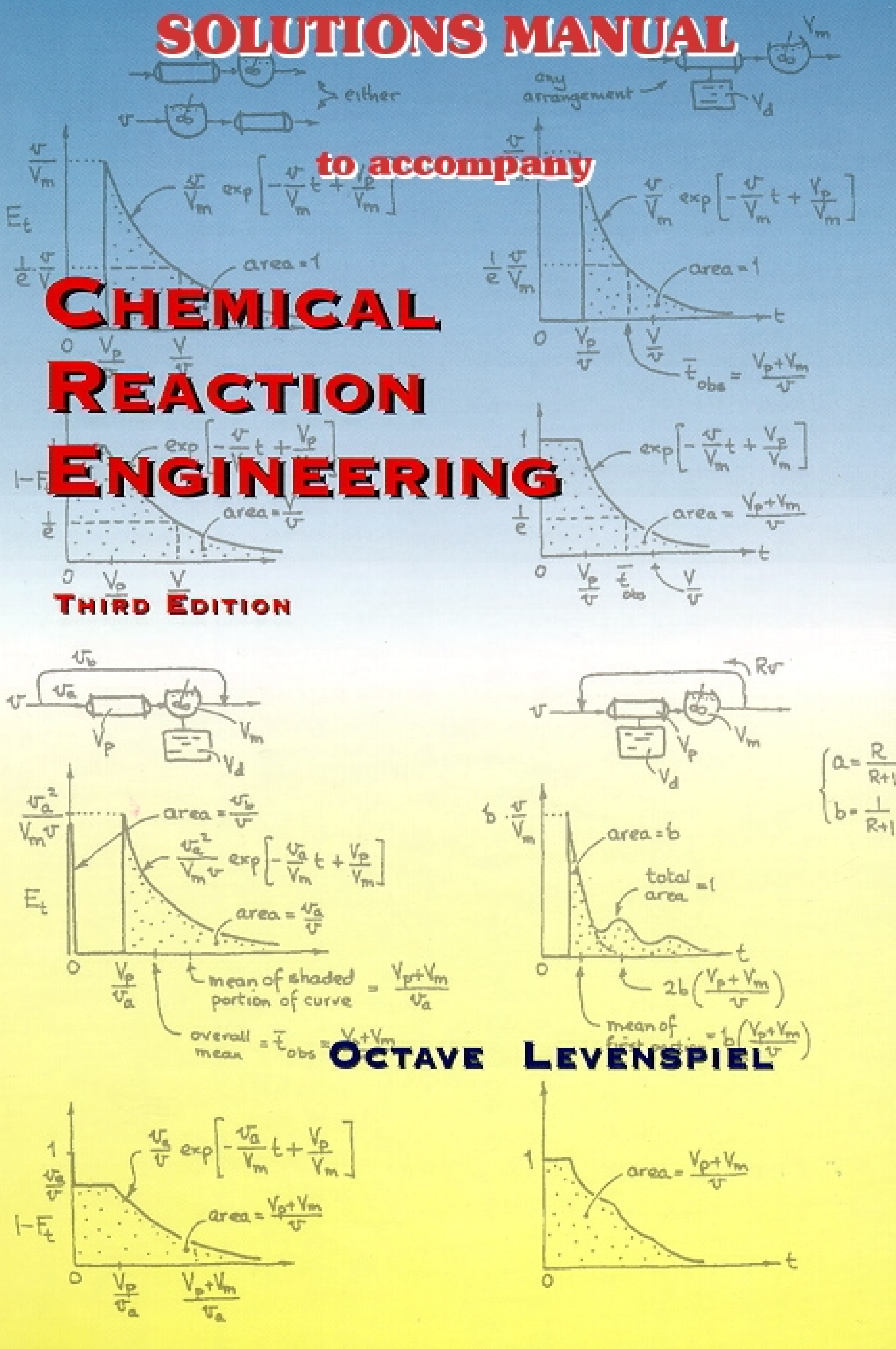
SOLUTIONS MANUAL

to accompany

CHEMICAL REACTION ENGINEERING

THIRD EDITION

OCTAVE LEVENSPIEL



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CHEMICAL REACTION ENGINEERING

THIRD EDITION

Includes Solutions to All 228 Odd-Numbered Problems

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JOHN WILEY & SONS, INC.
NEW YORK • CHICHESTER • WEINHEIM • BRISBANE • SINGAPORE • TORONTO

ISBN 0-471-31478-1

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

Printed and bound by Odyssey Press, Inc.

CONTENTS

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

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

or

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

O_2 used

$$\left(200\,\frac{\text{mg}}{\text{lit}}\right)\left(\frac{1\,\text{gm}}{1000\,\text{mg}}\right)\left(\frac{\text{mol}}{32\,\text{gm}}\right)\left(\frac{1000\,\text{lit}}{\text{m}^3}\right)\left(\frac{32000\,\text{m}^3}{\text{day}}\right) = 2\times10^5\,\frac{\text{mol } O_2}{\text{day}}$$

Thus the rate of reaction

$$\frac{2.0\times10^5\,\text{mol } O_2/\text{day}}{10667\,\text{m}^3} \left.\begin{aligned} &= 18.75\ \text{mol/m}^3\cdot\text{day} \\ &= 2.17\times10^{-4}\,\text{mol/m}^3\cdot\text{s} \end{aligned}\right\} \longleftarrow$$

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

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

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

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

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

So

$$-\frac{dN_{C_{20}H_{42}}}{dt} = \left(\frac{5\,400\,000\,\text{kg/day}}{0.282\,\text{kg/day}}\right)\left(\frac{\text{day}}{24(3600)\text{s}}\right)(0.6) = 133\ \text{mol reacted/s}$$

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

$$\left.\begin{aligned} -r' &= \frac{1}{W_{cat}}\frac{dN}{dt} = \frac{1}{50000}(133) = 0.0027\ \text{mol/kg cat}\cdot\text{s} \\ -r''' &= \frac{1}{V_{cat}}\frac{dN}{dt} = \frac{1}{62.5}(133) = 2.13\ \text{mol/m}^3\text{cat}\cdot\text{s} \end{aligned}\right\} \longleftarrow$$

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 <u>write</u> the stoichiometry affect the rate of reaction? The rate expression remains unchanged.

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

2.7 a) We are given $$-\underset{\text{atm/hr}}{\frac{dp_A}{dt}} = \underset{3.66}{k_p}\,\underset{(\text{atm})^2}{p_A^2}$$

Balancing dimensions we find $k_p = 3.66\,(\text{atm})^{-1}(\text{hr})^{-1}$ ⟵ a)

b) For an ideal gas $p_AV = n_ART$ or $p_A = C_ART$

Thus $-\frac{dp_A}{dt} = 3.66\,p_A^2$ … becomes … $-\frac{d(C_ART)}{dt} = 3.66\,(C_ART)^2$

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

b)

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

2.9 From Eq. 35 we write

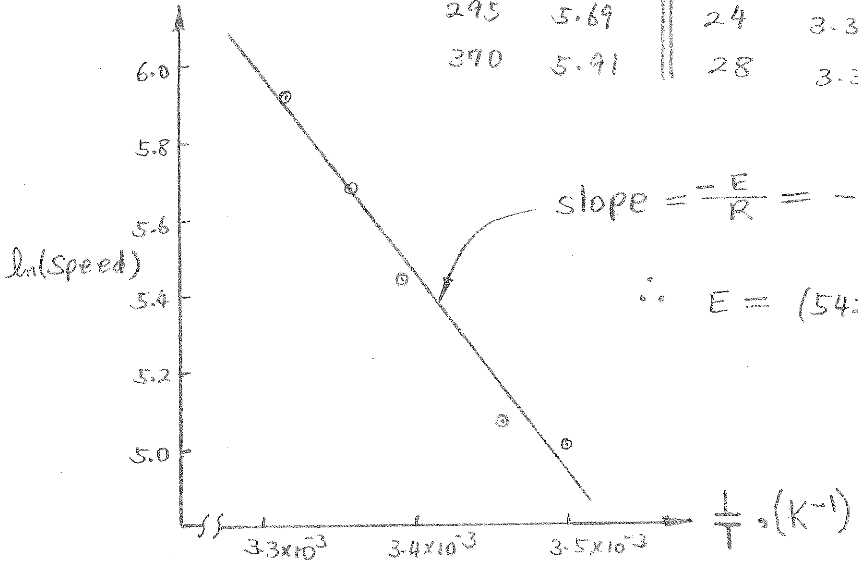
$$\frac{k_{650}}{k_{500}} = e^{-\frac{E}{R}\left(\frac{1}{T_{650}} - \frac{1}{T_{500}}\right)}$$

$$= e^{-\frac{300\,000}{8.314}\left(\frac{1}{923} - \frac{1}{773}\right)}$$

$$= 1971$$ ⟵

2.11

Speed	lnS	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



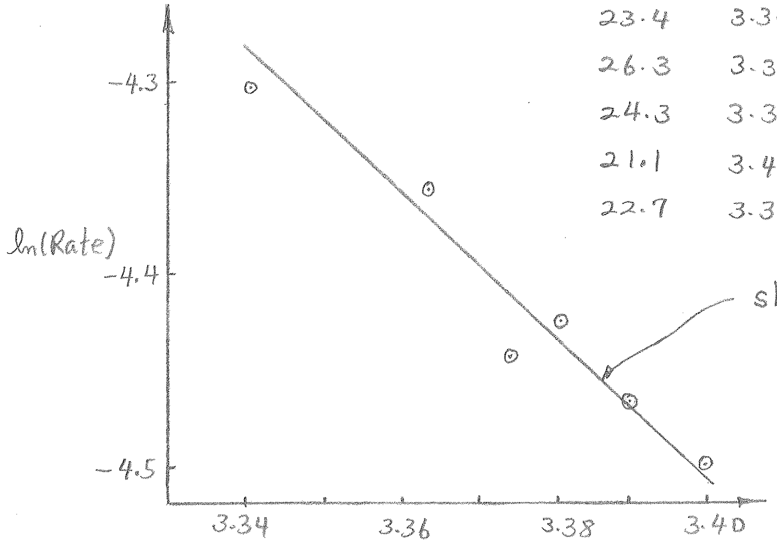
slope $= -\frac{E}{R} = -5420$

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

$\cong \underline{45\ kJ}$

2.13

T	$\frac{1}{T}\times10^{-3}$	Days	$\ln(Rate) = \ln(\frac{1}{days})$
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



slope $= -\frac{E}{R} = -3392$

$E = (3392)(8.314)$

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

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

2.15 $-r_A = kC_A^n$ $\therefore$ $\frac{-r_2}{\underset{\nwarrow 3}{-r_1}} = \frac{k(2C_A)^n}{kC_A^n} = 2^n$ $\therefore n = 1.585$ ←

2.17 Guess that $-r_A = kC_A^a C_B^b$

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

$$50 = k(2)^a(125)^b \quad \text{---(i)}$$
$$32 = k(2)^a(64)^b \quad \text{---(ii)}$$
$$48 = k(3)^a(64)^b \quad \text{---(iii)}$$

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

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

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

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

2.19 a) Consider the mechanism

$$\left.\begin{array}{l} 2A \underset{2}{\overset{1}{\rightleftharpoons}} A + A^* \\ A^* \xrightarrow{3} R + S \end{array}\right\} \dots$$

and let us find its rate expression.

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

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

from which $[A^*] = k_1[A]^2 / k_2[A] + k_3$ ----(ii)

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

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

And when $k_2[A] \gg k_3$

$$-r_A = \frac{k_1 k_3}{k_2}[A]$$

.... or first order rx ← 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

$$-r_A = k_1[A]^2$$

... or 2nd 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. ← b)

2.21 Hypothesize:

$$\left.\begin{array}{l} H_3PO_2 + H^+ \underset{k_2}{\overset{k_1}{\rightleftharpoons}} X^* + H^+ \\ X^* + O_x \underset{k_4}{\overset{k_3}{\rightleftharpoons}} H_3PO_3 \end{array}\right\} \text{... where } X^* \text{ is an unstable intermediate}$$

Then as in the example, pg 19, we write

$$r_{H_3PO_3} = k_3[X^*][O_x] - k_4[H_3PO_3] \quad \text{-------- (i)}$$

steady state assumption

$$r_{X^*} = k_1[H_3PO_2][H^+] - k_2[X^*][H^+] - k_3[X^*][O_x] + k_4[H_3PO_3] = 0$$

Thus

$$[X^*] = \frac{k_1[H_3PO_2][H^+] + k_4[H_3PO_3]}{k_2[H^+] + k_3[O_x]} \quad \text{------ (ii)}$$

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

$$r_{H_3PO_3} = \frac{k_1 k_3 [H_3PO_2][H^+][O_x]}{k_2[H^+] + k_3[O_x]} \quad \text{---------- (iii)}$$

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

$$r_{H_3PO_3} = k_1[H_3PO_2][H^+] \quad \text{------------ (iv)}$$

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

$$r_{H_3PO_3} = \frac{k_1 k_3}{k_2}[H_3PO_2][O_x] \quad \text{------------ (v)}$$

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

2.23

$$\left.\begin{array}{ll} A + E \underset{2}{\overset{1}{\rightleftharpoons}} X & \text{... ①} \\ X \longrightarrow R + E & \text{... ②} \\ \text{with} \quad E_0 = E + X & \text{... ③} \end{array}\right\}$$

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

$$K = \frac{X}{AE} = \frac{k_1}{k_2} \quad \text{... ④}$$

B-H assume that quickly

$$dX/dt = 0 \quad \text{.. ⑤}$$

2.23
(continued)

For M·M

From ②

$$r_R = k_3 X \quad \cdots\cdots \textcircled{6}$$

From ⑤

$$X = \frac{k_1}{k_2} A E$$

Eliminate E with ③

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

or

$$X = \frac{\frac{k_1}{k_2} A E_0}{1 + \frac{k_1}{k_2} A} \quad \cdots\cdots \textcircled{7}$$

Eq ⑦ in ⑥ gives

$$r_R = \frac{k_3 A E_0}{\frac{k_2}{k_1} + A}$$

For B-H

From ②

$$r_R = k_3 X \quad \cdots\cdots \textcircled{8}$$

From ⑤

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

Eliminate E with ③

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

or

$$X = \frac{k_1 A E_0}{k_1 A + k_2 + k_3} \quad \cdots\cdots \textcircled{9}$$

Eq ⑨ in ⑧ gives

$$r_R = \frac{k_3 A E_0}{\frac{k_2 + k_3}{k_1} + A}$$

These equations give essentially the same result

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

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

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

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

We also can find the rate constant. Thus replacing values

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

Hence the rate of disappearance of monomer is given by

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

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

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

Now at $t=0 \cdots \$_0 = 180$
$t = 2\text{ hrs} \cdots \$ = 135$ } 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 (Continued) After his raise we have $\left.\begin{matrix} t=0 \cdots \$_0 = ? \\ t = 3\text{ hrs} \quad \$ = 135 \end{matrix}\right\}$ ... from this find $\$_0$

For unchanged betting habits

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

Hence his raise is 208 − 180 ... or \$28

3.9 For a first order reversible reaction

$$A \underset{k_2}{\overset{k_1}{\rightleftarrows}} R \begin{cases} C_{A0} = 0.5 \text{ mol/lit} \\ C_{R0} = 0 \end{cases} \quad \cdots \quad X_{Ae} = 0.667$$

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

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

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 $\begin{cases} k_2 = \dfrac{0.086625}{3} = 0.028875 \\ k_1 = 0.057750 \end{cases}$

Thus the rate expression for the disappearance of A.

$$\underset{\text{mol/lit}\cdot\text{min}}{-r_A} = \underset{\text{min}^{-1}}{0.05775}\ \underset{\text{mol/lit}}{C_A} - \underset{\text{min}^{-1}}{0.028875}\ \underset{\text{mol/lit}}{C_R} \longleftarrow$$

3.11 From the table of data

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

Thus

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

$$C_A = 200\,\frac{\text{mol}}{\text{m}^3} \quad \cdots \text{ or } \quad X_A = 0.6 \longleftarrow$$

3.13

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

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

Playing A & B simultaneously $-\frac{d\$}{dt} = -\left(\frac{d\$}{dt}\right)_A - \left(\frac{d\$}{dt}\right)_B = (k_A + k_B)\$$ .... (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 $\ln \frac{\$_0}{\$} = k_A t$ ... or ... $k_A = \frac{1}{t} \ln \frac{\$_0}{\$}$

and with the data given. $k_A = \frac{1}{4} \ln 2$ .... (iv)

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

Integrating (iii) gives $\ln \frac{\$_0}{\$} = (k_A + k_B) t$ ... or ... $t = \frac{1}{k_A + k_B} \ln \frac{\$_0}{\$}$

and with (iv) & (v)

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

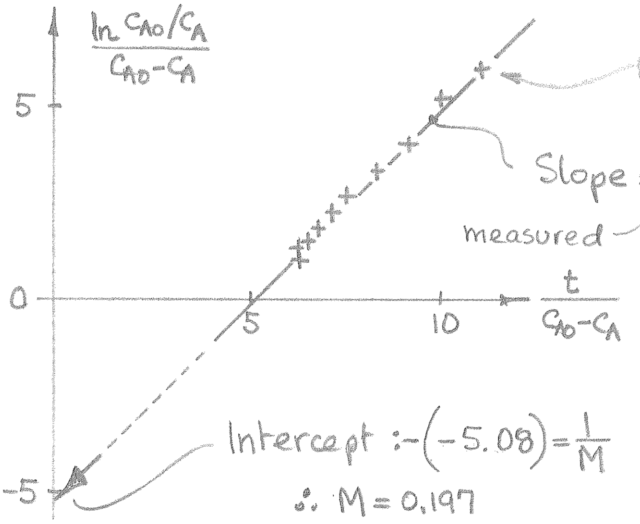
Note: This is simply a case of two "1st order reactions" in parallel, see pg. 49.

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

$$-r_A = \frac{k_3 C_{E0} C_A}{C_A + M} = \underset{\nwarrow \text{ use this form}}{\frac{k_4 C_A}{1 + k_5 C_A}} \quad \cdots \text{where} \begin{cases} k_4 = \dfrac{k_3 C_{E0}}{M} \\ k_5 = \dfrac{1}{M} \end{cases} \quad \cdots\cdots\cdots (i)$$

Integral method Integrating (i) gives

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



Plot the data from the table on the next page

$\text{Slope} = 1 = \frac{k_3(0.01)}{(0.197)}$, or $k_3 = 19.7$

measured

from below

$\text{Intercept}: -(-5.08) = \frac{1}{M}$

$\therefore M = 0.197$

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

$$\left.\begin{aligned} k_3 &= 19.7 \text{ hr}^{-1} \\ M &= 0.197 \frac{\text{millimol}}{\text{lit}} \end{aligned}\right\} \text{thus} \quad r_A = \frac{19.7\, C_A C_{E0}}{0.197 + C_A} \longleftarrow$$

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

$$k = \frac{0.6931}{t_{1/2}} = \frac{0.6931}{76\,\text{min}} = 9.12\times10^{-3}\,\text{min}$$

After one day

$$\frac{C_A}{C_{A0}} = e^{-kt} = e^{-(9.12\times10^{-3})(24\times60)} = 1.98\times10^{-6} \longleftarrow$$

Thus the radioactivity drops to 2×10^{-6} of the original value.

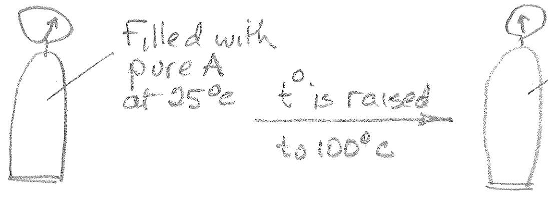
3.19 The time for complete conversion of an n^{th} order reaction from Eq. 29, is

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

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

3.21

Given



$\pi = 1\,\text{atm}\left(\frac{373}{298}\right) = 1.252\,\text{atm}$

$2A \rightarrow B$

Tabulate

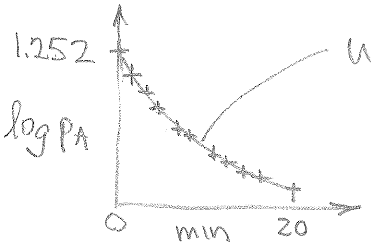
① time (min)	② π (atm)	③ p_A (atm)	④ $1/p_A$ (atm^{-1})
0	(1.252)	(1.252)	(0.800)
1	1.14	1.028	0.975
2	1.04	0.828	1.208
3	0.982	0.712	1.404
4	0.940	0.628	1.592
5	0.905	0.558	1.792
6	0.870	0.488	2.049
7	0.850	0.448	2.232
8	0.832	0.412	2.427
9	0.815	0.378	2.646
10	0.800	0.348	2.873
15	0.754	0.256	3.90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

given — calc'd.

