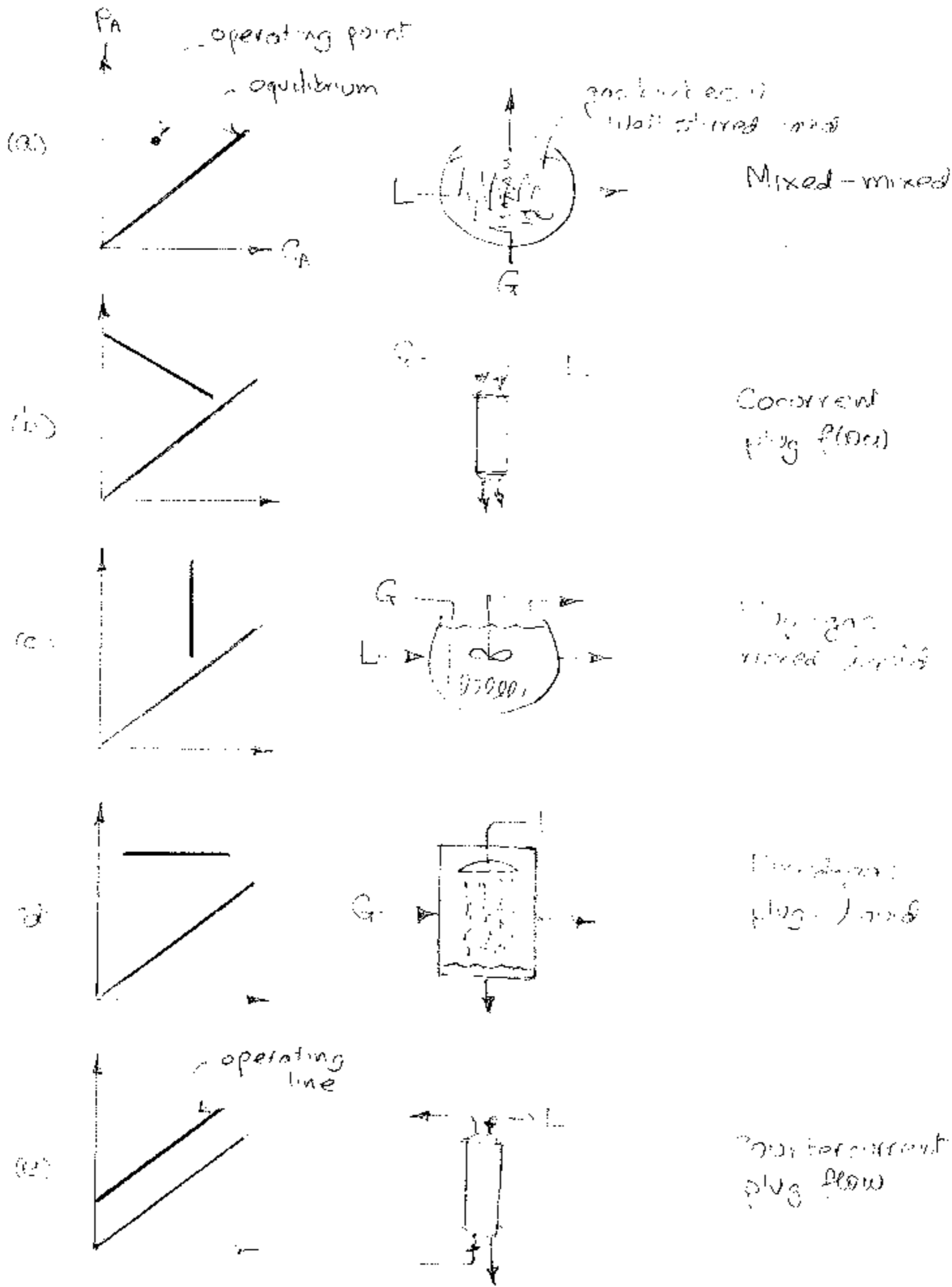
$$-r_A''' = \frac{1}{\frac{1}{k_{Ag} a} + \frac{H_A}{k_{L0} a}} (P_A - 0) = \frac{P_A}{\frac{1}{60} + \frac{10^{-4}}{0.02}} = \frac{P_A}{16.67 \times 10^{-3} + 5 \times 10^{-3}}$$

$$= 50 P_A = 50(0.02) = 1 \text{ mol/m}^3 \cdot \text{s}$$

82% in gas phase

∴ the rate is raised by 20% by adding MEA

24-1



24.3

Straight mass transfer counter current $H_A = 18$

$F_{A2} = 100$
 $F_2 = 900000$
 $C_{A2} = 10$

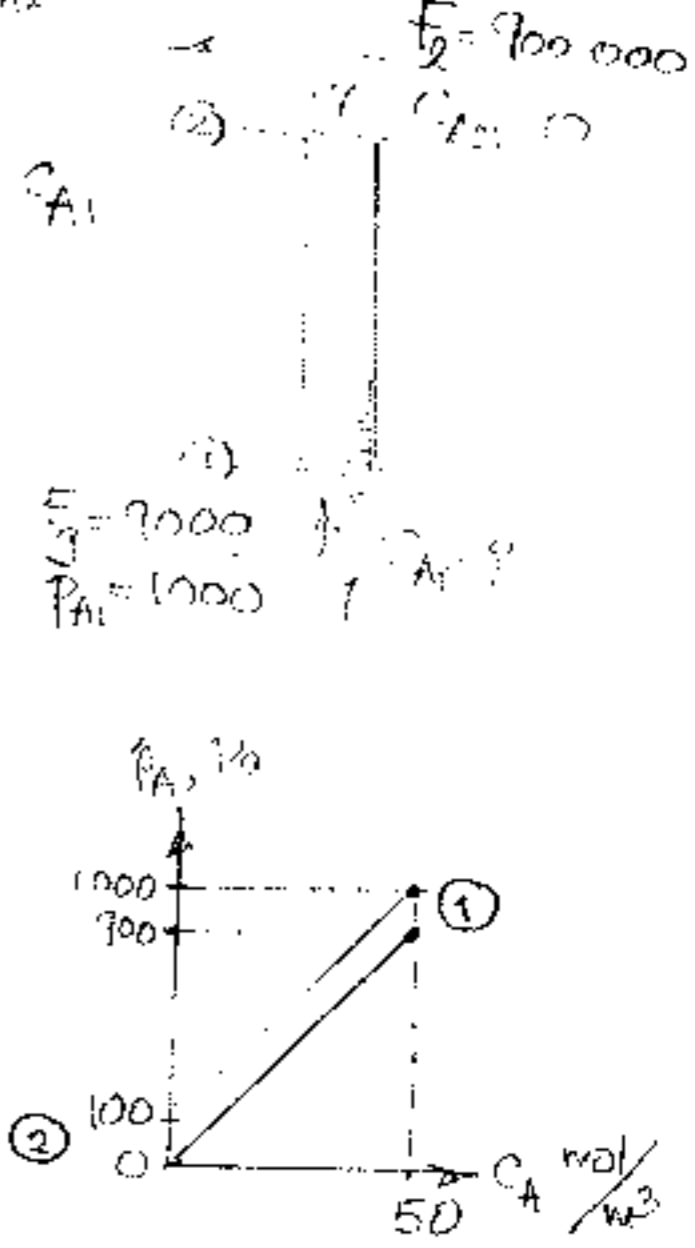
By material balance between (1) & (2) we find C_{A1}

$$\frac{90000}{10^5} (1000 - 100) = \frac{900000}{55556} (C_{A1} - 5)$$

or $C_{A1} = 50 \text{ mol/m}^3$

At equilibrium, $P_A^* = H_A C_A$ or $P_{A1}^* = 18 \times 50 = 900$

Now draw the P_A vs C_A diagram. We see that the operating & equilibrium lines are parallel. Thus the rate of transfer is the same everywhere. So we find

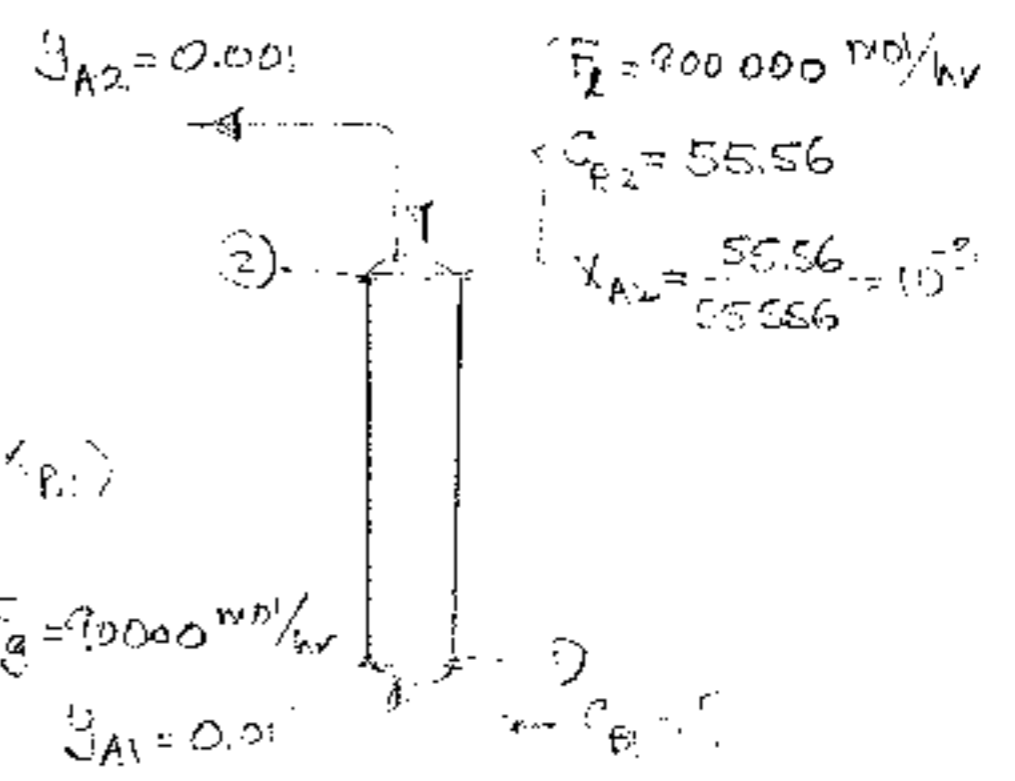


$$-r_A''' = \frac{1}{\frac{1}{k_{gA} a} + \frac{1}{H_A}} (P_A - P_A^*) = \frac{1}{0.56 + \frac{18}{72}} (1000 - 900) = ??$$

$$\therefore V_r = \frac{F_g \cdot dP_A}{\pi \cdot (-r_A''')} = \frac{90000 (1000 - 100)}{10^5 \cdot 33} = 24.5 \text{ m}^3$$

24.5

By material balance find C_{B1} (see diagram on right)



$$F_g \cdot Y_{A1} - F_{l2} \cdot y_{A2} = F_l \cdot (X_{A2} - X_{A1})$$

or $90000 \frac{0.01}{0.99} - \frac{90000}{0.99} = 900000 (0.001 - X_{B1})$

or $C_{B1} = 5 \text{ mol/m}^3$

We need to estimate E_i & M_H to find the rate

$$E_i = 1 + \frac{D_{e2} \cdot E_c}{b D_{e1} F} = 1 + \frac{C_e}{C_A} = 1 + \frac{C_e H_A}{P_{A1}} = 1 + \frac{10^5 C_e}{P_{A1}}$$

$$M_H = \sqrt{\frac{D_A k_{cB}}{k_{cA}}} = \infty$$

Since $E_i \ll M_H$
 Fig 22.4 shows that $E = E_i$

24.5
continued

Now determine the rate at top, bottom and intermediate point

At top, ②

$$E_i = 1 + \frac{55.56 \times 10^5}{100} = 5.556 \times 10^4$$

Here I am guessing that all the resistance is in the gas film, so I put $p_{A2}^* = p_{A2}$

Because $E_i \ll M_H$ we say that $E = E_i = 5.556 \times 10^4$. Now to the rate

$$-r_A''' = \frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{AL}aE} + \frac{H_A}{k^s E \delta_L}} \cdot p_A = \frac{1}{\frac{1}{0.36} + \frac{10^5}{72(5.556 \times 10^4)} + \frac{10^5}{\infty}} \cdot p_A = 0.36 p_A$$

$\leftarrow 99\%$ $\leftarrow < 1\%$ of resistance

At bottom, ①

$$E_i = 1 + \frac{55.56 \times 10^5}{100} = 501$$

I am again guessing that all resistance is in the gas film

so

$$-r_A''' = \frac{1}{\frac{1}{0.36} + \frac{10^5}{72(501)} + 0} \cdot p_A = \frac{1}{\frac{1}{0.36} + \frac{1}{0.36}} \cdot p_A = 501$$

this shows that 50% of resistance is in the liquid film. This is not what we

Try again

Guess $p_{A1} = 500$, repeat the procedure. We find $E_i = 1001$

and from the rate $1/3$ of the resistance is in the gas film. Wrong guess

Try once again

Guess $p_{A1} = 100$, or 10% resistance in the gas film. Then $E_i = 5001$ &

$$-r_A''' = \frac{1}{\frac{1}{0.36} + \frac{1}{360}} \cdot p_A = 0.33 p_A$$

9% of resistance is gas film - close enough

$$\text{So } (-r_A''')_{\text{mean}} = \frac{0.36 + 0.33}{2} = 0.345 p_A$$

Hence

$$V = \frac{F_A}{\bar{r}_A} \int \frac{dp_A}{-r_A'''} = \frac{90000 \cdot 10^2}{10^5} \frac{dp_A}{0.345 p_A} = \frac{90000}{34500} \cdot \frac{10}{1} = 6 \text{ m}^3$$

Gas film resistance is 91% of total, 9% is from liquid

24.7 First determine C_{Bout} ... see sketch at right

$$F_g(Y_{out} - Y_{in}) = F_l(X_{in} - X_{out})$$

or

$$90000 \left(\frac{0.01}{0.99} - \frac{0.001}{0.999} \right) = 9000 \left(\frac{5556}{5556} - \frac{C_{Bout}}{5556} \right)$$

so $C_{Bout} = 500 \text{ mol/m}^3$

Next determine the rate (note, at the exit conditions)

$$M_H = \sqrt{\frac{D k_{CB}}{k_{AL}}} = \sqrt{\frac{3.6 \times 10^{-6} (2.6 \times 10^5) 500}{0.72^2}} = 30$$

$$E_i = 1 + \frac{C_{BHA}}{PAI} = 1 + \frac{500(10^5)}{100} = 5 \times 10^5, \text{ or higher}$$

↑
or lower

Since $E_i \gg M_H$, Fig 23.4 shows that $E = M_H = 30$

$$-r_A''' = \frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{E} + \frac{H_A}{k'_{BL}E}} \cdot P_A = \frac{1}{\frac{1}{0.72} + \frac{10^5}{144(30)} + \frac{10^5}{2.6 \times 10^5 (500)(0.9)}} \cdot P_A$$

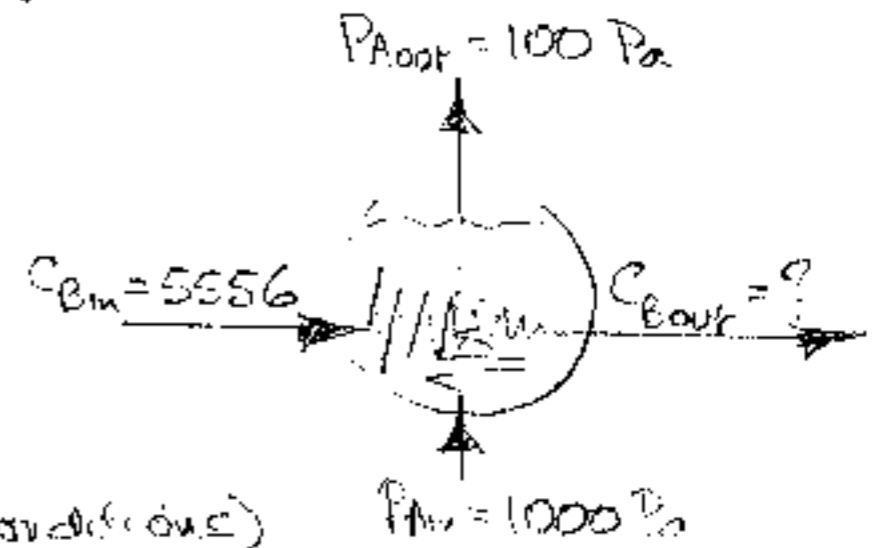
$$= \frac{1}{1.389 + 23.15 + 0} = 0.041 \text{ PA}$$

5.7% of the resistance 94% of the resistance

∴

$$V_r = \frac{F_g \Delta P_A}{P_A (-r_A''')} = \frac{90000 (1000 - 100)}{10^5 (0.041) 100} = 197.6 \text{ m}^3$$

Liquid film contributes 94.3% of the resistance.