Column ③ is obtained from Eq 5, or

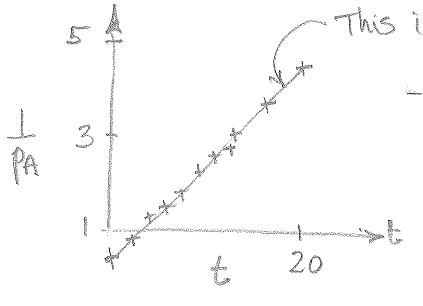
$$p_A = p_{A0} - \frac{a}{\Delta n}(\pi - \pi_0) = 1.252 - \frac{2}{(-1)}(\pi - 1.252) = 2p_A - 1.252$$

Try first order kinetics. For this plot as shown



We do not get a straight line so the reaction is not first order

Try second order kinetics. For this plot as shown



This is a good fit so find the slope

$$-\frac{dC_A}{dt} = k_c C_A^2 \quad \text{or} \quad \frac{dp_A}{dt} = \frac{k_c}{RT}p_A^2 \quad \cdots \quad \text{or} \quad \frac{1}{p} = \left(\frac{k_c}{RT}\right)t + \frac{1}{p_0}$$

$$\text{slope} = \frac{k_c}{RT} = \frac{4.92 - 0.8}{20} = 0.206\ \text{atm}^{-1}\,\text{min}^{-1}$$

or $k_c = 6.3$ lit/mol min

$$\therefore -r_A = \underset{\text{lit/mol·min}}{6.3}\, C_A^2 \ \text{mol/lit·min}$$

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

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

Replacing values give

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

Replacing in Eq 33a gives

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

or

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

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

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

(a) We could first transform all pressure readings into concentrations and then solve, or

(b) 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=∞ there is still some unreacted p_A. So the rate equation we will test is

$$A \underset{2}{\overset{1}{\rightleftarrows}} R, \quad \frac{dC_A}{dt} = k_1C_A - k_2C_R \quad \text{----} (53)$$

On integration we get

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

3.25
(continued)

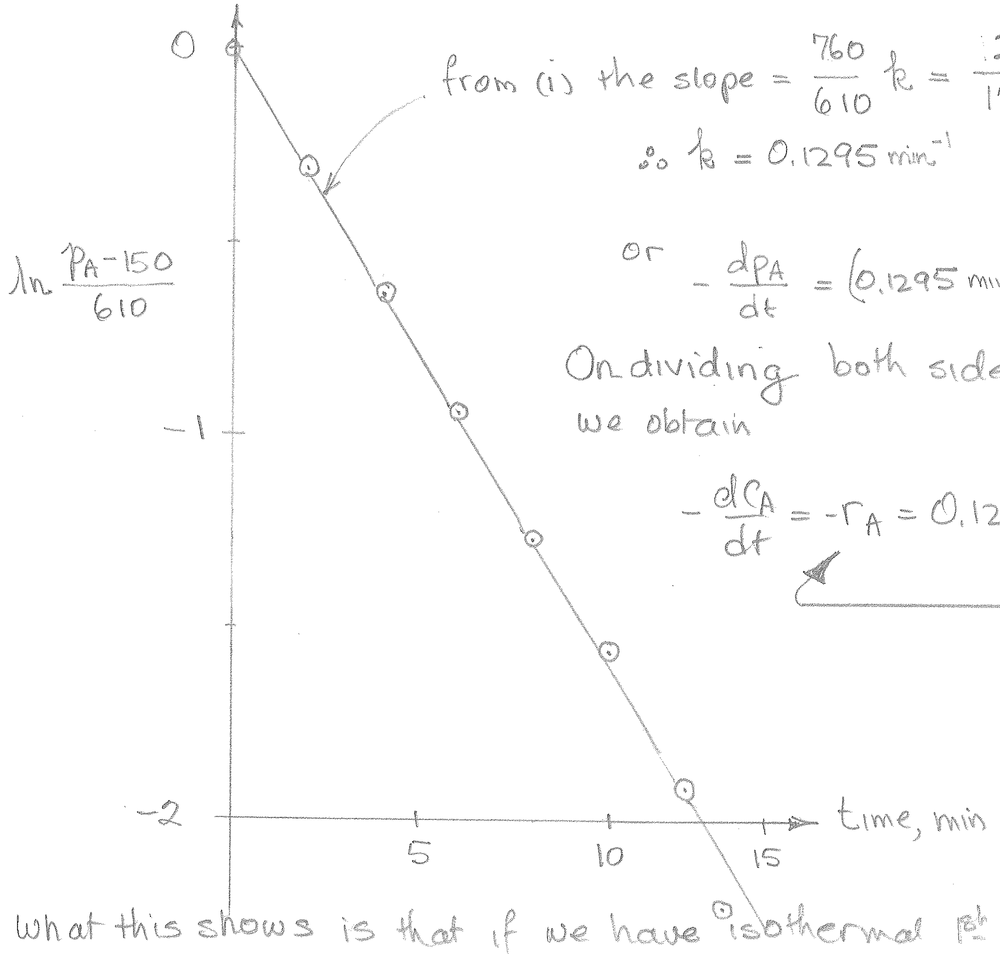
In pressure units this integrated expression becomes

$$\ln \frac{p_A - p_{Ae}}{p_{A0} - p_{Ae}} = \frac{k_1 t}{(p_{A0} - p_{Ae})/p_{A0}} \quad \cdots (i)$$

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	-1.9136
14	215	65/610	-2.2391
∞	150	0	-∞

<u>Note</u>: For 1st order rxs k_c and k_p have the same value, time^{-1}



from (i) the slope $= \frac{760}{610} k = \frac{2}{12.4}$

$\therefore k = 0.1295 \text{ min}^{-1}$

or $-\frac{dp_A}{dt} = (0.1295 \text{ min}^{-1})\, p_A$

On dividing both sides by RT we obtain

$$-\frac{dC_A}{dt} = -r_A = 0.1295\, C_A, \ \frac{\text{mol}}{\text{lit.min}}$$

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

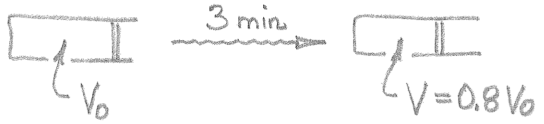
3.27 Since we are told that the reaction is elementary the stoichiometric equation shows that the reaction is 2nd order. So ~~for~~ a small relative concentration change we can write

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

or $$k = -\frac{\Delta C_A}{\Delta t}\,\frac{1}{\bar{C}_A^{2}} = \frac{-0.2\ \text{mol/lit}}{7\frac{2}{3}\ \text{hr}}\cdot\frac{1}{(19.9\ \text{mol/lit})^{2}} = 6.6\times10^{-5}\ \text{lit/mol}\cdot\text{hr}$$

$$\therefore\ -r_{NH_2\text{-}CO\text{-}NH_2} = (6.6\times10^{-5})\,C^{2}_{NH_2\text{-}CO\text{-}NH_2}\ ,\ \frac{\text{mol}}{\text{lit}\cdot\text{hr}} \longleftarrow$$

3.29



	2A →	B
Amount of A or B :	0.8	0.4
Amount of inert :	0.2	0.2
Total :	1.0	0.6

$\therefore\ \varepsilon_A = -0.4$

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

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

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

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

$$-r_A = kC_A^{2} = k_0 e^{-E/RT}\,C_A^{2}$$

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

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

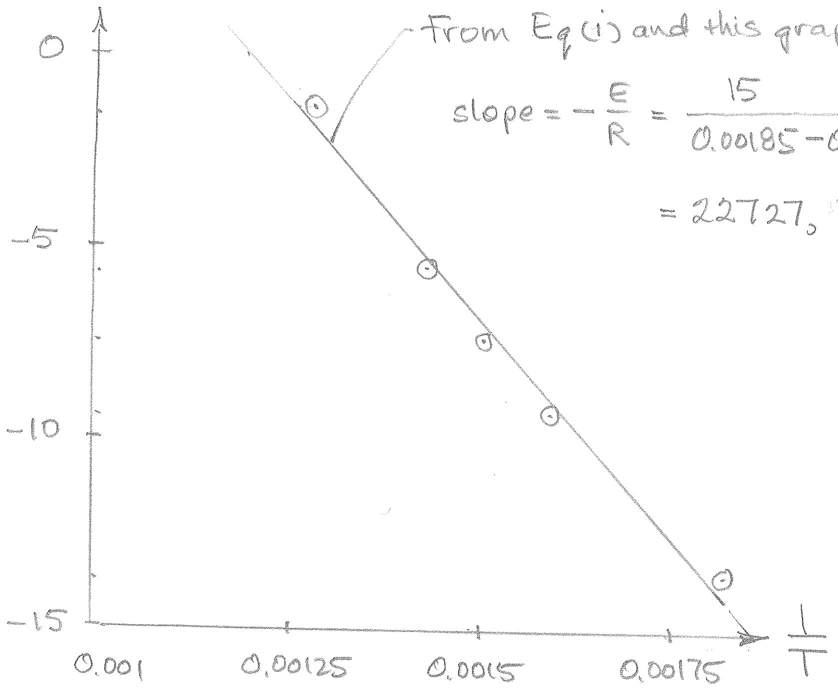
So to find the value of the rate constant, or k_0 and E/R, we must plot $\ln k$ vs $1/T$. The slope gives E/R and the intercept gives k_0. Let us follow this procedure

3.31
(continued)

First let us tabulate

T, °C	T, K	1/T, 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	0.000598	−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



From Eq (i) and this graph

$$\text{slope} = -\frac{E}{R} = \frac{15}{0.00185 - 0.00119}$$

$$= 22727, \text{K}^{-1}$$

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

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

$$= 5.7764 - 22727\left(\frac{1}{700}\right) = 38.2439$$

$$\text{or } k_0 = e^{38.2439} = 4.06 \times 10^{16}$$

So for the temperature range covered in the reported data

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

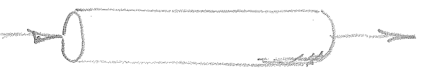
4.1

gas

$A + B \rightarrow R + S$

$C_{A0} = 100$

$C_{B0} = 100$



$\rightarrow X_A = 0.8$

$\left\{ \begin{array}{l} \varepsilon_A = 0 \\ \varepsilon_B = 0 \end{array} \right.$

$\left. \begin{array}{l} X_B = 0.8 \\ C_A = 0.2 \\ C_B = 0.2 \end{array} \right\} \longleftarrow$

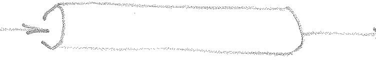
4.3

gas

$A + B \rightarrow R$

$C_{A0} = 200$

$C_{B0} = 100$



$\rightarrow C_A = 50$

Take 300 moles of feed gas. Consider A

$$\left. \begin{array}{ll} \text{at } X_A = 0 & V = 200A + 100B + 0R = 300 \\ \text{at } X_A = 1 & V = 0A - 100B + 200R = 100 \end{array} \right\} \varepsilon_A = \frac{100-300}{300} = -\frac{2}{3}$$

Now consider B

$$\left. \begin{array}{ll} \text{at } X_B = 0 & V = 300 \\ \text{at } X_B = 1 & V = 100A + 0B + 100R = 200 \end{array} \right\} \varepsilon_B = \frac{200-300}{300} = -\frac{1}{3}$$

∴ from Eq. 5

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

$$X_B = \frac{200 \times 0.9}{100} = 1.8 \text{ ... impossible} \longleftarrow$$

4.5

$C_{A0} = 100$

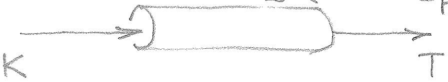
$C_{B0} = 200$

$T_0 = 400\text{K}$

$\pi_0 = 4\text{atm}$

gas

$A + B \rightarrow 2R$



$C_A = 20$

$T = 300\text{K}$

$\pi = 3\text{ atm}$

Since the number of moles is unchanged $\varepsilon_A = 0$ and $\varepsilon_B = 0$

4.5
(continued)

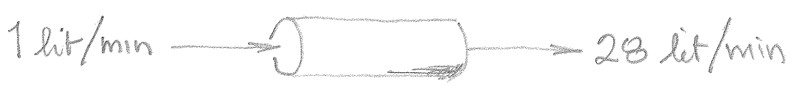
$$X_A = \frac{1 - \frac{C_A}{C_{A0}}\left(\frac{T\pi_0}{T_0\pi}\right)}{1+\varepsilon_A \frac{C_A}{C_{A0}}\left(\frac{T\pi_0}{T_0\pi}\right)} = \frac{1 + \left(\frac{20}{100}\right)\left(\frac{300\times4}{400\times3}\right)}{1+0} = 0.8 \longleftarrow$$

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

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

4.7

$A \rightarrow 31R$



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

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

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

the fraction popped.

5.1 By the definition of Eq 7 or 8 we have

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

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

$$\bar{t} > 1\ \text{min} \longleftarrow$$

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

$$\left.\begin{aligned} dt &= \frac{dV}{v} \\ dV &= \frac{F_{A0}\,dX_A}{(-r_A)} \end{aligned}\right\}$$

combining and integrating gives the expression for $\bar{t}$, or with $(F_{A0}, \text{mol/s}) = (C_{A0}, \text{mol/m}^3)(v_0, \text{m}^3/\text{s})$

$$\bar{t} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{(-r_A)\frac{v}{v_0}} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)} \quad \cdots \quad \cdots (24)$$

changes with conversion

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

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

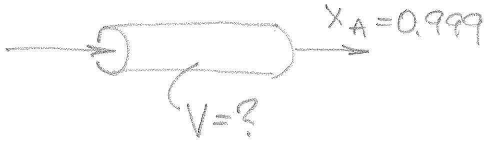
and

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

5.5 $C_{A0} = 100$ mmol/lit

$C_{B0} = 200$ mmol/lit

$v = 400$ lit/min



$A + B \rightarrow R$

$-r_A = 200 C_A C_B$

mol/lit·min

For a 2nd order reaction, Eq 3.14 gives

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

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 $\tau = 0.31$ min

Therefore $V = \tau v = (0.31)(400) = 124$ lit ←

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

Then for mixed flow, Eq 14a gives

$$\frac{a}{a_0} = \frac{1}{1+k\bar{t}} = \frac{1}{1+(0.1333)30} = 0.2$$

∴ Fraction of activity removed = 1-0.2 = 0.8 = 80% ←

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

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

$= 986$ lit $\approx 1\ m^3$ ←

5.11

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

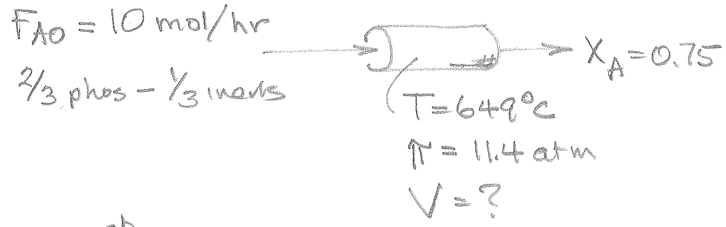
mol/lit·min

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

Then for mixed flow

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

5.13



$PH_3 \rightarrow P_4(g) + 6H_2$

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

For a 1st order reaction

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

Evaluate terms

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

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

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

$\varepsilon_A = 0.5 \longleftarrow$

$4A \longrightarrow 7R$

reactants: $40 \longrightarrow 70$

inerts: $20 \longrightarrow 20$

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

Replacing in (i) gives

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

5.15 $2A \rightarrow R$ with $-r_A = 0.05C_A^2$, mol/lit·s

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

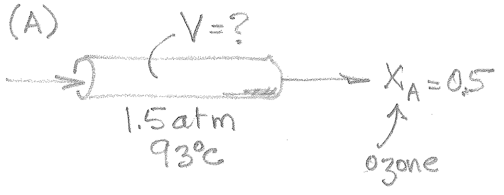
$$X_A = \frac{C_{A0}-C_A}{C_{A0}+\varepsilon_A C_A} = \frac{1-0.5}{1+(-0.5)(0.5)} = \frac{2}{3}$$

So for mixed flow

$$v = \frac{V(-r_A)}{C_{A0}X_A} = \frac{(2)(0.05\times0.5^2)}{1(2/3)} = 0.0375\,\text{lit/s} = 2.25\,\text{lit/min} \longleftarrow$$

5.17

20% ozone (A)
80% air
$v = 1$ lit/s



$2O_3 \rightarrow 3O_2$

$-r_A = kC_A^2$

$k = 0.05$ lit/mol·s

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

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

Evaluate terms

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

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

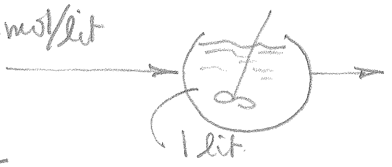
Replacing in (i) gives

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

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

5.19

$C_{A0} = 120$ mmol/lit
3 atm
30°C
various v_0



$A \rightarrow 3R$

Find a rate equation

For each run

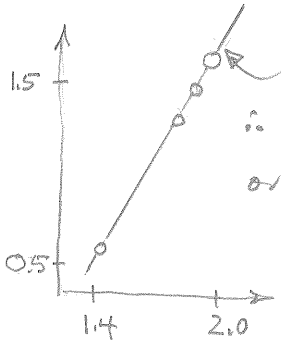
$$-r_A = \frac{C_{A0}X_A v_0}{V} = \frac{C_{A0}(C_{A0}-C_A)v_0}{(C_{A0}+\varepsilon_A C_A)V} = \frac{120(120-C_A)v_0}{(120+2C_A)}$$

$\varepsilon_A = \frac{3-1}{1} = 2$

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

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

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

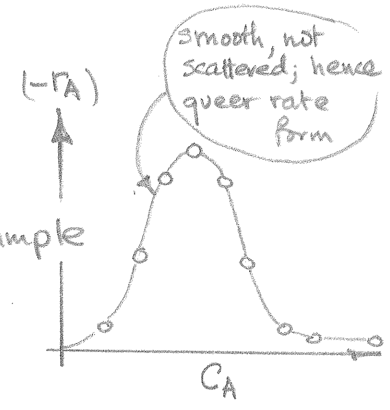
$\therefore k = 0.004$

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

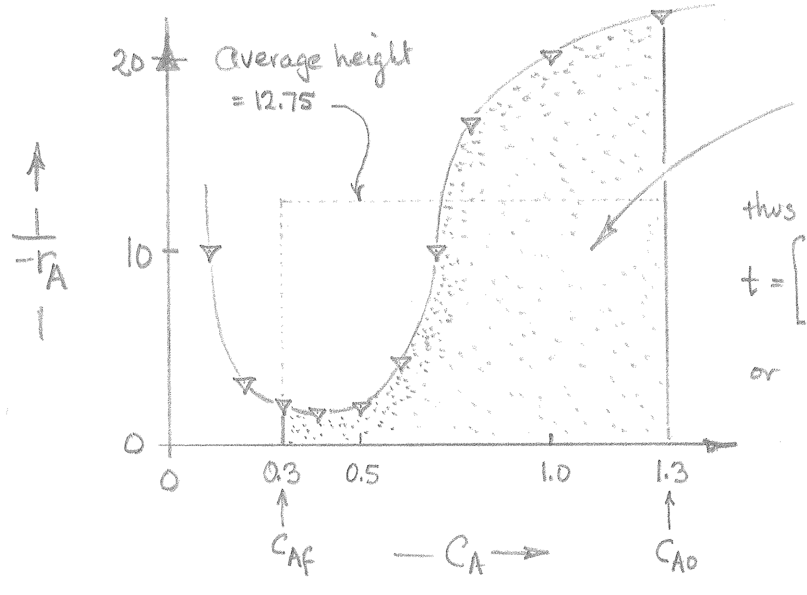
5.21 The approach which probably first comes to mind is to find a rate equation to represent the data, first order, second, etc., and then integrate it to give the time; thus

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

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



$$\text{Area} = t = +\int_{C_{Af}}^{C_{A0}} \frac{dC_A}{-r_A}$$

thus

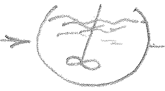
$$t = \left[12.75\ \frac{\text{lit}\cdot\text{min}}{\text{mol}}\right]\cdot\left[1.3 - 0.3\ \frac{\text{mol}}{\text{lit}}\right]$$

or

$$t = 12.75\ \text{min} \longleftarrow$$

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

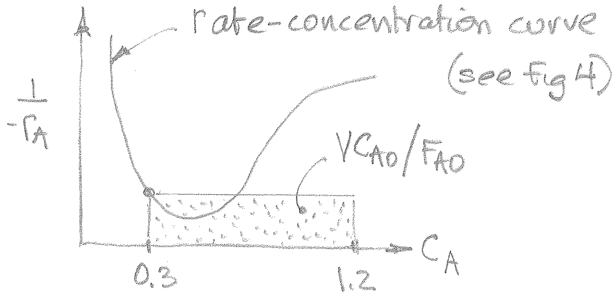
5.23 a) Given

$C_{A0} = 1.2$ mol/lit
$F_{A0} = 1000$ mol/hr $\longrightarrow$  $\longrightarrow X_A = 0.75$

Since this is a liquid reaction $\varepsilon_A = 0$, so $\frac{C_{Af}}{C_{A0}} = 1 - X_A$

or $C_{Af} = C_{A0}(1 - X_{Af}) = 1.2\,(1 - 0.75) = 0.3$ mol/lit

From the performance equation for mixed flow, Eq 13,



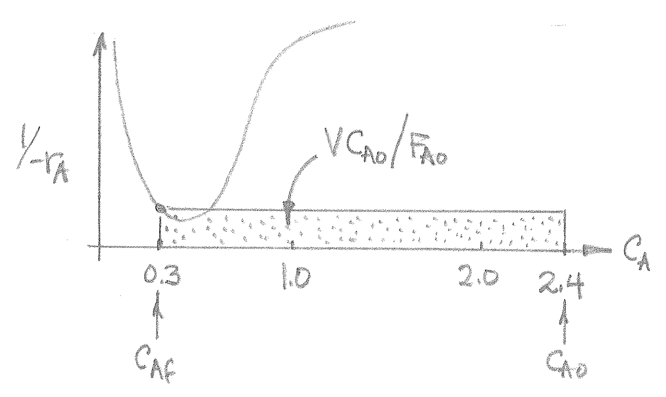
$$V = \frac{F_{A0}}{C_{A0}} \cdot \frac{C_{A0} - C_{Af}}{-r_{Af}}$$

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

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

$$V = \frac{F_{A0}}{C_{A0}} \cdot \frac{C_{A0} - C_{Af}}{-r_{Af}}$$ ... that V is doubled,

or $V = 50$ lit. $\longleftarrow$ b)



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

$$V = \frac{F_{A0}}{C_{A0}} \cdot \frac{C_{A0} - C_{Af}}{-r_A}$$

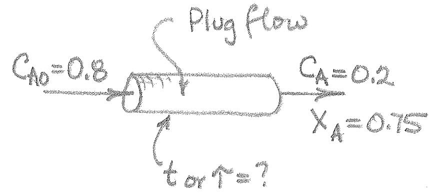
$$= \frac{1000}{2.4} \cdot \frac{(2.4 - 0.3)}{0.5} \cdot \frac{1}{60}$$

or $V = 29.167$ lit $\longleftarrow$ c)

5,25 For a mixed flow reactor, with $\varepsilon_A = 0$, we find the rate of reaction from Eq 13. Thus we tabulate as follows

t, sec	C_{A0}	$C_{A,out}$	$-\frac{1}{r_A} = \frac{t}{C_{A0} - C_{A,out}}$ … at $C_{A,out}$
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

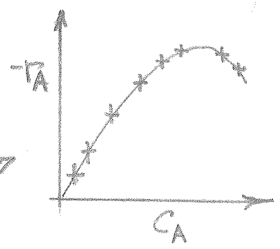
Holding time for plug flow.



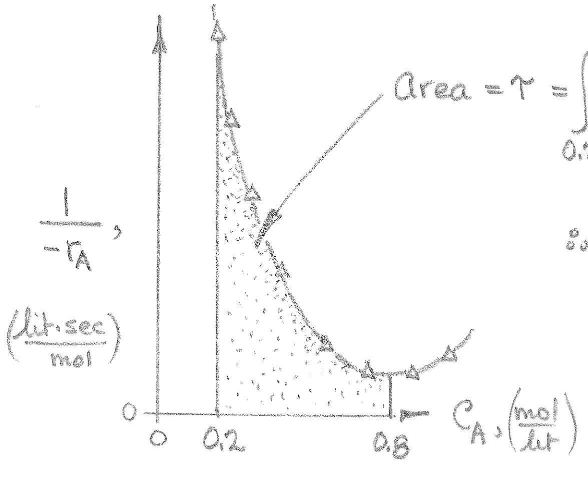
We may solve this by using conversions as suggested in the text. However since $\varepsilon_A = 0$ the use of concentrations poses no problems.
Let us use this. Then the performance expression is Eq. 19, or

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

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.



$$\text{Area} = \tau = \int_{0.2}^{0.8} \frac{dC_A}{-r_A} = 300 \text{ sec}$$

$\therefore$ for a plug flow reactor

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

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 googliox.