24.9 First determine C_{Bout} by a material balance

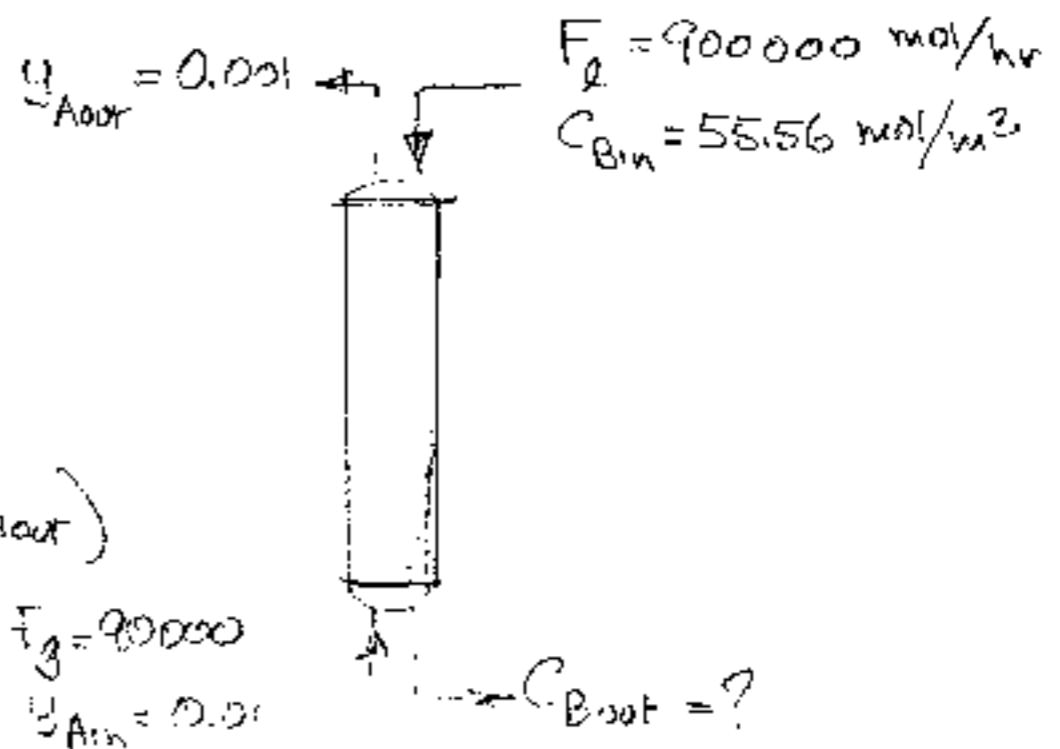
$$F_g(Y_{Ain} - Y_{Aout}) = F_l(X_{Bout} - X_{Bin})$$

or

$$90000 \left(\frac{0.01}{0.99} - \frac{0.001}{0.999} \right) = \frac{900000}{5556} (55.56 - C_{Bout})$$

From which

$$C_B = 5 \text{ mol/m}^3$$



24.9
continued

At top $M_H = \sqrt{\frac{9k_p C_B}{k_A}} = \sqrt{\frac{3.6 \times 10^{-6} (2.6 \times 10^7) 55.56}{0.72^2}} = 100$

$E_i = 1 + \frac{50.56 (10^5)}{100} = 55561 \gg M_H \dots \therefore E = M_H = 100$

$-\dot{r}_A''' = \frac{1}{\frac{1}{k_{Ag} a} + \frac{p_A}{k_{AL} E} + \frac{p_A}{k C_B^2}} \cdot p_A = \frac{1}{\frac{1}{0.36} + \frac{10^5}{72(100)} + \frac{10^5}{2.6 \times 10^7 (55.56)(0.72)}} \cdot 10^2 = 6$

liquid film = 82% of total resistance

At bottom $M_H = \sqrt{\frac{3.6 \times 10^{-6} (2.6 \times 10^7) 5}{(0.72)^2}} = 30$

$E_i = 1 + \frac{5(10^5)}{1000} = 501 \gg M_H \dots \therefore E = M_H = 30$

$-\dot{r}_A''' = \frac{1}{\frac{1}{0.36} + \frac{10^5}{72(30)} + \frac{10^5}{2.6 \times 10^7 (5) 0.72}} \cdot 10^3 = 20.4$

liquid film = 94%

Near the middle where $C_B = 30.56$. A mat. balance then gives $\begin{cases} p_A = 547 \text{ Pa} \\ Y_A = 0.0055 \end{cases}$

$M_H = \sqrt{\frac{3.6 \times 10^{-6} (2.6 \times 10^7) 30.56}{(0.72)^2}} = 74$

$\therefore E = M_H = 74$

$E_i = \text{large}$

$-\dot{r}_A''' = 25.4$

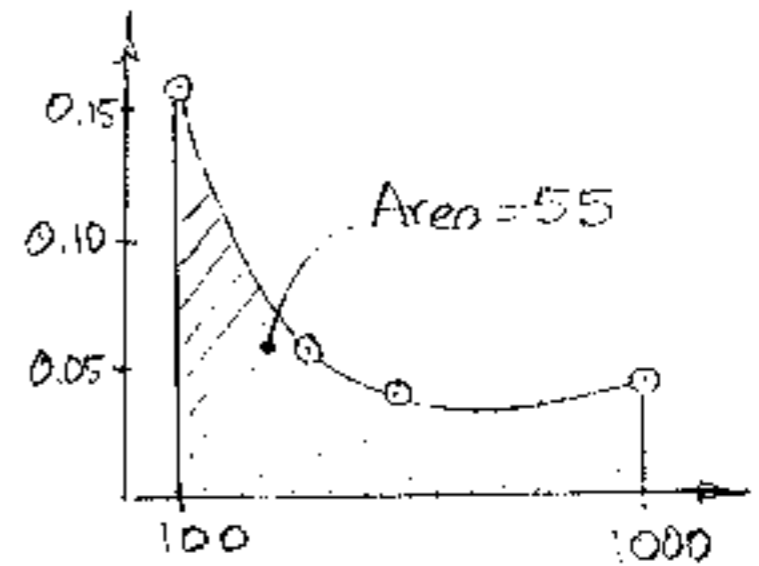
About 1/4 from the top where $p_A = 300 \text{ Pa}$ & $C_B = 44.4$ we find

$M_H = 89.5, E_i = \text{very large}, \therefore E = M_H = 89.5, -\dot{r}_A''' = 16.4$

So now to the performance of the reactor

| | p_A | $-\dot{r}_A'''$ | $1/-\dot{r}_A'''$ |
|--------------|-------|-----------------|-------------------|
| Top | 100 | 6 | 0.1667 |
| 1/4 from top | 300 | 16.4 | 0.0610 |
| Middle | 547 | 25.4 | 0.0394 |
| Bottom | 1000 | 20.4 | 0.0490 |

$\frac{1}{-\dot{r}_A'''}$



$V_R = \frac{F_B}{r_A''} \int \frac{dp_A}{-\dot{r}_A'''} = \frac{90000}{10^5} (\text{area}) = \frac{90000}{10^5} (55) = 49.5 \text{ m}^3$

Liquid film resistance dominates, 82 ~ 94%

24.11

$C_A = ?$ $C_B = 200 \text{ mol/m}^3$

$V_R = 0.6041$
 $\frac{V_R}{\tau} = 0.08$

$C_{Ain} = 1 \text{ atm}$
 $\sigma_0 = 0.0362 \text{ m}^3/\text{s}$

20°C

Let us start by evaluating C_A & C_B , and then the rate.

$$C_{Ain} = \frac{P_{Ain}}{RT_A} = \frac{101325}{3500} = 28.95 \text{ mol/m}^3$$

$C_B = 300 \text{ mol/m}^3$

Since $C_B \gg C_A$ we have an excess of B

so we can take $C_B \approx \text{constant} = 300$

Now to the rate of rx

$$M_H = \frac{0.4 \times 10^{-4} (0.433) 300}{0.05/20} = 2.05$$

since $E_a > 5 M_H$ we have

$$E_c = \frac{500(3500)}{350} = 1136$$

$E = M_H = 2.05$

so

$$-r_A''' = \frac{1}{0 + \frac{3500}{0.05 - (2.05)} + \frac{3500}{0.433(300)0.09}} \cdot \frac{1}{A}$$

$$= \frac{1}{0 + 68292 + 3727} = 1.457 \times 10^{-5} \text{ mol/m}^3 \text{ s} = 1.4764$$

(91.5% of the resistance)

(pure CO₂ at 1 atm, so $p_A = \text{constant}$, and $r_A''' = \text{const}$)

because $-r_A''' = \text{constant}$

From Eq 15

$$\frac{V_R}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A'''} = \frac{V_R}{F_{A0}} \cdot \frac{X_A}{-r_A'''}$$

$$\text{so } X_A = \frac{V_R}{F_{A0}} (-r_A''') = \frac{0.6041}{1.05} (1.48) = 0.8517 = 85\%$$

$$-F_{A0} = \sigma_0 C_{A0} = 0.0362(28.95) = 1.05$$

24.13 Here we have a batch agitated tank $V = 2.5 \times 10^5 \text{ m}^3$ $\mu_A = 10^5$

At the beginning $C_0 = 555.6$

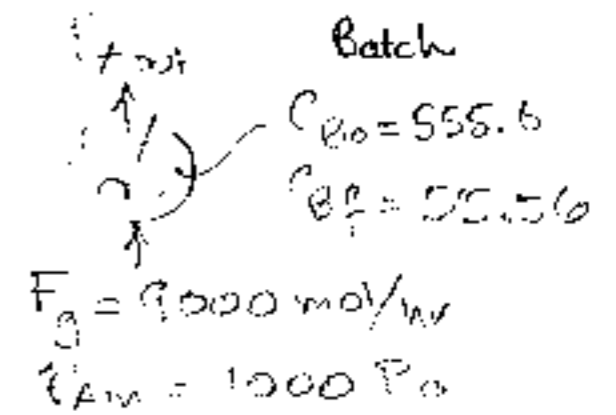
$$M_H = \frac{\sqrt{3.6 \times 10^{-6} (2.5 \times 10^5) 555.6}}{k_H/100} = 15.34$$

$$E_i = 1 + \frac{555.6 (10^5)}{10^3} = 5561$$

guess this or something smaller

whatever we guess is ok.

24.13.13.13



Now $M_H \ll E_i$ so $E = M_H = 15.34$.

Next, since $E = M_H$ and $\mu_A \ll P$ we can use the shortcut just above Eq 19 to evaluate the rate. So

$$\begin{aligned} -r_A^{III} &= \frac{1}{\frac{P_A}{k_g} + \frac{1}{k_{f,A}} + \frac{M_H}{k_{A,eff}} + \frac{M_H}{k_{C,eff}} \frac{P_{Ain}}{P}} \\ &= \frac{1}{\frac{10^5 (1.62/0.7)}{9000} + \frac{1}{0.72} + \frac{10^5}{104 (15.34)} + \frac{10^5}{2.5 \times 10^5 (555.6) 0.9}} \cdot 10^3 \text{ PA} \\ &= \frac{1}{20 + 1.3889 + 43.8417 + 0.0008} \cdot 1000 = 15.33 \end{aligned}$$

main resistances
negligible

$$\text{or } \frac{1}{-r_A^{III}} = 0.06523$$

At the end of the run $C_0 = 55.56$

$$M_H = 5.01$$

$$E_i = 1 + \frac{55.6 (10^5)}{10^3} = 5561$$

$$E = M_H$$

and again use the shortcut

$$-r_A^{III} = \frac{1}{20 + 1.3889 + \frac{10^5}{104 (5.01)} + 0.0008} \cdot 1000 = 6.25$$