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

$$\left.\begin{aligned} k\tau_1 &= \frac{X_{A1}}{1-X_{A1}} = \frac{0.8}{1-0.8} = 4 \\ k\tau_2 &= \frac{X_{A2}}{1-X_{A2}} = \frac{0.75}{1-0.75} = 3 \end{aligned}\right\}$$

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

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

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

or $$(25 \text{ Imp. gal})\left(\frac{10 \# H_2O}{1 \text{ Imp.gal}}\right)\left(\frac{1 ft^3}{62.4 \# H_2O}\right) = \underline{4.01 ft^3}$$

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

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

These volumes agree so Imbibit could well be in the vat. This hypothesis, or guess does fit the facts } ←

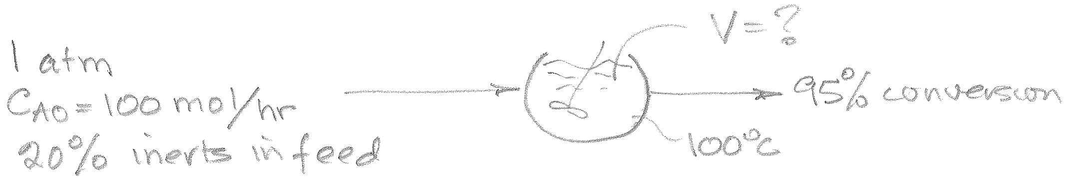
b) Why did Watson never come up with this explanation? Because smoking near 99% alcohol was not really cool. ←

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 # H_2O, and that 1 stone weighs 14 #.

5.29 (extension of problem 5.28)

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

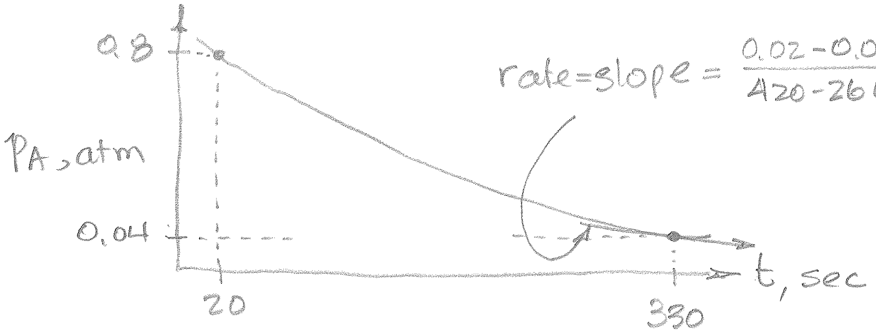


$\therefore \dot{n}_{feed} = 100\left(\frac{100}{80}\right) = 125$ mol/hr

$p_{A0} = 0.8$ atm

From the given
$p_{Af} = 0.04$ atm

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 $p_A = 0.04$ atm



$$\text{rate} = \text{slope} = \frac{0.02 - 0.08}{420 - 260} = -\frac{0.06}{160} \text{ atm/s}$$

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

$$\tau = \frac{V}{v} = \frac{p_{A0} - p_A}{-r_A} = \frac{0.8 - 0.04}{(0.06/160)} = 2\,026.67 \text{ s}$$

But $\tau = \frac{V}{v}$ so evaluate v from $pv = nRT$. Thus

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

$$\therefore V = \tau v = (2026.67 \text{ s})(3826 \text{ lit/hr})(1 \text{ hr}/3600 \text{ s})$$

$$= 2150 \text{ lit} = 2.15 \text{ m}^3 \longleftarrow$$

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

$$\frac{V_2}{V_1} = 2 = \frac{k\tau_2}{k\tau_1} = \frac{(C_{A1}-C_{A2})/C_{A2}^2}{(C_{A0}-C_{A1})/C_{A1}^2} = \frac{(0.5-C_{A2})/C_{A2}^2}{(1-0.5)/0.5^2}$$

or

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

therefore $C_{A2} = 0.25$ mol/lit. $\longleftarrow$

6.3 For the second order reaction

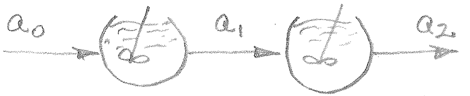
for the mixed flow reactor: $k\tau_m = \frac{C_{A0}-C_{A1}}{C_{A1}^2} = \frac{4-1}{1} = 3$

so for the plug flow reactor: $k\tau_p = 3k\tau_m = 9$

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

$\therefore$ $C_{A2} = 0.1\,(C_{A1}) = 0.1$ mol/lit $\longleftarrow$

6.5



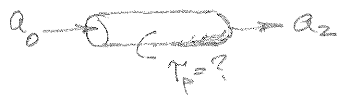
$\therefore\ \bar{t}_i = 2$ weeks $= 20160$ min

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 $\frac{a_2}{a_0} = \frac{a_2}{a_1}\cdot\frac{a_1}{a_0} = \frac{1}{(1+k\bar{t}_i)} = \frac{1}{[1+0.0495(20160)]^2} = 1.0017\times10^{-6}$

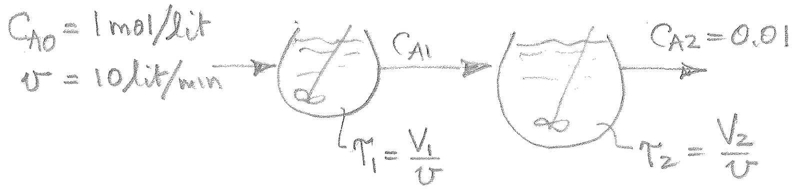
For plug flow



$$\frac{a_2}{a_0} = 1.0017\times10^{-6} = e^{-k\tau_p} = e^{-0.0495\,\tau_p}$$

$$\tau_p = \frac{\ln(1.0017\times10^{-6})}{-0.0495} = 279\text{ min} = \overset{\text{instead of 2 weeks for the MFR}}{4.65\text{ hr}} \longleftarrow$$

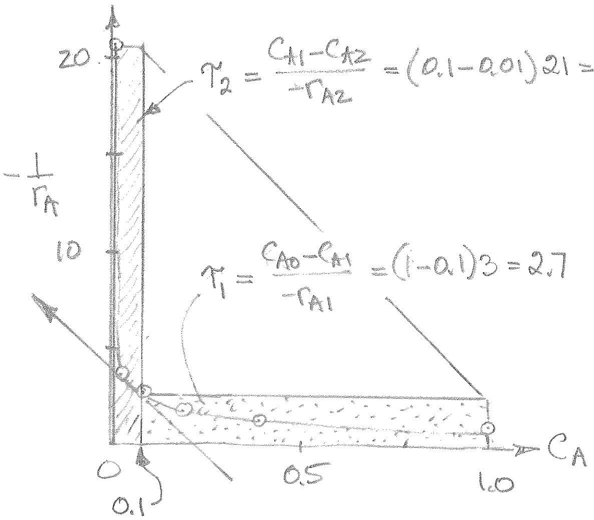
6.7



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

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



$$\tau_2 = \frac{C_{A1} - C_{A2}}{-r_{A2}} = (0.1 - 0.01)21 = 1.9$$

$$\tau_1 = \frac{C_{A0} - C_{A1}}{-r_{A1}} = (1 - 0.1)3 = 2.7$$

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

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

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

$$\frac{v_{\text{without}}}{v_{\text{with}}} = \frac{\tau_{\text{with}}}{\tau_{\text{without}}} = \frac{3\ln 4}{\ln 10} = \overset{\text{no recycle is better}}{1.8} \longleftarrow$$

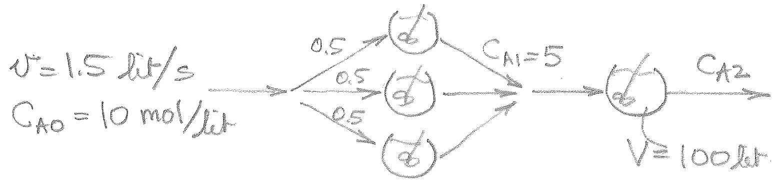
6.11 For this autocatalytic reaction the maximum rate occurs where $C_A = C_R$. Thus operate at $C_A = 5$, if possible. Here

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

So for mixed flow

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

Thus $V = 300$ 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

$$66.7s \rightarrow \tau = \frac{5 - C_{A2}}{k C_{A2} C_{R2}} = \frac{5 - C_{A2}}{0.001\, C_{A2}(10 - C_{A2})} \text{, or } C_{A2} = 3.486 \frac{\text{mol}}{\text{lit}} \longleftarrow$$

6.13 From ½ life data for radioactive decay (first order kinetics) we have

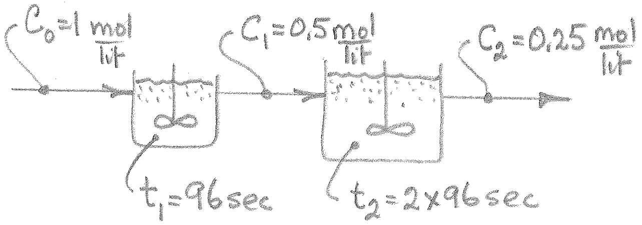
$$-\frac{dC}{dt} = kC \quad \cdots \text{or} \cdots \quad \ln\frac{C_0}{C} = kt \quad \cdots \text{or} \cdots \quad \ln 2 = k(20\,\text{hrs}) \quad \cdots \text{or} \cdots \quad k = \frac{\ln 2}{20\,\text{hr}}$$

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.

$$\left.\begin{aligned} &\text{For } 1^{st} \text{ reactor: } \quad \tau_1 = \frac{C_0 - C_1}{kC_1^n} \\ &\text{For } 2^{nd} \text{ reactor: } \quad \tau_2 = \frac{C_1 - C_2}{kC_2^n} \end{aligned}\right\} \text{ combining} \dots \quad \frac{\tau_1}{\tau_2} = \frac{C_0 - C_1}{C_1 - C_2}\left(\frac{C_2}{C_1}\right)^n$$

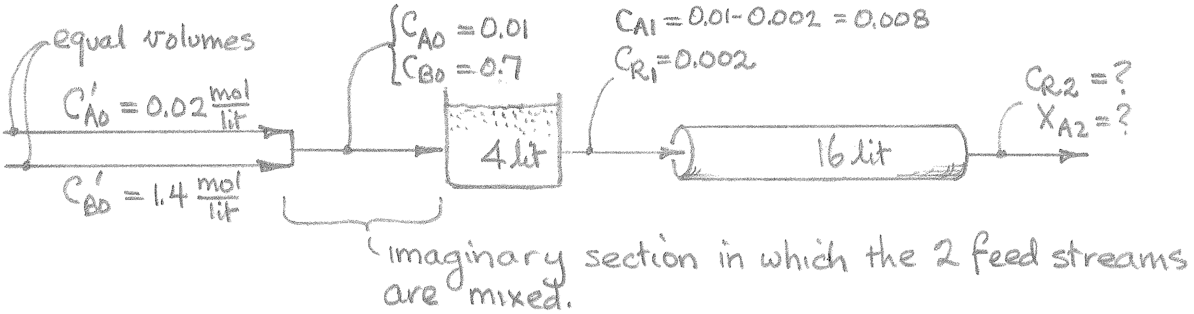
$$\therefore n = \frac{\log\frac{\tau_1}{\tau_2} + \log\frac{C_1 - C_2}{C_0 - C_1}}{\log\frac{C_2}{C_1}} = \frac{\log\frac{1}{2} + \log\frac{1}{2}}{\log\frac{1}{2}} = 2$$

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

Hence the rate

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

6.17



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

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

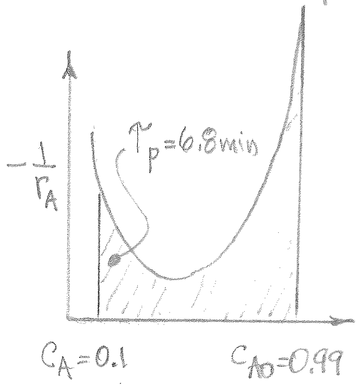
For the reactor: $k\tau_p = 4(k\tau_m) = 4(\frac{1}{4}) = -\int_{0.008}^{C_{A2}} \frac{dC_A}{C_A} = \ln\frac{0.008}{C_{A2}}$ ... or $C_{A2} = 0.00293$

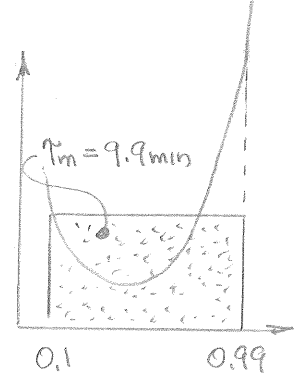
$$\therefore X_A = 0.707 \quad \& \quad C_{R2} = 0.00793 \longleftarrow$$

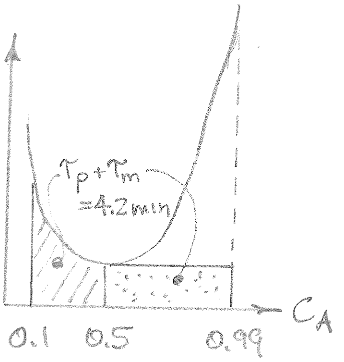
6.19 Let us solve by using the graphical procedure, and let's use concentrations, not conversions. First prepare the $1/-r_A$ vs C_A curves from the data of the table, below

C_A	C_R	$-r_A = kC_AC_R$	$\frac{1}{-r_A}$
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

$\tau_p = 6.8$ min $\longleftarrow$ a)

$\tau_m = 9.9$ min $\longleftarrow$ b)

$\tau_{best} = \tau_m + \tau_p = 2 + 2.2 = 4.2$ min $\longleftarrow$ c)

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

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

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

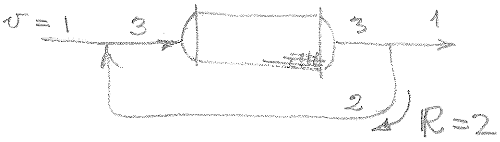
With recycle

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

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

$C_{Af} = 2.24$, or $X_{Af} = 0.776$ ←

7.1 a) Use a MFR with some particular concentration of A

b) Use a PFR, with low X_A

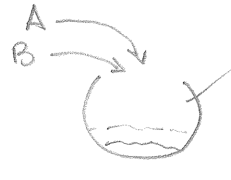
c) Use a MFR, with high X_A

7.3 For

$A+B \rightarrow R$
$2A \rightarrow S$
$2B \rightarrow T$

for A use low C_A
for B use low C_B

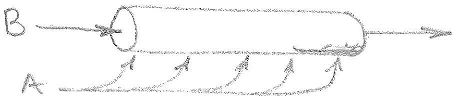
Thus



drip A and B in slowly
keep X_A high
keep X_B high
Don't have an excess of either A or B

7.5 For

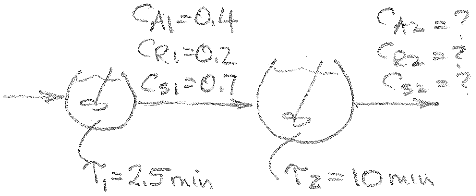
$A+B \rightarrow R$
$2A \rightarrow S$ } keep C_A low, but C_B high



7.7 Given

$$A \xrightarrow{1} R, \quad r_R = k_1 C_A^2 \qquad \text{and}$$
$$A \xrightarrow{2} S, \quad r_S = k_2 C_A$$

$C_{A0}=1$
$C_{R0}=0$
$C_{S0}=0.3$



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

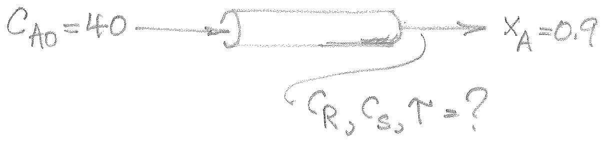
$$\tau_2 = \frac{C_{A1}-C_{A2}}{k_1 C_A^2 + k_2 C_A} = \frac{0.4 - C_{A2}}{0.5\,C_{A2}^2 + 0.4\,C_{A2}} = 10 \quad \therefore C_{A2} = 0.0745 \longleftarrow$$

Also

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

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

7.9



$A \overset{1}{\nearrow} R \quad r_R = k_1 C_A^2 \quad k_1 = 0.4\ \mathrm{m^3/mol \cdot min}$

$ \overset{2}{\searrow} S \quad r_S = k_2 C_A \quad k_2 = 2\ \mathrm{min^{-1}}$

First determine $\varphi(S/A)$..

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

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

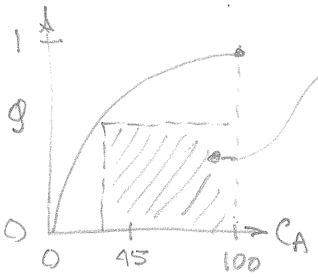
$$\left.\begin{aligned} \therefore\ C_A &= 4 \\ C_S &= 8 \\ C_R &= 28 \end{aligned}\right\} \longleftarrow$$

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

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

C_A	$\varphi(R/A)$
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

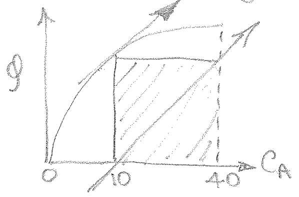
$$\left[\varphi(R/A) = \frac{0.4C_A^2}{0.4C_A^2 + 2C_A} = C_A / C_A + 5 \right]$$

Method 1 Solve analytically

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

$$\frac{dC_R}{dC_A} = \frac{(40-2C_A)(C_A+5) - (40C_A - C_A^2)}{(C_A+5)^2} = 0 \quad \text{-- or} \quad \left.\begin{aligned} C_A &= 10 \\ C_R &= 20 \\ C_S &= 10 \end{aligned}\right\} \longleftarrow$$

Method 2 Solve graphically by maximizing the shaded rectangle



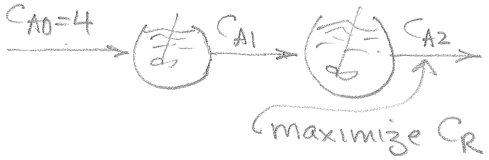
For τ:

$$\tau = \frac{C_{A0} - C_{Af}}{-r_A} = \frac{C_{A0} - C_{Af}}{0.4C_{Af}^2 + 2C_A} = \frac{40-10}{0.4(10)^2 + 2(10)}$$

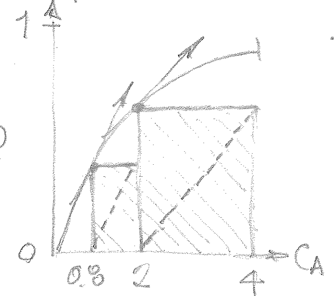
$$= \frac{30}{60} = \frac{1}{2}\ \text{min} \longleftarrow$$

7.13

$$A \nearrow R \quad r_R = C_A, \qquad A \searrow S \quad r_S = 1 \quad \Bigg\} \quad \varphi\left(\frac{R}{R+S}\right) = \frac{C_A}{C_A+1}$$



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

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

$$\therefore \tau_1 = \frac{V_1}{v} = \frac{C_{A0}-C_{A1}}{-r_{A1}} = \frac{C_{A0}-C_{A1}}{1+C_{A1}} = \frac{4-2}{1+2} = \frac{2}{3}$$

and $$\tau_2 = \frac{V_2}{v} = \frac{C_{A1}-C_{A2}}{-r_{A2}} = \frac{2-0.8}{1+0.8} = \frac{2}{3}$$

$$\Bigg\} \therefore \frac{V_1}{V_2} = 1$$

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

and

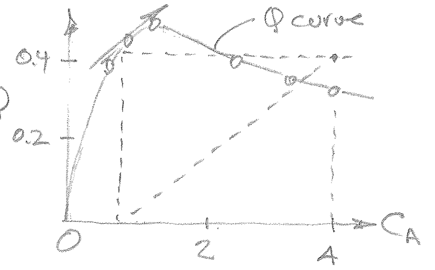
$$C_{R1} = \varphi \cdot \Delta C_A = \frac{C_{A1}}{C_{A1}+1}(C_{A0}-C_{A1}) = \frac{2}{2+1}(4-2) = 1.33$$

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

$$\Bigg\} \therefore C_{R\,max} = 1.86 \, \frac{mol}{lit} \longleftarrow$$

7.15

$$A \nearrow R \quad r_R = 1, \qquad A \rightarrow S \quad r_S = 2C_A, \qquad A \searrow T \quad r_T = C_A^2 \quad \Bigg\} \quad \varphi(S/A) = \frac{r_S}{-r_A} = \frac{2C_A}{(1+C_A)^2}$$



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

$$C_S = \int_0^4 \frac{2C_A}{(1+C_A)^2}\, dC_A \overset{\text{graphical integration}}{\cong} (0.3984)4 = 1.59$$

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

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

differentiating & setting to zero gives

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

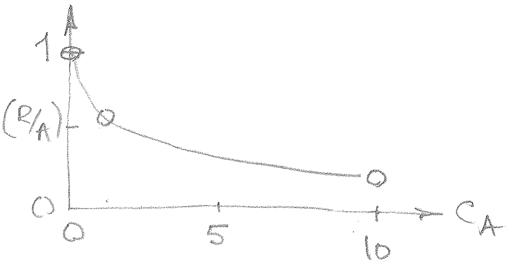
$$\therefore C_A(\text{at } C_{S\,opt}) = \frac{2}{3}$$

$$\varphi(\text{at } C_A = \tfrac{2}{3}) = 2\left(\tfrac{2}{3}\right)\Big/\left(1+\tfrac{2}{3}\right)^2 = \frac{12}{25}$$

$$\Bigg\} \therefore C_{S\,max} = \frac{12}{25}\left(4-\frac{2}{3}\right) = 1.6 \longleftarrow$$

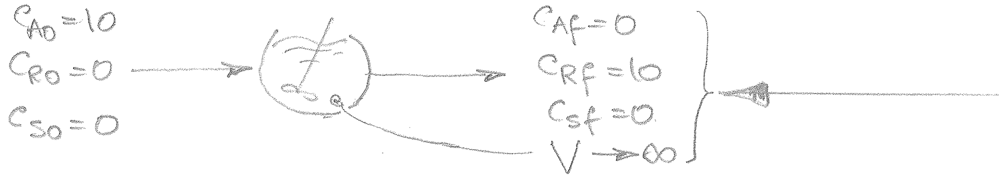
7.17 For reactions in parallel first evaluate & draw the φ vs C_A curve

C_A	$\varphi(R/A) = \dfrac{16C_A^{1/2}}{16C_A^{1/2}+12C_A+C_A^2}$
10	0.185
1	0.55
0	1.0



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

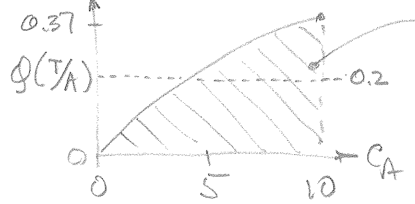
$\therefore$ operate the mixed flow reactor at $X_A \to 1$. Here