main resistances
negligible

$$\text{so } \frac{1}{-r_A^{III}} = 0.16$$

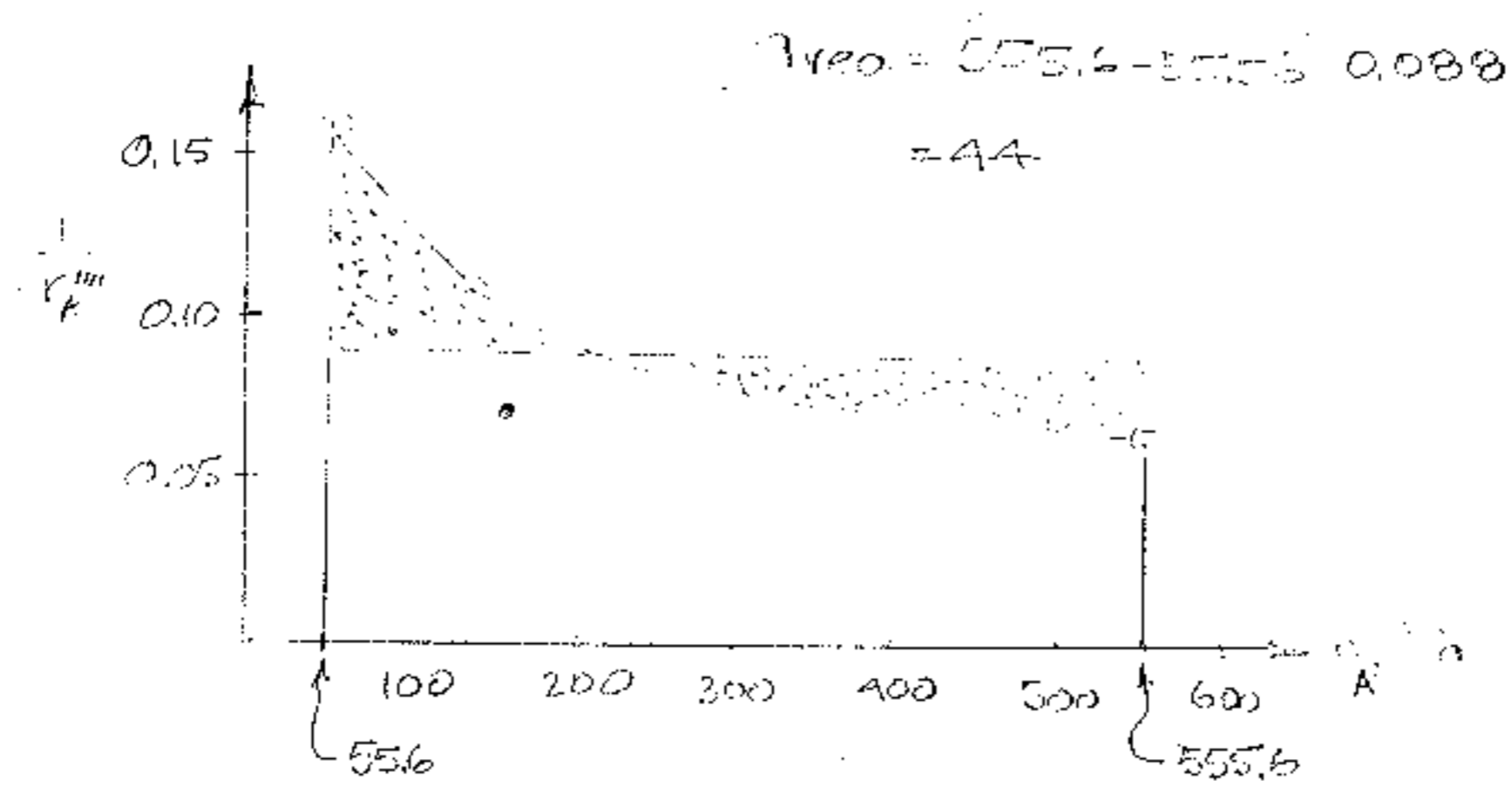
Prob. 13
continued

At some intermediate condition, say at $C_E = \frac{555.6}{4} = 138.9$

$$\left. \begin{aligned} M_{11} &= \frac{15.84}{4} = 3.96 \\ E_1 &= \frac{555.6}{4} = 138.9 \end{aligned} \right\} \bar{E} = \bar{M}_{11} = 3.96$$

$$\therefore -r_A^{III} = \frac{1}{20 + 138.9 \times \frac{10^5}{1000000}} \times 1000 = 7.168$$

$$\text{and } \frac{1}{-r_A^{III}} = 0.1407$$



The length of time that we have to utilize is τ_{eq} .

$$\frac{1}{\tau_{eq}} = \frac{r_A^{III}}{C_E} = \frac{1}{2} (1000 \times 0.9 \times 44) = 19.8 \text{ hr}^{-1}$$

The minimum time needed if all the A reacts with 12%

$$\tau_{min} = \frac{1}{r_A^{III}} \frac{C_{A0} - C_A}{C_A} = \frac{1.62 (555.6 - 55.56)}{1000 (1000/37000)} = 8.91 \text{ hr} \quad a)$$

$$\therefore \text{Efficiency of use of A} = \frac{8.91}{39.6} = 22.5\% \quad b)$$

24.15 Here we have a batch agitated tank with $k=2.6 \times 10^3$, $t_g=10^5$

At the beginning $C_B = 555.6 \text{ mol/m}^3$

$$M_H = \frac{\sqrt{2.6 \times 10^3 (2.6 \times 10^{-6}) 555.6}}{1.4/100} = 1.584$$

$$E_i = 1 + \frac{555.6 (10^5)}{10^2} = 55561$$

↑
- guess

$$\left. \begin{array}{l} M_H = 1.584 \\ E_i = 55561 \end{array} \right\} E = M_H = 1.584$$

Use the shortcut formula just above Eq. 19, thus

$$\tau_A^{III} = \frac{1}{\frac{V_R T}{t_g} + \frac{1}{k_A C_B^2} + \frac{E_i}{V_R T} + \frac{1.4}{k C_B}} \cdot 1000$$

$$= \frac{1}{\frac{1.62/0.9 \cdot 10^5}{1000} + \frac{1}{0.72} + \frac{10^5}{1.4 (1.584)} + \frac{10^5}{2.6 \times 10^3 (555.6) 0.9}} \cdot 1000$$

$$= \frac{1}{20 + 1.3889 + 438.4 + \sim 0} \cdot 1000 = 2.175$$

$$\frac{C_B}{C_{B0}} = \frac{1}{\tau_A^{III}} = 0.460$$

At the end of the run, $C_B = 55.56$

$$M_H = 1.584 / \sqrt{10} = 0.5$$

$$E_i = 1 + \frac{55.56 (10^5)}{10^2} = \text{big or bigger}$$

↑
- or smaller

$$\left. \begin{array}{l} M_H = 0.5 \\ E_i = \text{big or bigger} \end{array} \right\} \therefore E = M_H = 0.5$$

Shortcut

$$\tau_A^{III} = \frac{1}{20 + 1.3889 + 438.4 + \sqrt{10}} \cdot 1000 = 0.7096$$

↑
1388

$$\frac{C_B}{C_{B0}} = \frac{1}{\tau_A^{III}} = 1.41$$

(23)

24.15 At some intermediate condition, say $C_e = 555.6/4 = 138.9$
continued

$$M_H = 1.584/4 = 0.396$$

$$E_i = 1 + \frac{555.6(10^5)}{10^3} = 55660$$

$$E = 1 + \frac{M_H^2}{E_i} = 1.0000014$$

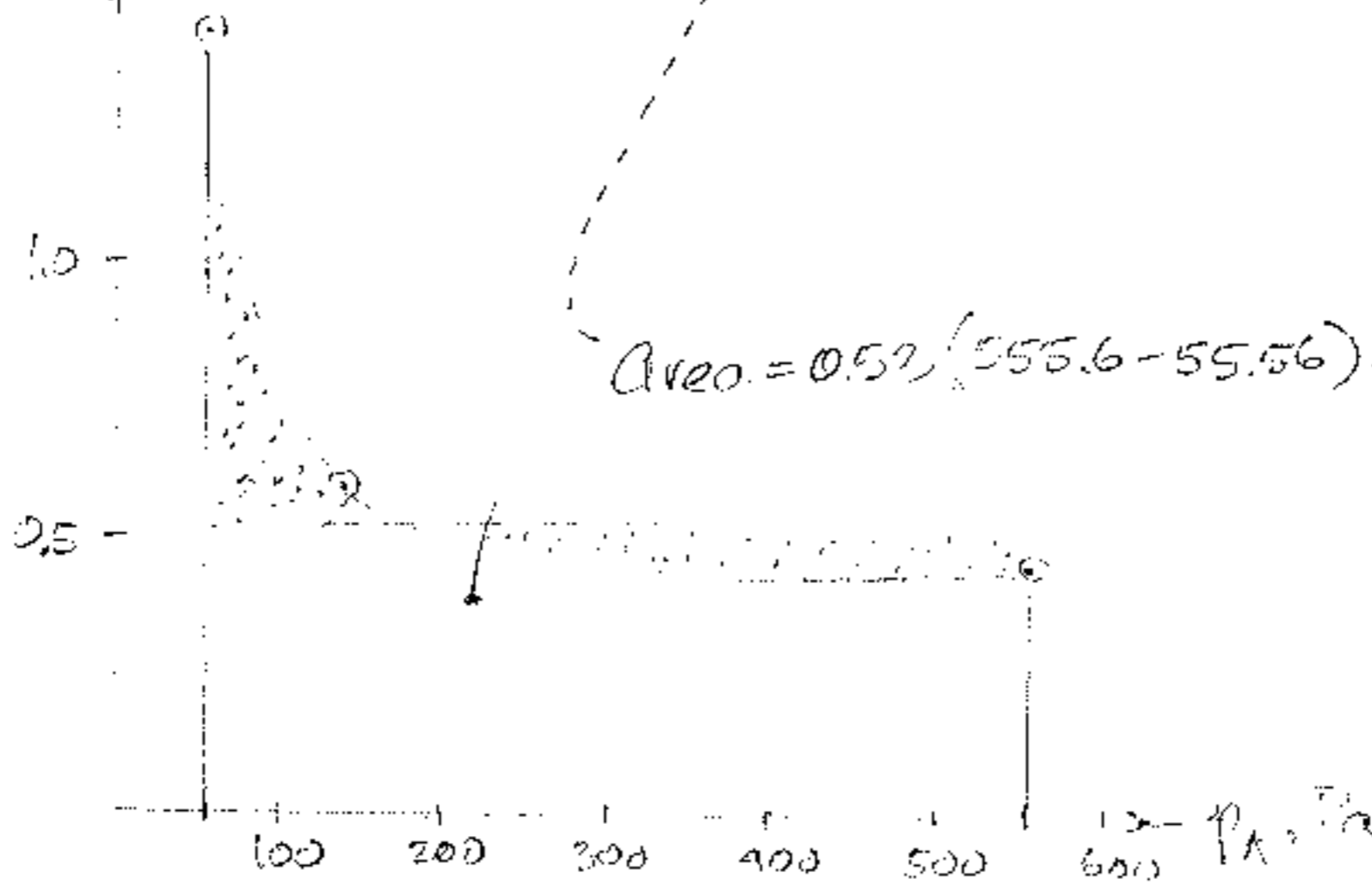
$$\therefore -r_A''' = \frac{1}{20 + 13889 + 10^5/12 + (1.2)} \cdot 1000 = 1.666$$

$$\therefore \frac{1}{-r_A} = 0.600$$

main resistance

The length of time needed to bubble gas through the reactor is

$$t = \frac{V}{Q} \int_{C_2}^{C_1} \frac{dC_e}{-r_A'''} = \frac{V}{Q} (\text{area}) = 0.9(265) = 238.5 \text{ hr} \quad (a)$$



$$t_{\text{min}} = \frac{V_e (C_{e0} - C_{e2})}{\frac{1}{Q} (P_{A0} - P_{A2})} = \frac{1.62(555.6 - 55.56)}{3000(1000/92000)} = 3.7 \text{ hr}$$

$$\therefore \text{Efficiency of use of A} = \frac{3.7}{238.5} = 3.7\% \quad (b)$$

25.1 Test the 3 possible shrinking-core mechanisms to see which is consistent with the following reported data

$$\left. \begin{array}{l} X_B = 0.875 \text{ at } t = 1 \text{ hr} \\ X_B = 1.000 \text{ at } t (= \tau) = 2 \text{ hr} \end{array} \right\} \dots \text{ or } X_B = 7/8 \text{ at } \frac{t}{\tau} = 0.5$$


Since the shape of the solids is not specified assume to start with that they are spherical. Then from Table 1

If film diffusion controls: $\frac{t}{\tau} = X_B$
 but from the data: $0.5 \stackrel{?}{=} 0.875$... this doesn't agree, so we reject this mechanism

If ash diffusion controls: $\frac{t}{\tau} = 1 - 3(1 - X_B)^{2/3} + 2(1 - X_B)$
 again from the data $0.5 \stackrel{?}{=} 1 - 3(1/8)^{2/3} + 2(1/8) = 0.5$... this agrees

Now before we feel that all is solved let us try the third mechanism. Who knows, maybe it too will fit. So

If surface reaction controls: $\frac{t}{\tau} = 1 - (1 - X_B)^{1/3}$
 & again from the data: $0.5 \stackrel{?}{=} 1 - (1/8)^{1/3}$... amazing, this also fits!

So here we have a coincidence where both reaction & ash diffusion mechanisms fit the data } 

Note - Figure 9 or 10 shows that the data were taken at the precise point where the ash diffusion curve crosses the reaction controlling curve.

- If we try the equations for flat plate or cylindrical pellets we find that neither will fit the data.

2.5.3 Here we have shrinking particles, hence only 2 possible resistances, film diffusion & surface reaction. Since we are told that we can ignore film diffusion we are left with reaction controlling alone. So solve for this case.

From Table 1 pg 580 we have for reaction controlling

$$\frac{t}{\tau} = 1 - (1 - X_B)^{3/2} \quad \dots \text{ where } \tau = \frac{\rho_B R_0}{b k_s C_{Ag}}$$

but $\rho_B = \frac{2.2 \text{ gm/cm}^3}{12 \text{ gm/mol}} = 0.183 \text{ mol/cm}^3$

$$C_{Ag} = \frac{1 \text{ mol}}{22400 \text{ cm}^3} \cdot \frac{273}{273+900} \cdot 0.08 = 8.30 \times 10^{-7} \text{ mol/cm}^3$$

for the reaction $C + O_2 \rightarrow CO_2 \quad \dots b = 1$

Replacing these quantities in the τ expression gives

$$\tau = \frac{(0.183)(0.5)}{(1)(20)(8.3 \times 10^{-7})} = 5510 \text{ sec} = 1.53 \text{ hr} \quad \leftarrow$$

2.5.5 Let 1 refer to particles of size R_1 and 2 refer to particles of size $2R_1$. Then $\tau_2 = 2\tau_1 \dots (i)$

Now $\tau_1 = \tau_{1ash} + \tau_{1rxn} \quad \dots (ii)$

$\tau_2 = \tau_{2ash} + \tau_{2rxn} \quad \dots (iii)$

Put $\tau_{2ash} = 4\tau_{1ash} \quad \dots (iv)$

$\tau_{2rxn} = 2\tau_{1rxn} \quad \dots (v)$

So (iii) & (iv) & (v) in (iii) gives $3\tau_1 = 4\tau_{1ash} + 2\tau_{1rxn} \quad \dots (vi)$

From (ii) and (vi) we find $\tau_{1ash} = \tau_{1rxn}$

so the % contribution of ash diffusion for $R_1 = 50\% \quad \leftarrow$

25.7

guess → ash diffusion controls
guess reaction controls

| d_t | X_e | t | $\frac{R}{t} \left[1 - 2(1-X_e)^{2/3} + 2(1-X_e) \right]$ | $\frac{R}{t} \left[1 - (1-X_e)^{1/3} \right]$ |
|-------|-------|-----|--|--|
| 1 | 1 | 4 | 0.0625 | 0.125 ← |
| 1.5 | 1 | 6 | 0.0938 | 0.125 ← |

(same value)

∴ chemical reaction controls

25.9

ash
reaction controls

| d_t | X_e | t | $\frac{R}{t} \left[1 - 3(1-X_e)^{2/3} + 2(1-X_e) \right]$ | $\frac{R}{t} \left[1 - (1-X_e)^{1/3} \right]$ |
|-------|-------|-----|--|--|
| 1 | 1 | 200 | 1.25×10^{-3} ← | 2.5×10^{-3} |
| 1.5 | 1 | 450 | 1.25×10^{-3} ← | 1.67×10^{-3} |

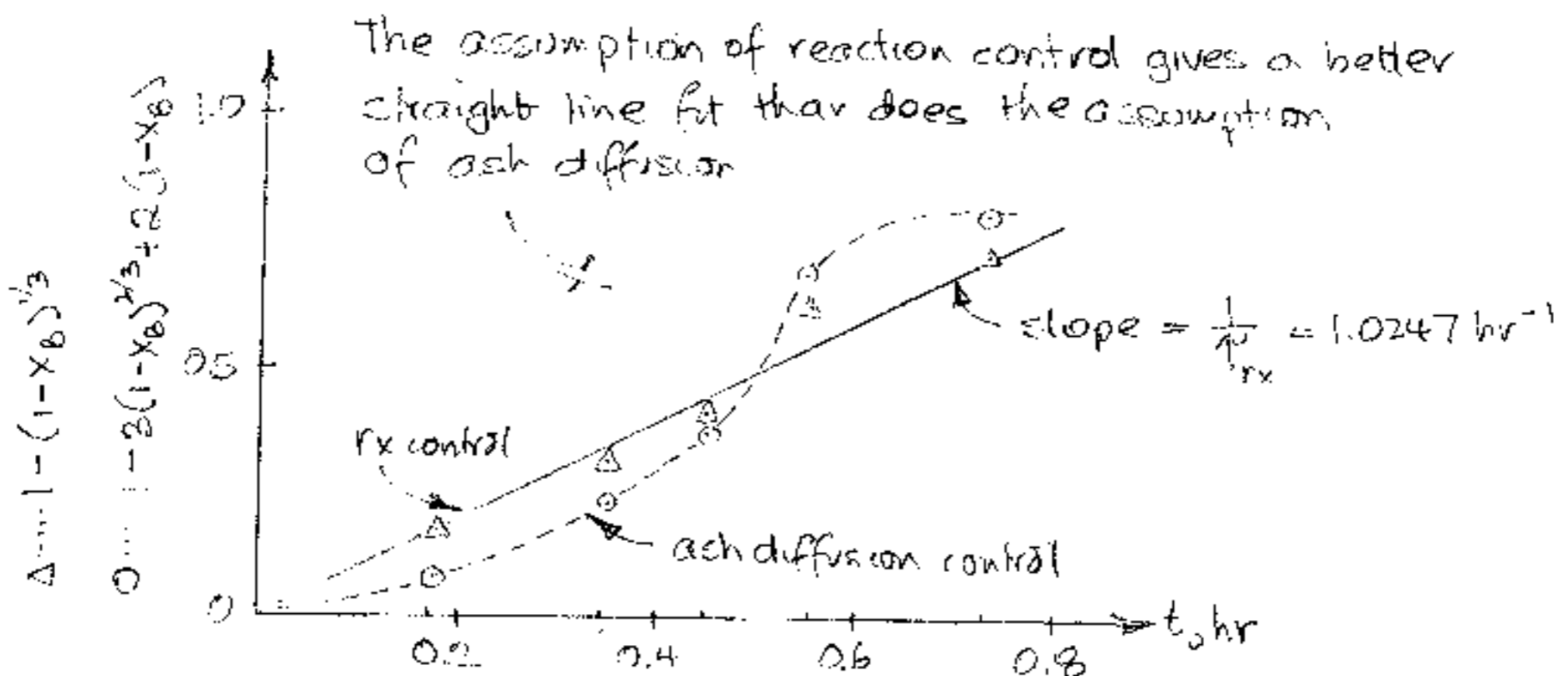
(same)

∴ ash diffusion controls

25.11

Plot assuming that reaction, and then ash diffusion controls

| | | | | | |
|-------------------------------------|--------|--------|--------|--------|--------|
| t, hr | 0.180 | 0.247 | 0.453 | 0.567 | 0.733 |
| X_e | 0.45 | 0.68 | 0.80 | 0.95 | 0.98 |
| $1 - (1 - X_e)^{1/3}$ | 0.1807 | 0.2160 | 0.4152 | 0.5216 | 0.7296 |
| $1 - 3(1 - X_e)^{2/3} + 2(1 - X_e)$ | 0.0861 | 0.2265 | 0.2740 | 0.6422 | 0.8190 |



From the above plot $\frac{t}{r_x} = 1 - (1 - X_e)^{1/3}$
 $r_x = \tau = 0.98 \text{ hr}$

26.1 For plug flow, SCM/each diffusion control, in the original reactor

$$\frac{t}{\tau} R = 1 - 3(1 - X_B)^{2/3} + 2(1 - X_B) = 1 - 3(1 - 0.8)^{2/3} + 2(1 - 0.8) = 0.374$$

Now double t_p . Then the conversion X'_B is

$$2 \frac{t_p}{\tau} R = 2(0.374) = 1 - 3(1 - X'_B)^{2/3} + 2(1 - X'_B)$$

or $X'_B = 16.5\%$ ←

26.3 For plug flow SCM/reaction control $\tau_{min} R$, therefore

$$\tau_{4mm} = 4 \text{ hr (given)}$$

$$\tau_{2mm} = 2 \text{ hr (calculated)}$$

$$\tau_{1mm} = 1 \text{ hr (calculated)}$$

So for 100% conversion, the residence time must be longer than

τ_{4mm} . Therefore $\tau_{\text{reactor}} = 4 \text{ hr or more}$ ←

26.5 We are given that: $W_1 = W_2$, $C_{A0,1} = C_{A0,2}$, $\bar{t}_1 = \bar{t}_2$, $F_{A0,1} = F_{A0,2}$

so we end up with the same conversion. ←

Note: Size of reactor is unimportant, weight of solids is.

26.7 Following the procedure of Example 3 we have

$$\bar{t} = 10 \text{ min} \quad \begin{array}{l} \tau(50 \mu\text{m}) = 2.5 \text{ min} \\ \tau(100 \mu\text{m}) = 10 \text{ min} \\ \tau(200 \mu\text{m}) = 40 \text{ min} \end{array} \quad \begin{array}{l} \text{from eq 25.37} \\ \text{for each diff} \end{array}$$

So from Eq 11

$$1 - \bar{X}_B = \left[\frac{1}{5} \left(\frac{2.5}{10} \right) - \frac{19}{420} \left(\frac{2.5}{10} \right)^2 + \frac{1}{10} \left(\frac{2.5}{10} \right) + \frac{1}{5} \left(\frac{10}{10} \right) - \frac{19}{420} \left(\frac{10}{10} \right)^2 + \frac{41}{4620} \left(\frac{10}{10} \right)^3 + \dots \right] \frac{4}{10}$$

$$+ \left[\frac{1}{5} \left(\frac{40}{10} \right) - \frac{19}{420} \left(\frac{40}{10} \right)^2 + \frac{41}{4620} \left(\frac{40}{10} \right)^3 - 0.00149 \left(\frac{40}{10} \right)^4 + \dots \right] \frac{5}{10}$$

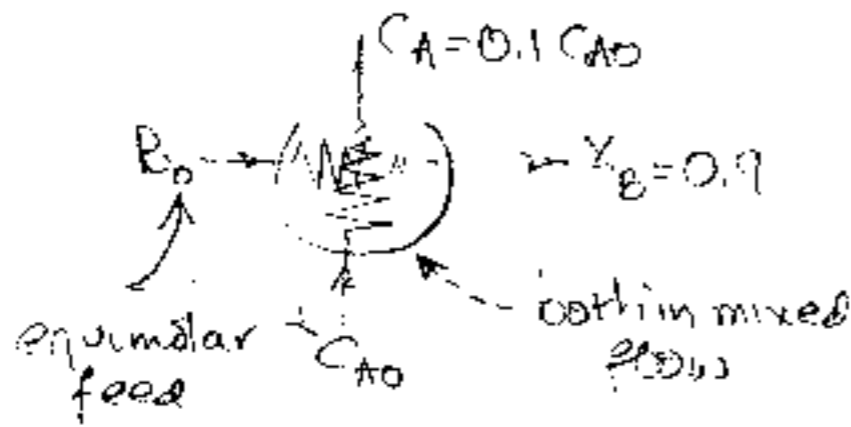
converges too slowly, so use Fig. 4. This gives $1 - \bar{X}_B = 0.35$

$$= 0.0141 + 0.0654 + 0.105 = 0.1845$$

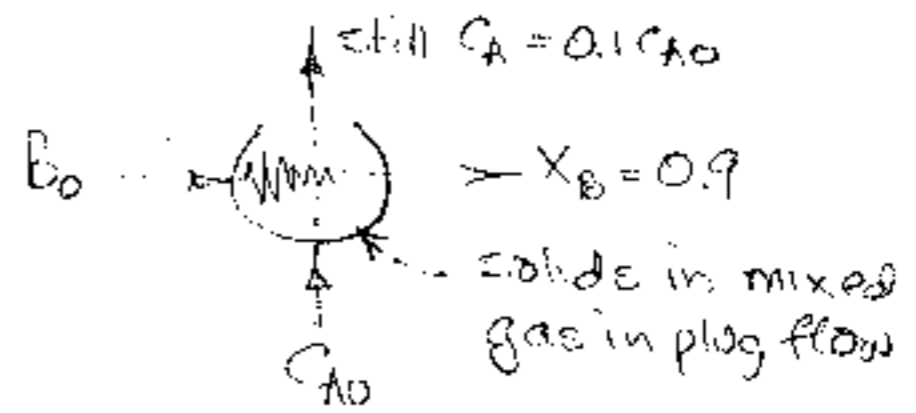
so the conversion for each resistance control is $\bar{X}_B = 18.5\%$

(for reactor control Example 3 gives $\bar{X}_B = 77.8\%$) ←

26.9 In Example 4 we have:



Here we have:



Here $\bar{C}_A = \frac{C_{A0} - C_{Af}}{\int_0^{\tau} C_{A0}/\tau dt} = \frac{C_{A0} - 0.1 C_{A0}}{\int_0^{\tau} C_{A0}/0.1 C_{A0} dt} = \frac{0.9}{\int_0^{\tau} 10 dt} = 0.09$

\therefore Wt of solids needed = $\frac{25 \text{ tons}}{3.9}$

= 5.98 tons

instead of 0.1, as in Example 4

26.11 For SCM/reaction control, $1 - X_B = (1 - t/\tau)^2$

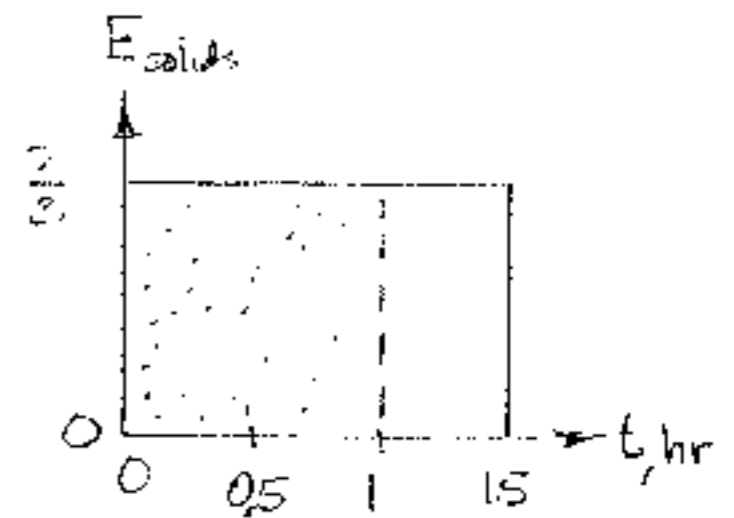
So from Eq 16, with $\tau = 1$ hr

$$1 - \bar{X}_B = \int_0^{\tau} (1 - X_B)_{\text{part}} E_{\text{solids}} dt$$

$$= \int_0^{\tau} \left(1 - \frac{t}{\tau}\right)^2 \frac{2}{3} dt$$

$$= \frac{2}{3} \int_0^1 (1-t)^2 dt = \frac{2}{3} \cdot \frac{1}{3} = \frac{1}{6}$$

$\therefore \bar{X}_B = 83.3\%$



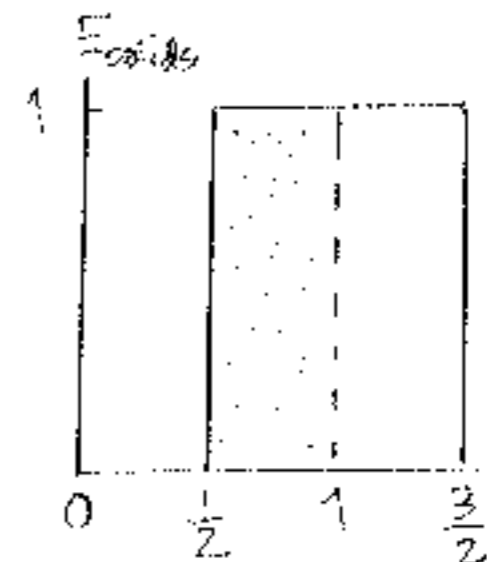
26.13 For SCM/reaction control, $1 - X_B = (1 - t/\tau)^3$

So from Eq 16, with $\tau = 1$

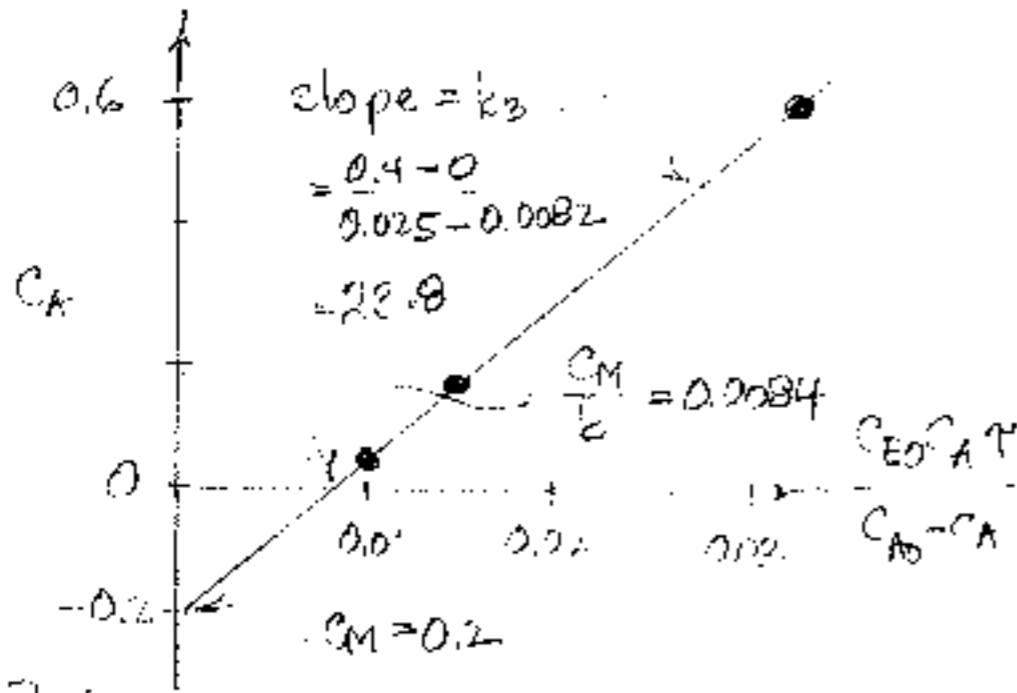
$$1 - \bar{X}_B = \int_{1/2}^1 (1-t)^3 (1) dt$$

$$= -\frac{(1-t)^4}{4} \Big|_{1/2}^1 = \left[-\frac{1}{4} - \left(-\frac{1}{64}\right) \right] = 0.0156$$