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

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

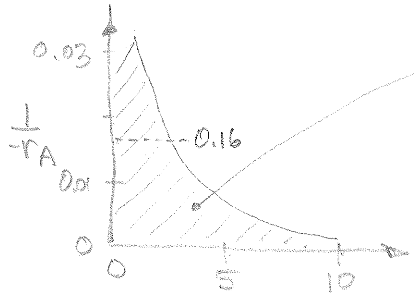
Now plot



$$C_R = \begin{pmatrix}\text{shaded}\\ \text{area}\end{pmatrix} = \int \varphi \, dC_A = 0.2(10-0) = 2 \ \frac{\text{mol}}{\text{lit}} \longleftarrow$$

[Note that plug flow is best since it gives most T]

Next, to find τ plot $-1/r_A$ vs C_A



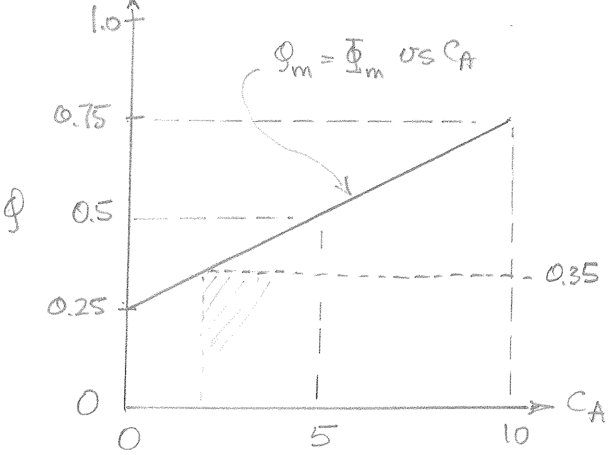
$$\tau = \int_{10}^{0} \frac{dC_A}{-r_A} = 0.016(10) = 0.16 \text{ min}$$

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

$= 160$ lit $\longleftarrow$

7.21 First let us calculate φ, the instantaneous fractional yield. This is obtained directly from the mixed flow run because $\varphi_m = \Phi_m$

C_{A0}	C_A	C_R	$\varphi = \Phi = \frac{C_R}{C_{A0}-C_A}$
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	$25/100 = 0.25$

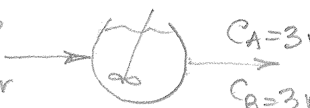


So for mixed flow with $C_{A0} = 100$

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

7.23

$F_{A0} = 300$ mol/hr
$C_{A0} = 30$ mol/m^3
$F_{B0} = 300$ mol/hr
$C_{B0} = 30$ mol/m^3



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

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

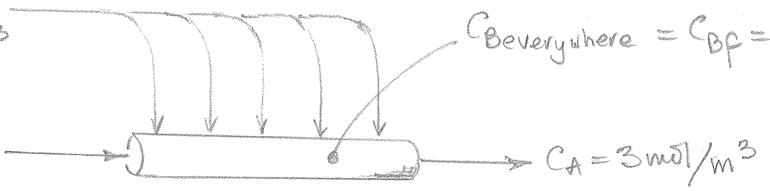
$$\therefore C_R = \varphi(R/A)(-\Delta C_A) = \frac{1}{3}(30-3) = 9 \text{ mol/m}^3 \quad \therefore R/S = 1/2 \longleftarrow$$

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

7.25

$F_{B0} = 300$ mol/hr
$C_{B0} = 30$ mol/m^3

$F_{A0} = 300$ mol/hr
$C_{A0} = 30$ mol/m^3



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

7.25 (continued)

$$\therefore\ C_{Rf} = \int_{C_{Af}}^{C_{A0}} \varphi(R/A)\, dC_A = \int_3^{30} \frac{C_A}{C_A + 2\underset{\uparrow\,=3}{C_B}}\, dC_A = \Big[C_A - 6\ln(C_A+6)\Big]_3^{30} = 18.68$$

$$C_{Sf} = \int_{C_{Af}}^{C_{A0}} \varphi(S/A)\, dC_A = \int_3^{30} \frac{2C_B}{C_A + 2\underset{\uparrow\,=3}{C_B}}\, dC_A = \Big[6\ln(C_A+6)\Big]_3^{30} = 8.32$$

So $\dfrac{C_{Rf}}{C_{Sf}} = \dfrac{18.68}{8.32} \cong 2.25 \longleftarrow$

Finally $V = \dfrac{F_{A0}}{C_{A0}} \displaystyle\int_{C_{Af}}^{C_{A0}} \frac{dC_A}{-r_A} = \frac{300}{30} \int_{30}^{300} \frac{dC_A}{50C_A + 100(3)} = \Big[(10)\big(\tfrac{1}{50}\big)\ln(50C_A + 300)\Big]_3^{30}$

$= 0.2773\ m^3 = 277.3\ lit \longleftarrow$

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

$$\left.\begin{aligned} -\frac{dF}{dt} &= kB \\ -\frac{dB}{dt} &= kF \end{aligned}\right\}$$

dividing one by the other to eliminate the time variable (as with multiple reactions) we see

$$\frac{dF}{dB} = \frac{B}{F} \quad \text{-----}(1)$$

Separating and integrating gives

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

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

$$F^2 = 33^2 - 27^2 = 360 \quad \text{---- or} \quad F = 19 - \varepsilon \text{ ships} \longleftarrow$$

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

For the 1st battle : $B_0^2 - B_1^2 = f^2 - 0$

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

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

To maximize B_2 take $\frac{dB_2}{df} = 0$ from which we find $f = \frac{F_0}{2}$.
Thus the British should fight ½ the French fleet in each battle.
So for f=16 or 17 we find that the British are left with

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

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.

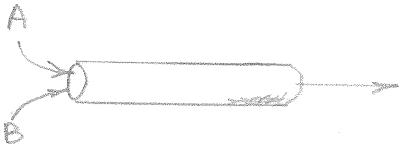
The British war office had a couple of mathematicians on their staff who in essence did the above calculation. The French military probably were more "practical", and didn't spend money on "useless" activities.

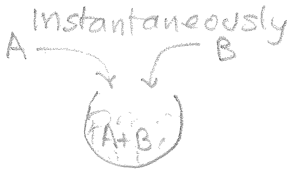
It would be interesting to consider historical battles (Thermopolae, Jutland, Coral sea, guerrila warfare) from the standpoint of this law. For more on this subject see the section on *Mathematics & Warfare* in "World of Mathematics" by James Newman. This problem has many interesting extensions: suppose 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) $r_1 = k_1 C_A C_B^2$

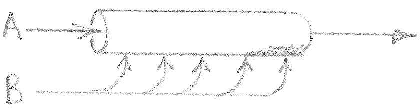
$r_2 = k_2 C_R C_B$

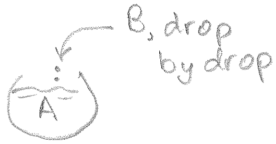




b) $r_1 = k_1 C_A C_B$

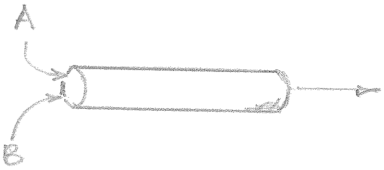
$r_2 = k_2 C_R C_B^2$

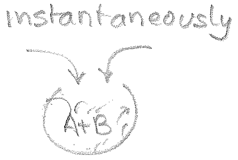




c) $r_1 = k_1 C_A C_B$

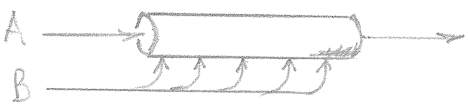
$r_2 = k_2 C_R^2 C_B$





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 $A \begin{matrix} \nearrow R \\ \searrow S \end{matrix}$ ·· $r_R = k_1 C_A$, $r_S = k_2 C_A$ } Then for mixed flow

$$\left.\begin{aligned} \tau &= \frac{C_R - C_{R0}}{k_1 C_A} \\ \tau &= \frac{C_S - C_{S0}}{k_2 C_A} \end{aligned}\right\} \text{dividing gives} \quad \frac{C_R}{C_S} = \frac{k_1}{k_2} = \text{constant}$$

This agrees with the observed so we conclude that

$$A \begin{matrix} \nearrow R \text{ ·· } r_R = k_1 C_A \\ \searrow S \text{ ·· } r_S = k_2 C_A \end{matrix} \Bigg\} \quad k_1 = 1.5\, k_2 \longleftarrow$$

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

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

8.5 (continued)

Let us next evaluate the rate constants

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

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

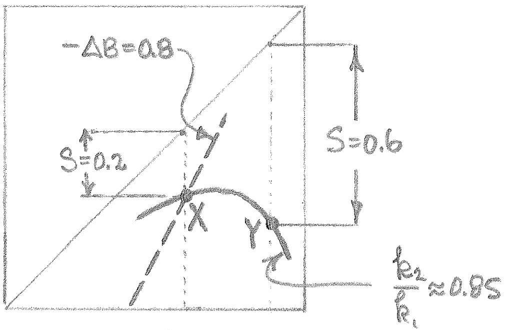
these results are consistent

Therefore the kinetics are

$$A \xrightarrow[n_1=1]{k_1=0.2\,\text{min}^{-1}} R \xrightarrow[n_2=1]{k_2=0.05\,\text{min}^{-1}} S \longleftarrow$$

8.7 a) At the start $\begin{cases} A_0 = 1 \\ B_0 = 3 \end{cases}$

After some time $\begin{cases} B = 2.2 \\ S = 0.2 \end{cases}$



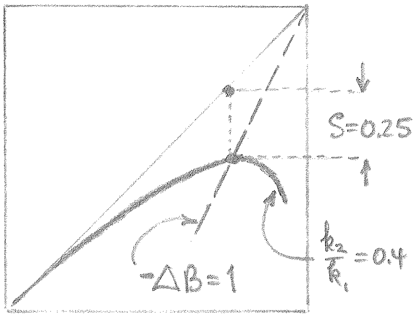
By material balance $-\Delta B=0.8$, and using ΔB & S locates point X on Fig. 7.15.

At this point $k_2/k_1 = 0.85$

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

b) Nothing $\longleftarrow$ b)

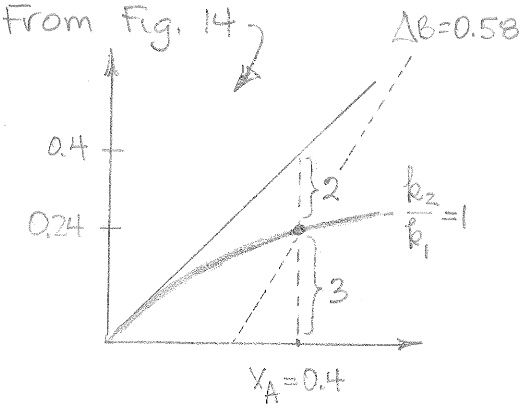
c)



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.

$\therefore k_2/k_1 \le 0.4 \longleftarrow$ c)

8.9 From Fig. 14



Thus

$$\text{given} \longrightarrow \left.\begin{array}{l} \frac{C_A}{C_{A0}} = 0.6 \\ \frac{C_R}{C_{A0}} = 0.24 \\ \frac{C_S}{C_{A0}} = 0.16 \\ \frac{C_B}{C_{A0}} = 0.42 \end{array}\right\} \frac{k_2}{k_1} = 1 \longleftarrow$$

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

$$C_A=0 \quad C_R=20 \quad C_S=20 \quad C_T=20 \text{ and } C_U=40 \longleftarrow \text{a)}$$

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

$$C_A=10 \quad C_R=0 \quad C_S=20 \quad C_T=30 \text{ and } C_U=40 \longleftarrow \text{b)}$$

8.15 Our reaction scheme is

$$\begin{tikzcd} & R \arrow[dr, "\text{fast}", "③"'] & & \\ A \arrow[ur, "\text{medium}", "①"'] \arrow[rr, "\text{medium}", "②\ \text{rate}"'] & & S \arrow[r, "\text{slow}", "④"'] & T \end{tikzcd}$$

Combining gives $\frac{1}{k_{13}} = \frac{1}{k_1} + \frac{1}{k_3} = \frac{1}{0.21} + \frac{1}{4.2} = \frac{1}{0.2}$

$$\begin{tikzcd} A \arrow[r, bend left] \arrow[r, "0.2"] & S \arrow[r, "0.004"] & T \end{tikzcd}$$

thus $A \xrightarrow[k_{123}]{0.4} S \xrightarrow[k_4]{0.004} T$ ··· or $\frac{k_{123}}{k_4} = 100$

Since S is desired use plug flow. Then an extension of Eq. 49 gives

$$\frac{C_{S\max}}{C_{A0}} = \left(\frac{k_{123}}{k_4}\right)^{k_4/(k_4-k_{123})} = \left(\frac{0.4}{0.004}\right)^{0.004/(0.004-0.4)}$$

$$= 0.955 \quad \cdots \text{or} \quad C_{S\max} = 0.955\, C_{A0} \longleftarrow$$

8.17 Since this is a course on chemical reactors let us make the analogy of this process to a chemical process, so

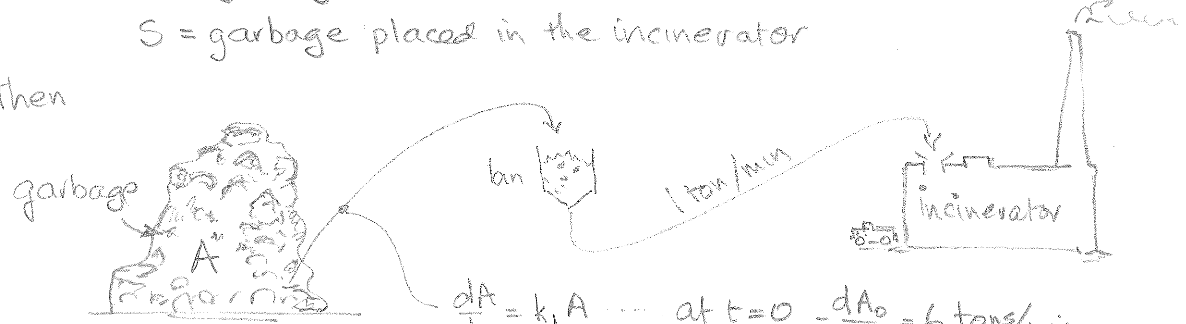
Let A = garbage still to be collected

A_0 = 1440 tons

R = garbage in the bin

S = garbage placed in the incinerator

Then



$\frac{dA}{dt} = k_1 A$ ··· at t=0 $-\frac{dA_0}{dt} = 6$ tons/min

$\therefore\ k_1 = \frac{-dA/dt}{A} = \frac{6}{1440} = \frac{1}{240}\ \text{min}^{-1}$

Then

$$A \xrightarrow[k_1 = \frac{1}{240}\ \text{min}^{-1}]{n_1 = 1} R \xrightarrow[k_2 = 1\ \text{ton/min}]{n_2 = 0} S$$

with

$$-\frac{dA}{dt} = k_1 A \quad \text{and} \quad \frac{dR}{dt} = k_1 A - k_2 \quad \text{--------- (i)}$$

8.17 (continued)

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

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

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

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

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

or

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

$$\left.\begin{array}{l}\therefore \text{ at 6pm 95\% of the days garbage} \\ \quad \text{will have been collected}\end{array}\right\} \longleftarrow \text{a)}$$

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

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

The time, from Eq. (ii)

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

$$\text{or } 1.20 \text{ pm} \longleftarrow \text{c)}$$

(b) Max contents of the bin

$$R_{max} = 1440\left(1-e^{-430/240}\right) - 430 \quad \cdots \text{ or } R_{max} = 430 \text{ tons} \longleftarrow \text{b)}$$

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

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

or

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

Solve by trial & error

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

$$\nwarrow 5.56 \text{ am} \longleftarrow \text{d)}$$

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

-- It is well designed, but with nothing to spare

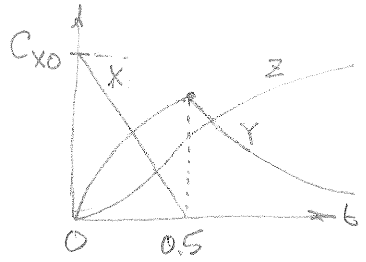
8.19 Let us follow the text. From Eq 22

$$X \xrightarrow{n_1=0} Y \xrightarrow[k_2=1.5\,hr^{-1}]{n_2=1} Z \qquad C_{X0} = 100\ mol/m^3$$

we are given

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

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



(a) at half an hour one gets Ymax (see Fig 8.8)

$$\frac{C_{Y max}}{C_{X0}} = \frac{1}{K}\left(1-e^{-K}\right) = \frac{1}{0.75}\left(1-e^{-0.75}\right) = 0.7035 \longleftarrow a)$$

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

$$\frac{C_Y}{C_{X0}} = \frac{1}{K}\left(e^{+K-k_2t} - e^{-k_2t}\right)$$

$$= \frac{1}{0.75}\left(e^{-0.75-1.5} - e^{-1.5}\right) = 0.3323$$

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

8.21 The reaction is $A \xrightarrow{6} R \genfrac{}{}{0pt}{}{\xrightarrow{3} S}{\xrightarrow{1} T}$ for which from Eq 49

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

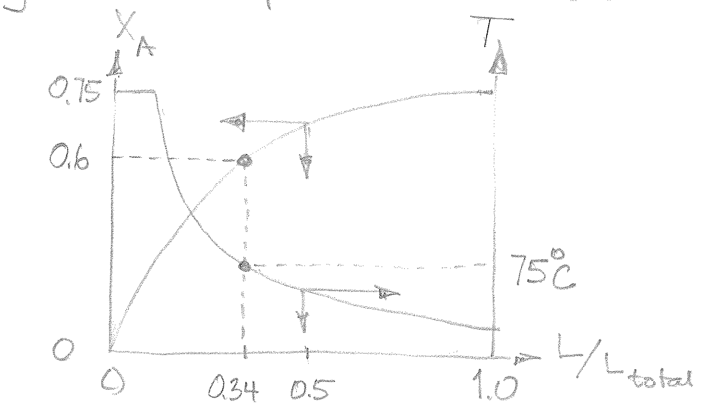
or $C_{Rmax} = 0.444\ mol/lit \longleftarrow$

From Eq.50

$$t_{R,max} = \frac{\ln(k_{34}/k_1)}{k_{34}-k_1} = \frac{\ln 4/6}{4-6} = 0.2027\,h = 12.2\ min \longleftarrow$$

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

9.1 Figure E4c presents the solution to this problem



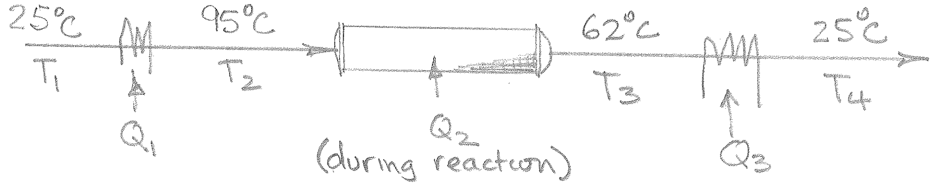
From Fig. E4c we find $\tau_{X_A=0.6} = 0.34\,\tau_{X_A=0.8}$

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

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

Also $T_{exit} = 75°C \longleftarrow$

9.3 From Fig E4a we find



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

So the heat added to the flowing stream is

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

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

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

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

9.5 (a) Redo Example 4 with one change: $C_{A0}=4 \longrightarrow C_{A0}=1$ 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

$$\frac{\tau}{C_{A0}} = \frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A} = \left(\begin{array}{c}\text{area under the}\\ 1/{-r_A} \text{ vs } X_A \text{ curve}\end{array}\right) \quad \cdots\cdots (i)$$

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

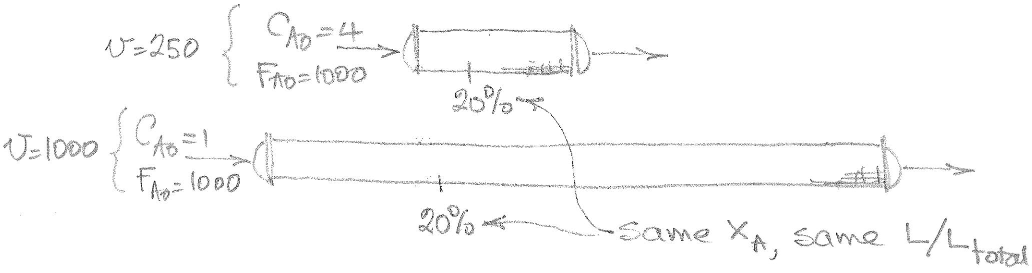
also, from Eq (i)

$$\left.\begin{array}{r} V = F_{A0}(\text{area}) = 1000(1.62) = 1620 \text{ lit} \\ = 1.62 \text{ m}^3 \end{array}\right\} \longleftarrow \text{a)}$$

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 $\longleftarrow$ b)



9.7 Redo Example 6 with one change: $C_{A0}=4 \longrightarrow C_{A0}=1$

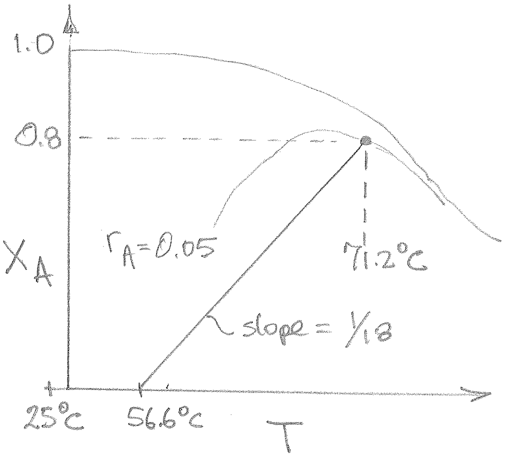
Here $\mathbf{C}_p = 1000\,\text{cal/mol A}$