$\therefore \bar{X}_B = 98.44\%$



Q7.1



For mixed flow & Monod kinetics
Eq 8 gives

$$C_A = -C_M + k_3 \frac{C_{E0} C_A \tau}{C_{A0} - C_A}$$

$$y = a + b x$$

Plotting gives: (see Fig. 6)

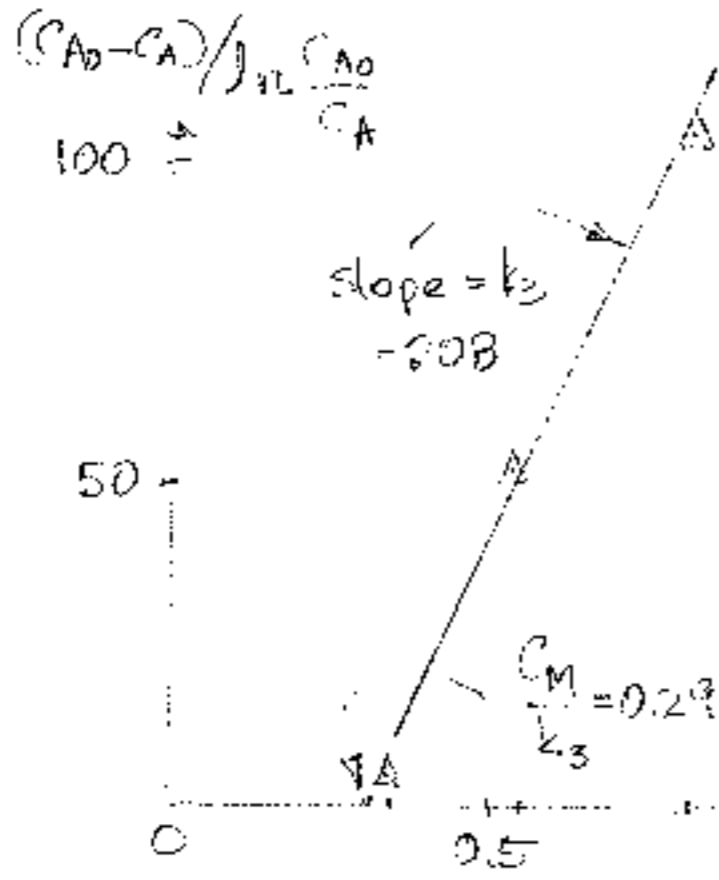
$$-r_A = \frac{28.8 C_A C_{E0}}{0.2 + C_A} \text{ mol/lit} \cdot \text{hr}$$

Tabulate

| C_{E0} | C_{A0} | C_A | τ | $\tau = V/v$ | $C_{E0} C_A \tau / (C_{A0} - C_A)$ |
|----------|----------|-------|--------|--------------|------------------------------------|
| 0.02 | 0.3 | 0.04 | 3.0 | 2 | 0.01 |
| 0.01 | 0.2 | 0.15 | 4.0 | 1.5 | 0.015 |
| 0.001 | 0.69 | 0.60 | 1.2 | 5 | 0.0323 |

given data calculated

Q7.3



For plug flow & Monod kinetics
Eq 6 gives

$$C_{A0} - C_A = -C_M + k_3 \frac{C_{E0} \tau}{\frac{1}{\mu} \frac{C_{A0}}{C_A}}$$

From the plot & table below
we find

$$-r_A = \frac{208 C_A C_{E0}}{60.2 + C_A} \text{ mol/lit} \cdot \text{hr}$$

Tabulate

| C_{E0} | C_{A0} | C_A | t | $(C_{A0} - C_A) / (\tau \frac{C_{A0}}{C_A})$ | $t C_{E0} / (\tau \frac{C_{A0}}{C_A})$ |
|----------|----------|-------|-----|--|--|
| 3 | 400 | 10 | 1 | 105.7 | 0.81 |
| 2 | 200 | 5 | 1 | 52.9 | 0.54 |
| 1 | 50 | 1 | 1 | 6.34 | 0.32 |

given data calculated

27.5

Run 1 $C_{A0} = 600 \text{ mol/m}^3$
 $C_{E0} = 8 \text{ gm/m}^3$
 $C_{B0} = 0$

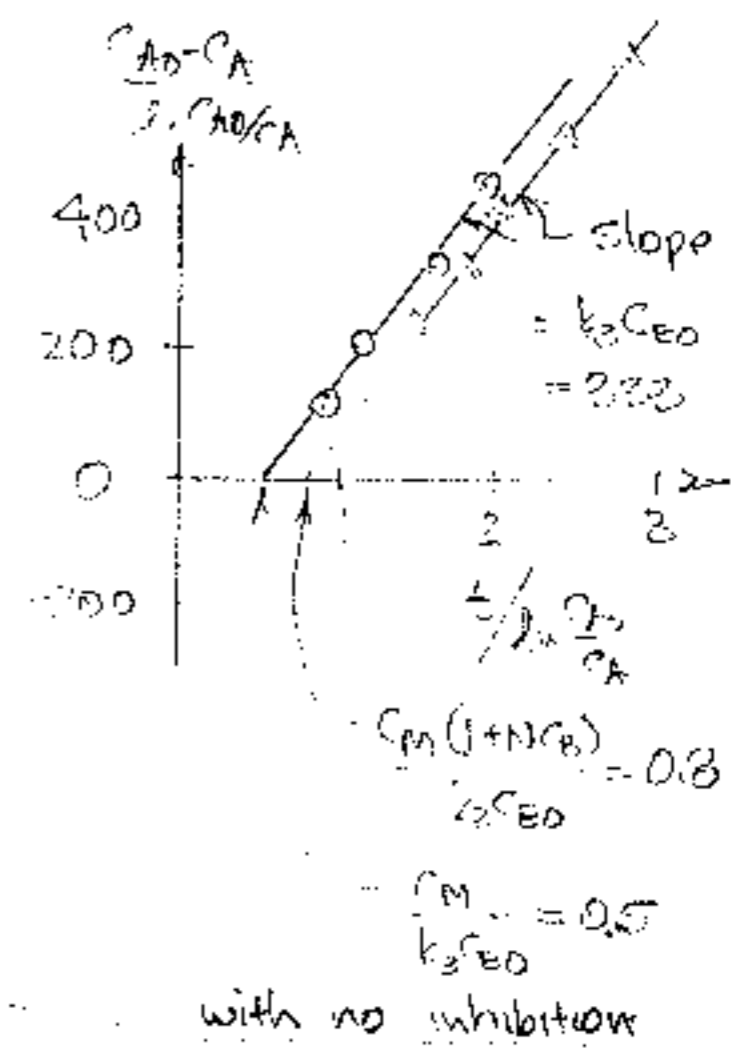
| t | C_A | $\frac{C_{A0}-C_A}{\int_0^t C_A dt}$ | $\frac{t}{\int_0^t C_A dt}$ |
|---|-------|--------------------------------------|-----------------------------|
| 0 | 600 | | |
| 1 | 250 | 464 | 1.3 |
| 2 | 160 | 733 | 1.5 |
| 3 | 40 | 207 | 1.1 |
| 4 | 10 | 144 | 0.97 |

Run 2 $C_{A0} = 800 \text{ mol/m}^3$
 $C_{E0} = 8 \text{ gm/m}^3$
 $C_{B0} = C_B = 100 \text{ mol/m}^3$

| t | C_A | $\frac{C_{A0}-C_A}{\int_0^t C_A dt}$ | $\frac{t}{\int_0^t C_A dt}$ |
|---|-------|--------------------------------------|-----------------------------|
| 0 | 800 | | |
| 1 | 560 | 672 | 2.8 |
| 2 | 340 | 538 | 2.5 |
| 3 | 180 | 416 | 2.0 |
| 4 | 80 | 318 | 1.7 |
| 5 | 30 | 235 | 1.5 |

Run #1. For Monod kinetics (plug flow)
 fit Eq. 6. From the figure

$C_{E0} = 8$ (given data)
 slope = $k_3 C_{E0} = 222$
 $\therefore k_3 = 222/8 = 41.63$
 Intercept = $\frac{C_M}{k_3 C_{E0}} = 0.5$
 $\therefore C_M = 0.5 (222) = 111$



the rate equation is

$$r_R = \frac{41.63 C_{E0} C_A}{C_A + 111} = \frac{222 C_A}{111 + C_A}$$

with no inhibition

Run #2. Parallel slopes means competitive inhibition. From run #1

$C_{E0} = 8, k_3 = 41.63, C_M = 111$
 Intercept = $\frac{C_M(1 + N C_B)}{k_3 C_{E0}} = \frac{111(1 + N \times 100)}{222} = 0.23 \quad \therefore N = 0.006$

The rate equation is

$$r_R = \frac{k_3 C_{E0} C_A}{C_M + C_A + N C_B C_A} = \frac{41.63 C_{E0} C_A}{111 + C_A + C_B} = \frac{222 C_A}{251 + C_A}$$

with competitive inhibition

27.7

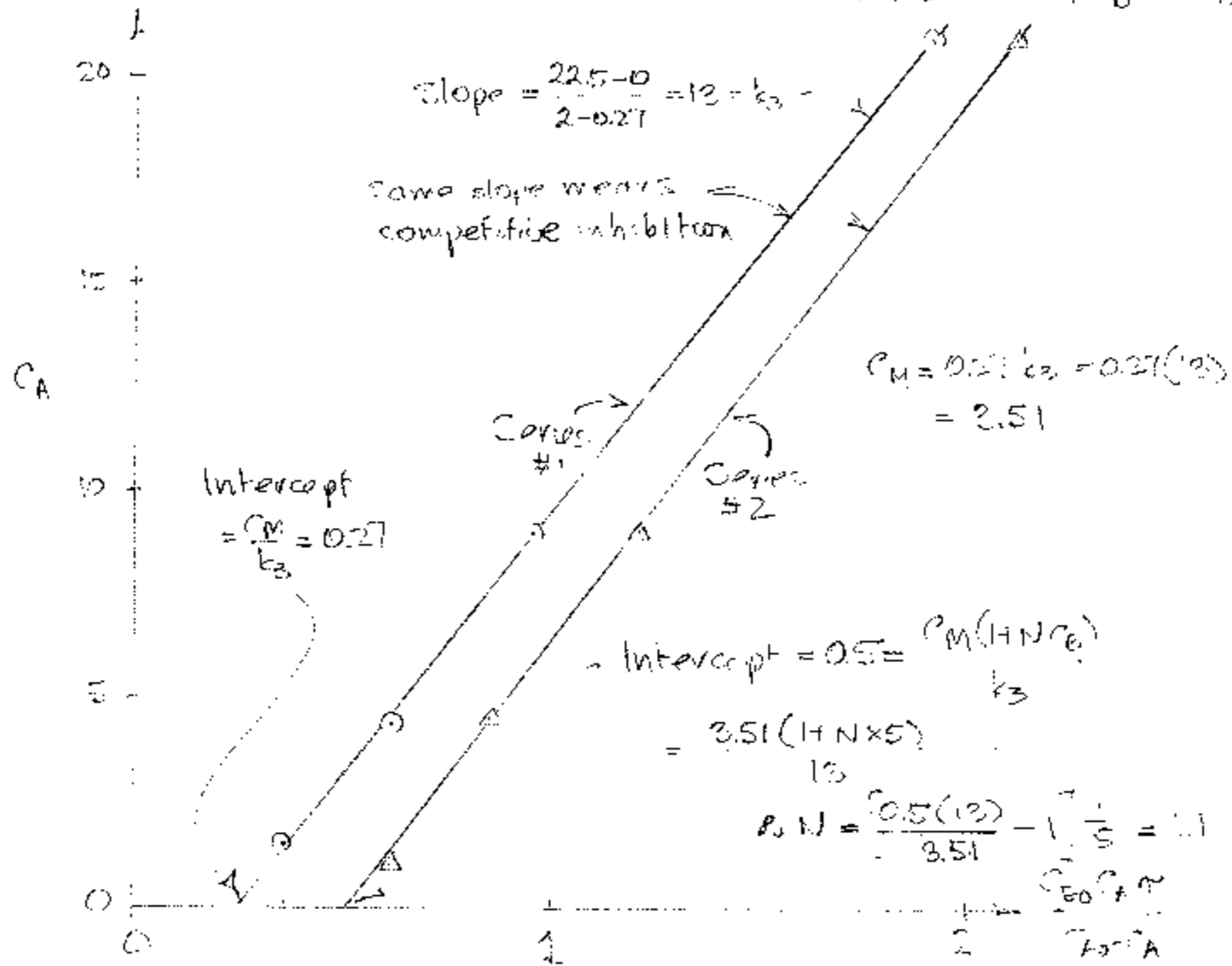
Cellulose $\xrightarrow{\text{cellulase}}$ sugar, Monod kinetics, mixed flow

Series 1 has no inhibitor, series 2 has $C_B = 5 \frac{kg}{m^3}$. To see which form of inhibition applies, if any, try to fit Eq 11 or 15 in Fig 9.

| C_{A0} | C_A | τ | $\frac{C_{E0} C_A \tau}{(C_{A0} - C_A)}$ | C_{A0} | C_A | τ | $\frac{C_{E0} C_A \tau}{(C_{A0} - C_A)}$ |
|----------|-------|--------|--|----------|-------|--------|--|
| 25 | 1.5 | 587 | 0.2747 | 25 | 1.5 | 587 | 0.6 |
| 25 | 4.5 | 279 | 0.6124 | 25 | 4.5 | 287 | 0.80 |
| 25 | 9 | 171 | 0.9616 | 25 | 9 | 213 | 1.2 |
| 25 | 21 | 86 | 1.890 | 25 | 21 | 40 | 2.1 |

Series #1: without B

Series #2: with $C_B = 5 \frac{kg}{m^3}$



From the plot

With no inhibition: $r_R = \frac{k_3 C_{E0} C_A}{C_M + C_A} = \frac{65 C_A}{3.51 + C_A}$

With inhibition (competitive): $r_R = \frac{k_3 C_{E0} C_A}{C_M(1 + N C_B) + C_A} = \frac{65 C_A}{3.51(1 + N \times 5) + C_A} = \frac{65 C_A}{3.67 + C_A}$

27.9 For M.M kinetics the reaction rate is

1st order with respect to E

1st order with respect to A

∴ the dependence on E is of higher order than that of A
Thus it is more important to keep E at high concentration than A.