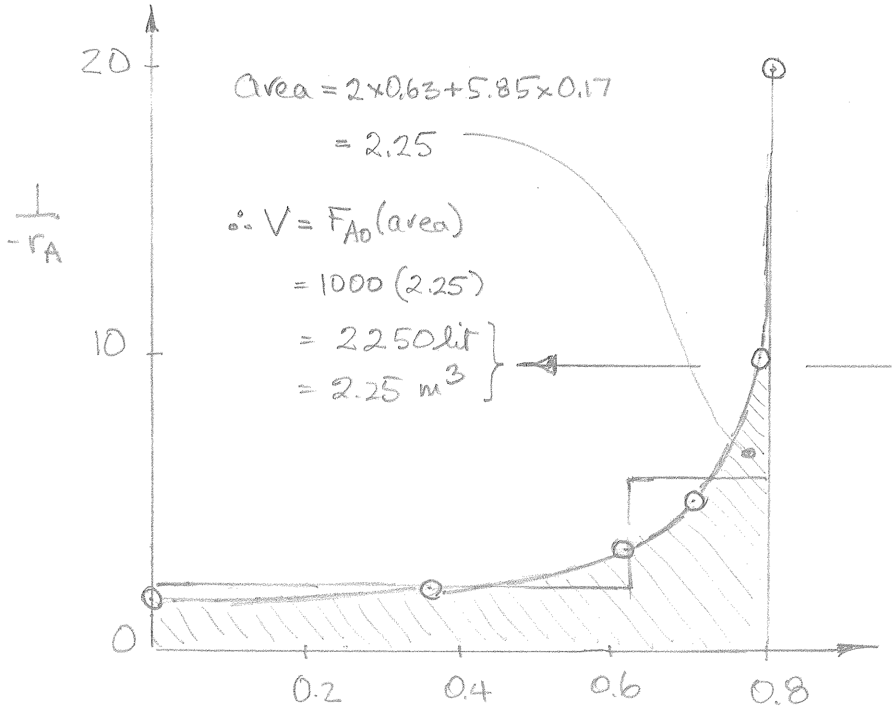
Therefore the slope of the adiabatic

$$\text{slope} = \frac{\mathbf{C}_p}{\Delta H_r} = \frac{1000}{-18000} = -\frac{1}{18}$$

Next, from Fig E3 directly we get

X_A	$-r_A$	$-1/r_A$
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

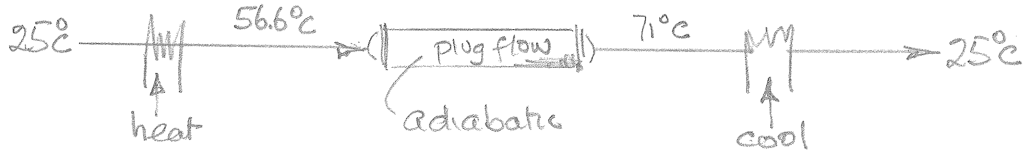




area $= 2\times0.63 + 5.85\times0.17$
$= 2.25$

$\therefore V = F_{A0}(\text{area})$
$= 1000\,(2.25)$
$= 2250\,\text{lit}$
$= 2.25\ \text{m}^3$

Here the feed must be heated, not cooled



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

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

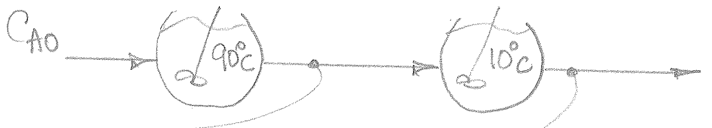
$$= 11.9 \sim 12.7 \text{ m}^3 \longleftarrow$$

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°C = 283K	90°C = 363K
k_1	0.6199	66.31
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 ~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



$$\frac{C_R}{C_R + C_T} = \frac{66.31}{66.31 + 163.83} = 0.288$$

$$\frac{C_S}{C_S + C_U} = \frac{15.4}{15.4 + 3.84} = 0.800$$

fraction which forms R

$$\frac{C_S}{\Delta C_A} = 0.288(0.8) = 0.23 \longleftarrow$$

10.1 For the 4 schemes: G, N, N, Good ◄———

10.3 Here we have: N, N, N, G ◄———

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

$$E_1 > E_2 \text{ and } E_1 > E_3$$ ◄——— a)

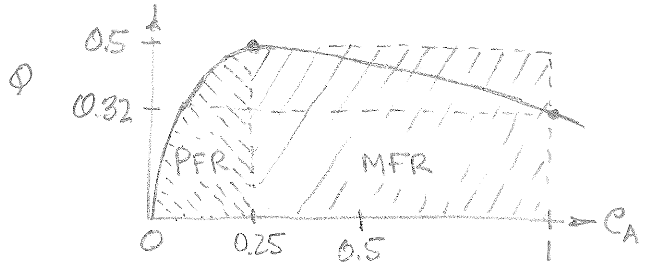
b) We should have a falling temperature when

$$E_1 > E_3 \text{ and } E_1 < E_2$$ ◄——— b)

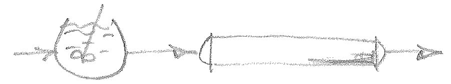
10.7 From Example 1

$$\varphi(S/A) = \frac{0.2C_A}{0.025 + 0.2C_A + 0.4C_A^2}, \text{ and } \begin{cases} C_A = 0.25 \\ C_S = 0.375 \\ \varphi_{max} = \frac{0.375}{1-0.25} = 0.5 \end{cases}$$

The φ vs C_A curve is



so use MFR followed by PFR



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

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

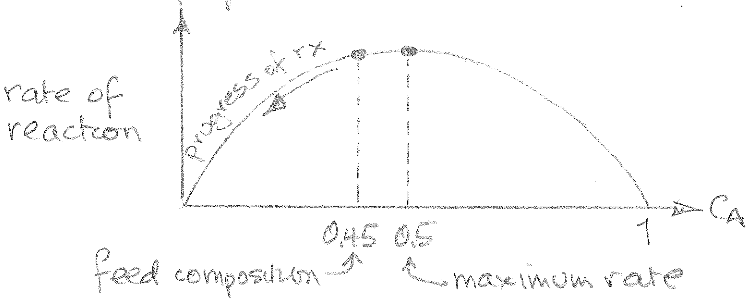
But from a table of integrals: $\int_1^2 \frac{x}{(a+bx)^2} dx = \frac{a}{b^2(a+bx)} + \frac{1}{b^2}\ln(a+bx)\Big|_1^2$

So

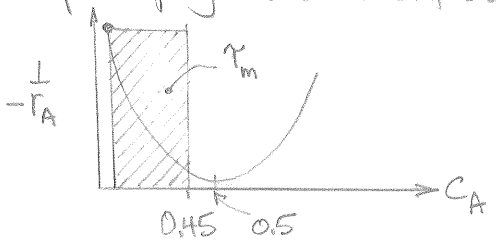
$$C_{Sp} = \left[\frac{1}{16}\cdot\frac{1}{1+4x} + \frac{1}{16}\ln(1+4x)\right]_0^{0.25} = \frac{1}{2}\left[\frac{1}{2} + \ln 2 - 1\right] = 0.0966$$

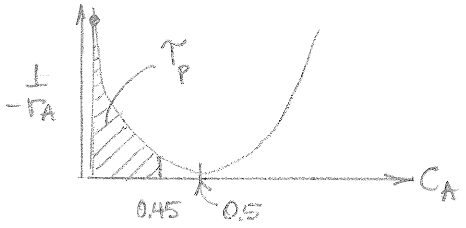
$\therefore C_{S\,total} = C_{Sm} + C_{Sp} = 0.375 + 0.0966 = 0.4716$ ◄———

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



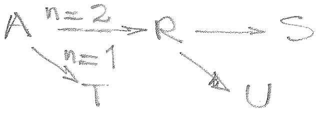
compare plug with mixed flow performance





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

10.11



$C_{A0} = 6$
$C_{R0} = 0.6$
$C_{T0} = 0$

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

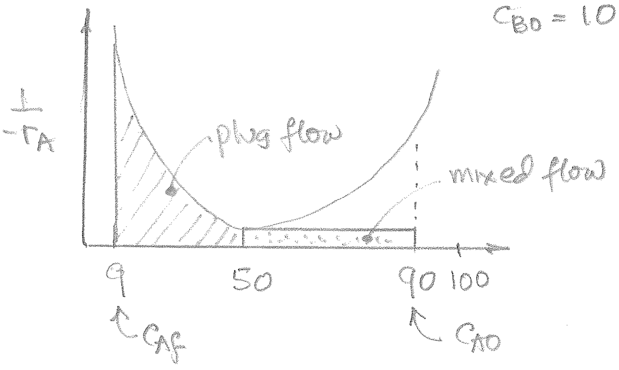
(a) So to maximize C_R/C_T do not react at all
The design of Fig P11 is no good } ← a)

(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 $A+B \longrightarrow B+B \qquad -r_A = kC_AC_B \qquad C_{A0}=90 \quad C_{B0}=10 \qquad C_{Af}=9 \quad C_{Bf}=91$



Use a MFR followed by a PFR ←

10.15 Since $E_1 > E_2$ use a high temperature, or $T = 90°C$

at $90°C = 363K$ $\quad k_1 = 30\, e^{-20000/8.314(363)} = 0.0397\ \text{min}^{-1}$

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

$\therefore\ k_2/k_1 = 0.3322$

From Fig 8.13 or Eqs 8.8 & 8.9 $\quad \frac{C_{R\,max}}{C_{A0}} = 0.58$ ←

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

10.17 Let $A = C_3H_6$
$B = O_2$
$R = C_3H_4O$ (desired)

then
$A + B \longrightarrow R$
$A + 4.5B \longrightarrow S$
$R + 3.5B \longrightarrow S$

$k_2/k_1 = 0.1$
$k_3/k_1 = 0.25$

Rewrite the rates

$$\begin{tikzcd} A \arrow[r, "k_1=10"] \arrow[rr, bend right, "k_2=1"'] & R \arrow[r, "k_3=2.5"] & S \end{tikzcd}$$

From the Denbigh reaction set, eq 49 gives

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

Use plug flow ←

10.19 Given

$$\left.\begin{aligned} k_1 = k_2 &= 2\times10^{13}\exp(-159000/RT) \\ k_3 &= 8.15\times10^{17}\exp(-209000/RT) \\ k_4 &= 2.1\times10^{5}\exp(-83600/RT) \end{aligned}\right\}$$

$$\begin{tikzcd} & S \arrow[dr, "3"] & & \\ A \arrow[ur, "2"] \arrow[rr, "1"] & & R \arrow[r, "4"] & T \end{tikzcd}$$

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

At 1200 K

$k_1 = 2.4\times10^6\ \text{hr}^{-1}$

$k_2 = 2.4\times10^6\ \text{hr}^{-1}$

$k_3 = 650\times10^6\ \text{hr}^{-1}$

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

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

$$\begin{tikzcd} A \arrow[r, "2.4\times10^6"] \arrow[r, bend left=50, "2.4\times10^6"] & R \arrow[r, "48.2"] & T \end{tikzcd} \Longrightarrow A \xrightarrow[\textcircled{5}]{4.8\times10^6} R \xrightarrow[\textcircled{6}]{48.2} T$$

Now find $C_{R\max}$ from Eq 8.8

$$\frac{C_{R\max}}{C_{A0}} = \left(\frac{k_5}{k_6}\right)^{k_6/k_6-k_5} = \left(\frac{4.8\times10^6}{48.2}\right)^{48.2/48.2-4.8\times10^6} = 0.99988 \longleftarrow$$

and

$$\bar{t}_{\text{plug}} = \frac{\ln(k_2/k_1)}{k_2-k_1} = 2.4\times10^{-6}\ \text{hr} = 0.0086\ \text{s} \longleftarrow$$

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 $C_{R\max}$. From Eq 8.7 we find, for this time

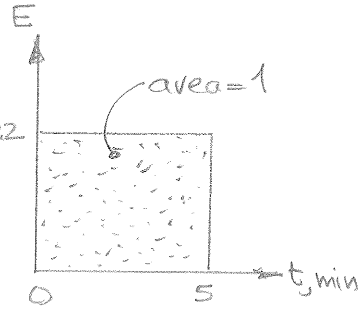
$$\frac{C_R}{C_{A0}} = \frac{k_5}{k_6-k_5}\left[e^{-k_1 t} - e^{-k_2 t}\right] = (-1)\left[0-0.9762\right] = 0.9762$$

11.1 a) Check to see if the results are consistent

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

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

So the results are consistent ← a)



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

c) Find the E curve. From t=0 to 5

$E = \frac{C}{M/v} = \frac{C}{1/4} = 4C = 0.2$ ← c)

11.3 a) Check for consistency

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

But from the experimental curve: compare

$\bar{t} = \frac{1}{3}(18\times1 + 21\times2) = 20\ \text{sec}$

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

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

From the material balance

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

$\therefore\ M = (A)v = \left(52.5\times10^{-6}\ \frac{\text{unit day}}{m^3}\right)\left(6000\ \frac{m^3}{s}\right)\left(\frac{3600\times24\ s}{\text{day}}\right) = 27216\ \text{units}$ ← a)

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

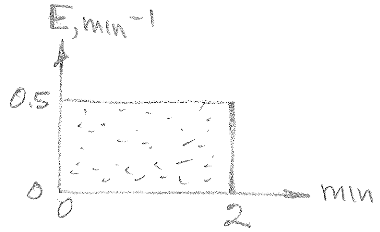
$V = (\bar{t})v = 60\ \text{days}\left(6000\ \frac{m^3}{s}\right)\left(\frac{3600\times24\ s}{\text{day}}\right) =$

$= 3.11\times10^{10}\ m^3$ —— b)

11.7 Calculate the conversion for

$A \rightarrow R$, $C_{A0} = 1\ \text{mol/lit}$

$-r_A = (2\ \text{mol}^{1/2}/\text{lit}^{1/2}\cdot\text{min})\, C_A^{\frac{1}{2}}$



The performance equation is

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

from Eq 3.29

$$(n-1)kC_{A0}^{n}t = \left(\frac{C_A}{C_{A0}}\right)^{1-n} - 1$$

or $$\left(-\tfrac{1}{2}\right)(2)(1)t = \left(\frac{C_A}{C_{A0}}\right)^{1/2} - 1$$ for a batch of material

or $$\frac{C_A}{C_{A0}} = (1-t)^2$$

$$\therefore \frac{C}{C_0} = \int_0^2 (1-t)^2 \left(\tfrac{1}{2}\right) dt = \frac{0.5}{3}(1-t)^3\Big|_2^0 = \frac{1}{6}(1+1) = \frac{1}{3}$$

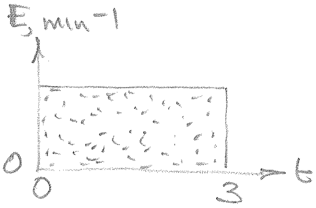
$$\therefore X_A = \frac{2}{3} \longleftarrow$$

11.9 Calculate the conversion for

$A \longrightarrow R$ $C_{A0} = 6$

$-r_A = 3\ \text{mol/lit}\cdot\text{min}$

zero order reaction



The performance equation is $\frac{C_A}{C_{A0}} = \int \left(\frac{C_A}{C_{A0}}\right) E\,dt$

from Eq 3.31 .... $\frac{C_A}{C_{A0}} = 1 - \frac{kt}{C_{A0}}$ for $t < \frac{C_{A0}}{k} = \frac{6}{3} = 2$

$\frac{C_A}{C_{A0}} = 0$ for $t > 2$

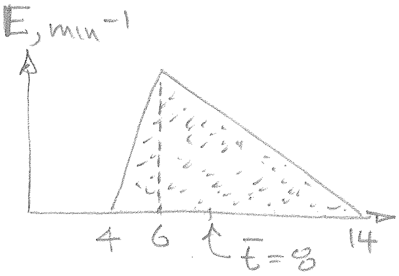
replace into above

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

$$= \frac{1}{6}\,\frac{(2-t)^2}{2}\Big|_2^0 = \frac{1}{6}\left[\frac{2^2}{2} - 0\right] = \frac{1}{3}$$

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

11.11 Calculate the conversion for



$A \rightarrow R$ $\quad C_{A0} = 0.1$ mol/lit

$-r_A = 0.03$ mol/lit·min

$\quad\uparrow$ zero order

Performance equation $\quad \frac{C_A}{C_{A0}} = \int \frac{C_A}{C_{A0}} E\, dt$

zero order

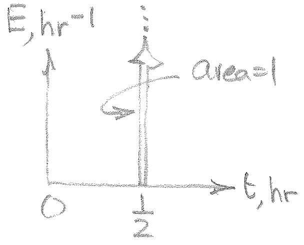
From Eq 3.31 ... $\frac{C_A}{C_{A0}} = 1 - \frac{kt}{C_{A0}} = 1 - \frac{0.03}{0.1} t$ ... for $t < \frac{C_{A0}}{k} = \frac{0.1}{0.03} = 3.33$ min

$\frac{C_A}{C_{A0}} = 0$ ... for $t < 3.33$ min

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

$C_{Af} = 0, \; X_{Af} = 1 \longleftarrow$

11.13 For the solid particles

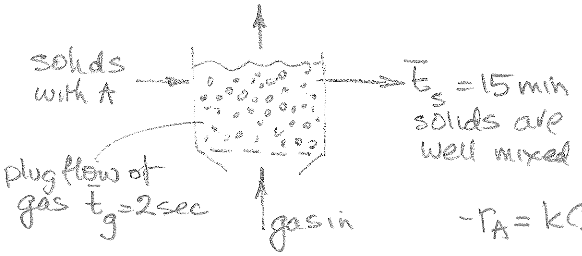


$$\overline{1-X} = \int (1-X) E\, dt = \int_0^1 (1 - \underset{\uparrow = 1\text{ hr}}{t})^3 \delta(t - t_0)\, dt$$

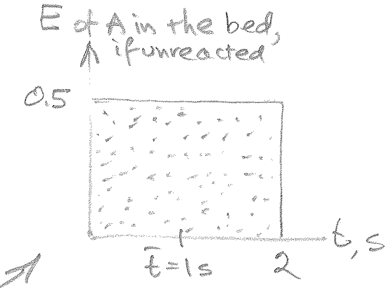
$$= (1-t)^3 \Big|_{\text{at } t = \frac{1}{2}} = \left(\tfrac{1}{2}\right)^3 = 0.125$$

$\therefore \overline{X} = 1 - 0.125 = 0.875 \longleftarrow$

11.15



$-r_A = kC_A = (1\,\text{sec}^{-1})C_A$



Conversion of A

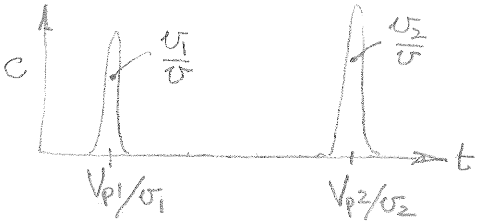
A is released uniformly by solids, so

$$\frac{C_A}{C_{A0}} = \int \left(\frac{C_A}{C_{A0}}\right) E\, dt = \int_0^2 e^{-kt}\, 0.5\, dt = 0.5 \int_0^2 e^{-t}\, dt = 0.5\, e^{-t} \Big|_2^0 = 0.4323$$

$\therefore X_A = 0.5677 \longleftarrow$

$\quad\uparrow$ 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 $v = 1\,m^3/s$ we have

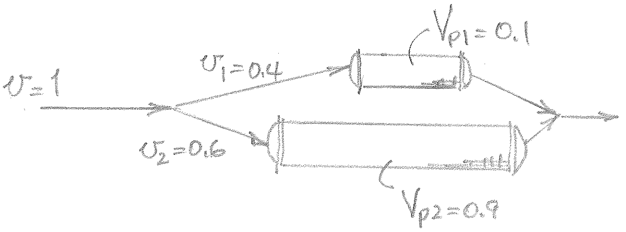


$$v_1 = \frac{16}{16+24} = 0.4\ m^3/min$$

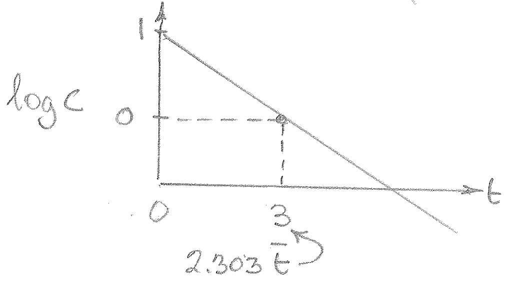
$$v_2 = \frac{24}{16+24} = 0.6\ m^3/min$$

$$V_{p1} = \bar{t}_1 v_1 = (0.25)(0.4) = 0.1\ m^3$$

$$V_{p2} = \bar{t}_2 v_2 = (1.5)(0.6) = 0.9\,m^3$$



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

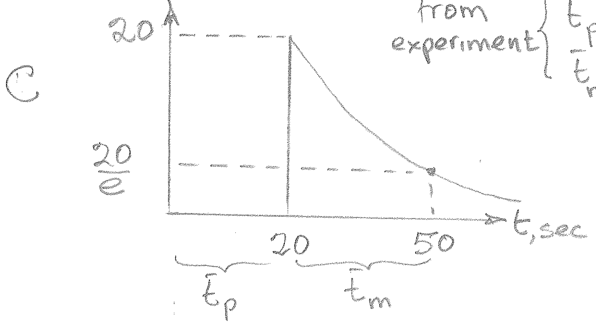
But we know that

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

← 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

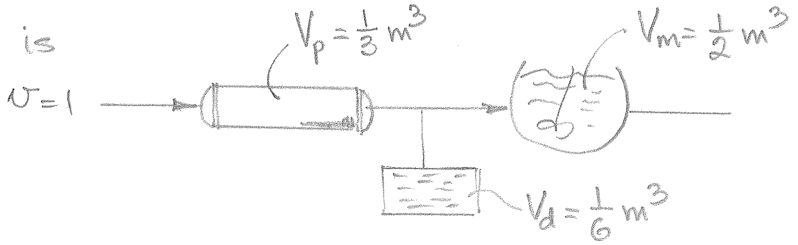


from experiment $\left\{ \begin{array}{l} \bar{t}_p = 20 \\ \bar{t}_m = 30 \end{array} \right\}$ $\bar{t}_{active} = 50\,s$

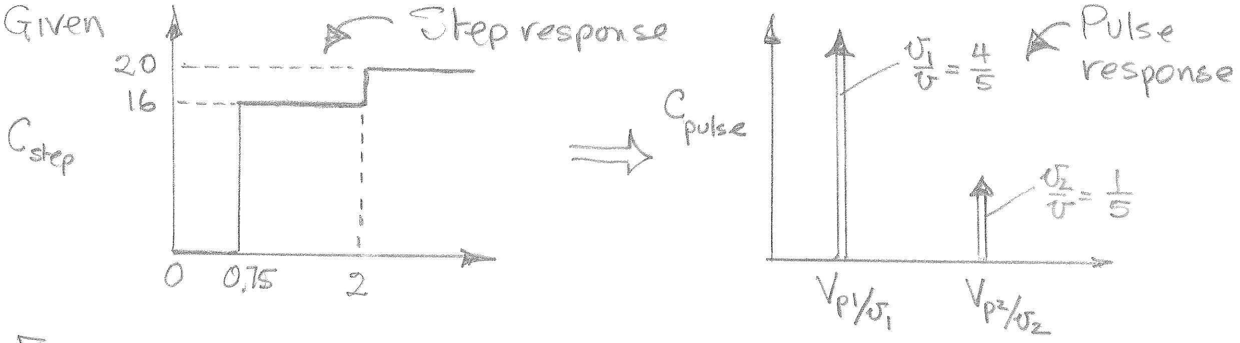
$\bar{t}_{total} = \frac{V}{v} = 60\,s$

$\therefore\ \bar{t}_{dead} = 10\,s$

Thus our model is



12.7 Given



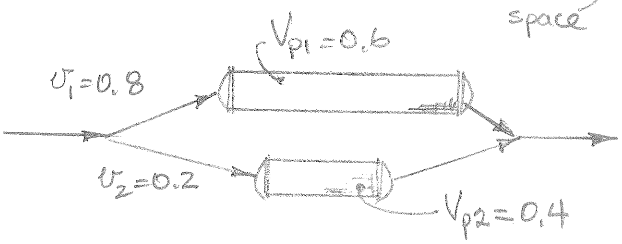
From the pulse response curve

$v_1 = \frac{4}{5} v = 0.8$ $\quad V_{p1} = v_1(0.75) = 0.8(0.75) = 0.6$

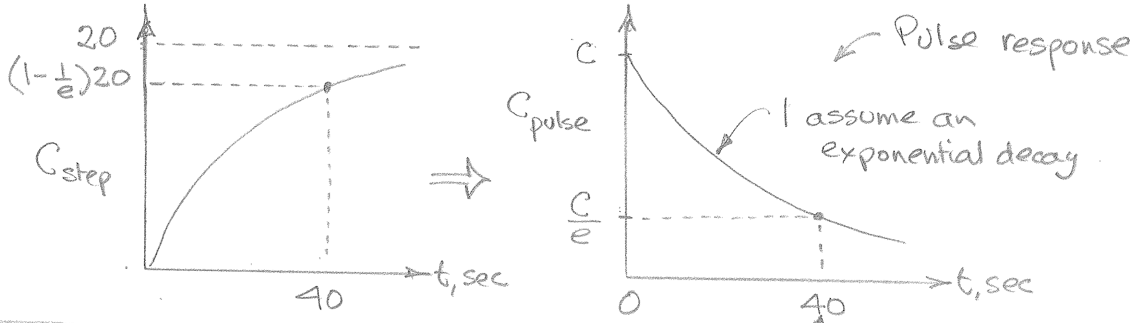
$v_2 = \frac{1}{5} v = 0.2$ $\quad V_{p2} = v_2(2) = 0.2(2) = 0.4$

note: no dead space

So the flow model is



12.9

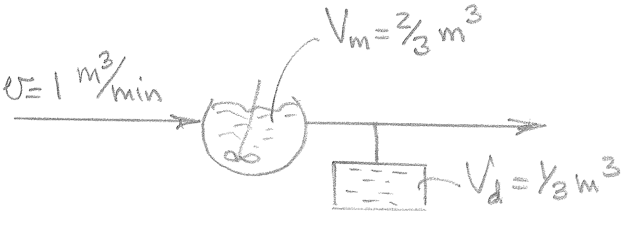


For mixed flow alone this should be 60 sec. However, this curve comes out early, meaning dead spaces are present. This tracer curve shows that $\bar{t} = 40$ sec, thus

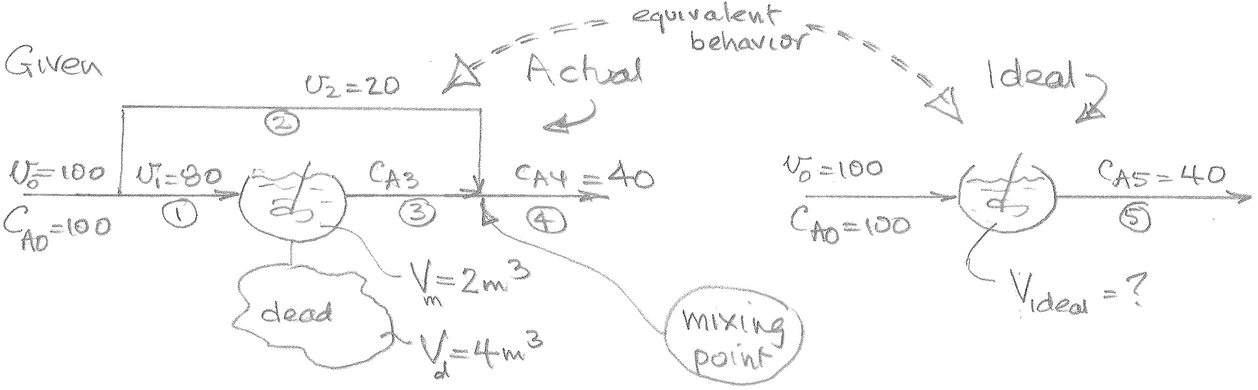
$V_m = 2/3\ m^3$

$V_d = 1/3\ m^3$

and our flow model is



12.11 Given



First let $C_{A0} = 100$, $v_0 = 100$ } It is not necessary to do this, but this assumption makes the calculations simpler.

Now take a material balance about the mixing point

$$v_2 C_{A2} + v_3 C_{A3} = v_4 C_{A4}$$

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 2^{nd} order reaction

$$A + B \longrightarrow R + S \quad \ldots \quad C_{A0} = C_B$$

we have
$$\tau = \frac{V}{v} = \frac{C_{A0} - C_{A3}}{k C_{A3}^2}$$

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

Finally, for the ideal reactor

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

or

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

This is so much smaller than $6 m^3$

13.1 Evaluate the intensity of dispersion for the middle section.

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

Width at 61% = 0.70

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

$$\sigma_2^2 = 0.1225$$

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

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

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

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

From the blast furnace experiment $\frac{D}{ud_p} = 10.1$

From the correlation for smaller solids, Fig 17 : $\frac{D}{ud_p} = 0.5$ ←

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 experiment:

t, sec	$\bar{t}$, sec	C
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:

$\Sigma C = 565$

$\Sigma tC = 17687.5$

$\Sigma t^2C = 573781.25$

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

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

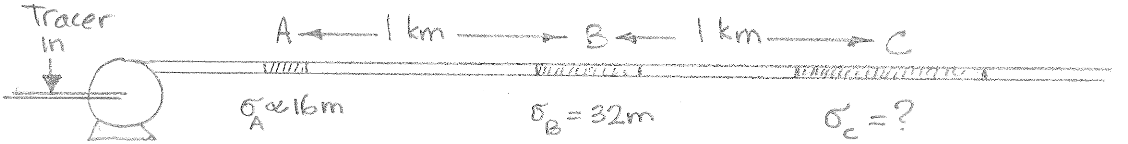
$$\frac{D}{uL} = \frac{\sigma^2}{2(\bar{t})^2} = 0.018 \longleftarrow$$

Now calculate the volume of the baffles

From mat. balance
$$\left.\begin{aligned} V &= (1.21\times10^2)(\pi\times1.75^2) = 1164\,cm^3 \\ v &= 1300\,cm^3/min = 21.67\,cm^3/s \end{aligned}\right\} \bar{t} = \frac{1164}{21.67} = 53.72 \text{ sec}$$

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

13.5



$\sigma_A \propto 16m$ $\quad\quad$ $\sigma_B = 32m$ $\quad\quad$ $\sigma_C = ?$

$\sigma_A^2 \propto 256$ $\quad\quad$ $\sigma_B^2 \propto 1024$ $\quad\quad$ $\sigma_C^2 \propto ?$

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

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

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

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

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

or $\sigma_C^2 = 1792$ $\quad\quad$ or Width $= k\,\sigma_C = 42.3\,m$ ←

13.7 First find the σ^2 for this flow

$$Re = \frac{du\rho}{\mu} = (0.255)(1.1)/0.9\times10^{-6} = 3.12\times10^{5}$$

From Fig 15: $\quad D/ud_t = 0.22$

From Eq 8: $\quad \dfrac{D}{uL} = \left(\dfrac{D}{ud_t}\right)\left(\dfrac{d_t}{L}\right) = 0.22\left(\dfrac{0.255}{1000000}\right) = 5.61\times10^{-8}$

$$\frac{\sigma^2}{\bar{t}^2} = \sigma_\theta^2 = 2\left(\frac{D}{uL}\right) = 2\,(5.61\times10^{-8}) = 11.22\times10^{-8}$$

$$\therefore \sigma = (11.22\times10^{-8})^{1/2}\ \frac{1000000}{1.1} = 304.5\ \text{sec}$$

∴ the width at $1\sigma = (304.5)(1.1) = 335\ m$

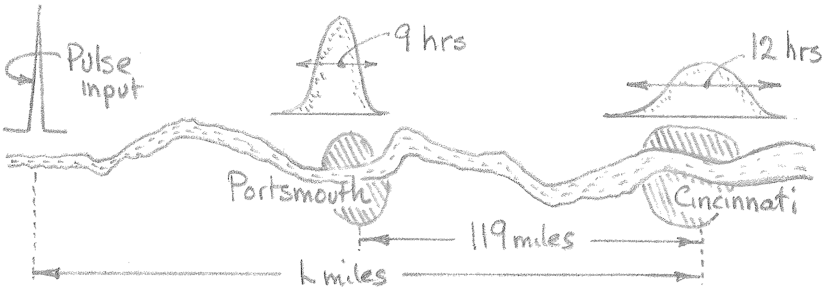
From 5/95 to 95/5 Fig 12 shows that this includes

$(1.656\times2)\sigma$ of width

∴ the 5/95 to 95/5% width is

$$\underset{\text{width of one }\sigma^2}{(335m)}(1.655\times2) = 1105\ m \longleftarrow$$

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)

$$\sigma^2_{\text{tracer curve}} \propto \begin{pmatrix}\text{distance from}\\ \text{point of injection}\end{pmatrix} \quad \text{--or--} \quad \begin{pmatrix}\text{spread}\\ \text{of curve}\end{pmatrix} \propto \sqrt{\begin{matrix}\text{distance downstream}\\ \text{from injection point}\end{matrix}}$$

$\therefore$ from the Cincinnati reading ... $12\text{ hrs} = kL^{1/2}$

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

Dividing one by the other & solving for L gives $L = 272$ miles

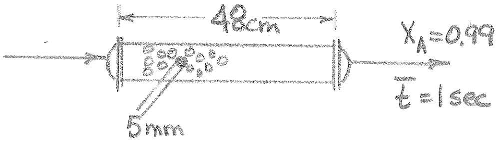
Since the dumping may not be instantaneous any location where $L \leq 272$ miles is suspect or

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, $\varepsilon_A = 0$, we have

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

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

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

$$\frac{D\epsilon}{ud_p} = 1 \quad \text{... thus} \quad \frac{D}{ud_p} = 2.5$$

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

$$\frac{L}{L_p} = \frac{k_{true}}{k_{measured}} = 1 + k\tau\left(\frac{D}{uL}\right) = 1 + k\tau\left(\frac{D}{ud_p}\right)\left(\frac{d_p}{L}\right)$$

$$= 1 + 4.6(2.5)\left(\frac{5\,mm}{480\,mm}\right) = 1.1198$$

$$\therefore k_{true} = (4.6\,sec^{-1})(1.1198) = 5.15\,sec^{-1} \longleftarrow \text{b)}$$

<u>Note</u>: 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.

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

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

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

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

So from Eq 21

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

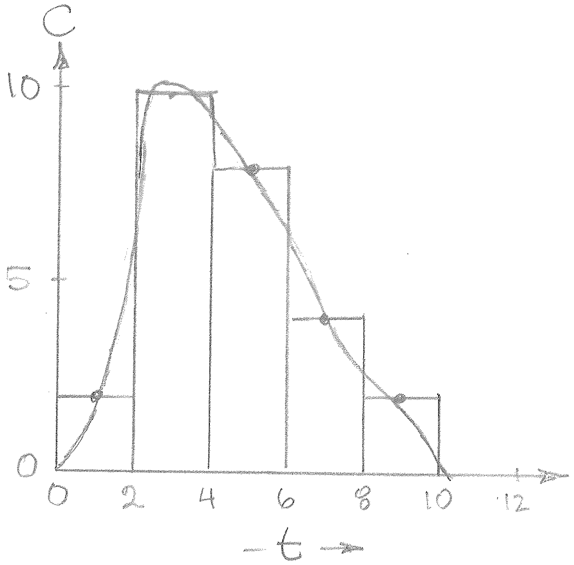
or $= 0.001172$

$$\therefore C_A = 1.17 \longleftarrow$$

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

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

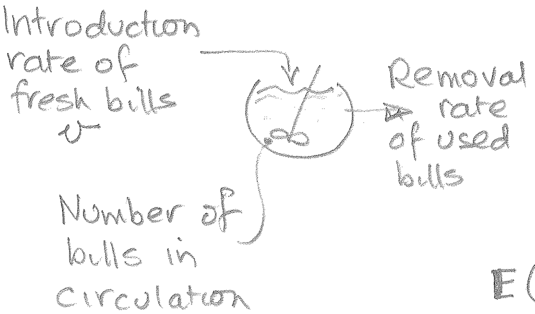
$$\sigma^2 = \frac{\Sigma t^2C}{\Sigma C} - \bar{t}^2 = \frac{1^2(2)+3^2(10)+\cdots}{2+10+\cdots} - (4.538)^2 = 4.4038$$

From Eq 3

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

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

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



$$\left.\begin{array}{l} v = 10^9 \text{ bills/yr} \\ V = 1.25\times10^9 \text{ bills} \end{array}\right\} \bar{t} = \frac{V}{v} = 1.25 \text{ yrs}$$

n = no. of bills

n_0 = total no. of bills.

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

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

$$F(t) = 1 - e^{-t/\bar{t}} = 1 - e^{-t/1.25} \qquad \left.\begin{matrix} t=0 & F(t)=0 \\ t=\infty & F(t)=1 \end{matrix}\right\} \longleftarrow$$

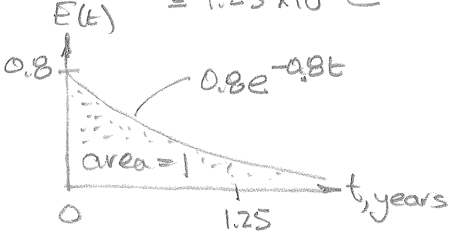
b) The number of bills in circulation which are over 21 yrs of age is given by the E(t) function. Thus

$$n = \int_{21}^{\infty} n_0 E(t)\,dt \quad \text{--- where} \quad n_0 = 1.25\times10^9$$

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

$$\therefore n = \int_{21}^{\infty} (1.25\times10^9)(0.8e^{-0.8t}) \longleftarrow$$

$$= 1.25\times10^9 e^{-0.8t}\Big|_{21}^{\infty} = (-1.25\times10^9)\left[\frac{1}{e^{\infty}} - \frac{1}{e^{0.8(21)}}\right] = 63.2 \text{ bills}$$



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

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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

$$\frac{1}{N} = \sigma_\theta^2 = \frac{\sigma^2}{\bar{t}^2} = \frac{2/3}{(10)^2} = 0.67\times10^{-2} \quad \cdots \therefore N = 150 \text{ tanks}$$

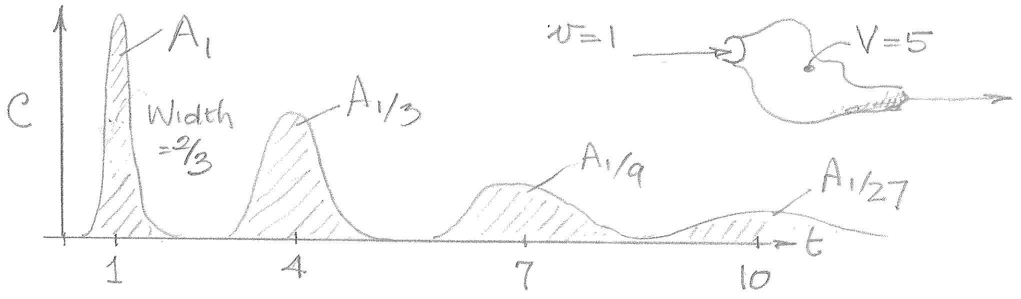
$$\therefore k\bar{t}_i = \frac{6.9078}{150} = 0.0461$$

For tanks in series

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

$$\therefore C_A = 1.16 \longleftarrow$$

14.7



First approximate each pulse by plug flow. Then from Fig 12·1

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

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

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

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

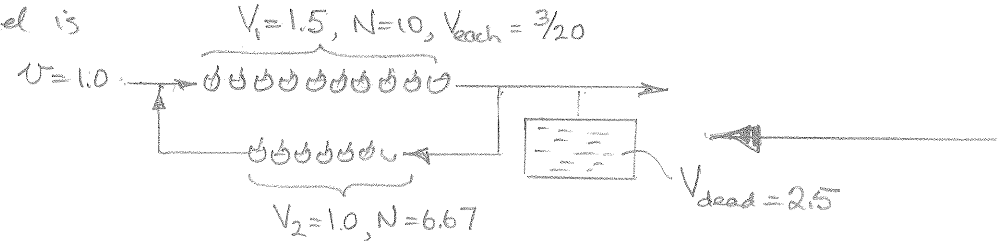
$\therefore V_{\text{dead}} = 5 - 2.5 = 2.5$

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

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

and $\quad N_2 = 2/3\, N_1 = 2/3\,(10) = 6.67$ tanks

Thus our model is



Verify

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

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

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

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

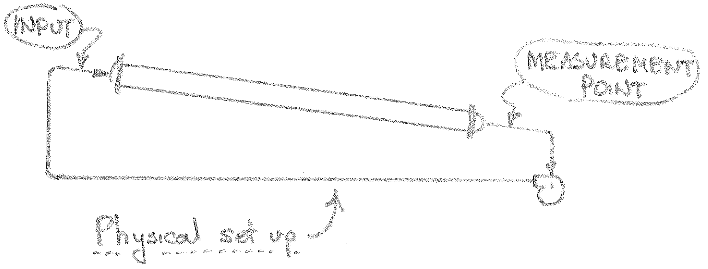
for 1st peak: $N_{1\,pass} = 1 + 4\left(\frac{16.2\,mm}{3.2\,mm}\right)^2 = 104$ tanks ... or N = 104 tanks/pass

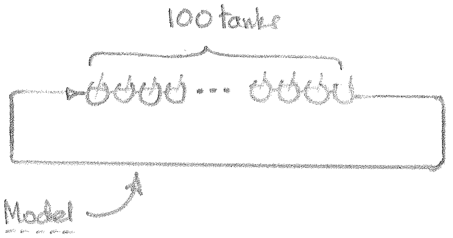
for 2nd peak: $N_{2\,passes} = 1 + 4\left(\frac{32.6}{4.6}\right)^2 = 202$ tanks ... or N = 101 tanks/pass

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

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

These values average to $N \cong 100$ 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

$\Sigma C = 213$ $\quad \bar{t} = 2149/213 = 10.09$ min

$\Sigma tC = 2149$ $\quad \sigma^2 = 37685/213 - (10.09)^2 = 75.1168$

$\Sigma t^2 C = 37685$

$$\therefore \sigma_\theta^2 = \frac{\sigma^2}{\bar{t}^2} = \frac{75.1168}{(10.09)^2} = 0.7378$$

Next determine the behavior in an ideal plug flow reactor

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

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

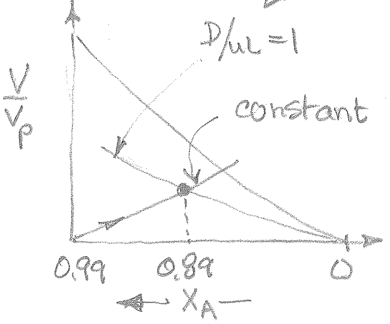
(a) Use the dispersion model

Here Eq. 13.15 relates σ_θ^2 with D/uL. So

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

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

Then from Fig. 13.19



From this figure

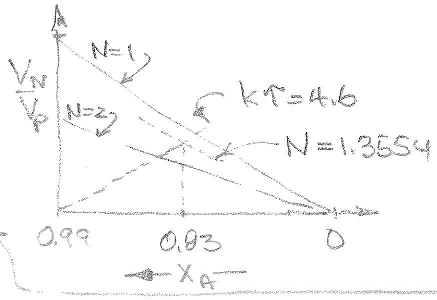
$X_{\text{disp.}} = 0.89 \longleftarrow$ a)

14.11 (continued) (b) Use the tanks-in-series model

from Eq. 3 we find

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

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



b)

(c) Use the tracer data directly

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

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

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

t, min	C	$e^{-0.456 t_i} C_i/213$
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	1×10^{-6} ≈ 0
25–27	3	-
29–31	2	-
33–45	1	-
	$\Sigma C = 213$	$\Sigma = 0.1191$

Now follow the method of Example 11.4

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

$$= \Sigma e^{-kt_i} \frac{C}{\Sigma C}$$

$$= \sum_i e^{-0.456 t_i} \cdot \frac{C_i}{213}$$

now tabulate

$X_{from\ curve} = 0.88$ ← c)

(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 D/uL = 1. Thus we'd expect that the answers to parts a) and c) should agree. They do.