∴ looking at the 6 contacting patterns we see that

a) .

c) . are not as good, while

d) .

e) .

b) }

f) }

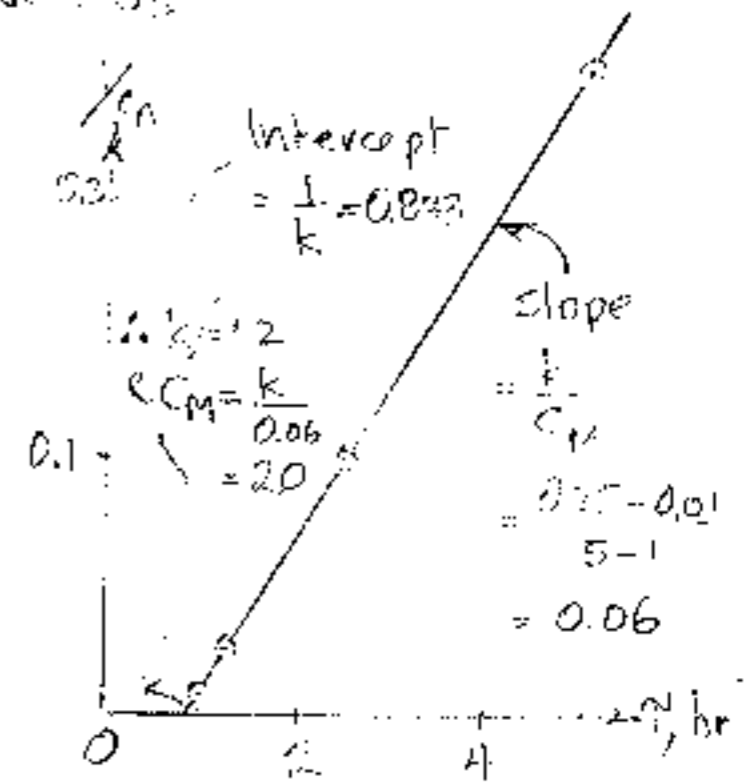
are the best ←

29.1 For mixed flow & Monod kinetics Eq 8 gives us

$$\frac{1}{C_A} = \frac{k}{C_M} \tau \frac{1}{C_A} \quad \text{or} \quad \tau_A = \frac{C_M}{k(C_A - 1)}$$

Test graphically

| τ | C_{A0} | C_A | C_C | $(C/A) = \frac{C_C}{C_{A0} - C_A}$ | $\tau = \frac{V}{v} = \frac{1}{v}$ | $\frac{1}{C_A}$ |
|--------|----------|-------|-------|------------------------------------|------------------------------------|-----------------|
| 0.2 | 100 | 4 | 15.6 | 0.1 | 5 | 0.25 |
| 0.4 | 100 | 10 | 15 | 0.1 | 2.5 | 0.1 |
| 0.3 | 100 | 40 | 12 | 0.1 | 1.25 | 0.025 |
| 1.0 | 100 | 100 | 0 | 0.1 | 1 | 0.01 |



$$r_A = \frac{1.2 C_A C_C}{20 + C_A} \text{ mg/lit} \cdot \text{hr}$$

29.3 For mixed flow see Eq 8

| τ | v | V | τ | $k\tau$ | $C_A = \frac{C_M}{(k\tau - 1)} = \frac{2}{(k\tau - 1)}$ |
|--------|-----|-----|--------|---------|---|
| 6 | 1 | 1 | 1 | 1.2 | 10 |

Because $C_A > C_{A0}$... we have without impossible data

29.5 Our reaction is

$$r_C = \frac{1.2 C_A C_C}{2 + C_A}, \text{ with } (C/A) = 0.1$$

For optimum operations

$$N = \sqrt{1 + \frac{C_A}{C_M}} = \sqrt{1 + \frac{6}{2}} = 2$$

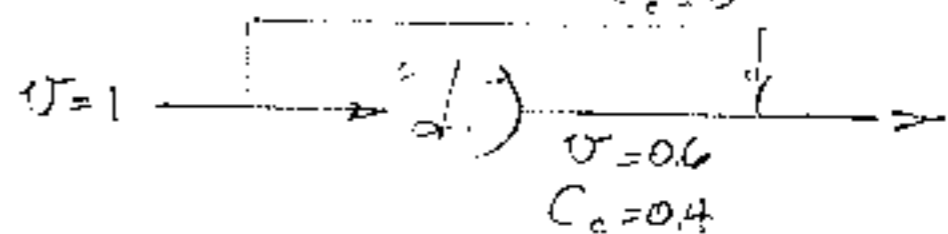
$$k\tau_{opt} = N/(N-1) = 2/1 = 2$$

$$\tau_{opt} = \frac{2}{1.2} = 1.67$$

Now for $V = 1 \text{ m}^3$ if all feed goes through the reactor

$$\tau = \frac{V}{v} = \frac{1}{v} = 1 < \tau_{opt} \text{ so bypass some feed}$$

$$\text{and } \tau_{opt} = \frac{V}{v_{opt}} = \frac{1}{1.67} = 0.6 \text{ so}$$



$$\therefore C_{C_{exit}} = 0.4 \times 0.6 + 0 = 0.24 \text{ gm/m}^3$$

29.7 We are given: $A \xrightarrow{c} F + C$, $r_c = \frac{k C_A C_c}{C_A + C_M} = \frac{2 C_A C_c}{C_A + 1}$ & $(c/A) = 0.5$
 for optimum operations with a single VFR ($C_{A0} = 3, C_{c0} = 0, v = \frac{1}{3}$)

$$N = \sqrt{1 + \frac{C_{A0}}{C_M}} = \sqrt{1 + \frac{3}{1}} = 2$$

$$k_1 \tau_{opt} = \frac{N}{N-1} = \frac{2}{1} = 2, \quad \therefore \tau_{opt} = 1$$

$$C_{Aopt} = \frac{C_{A0}}{N+1} = \frac{3}{2+1} = 1, \quad \therefore C_{copt} = (c/A)(C_{A0} - C_A) = 0.5(3-1) = 1$$

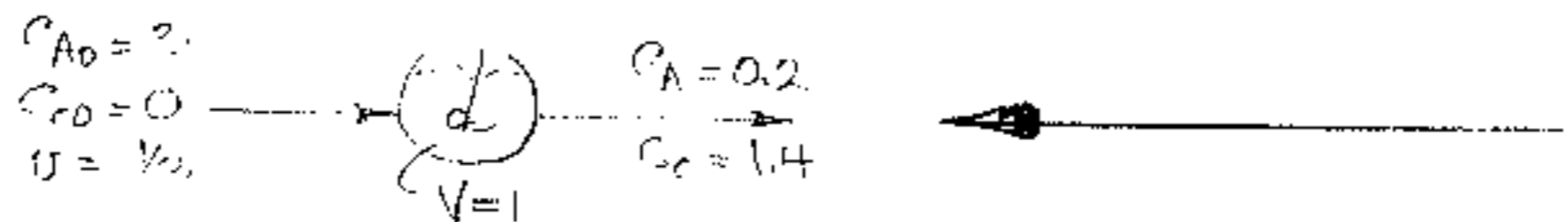
$$\tau_{washout} = \frac{N^2}{N^2 - 1} = \frac{4}{4-1} = \frac{4}{3}$$

Thus with $v = \frac{1}{3}, \tau = \frac{V}{v} = 3$... we are beyond the optimum τ

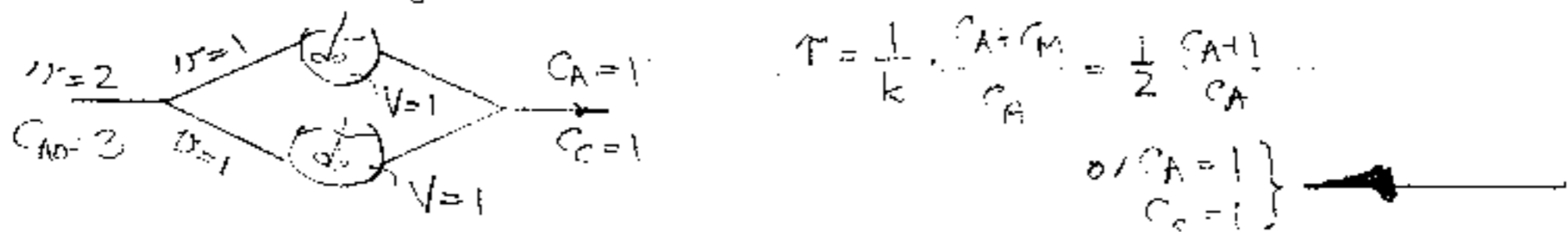
Hence $\tau_M = \frac{1}{k} \frac{C_M + C_A}{C_A} = \frac{1}{2} \frac{C_A + 1}{C_A} = 3 \dots$ or $C_{Aopt} = 0.2$

and $C_{copt} = (c/A)(C_{A0} - C_{Aopt}) = 0.5(3 - 0.2) = 1.4$

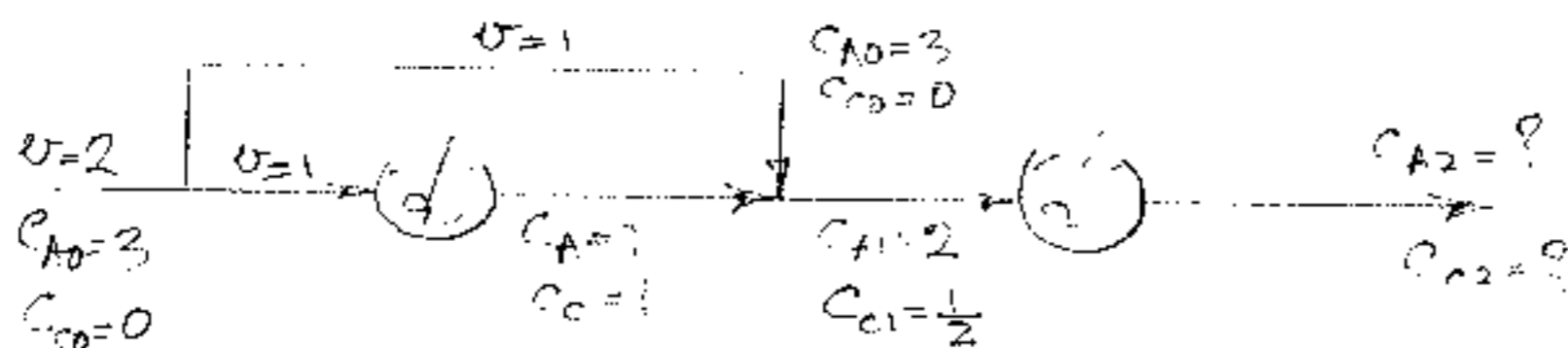
Thus



29.9 From the previous problems (see slides), we know that $\tau_{opt} = 1$
 So the best arrangement is



Alternative solution: (wonder whether the scheme below is equally good, or maybe better)



Let us check this

29.9
continued

For the second reactor, from Eq 12

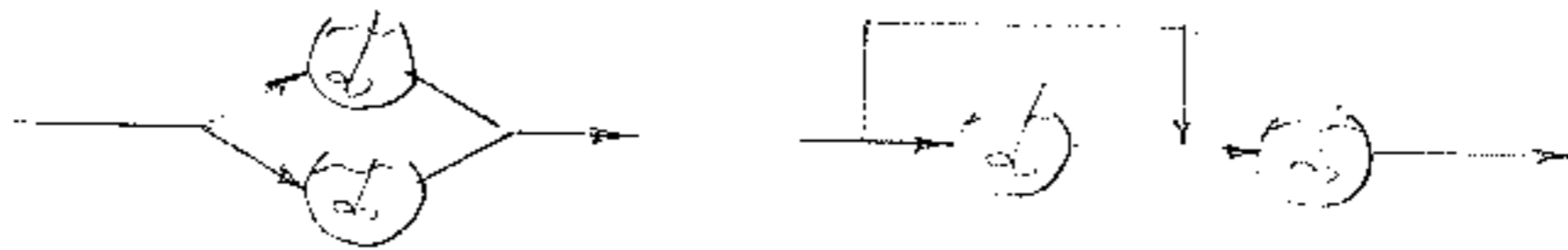
$$k\tau = \frac{(1-C_{A2})(C_{A2}+1)}{A \cdot C_{A2}} = \frac{1-C_{A2}}{(0.5)C_{A2} + (2-C_{A2})C_{A2}}$$

or $C_{A2} - C_{A2}^2 = 2 + C_{A2} - C_{A2}^2$

or $C_{A2} = 1$

$C_{A2} = \frac{1}{A} (C_{A1} - C_{A2}) + C_{A1} = 0.5 + 0.5 = 1$ comes as for the first arrangement