15.1 Given, a zero order reaction

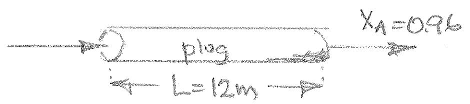
For plug flow: $\frac{C_A}{C_{A0}} = 1 - X_A = 0.2 = 1 - \frac{k\tau}{C_{A0}}$ ... or $\frac{k\tau}{C_{A0}} = 0.8$

For convective flow Eq 9 gives

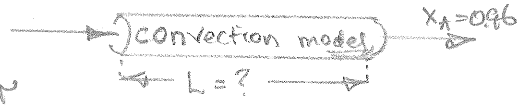
$$\frac{C_A}{C_{A0}} = \left(1 - \frac{k\tau}{2C_{A0}}\right)^2 = \left(1 - \frac{0.8}{2}\right)^2 = 0.36 \quad \therefore X_A = 0.64 \longleftarrow$$

15.3 For second order and plug flow

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



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



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

then Eq 11 gives

$$X_A = 1 - \frac{C_A}{C_{A0}} = \underbrace{y\left[1 - \frac{y}{2}\ln\left(1 + \frac{2}{y}\right)\right] = 0.96}_{\text{solve by trial \& error}} \longrightarrow$$

guess y	calculate X_A
24	0.9477
36	0.9644
30	0.9577
32	0.9602

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

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

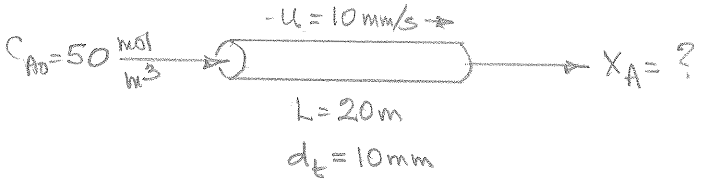
15.5

$A \rightarrow R \quad -r_A = kC_A^2$

$\rho = 1000\ kg/m^3$

$\mathcal{D} = 10^{-9}\ m^2/s$

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



First find which regime applies (see Fig 2)

$$\left.\begin{aligned} Re &= \frac{du\rho}{\mu} = \frac{0.01(0.01)1000}{10^{-3}} = 100 \\ Bo &= \frac{ud_t}{\mathcal{D}} = \frac{0.01(0.01)}{10^{-9}} = 10^5 \\ \frac{L}{d_t} &= \frac{20}{0.01} = 2000 \end{aligned}\right\}$$

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

$$\mathbf{D} = \frac{u^2 d_t^2}{192\,\mathscr{D}} = \frac{(0.01)^2(0.01)^2}{192(10^{-9})} = 5.21\times10^{-2}\ \frac{m^2}{s}$$

$$\left.\begin{aligned} \frac{\mathbf{D}}{uL} &= \frac{5.21\times10^{-2}}{(0.01)(20)} = 0.26 \\ kC_{A0}\tau &= (10^{-3})(50)(20/0.01) = 100 \end{aligned}\right\} \quad \begin{aligned} &\text{From Fig 13.20} \\ &\frac{C_A}{C_{A0}} = 0.022 \ \cdots \quad X_A = 0.978 \end{aligned}$$

Convection model

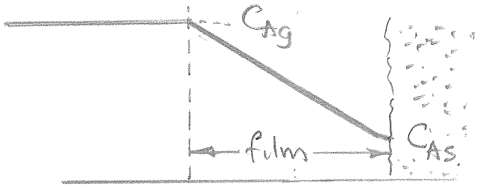
$$\frac{C_A}{C_{A0}} = 1 - kC_{A0}\tau\left[1 - \frac{kC_{A0}\tau}{2}\ln\left(1+\frac{2}{kC_{A0}\tau}\right)\right] = 1-100\left[1-\frac{100}{2}\ln\left(1+\frac{2}{100}\right)\right]$$

$$= 0.013$$

$$\therefore X_A = 0.987$$

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

17.1 For the mass transfer step



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

For the reversible reaction step

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

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

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

17.3 For the interface between gas bubbles and liquid

$$(-r) = -\frac{1}{V}\frac{dN}{dt} = k_{Al}\, a_i\left(C_{Ai}-C_{Al}\right) \quad \text{--- (i)}$$

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

$$(-r) = -\frac{1}{V}\frac{dN}{dt} = k'_{Al}\, a_s\left(C_{Al}-C_{As}\right) \quad \text{--- (ii)}$$

liquid-solid mass transfer coefficient

area of liquid-solid interface per volume of reactor

For surface reaction

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

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

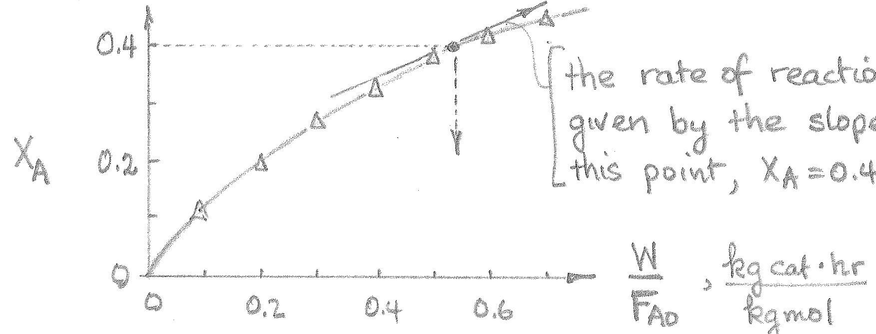
$$(-r) = -\frac{1}{V}\frac{dN}{dt} = \frac{1}{\dfrac{1}{k_{Al}a_i} + \dfrac{1}{k'_{Al}a_s} + \dfrac{1}{k_s}}\, C_{Ai} \longleftarrow$$

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



the rate of reaction at $X_A = 0.4$ is given by the slope of the curve at this point, $X_A = 0.4$

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

$$-r_A' = \frac{0.482 - 0.23}{0.8 - 0.1} = 0.36 \, \frac{\text{kmoles converted}}{\text{kg cat}\cdot\text{hr}} \longleftarrow \text{a)}$$

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

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

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

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

18.5 A → 3R, n=1 ··· 1st order

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

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

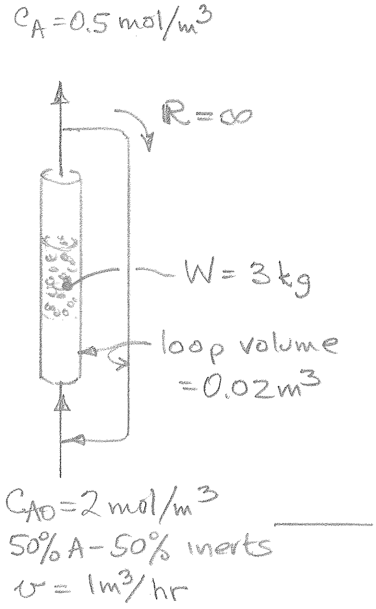
Mixed flow reactor

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

Thus

$$\underset{\text{mol/kg·hr}}{-r'_A} = \left(0.8\ \frac{m^3}{kg\cdot hr}\right)\left(C_A\ \frac{mol}{m^3}\right) \longleftarrow$$

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



18.7 Given A → R,

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

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

First find the rate at the 3 conditions

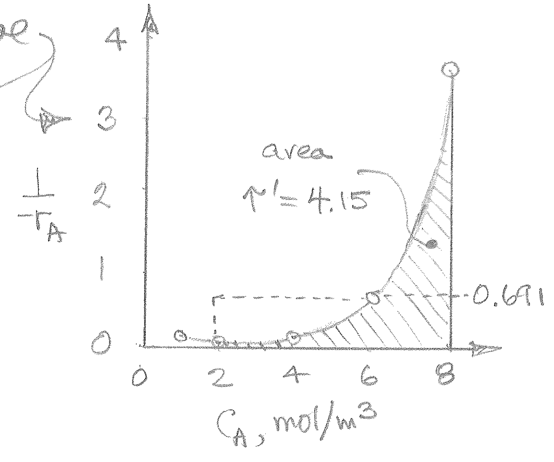
v	X_A	C_A	$-r'_A = C_{A0}X_A v/W$
3	0.2	8	10(0.2)(3)/4 = 1.5
2	0.3	7	10(0.3)(2)/4 = 1.5
1.2	0.5	5	10(0.5)(1.2)/4 = 1.5

Therefore Zero order

$$-r'_A = 1.5\ mol/kg\cdot hr \longleftarrow$$

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

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

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

18.11

$v = 1000\ \mathrm{m^3/hr}$

$C_{A0} = 100\ \mathrm{mol/m^3}$

W = ?

$X_A = 0.8$

$-r_A' = \frac{50C_A}{1+0.02C_A}$, $\mathrm{mol/kg\cdot hr}$

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)

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

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

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

18.13

$v_0 = 10\ \mathrm{m^3/hr}$

$C_{A0} = 0.1\ \mathrm{mol/m^3}$

$C_{B0} = 10\ \mathrm{mol/m^3}$

W = 4 kg

$X_A = ?$

$A + B \longrightarrow R + S$

$-r_A' = 0.6\,C_A C_B$, $\mathrm{mol/kg\cdot hr}$

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

$$\therefore\ -r_A' = 0.6\,C_A C_B = 0.6\,C_A(10) = 6C_A$$

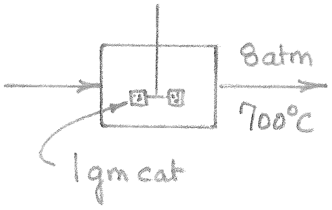
$$\tau' = \frac{W}{v} = \frac{4}{10} = 0.4\ \mathrm{kg\cdot hr/m^3}$$

For a first order reaction

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

therefore $$\left.\begin{aligned} X_A &= 90.9\% \\ X_B &= 0.909\% \end{aligned}\right\} \longleftarrow$$

18.15 Sketch out what we know at the start:—



$$A \longrightarrow 3R$$

$$1 \quad \text{"} \quad 3$$

$$\varepsilon_A = \frac{3-1}{1} = +2$$

$$\frac{C_A}{C_{A0}} = \frac{1-X_A}{1+2X_A}$$

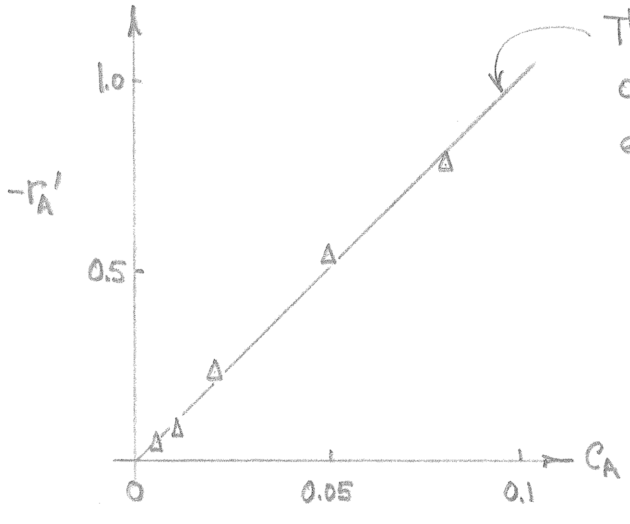
$$\overset{\text{gm cat}}{W} \over \underset{\text{mol/hr}}{F_{A0}} = \frac{X_A}{\underset{\text{mol/hr·gmcat}}{(-r_A')}} \quad \cdots (i)$$

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

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



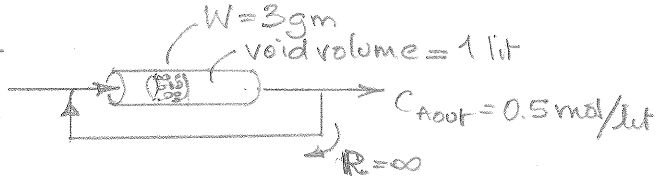
This gives a good straight-line fit of slope 10. thus our rate equation is

$$\underset{\text{mol/hr·gmcat}}{-r_A'} = \underset{\text{lit voids/hr·gmcat}}{10}\,\underset{\text{mol/lit voids}}{C_A}$$

18.17

$C_{A0} = 2$ mol/lit

$v_0 = 1$ lit/hr



$A \rightarrow R$

second order

$-r_A' = kC_A^2$

(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

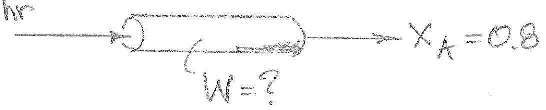
$$\therefore k' = \frac{v_0}{W} \cdot \frac{C_{A0}-C_A}{C_A^2}$$

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

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

$v_0 = 1000$ lit/hr

$C_{A0} = 1$ mol/lit



For plug flow

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

$$\therefore W = \frac{1000\ \text{lit/hr}}{2\ \text{lit}^2/\text{mol}\cdot\text{gmcat}\cdot\text{hr}}\left[\frac{1}{0.2\ \text{mol/lit}} - \frac{1}{1\ \text{mol/lit}}\right] = 2000\ \text{gm}$$

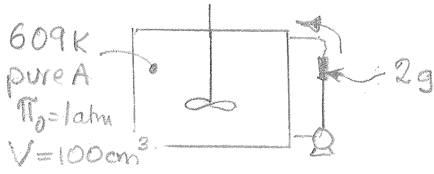
$$= 2\ \text{kg} \longleftarrow \text{b)}$$

(c) Add inert solids

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

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

18·19



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

$$2A \rightarrow R$$

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

$$p_A = p_{A0} + \frac{a}{\Delta n}(\pi_0 - \pi)$$
$$= 1 + \frac{2}{(-1)}(1 - \pi)$$
$$= 2\pi - 1 \quad \cdots\cdots (i)$$

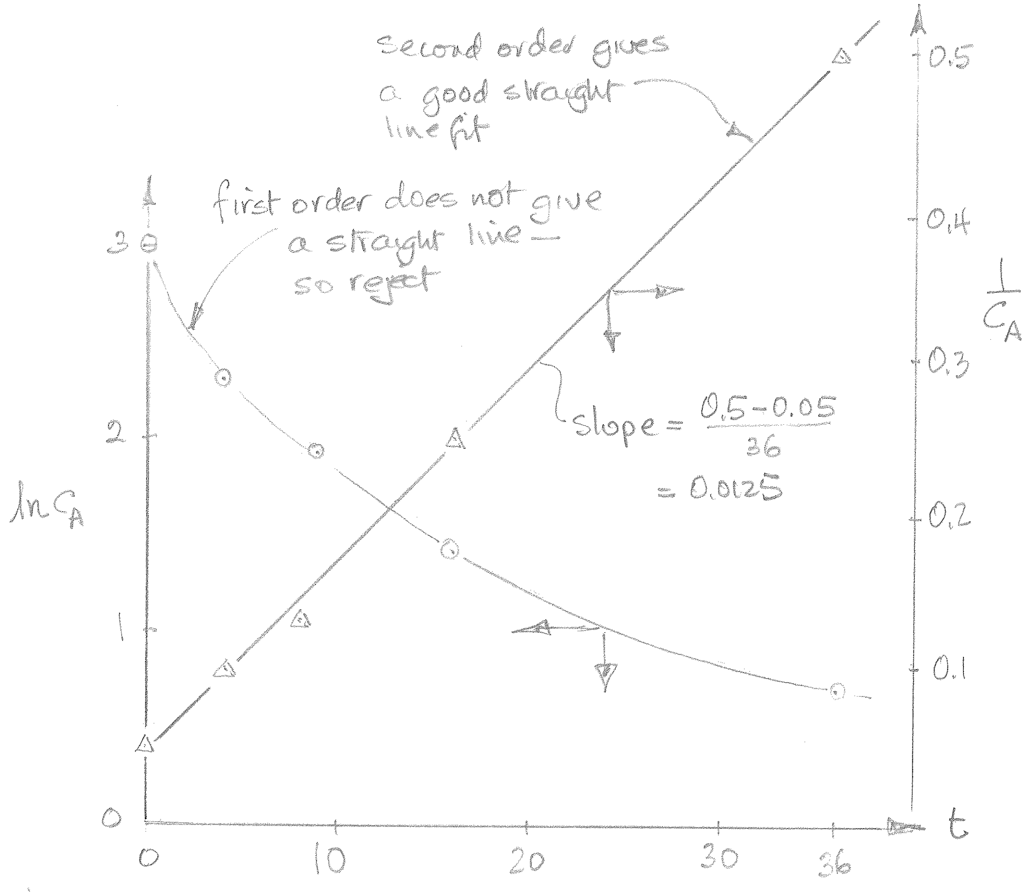
Tabulate the data

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 (i)

first order test

second order test



Therefore the rate equation is: $r_A = 0.0125\, C_A^2$ mol/m³·min

or $r_A' = \frac{V}{W} r_A = \frac{100 cm^3}{2 gm}\left(\frac{1000 gm}{1 kg}\right)\left(\frac{m^3}{10^6 cm^3}\right)(0.0125 C_A^2) = 6.25\times10^{-4} C_A^2$ $\boxed{\frac{mol}{kg \cdot min}}$

18.21

Given A → R, $-r_A''' = 0.1 C_A^2$, mol/m³·s

$d_p = 6$ mm
$\mathcal{D}_{eff} = 10^{-6}$ m³/m·s
$C_{A0} = 100$ mol/m³

Find the effectiveness factor & the amount slowed by diffusion

For nth order rx: $M_T = \frac{d_p}{6}\sqrt{\frac{n+1}{2}\cdot\frac{k'''C_A^{n-1}}{\mathcal{D}_{eff}}}$

$$= \frac{6\times10^{-3}}{6}\sqrt{\frac{2+1}{2}\cdot\frac{(0.1)(100)^{2-1}}{10^{-6}}} = 3.873$$

∴ from the chart of Fig 5 or 6: $\mathcal{E} = 0.23$ ◄

Note If we mistakenly assume 1st order kinetics

$$M_T = L\sqrt{\frac{k'''}{\mathcal{D}}} = \frac{6\times10^{-3}}{6}\sqrt{\frac{0.1}{10^{-6}}} = 0.3162 \quad \text{or} \quad \overset{\text{quite wrong}}{\mathcal{E} = 1}$$

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 $\tau' = \frac{W}{v} = \frac{C_{A0}-C_A}{k'C_A}$

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 infuence 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 ½ 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:

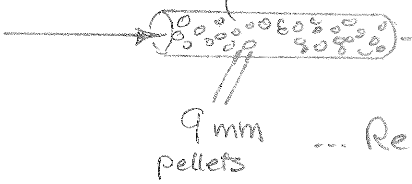
$\frac{k_2}{k_1} = 0.25$ ... and by eliminating pore diffusion in backmix flow we can get ... $\frac{C_R}{C_{A0}} = 0.44$

... and by eliminating pore diffusion & using plug flow we can get ... $\frac{C_R}{C_{A0}} = 0.63$

So use smaller pellets in a packed & we should be able to achieve as high as ... $\frac{C_R}{C_{A0}} = 0.63$ ⟵

18:31

first order, A ⟶ R, strong pore diffusion regime



$\longrightarrow X_A = 0.632$

... Replace with 18mm pellets

Note that in the regime of strong pore diffusion resistance doubling the pellet size halves the rate constant

For 9mm pellets, plug flow, $\varepsilon_A = 0$

$$\ln \frac{1}{1-X_A} = (k'_{obs}\tau')_1 \quad \cdots \text{ or } \quad X_A = 1 - e^{-k'_{obs,1}\tau_1}$$

$$\therefore k'_{obs,1}\tau_1 = \ln \frac{1}{1-0.632} = 1$$

For the 18 mm pellets

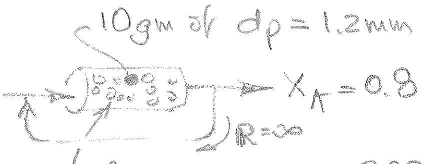
$$(k'_{obs}\tau)_2 = 2$$

$$\therefore \quad X_{A2} = 1 - e^{-(k_{obs}\tau)_2} = 1 - e^{-\frac{1}{2}}$$

or $X_{A2} = 0.393$ ⟵

18.33 From experiment

pure A
$v = 4\,cm^3/s$
1 atm
336°C



(for catalyst $\rho = 2000\,kg/m^3$
$\mathscr{D}_e = 10^{-6}\,m^3/m\,cat \cdot s$

Design a commercial unit for $X_A = 0.8$, either

- a fluidized bed (mixed flow) using $d_p = 1\,mm$ particles
- a packed bed (plug flow) using $d_p = 15\,mm$ particles

Which design needs less catalyst?

For the experimental run

$$\tau' = \frac{C_{A0}X_A}{-r'_{A,obs}} \quad \text{or} \quad -r'_{Aobs} = \frac{C_{A0}X_A}{W/v}$$

$$C_{A0} = \frac{p_{A0}}{RT} = \frac{101325}{(8.314)(336+273)} = 20\ mol/m^3$$

$$-r'_{Aobs} = \frac{20(0.8)}{0.01/4\times10^{-6}} = 0.0064\ mol/kg\cdot s \quad \cdots r'''_{Aobs} = -r'_{Aobs}\left(\frac{W}{v}\right) = 12.8\ mol/m^3\cdot s$$

$$\therefore M_W = \frac{-r'''_A L^2}{\mathscr{D} C_{As}} = \frac{12.8(1.2/6\times10^{-3})^2}{10^{-6}(20)(1-0.8)} = 0.128 \quad \cdots \varepsilon_{expt} = 1$$

For the packed bed

$$\left.\begin{aligned} &L = 2.5\times10^{-3}m \\ &M_T = 2.5\times10^{-3}\sqrt{3.2/10^{-6}} = 4.472 \end{aligned}\right\} \cdots \therefore \varepsilon = \frac{1}{M_T} = 0.2236$$

and $$\frac{W}{v} = \frac{1}{k'\varepsilon}\ln\frac{C_{A0}}{C_A} = \frac{1}{0.016(0.2236)}\ln\frac{20}{4} = 4500\ kg/m^3\cdot s \longleftarrow$$

For the fluidized bed

$$\left.\begin{aligned} &L = 1.67\times10^{-4}m \\ &M_T = 1.67\times10^{-4}\sqrt{3.2/10^{-6}} = 0.2987 \end{aligned}\right\} \cdots \therefore \varepsilon = 1$$

and $$\frac{W}{v} = \frac{1}{k'\varepsilon}\frac{C_{A0}X_A}{C_{A0}(1-X_A)} = \frac{1}{0.0016(1)}\cdot\frac{0.8}{1-0.8} = 2500\ kg/m^3\cdot s \longleftarrow$$

Conclusion : The fluidized bed is better because it needs only 56% of the packed bed catalyst $\longleftarrow$

18.35 Check for pore diffusion resistance. If it is important it will affect the observed rate constant

$$k''' = \left(2\ \frac{m^3}{m^3 bed \cdot s}\right)\left(\frac{2 m^3 bed}{1 m^3 catalyst}\right) = 4\ \frac{m^3}{m^3 cat \cdot s}$$

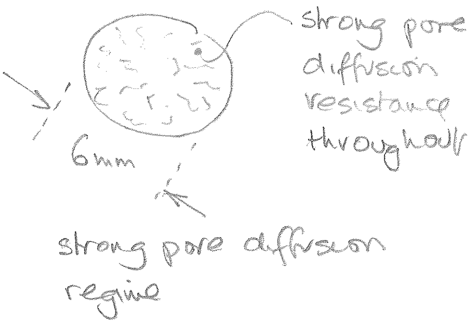
$$M_T = L\sqrt{\frac{k'''}{D}} = \frac{6\times10^{-3}}{6}\sqrt{\frac{4}{4\times10^{-8}}} = 10 \quad \cdots \therefore \text{ strong pore diffusion, and } \mathcal{E} = 0.1$$

$$\therefore\ \tau''' = \frac{C_{A0}V_{cat}}{F_{A0}} = \int\frac{dC_A}{k'''\mathcal{E}C_A} = \frac{1}{k'''\mathcal{E}}\ln\frac{C_{A0}}{C_A}$$

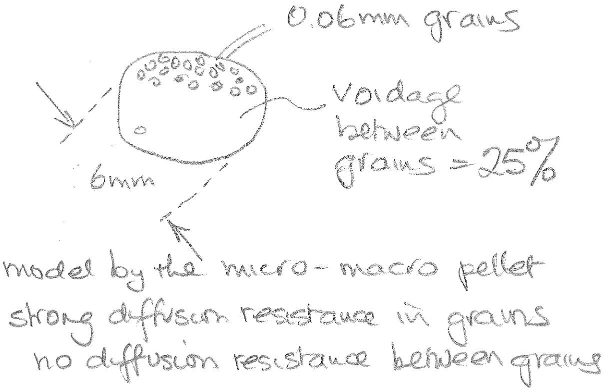
$$\text{or } V_{cat} = \frac{F_{A0}}{C_{A0}k'''\mathcal{E}}\ln\frac{C_{A0}}{C_A} = \frac{10^4/3600}{10^3(4)(0.1)}\ln\frac{10}{1} = 0.016$$

$$\therefore\ W = V_{cat}\,\rho_{cat} = V_{cat}\left(\frac{\rho_{bulk}}{\text{voidage}}\right) = 0.016\left(\frac{2000}{0.5}\right) = 64\text{ kg} \longleftarrow$$

18.37 Original pellet



Proposed pellet



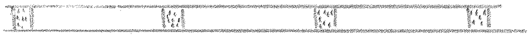
$$\therefore\ \frac{M_{T,new}}{M_{T,old}} = \frac{L_{new}\sqrt{k'''/\mathcal{D}_e}}{L_{old}\sqrt{k'''/\mathcal{D}_e}} = \frac{10^{-5}}{10^{-3}} = 0.01$$

$$\therefore\ \frac{\mathcal{E}_{new}}{\mathcal{E}_{old}} = 100 \qquad \text{or} \qquad W_{new} = \frac{1}{100}W_{old}$$

Considering the void volume between grains

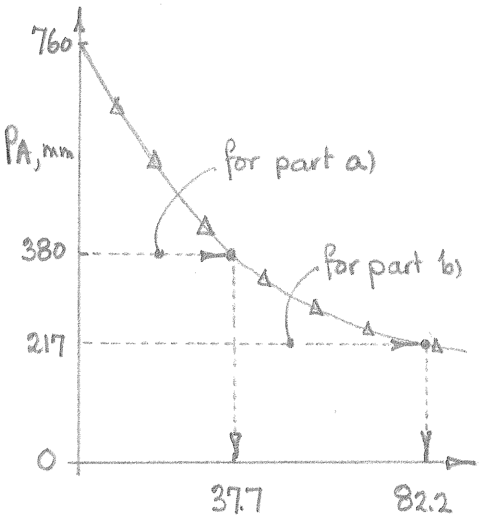
$$V_{new} = V_{old}\,\frac{1}{100}\cdot\frac{1}{1-0.25} = 0.0133\ V_{old}$$

∴ With this new catalyst we need
1% of weight of the original catalyst
or 1.33% the volume of the original reactor ⟵

18.39  

The system given ↑ should be equivalent to this ↑ 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 $F_{A0} = 10^5$ mol A/hr

$$V_r = \left(84{,}400\,\frac{\text{cm}^3\,\text{cat}\cdot\text{sec}}{\text{mol A}}\right)\left(\frac{10^5\,\text{mol A/hr}}{3600\,\text{sec/hr}}\right)$$

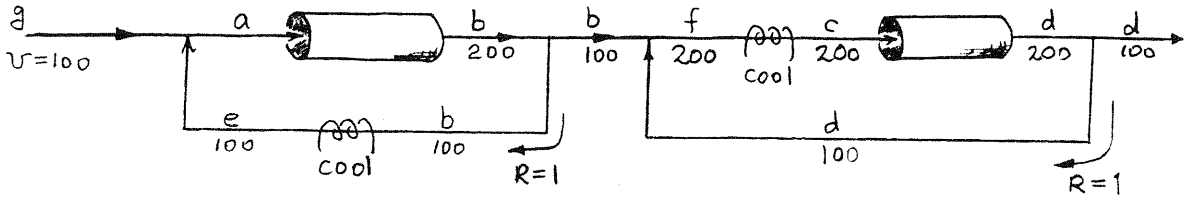
$$= 2.34\times10^6\,\text{cm}^3 = 2.34\,\text{m}^3 \longleftarrow \text{a)}$$

b) For $A \rightarrow 2.5R$ $\varepsilon_A = 1.5$ & from $\frac{C_A}{C_{A0}} = \frac{1-X_A}{1+\varepsilon_A X_A}$ we find $p_{A,out} = 760(0.2857)$ for $X_A = 0.5$.