∴ both are equally good

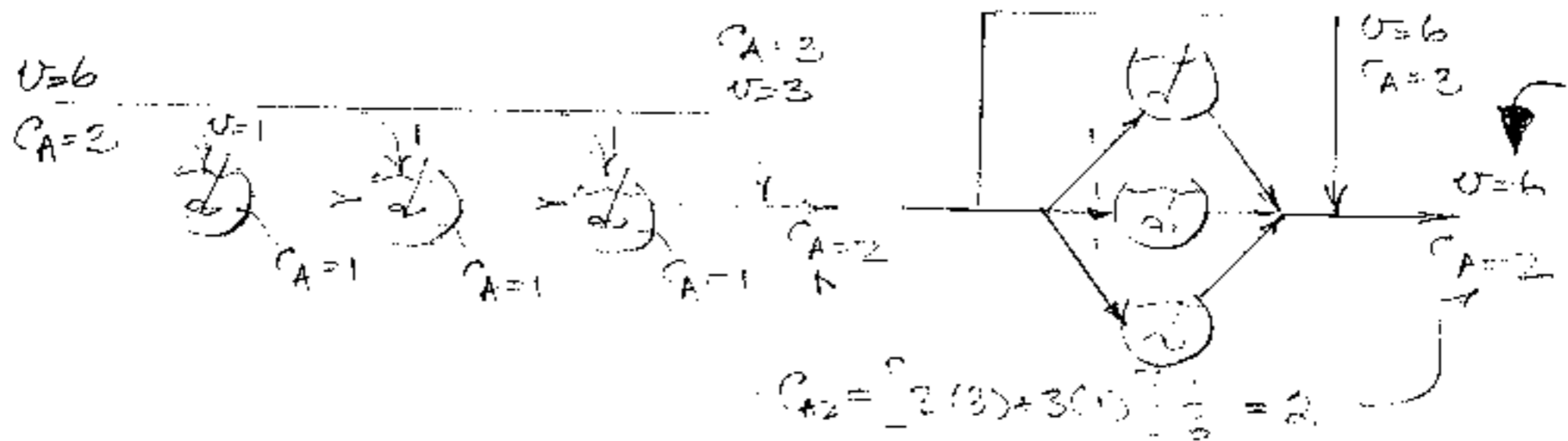


29.11

From the previous problems we have $\tau_{opt} = 1$ and $C_{Aopt} = 1$

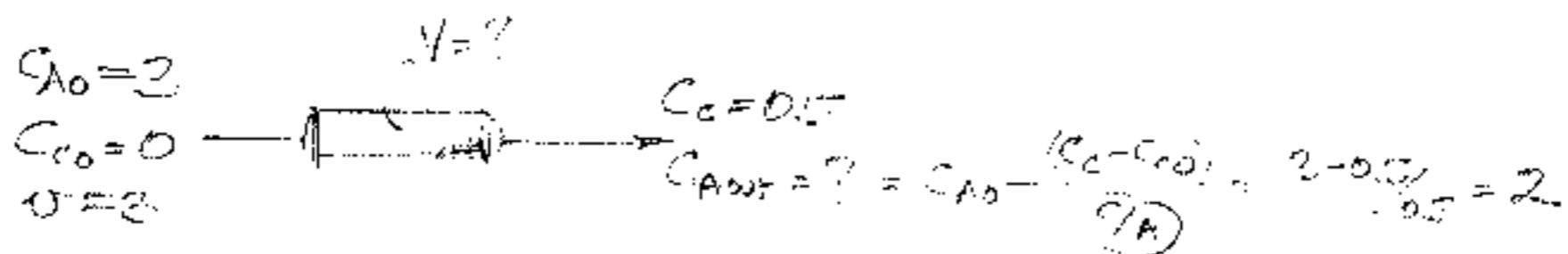
So for $U=6$

$V_{total} = 3$, we have the following good designs

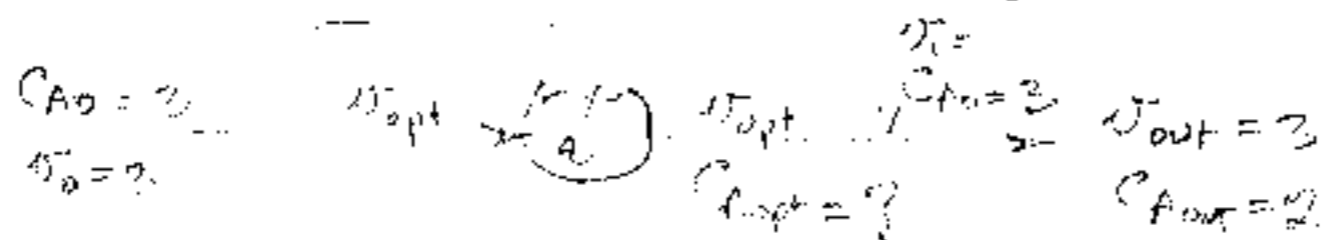


29.13

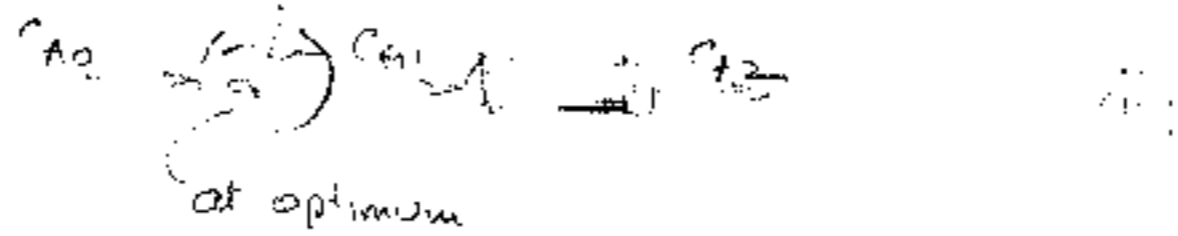
Here we have a PFR and we want the minimum volume



Now recall that if $C_{Aout} > C_{Aopt}$ use bypass with the reactor at C_{Aopt}



27.12 (continued) On the other hand if $C_{Aout} < C_{Aopt}$ then the best is to use



Here we want the design of (ii), not (i). So the size of the reactor should be such that

$$T_{opt} = 1 \quad \text{and} \quad C_{A2} = 1$$

Now evaluate the flows V_1 and V_{opt}

$$V_1 + V_{opt} = 2$$

$$V_1 C_{A0} + V_{opt} \times C_{Aopt} = C_{Aout} V_{out}$$

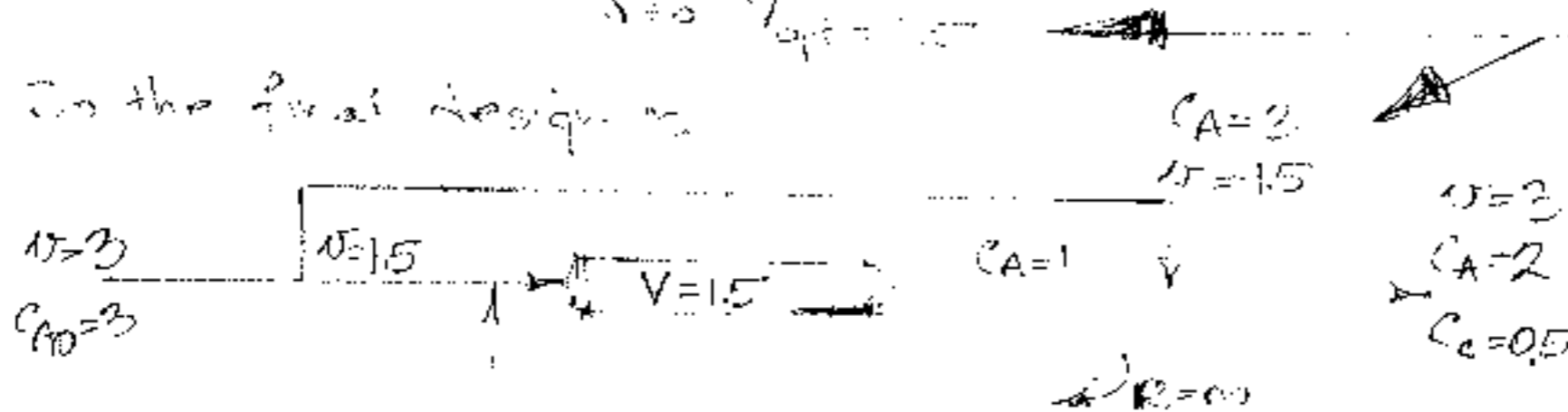
$$\therefore 1 \cdot 3 + (2 - V_1) \cdot 1 = 2 \cdot (3) \quad \text{-- solve}$$

$$\text{or } V_1 = 1.5$$

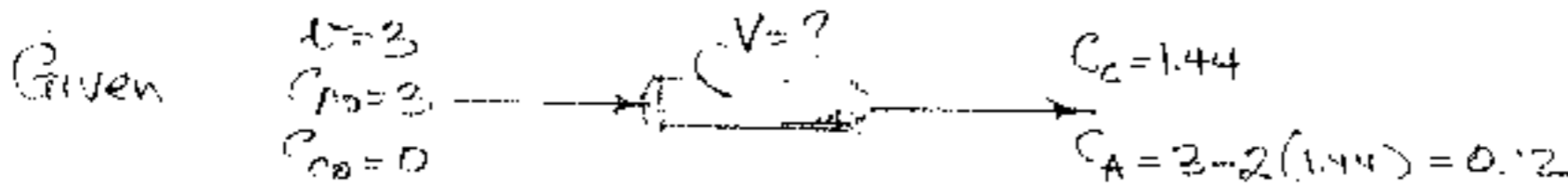
$$V_{opt} = 1.5$$

$$S = 0 \quad V_{opt} = 1.5$$

In the final design:



27.15



Find the optimum.

$$N = \frac{1}{1 + \frac{C_{A0}}{C_A}} = \frac{1}{1 + \frac{3}{1}} = \frac{1}{4} \quad \frac{C_c}{C_{cmax}} = \frac{N}{N+1} = \frac{1}{4+1} = \frac{1}{5} \quad \therefore C_{c,opt} = 1 \quad C_{A,opt} = 1$$

So use mixed flow up to $C_c = 1$ then use plug flow (so for mixed flow)

$$\tau_{RT} = \frac{C_{A0} - C_A}{C_A} = \frac{3-1}{1} = 2 \quad \text{or } V_m = \frac{2V}{k} = \frac{2 \times 3}{2} = 3$$

29.15
(continued)

For the rest of the reactor use plug flow

$$k\tau = \left(\frac{C_M}{(C_0 + k/c)C_0} + 1 \right) \ln \frac{C_0}{C_1} = \left(\frac{C_M}{(C_0 + k/c)C_0} + 1 \right) \ln \frac{C_0}{C_2}$$

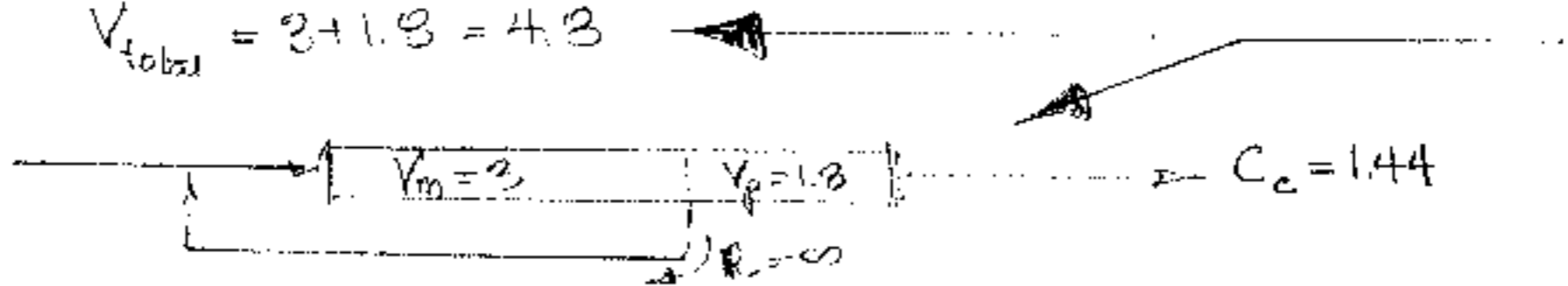
replacing values gives

$$\ln \left(\frac{C_1}{C_2} \right) = \left(\frac{1}{1+2 \times 1} + 1 \right) \ln \frac{1.44}{1} = \left(\frac{1}{1+2 \times 1} + 1 \right) \ln \frac{0.12}{1} = 1.1929$$

so

$$V_p = 2 \times \frac{1.1929}{2} = 1.3$$

$$\text{and } V_{\text{total}} = 2 + 1.3 = 4.3$$



29.17

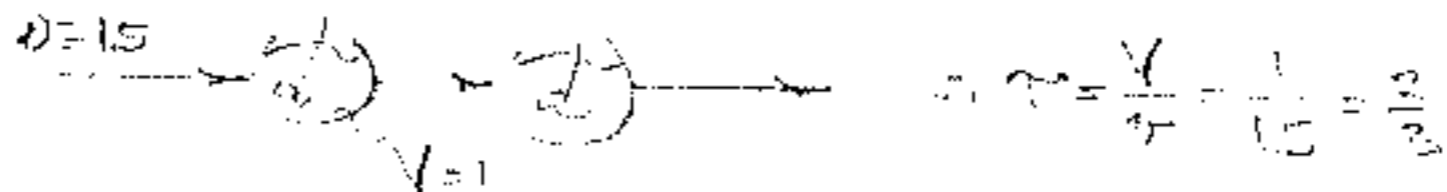
Reactor contacting patterns (a), (d), and (e) can never be optimum. I can always do better

Patterns (b), (c) and (f) could under certain conditions be optimum.

29.19

Calculate the conversion from the three flow sheets of Fig. 19.19

Pattern (a)



$$\text{Determine } M = \frac{C_M}{C_0} + 1 = \sqrt{\frac{3}{1}} + 1 = 2.2$$

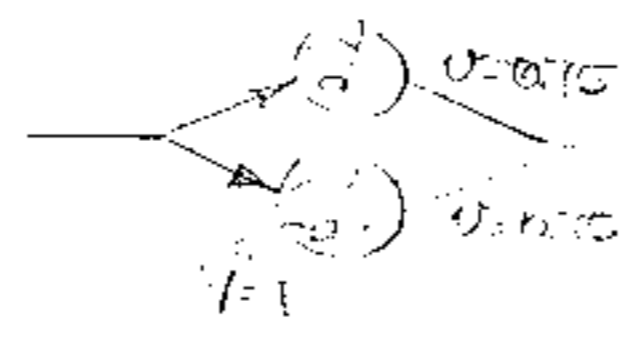
$$\text{then } k\tau_{\text{without}} = \frac{M^2}{M-1} = \frac{4}{1.2} = 4/3$$

$$\therefore \tau_{\text{without}} = \frac{4}{3} \times \frac{1}{1.5} = 1/3$$

But this is the τ value for this arrangement. So we have no outlet and no reaction with pattern (a)

2.19
(continued)

Pattern (b)



$\tau = 1.5 \rightarrow C_{Aout} = \frac{1}{3} = 0.333$

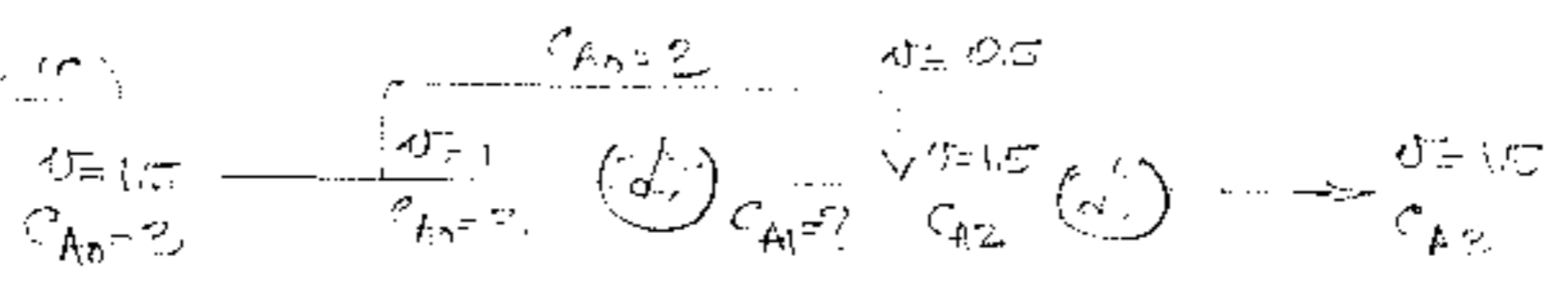
For each mixed flow unit

$$C_{Aout} = \frac{C_M}{k\tau + 1} = \frac{1}{2(\frac{1}{2}) + 1} = 0.6 \rightarrow \text{pretty good}$$

this is not bad

Let us try the third pattern

Pattern (c)



For reactor 1 (at the optimum) $\tau = 1$

By material balance

$$C_A = \frac{C_M}{k\tau + 1} = \frac{1}{2(1) + 1} = 1 \Rightarrow C_{A2} = \frac{2(0.5) + 1(1)}{1.5} = \frac{2}{3}$$

$$\Rightarrow C_{A1} = 2 \quad C_{A2} = \frac{2(1) + 0}{1.5} = \frac{4}{3}$$

For reactor 2 (not at optimum) $\tau = \frac{V}{v} = \frac{2}{3}$

Then from Eq 12,

$$k\tau = \frac{(C_{A2} - C_{A1})(C_{A2} + C_{A1})}{C_{A1} C_{A2} + C_{A2} (C_{A2} - C_{A1})}$$

$$2 \cdot \frac{2}{3} = \frac{(5/3 - C_A)(5/3 + 1)}{4/2 C_A + C_A(5/3 - C_A)}$$

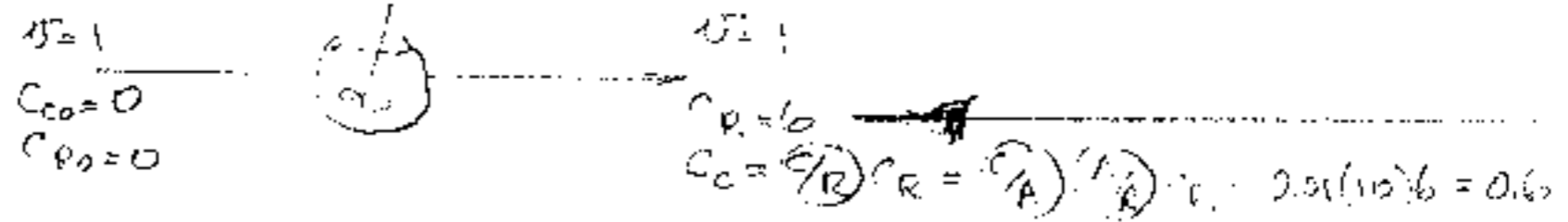
$$12 C_A - 4 C_A^2 = -3 C_A^2 + 2 C_A + 5$$

or $C_{Aout} = 5 - \sqrt{20} = 0.528 \rightarrow \text{this is best}$

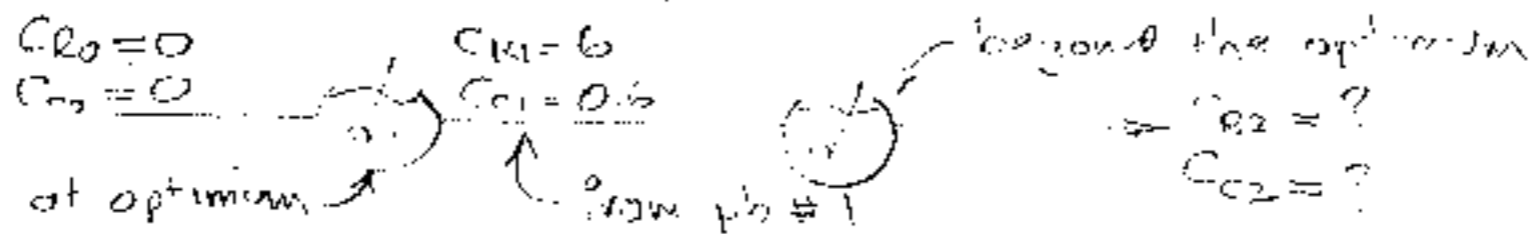
30.1 For a MFR, $n=1$, the best way to run the reactor is at $k\tau = 2$ where $C_{Ropt} = C_R^* / 2 = 1/2 = 0.5$... see after Eq 11.

In our system

$k\tau = k \frac{V}{v} = 2 \left(\frac{1}{1} \right) = 2$ which is optimum. So use the reactor, no recycle, no bypass



30.3 For each tank $k\tau = 2$, so put them in series



For the second reactor, from Eq 9

$$2 = k\tau = \frac{C_{R2} - C_{R1}}{1 - \frac{C_{R2}}{C_R^*} (C_{R2} - C_{R1} + \frac{v}{C} C_{C1})} = \frac{C_{R2} - 0.5}{1 - \frac{C_{R2}}{0.5} (C_{R2} - 0.5 + 0.01 C_{C1})}$$

$$\therefore C_{R2} = 0.97 \quad C_{C2} = \left(\frac{v}{A}\right) \left(\frac{v}{A}\right) C_{R2} = (0.01/0.1) 0.97 = 0.097$$

30.5 From the above problems $C_R = 0.5$ represents the optimum

Therefore $k\tau_{opt} = 2$

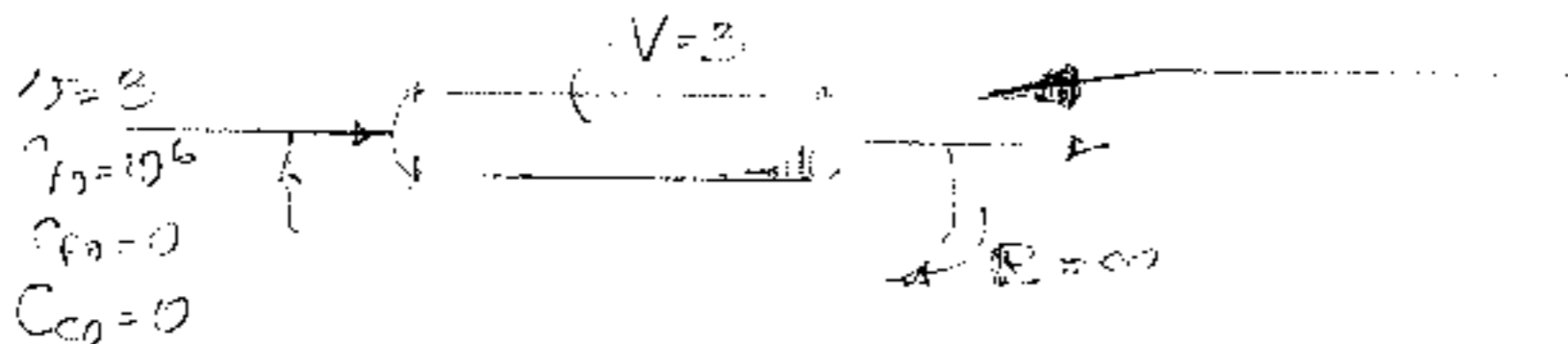
or $\tau_{opt} = 1 = \frac{V}{v}$

Since $v=3$ (given) we want

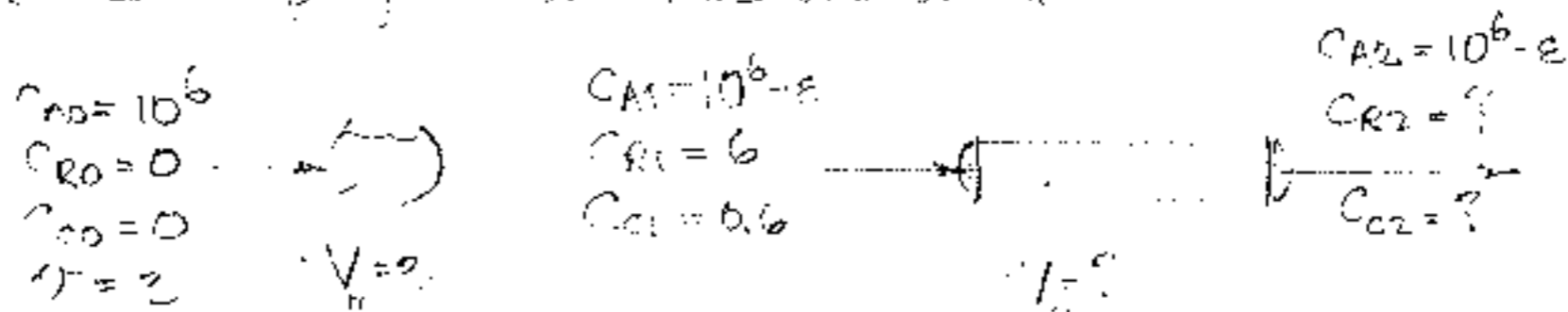
$V=3$, and fixed flow

Hint: but then you get series flow

Thus



30.8 The optimum is where $C_R = C_R^* = 0$, and $k\tau = 2$.
 But with $k=2$ this means that $\tau = 1$ hr. So for $\tau = 2$ our mixed flow reactor should have a volume $V_m = 2V_p$, the rest should be plug flow. Thus we want



From earlier problems the composition after the mixed flow reactor are as shown above.

For the plug flow reactor, Eq 5 gives

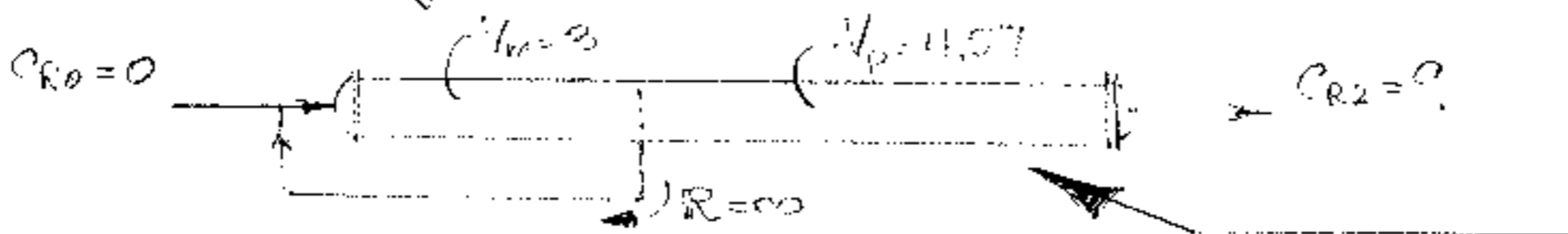
$$k\tau_p = k \frac{V_p}{F} = \frac{C_R^*}{(C_R^* - C_{R1} + R_1^2) C_{C1}} \int_{C_{C1}}^{C_{C2}} \frac{(C_{C1} + C_1)(C_{R2} - C_{R1})}{C_{C1}(C_R^* - C_{R2})} (C_R^* - C_{R1})$$

With $R_1/C_1 = R_2/C_2 = 0.1/0.01 = 10$, replacing all values in the above gives

$$2 \frac{V_p}{F} = \frac{12}{12 - 6 + 10(0.6)} \int_{0.6}^{12} \frac{(6 + 0.1(12 - 6))(12 - 6)}{0.6(12 - 9)}$$

$$V_p = \frac{F}{0.6} \ln \frac{6.2(6)}{2.6(2)} = 4.57$$

So the final design is



30.9 At the optimum $k\tau = \left(\frac{n+1}{n}\right)^n = \left(\frac{0.5+1}{0.5}\right)^{0.5} = 1.73$.

But $k = \sqrt{3}$, $\therefore \tau_{m,opt} = \frac{1.73}{\sqrt{3}} = 1$...

Or $v = \tau V = 1 \times 30 = 30 \text{ m}^3/\text{hr}$.

$$\therefore C_{Rmax} = \frac{C_R^*}{n+1} = \frac{0.12}{0.5+1} = 0.08 \frac{\text{kg alc}}{\text{kg sol}^n} \times \frac{1000 \text{ kg}}{\text{m}^3} \quad \therefore \text{production rate is } 80 \times 30 = 2400 \frac{\text{kg alc}}{\text{hr}}$$

20.11 Try first order poisoning and see if this fits the facts. So from Eq 10 we have

$$\text{for run \#1 } k\tau_1 = \frac{90}{90-54}$$

$$\text{for run \#2 } k\tau_2 = \frac{90}{90-75}$$

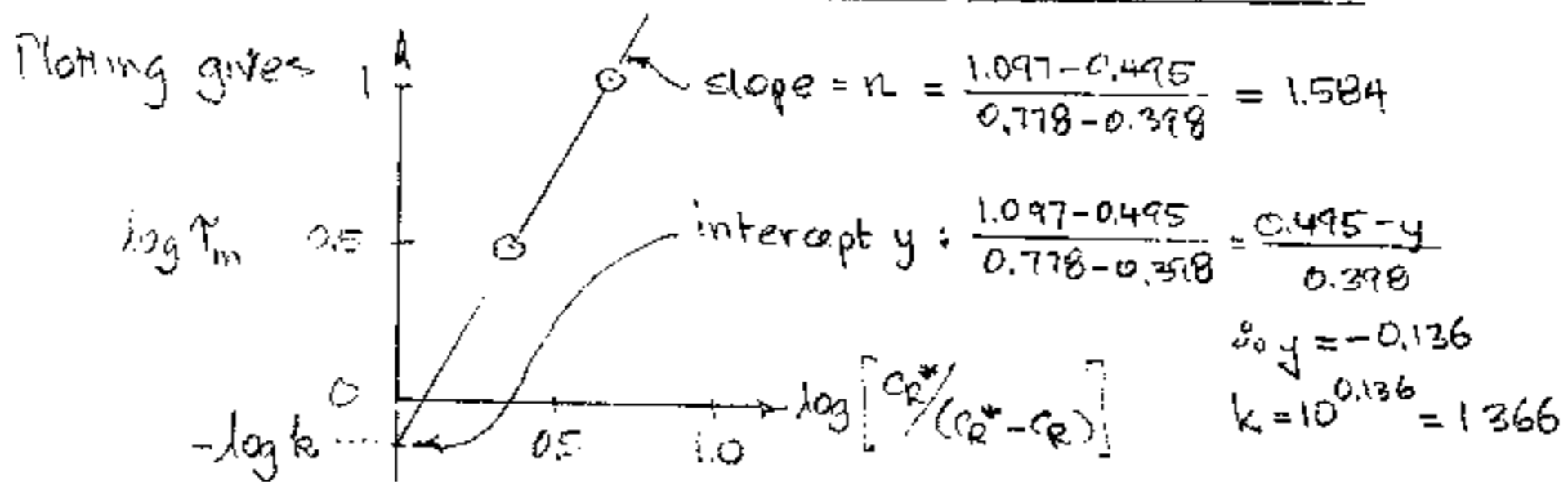
Taking ratios

$$\frac{\tau_1}{\tau_2} = \frac{15}{36} = 0.4167 \quad \dots \text{ if poisoning follows } n=1 \text{ kinetics}$$

But actually $\frac{\tau_1}{\tau_2} = \frac{3.125}{12.5} = 0.25$ these are too different so we have to try $n \neq 1$.

For n^{th} order poisoning test with the plot of Eq 15. First tabulate

| $\tau_m = V/v$ | C_R | $\log \tau_m$ | $C_R^*/(C_R^* - C_R)$ | $\log(C_R^*/(C_R^* - C_R))$ |
|----------------|-------|---------------|-----------------------|-----------------------------|
| 3.125 | 54 | 0.495 | 2.5 | 0.398 |
| 12.5 | 75 | 1.097 | 6 | 0.778 |



Thus the rate equation is

$$r_R = 1.366 \left(1 - \frac{C_R}{90}\right)^{1.584} C_R$$

Now to the optimum

$$v_{\text{opt}} = kV \left(\frac{n}{n+1}\right)^n = 1.366(50) \left(\frac{1.584}{2.584}\right)^{1.584} = 31.46 \text{ books/hr}$$

Maximum production rate

$$F_{R \text{ max}} = (C_R v)_{\text{opt}} = \frac{kV C_R^* n^n}{(n+1)^{n+1}} = \frac{1.366(50)90(1.584)^{1.584}}{(2.584)^{2.584}} = 1095 \mu\text{m/hr}$$