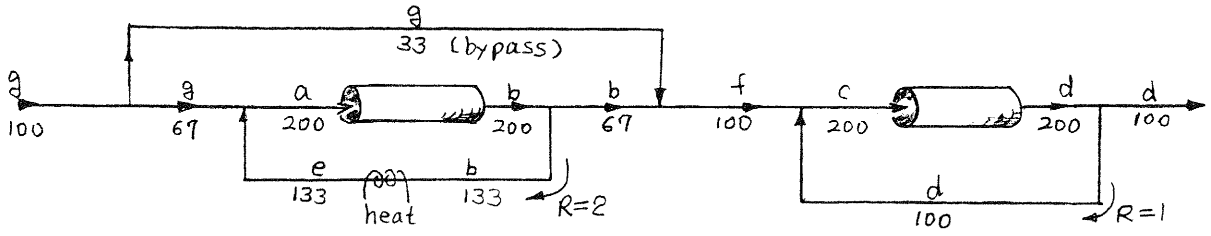
Thus the amount of catalyst needed is 82.2 m instead of 37.7 m. With all else unchanged

$$V_r = 2.34\,\text{m}\left(\frac{82.2}{37.7}\right) = 5.1\,\text{m}^3 \text{ of catalyst bed} \longleftarrow \text{b)}$$

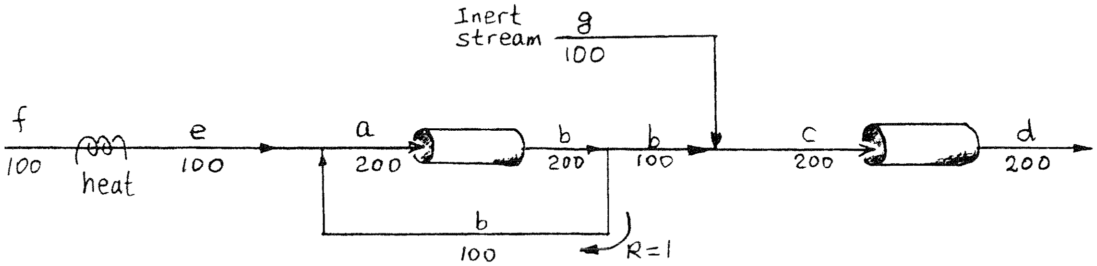
19.1



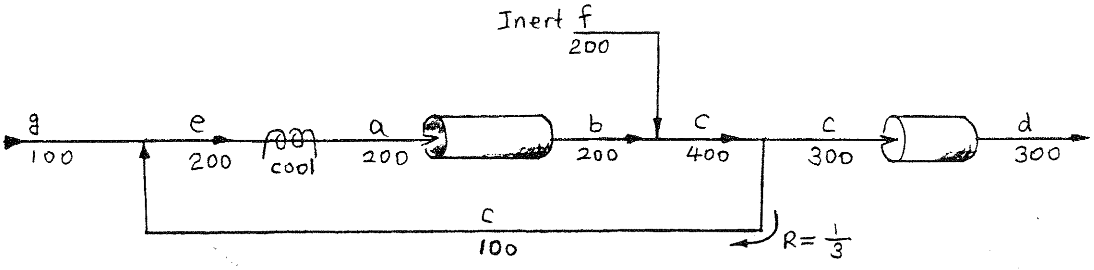
19.3



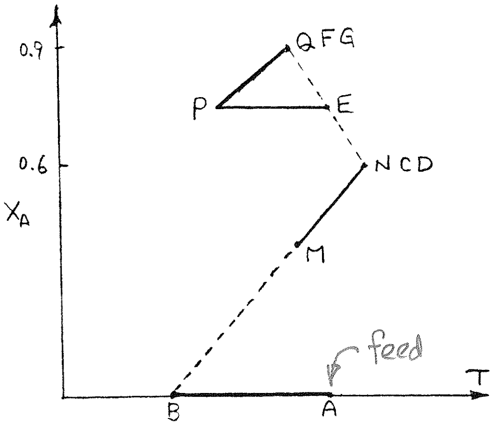
19.5



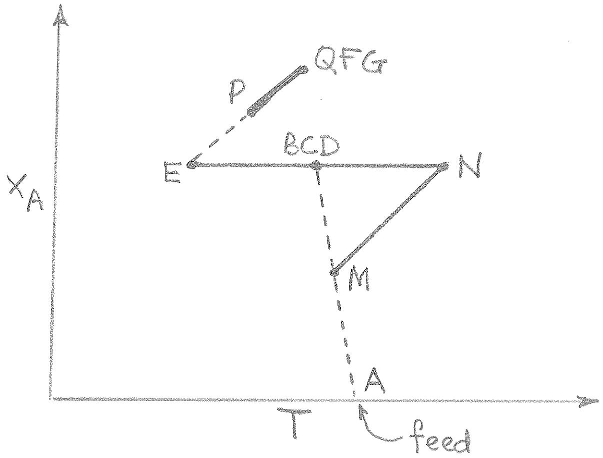
19.7



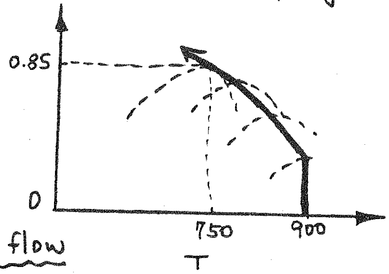
19.9



19·11



19·13 Optimal temperature progression



Plug flow

$$W = F_{A0}\int_0^{0.85}\frac{dX_A}{-r_A'} = (100)(2.124) = \underline{212.4\ \text{kg}}$$

Heat added ahead of the reactor

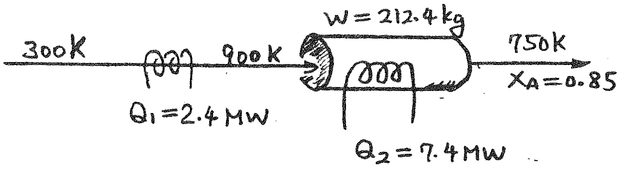
$$Q_1 = F_{A0}C_p\Delta T = (100)(40)(900-300) = \underline{2.4\times10^6\ \text{J/s}}$$

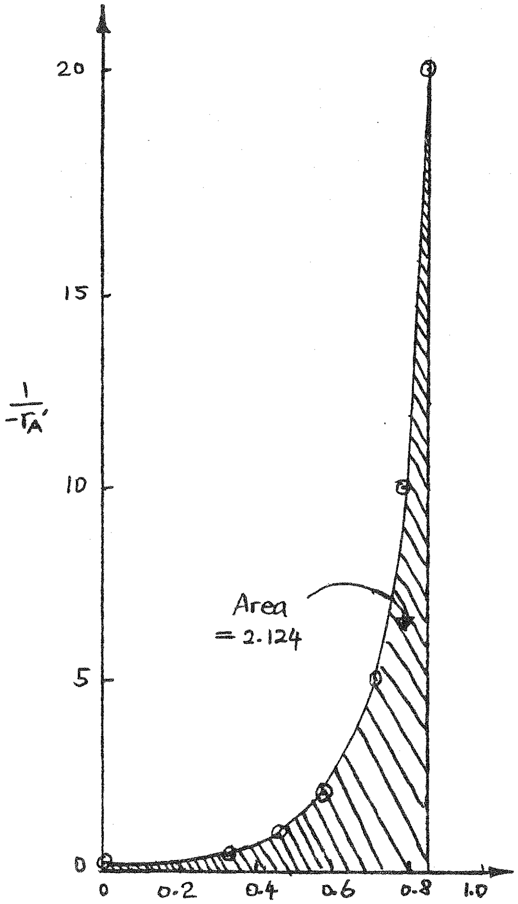
Heat removed from the reactor

$$Q_2 = F_{A0}X_A(-\Delta H_r) + F_{A0}C_p(\Delta T)$$

$$= (100)(0.85)(80000) + (100)(40)(900-750)$$

$$= \underline{7.4\times10^6\ \text{J/s}}$$





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

$$R = \frac{0.51}{0.75-0.51} = \underline{2.125}$$

$$W = F_{A_0}\frac{X_A}{-r_A'} = (100\times 0.2)(0.75)(22.8)$$

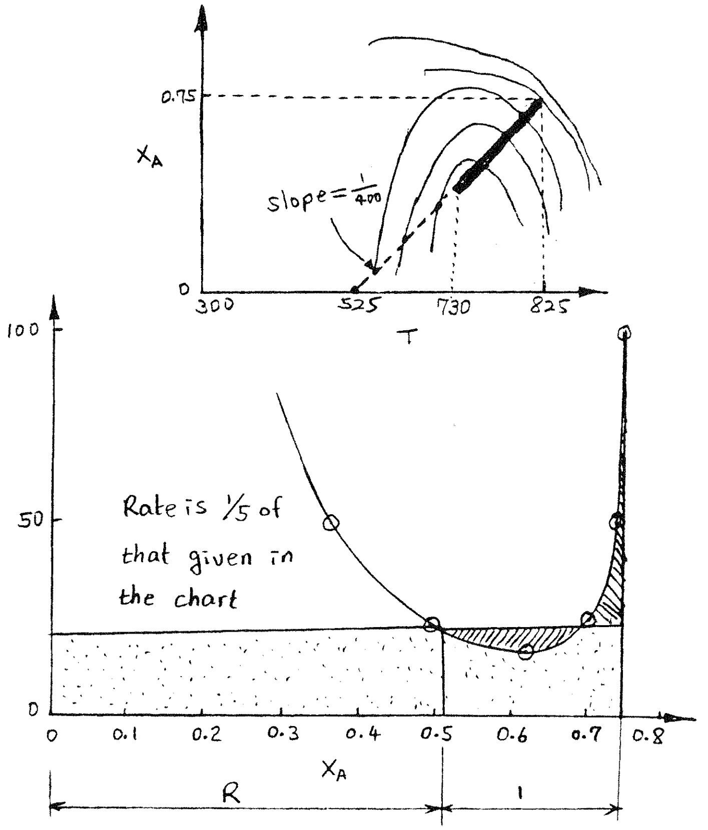
$$= \underline{342\text{ kg}}$$

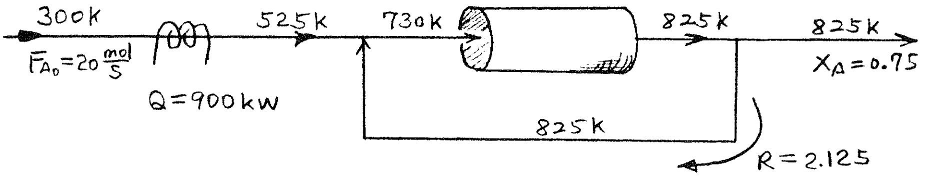
Heat duty

$$Q = F_{TOT}\cdot C_p\Delta T - F_{A_0}X_A(-\Delta H_r)$$

$$= (100)(40)(825-300) - (20)(0.75)(80000)$$

$$= \underline{9\times 10^5\text{ J/S}}\ \text{(heating)}$$





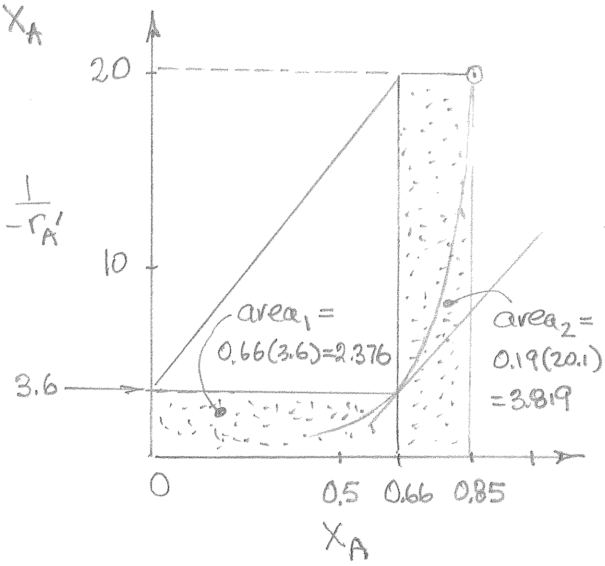
19.17 From Fig 11 plot the $1/-r'_{A,opt}$ vs X_A curve. By the optimization of rectangles we find the minimum amount of catalyst needed

$$W_1 = F_{A0}(\text{area}_1) = 100(2.376)$$

$$= 237.6\text{ kg}$$

$$W_2 = F_{A0}(\text{area}_2) = 100(3.819)$$

$$= 381.9\text{ kg}$$

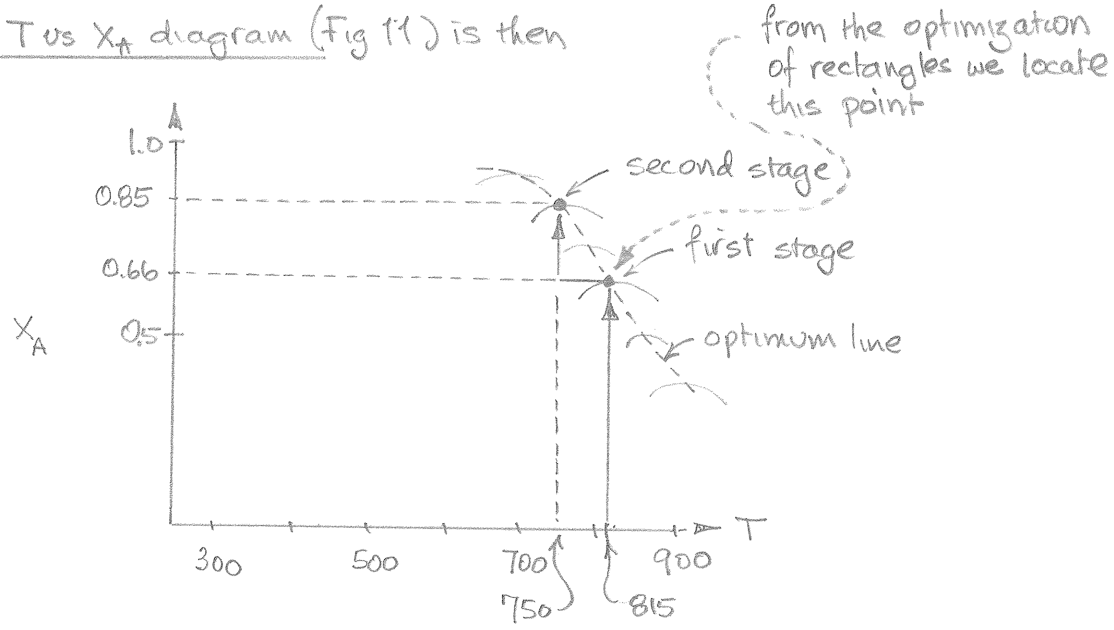


19.17 (continued) Heat duty

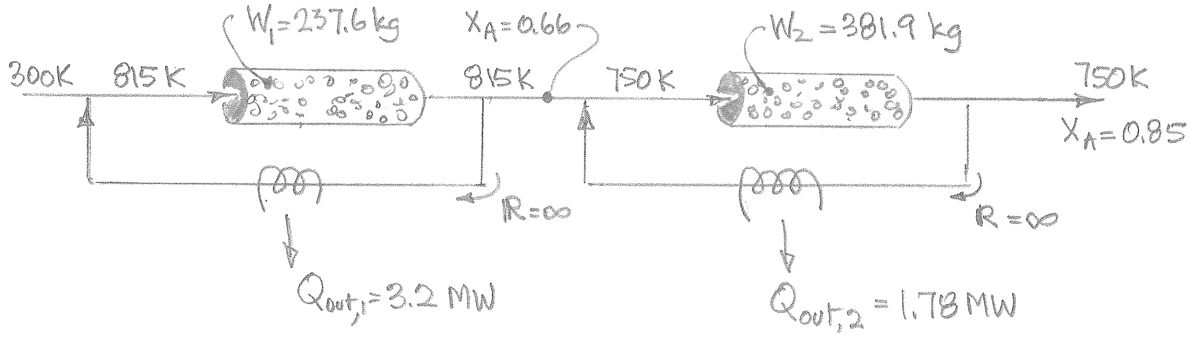
$$Q_1 = \left[F_{A0}(C_p \Delta T) - X_A(-\Delta H_r)\right]$$
$$= 100\left[40(815-300) - 0.66(+80000)\right]$$
$$= -3.2\ \text{MW}\ \text{(remove}$$

$$Q_2 = \left[F_{A0}(C_p \Delta T) - X_A(-\Delta H_r)\right]$$
$$= 100\left[40(750-815) - 0.19(+80000)\right.$$
$$= -1.78\ \text{MW}$$

The T vs X_A diagram (Fig 11) is then



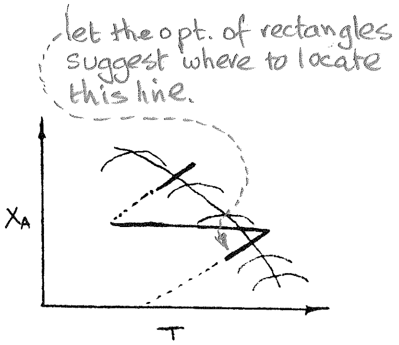
Final design

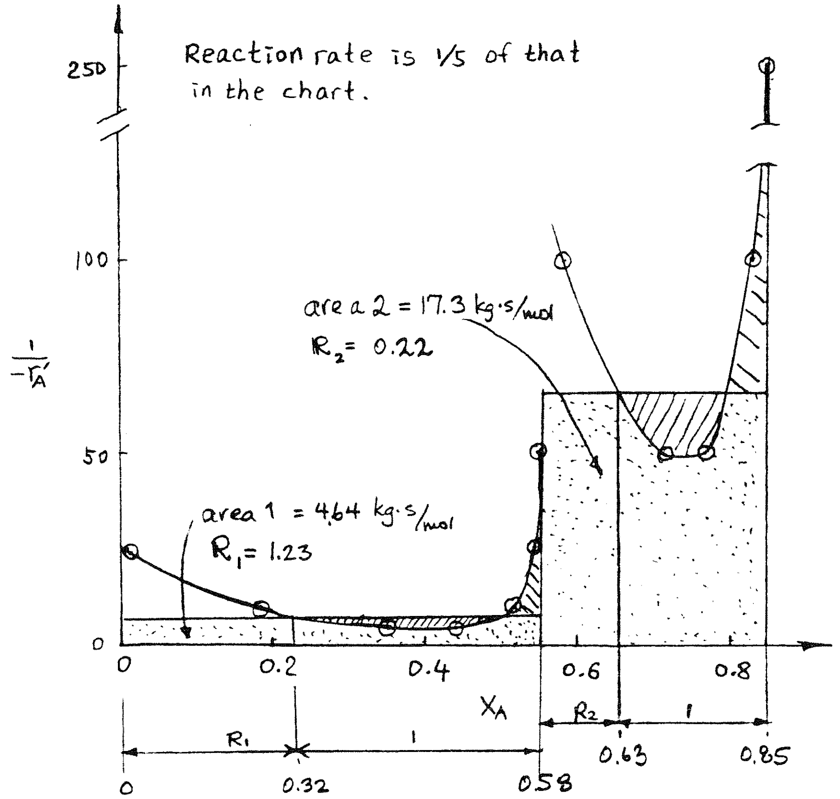


19.19 20% A – 80% B , $X_A = 0.85$

$$\text{slope} = \frac{C_p}{-\Delta H_r} = \frac{40\times5}{80000} = \frac{1}{400}$$

Plug flow with recycle is best.


let the opt. of rectangles suggest where to locate this line.


Reaction rate is 1/5 of that in the chart.

$W_1 = F_{A0} \cdot \text{area1} = (20)(4.64)$
$= \underline{92.8 \text{ kg}}$

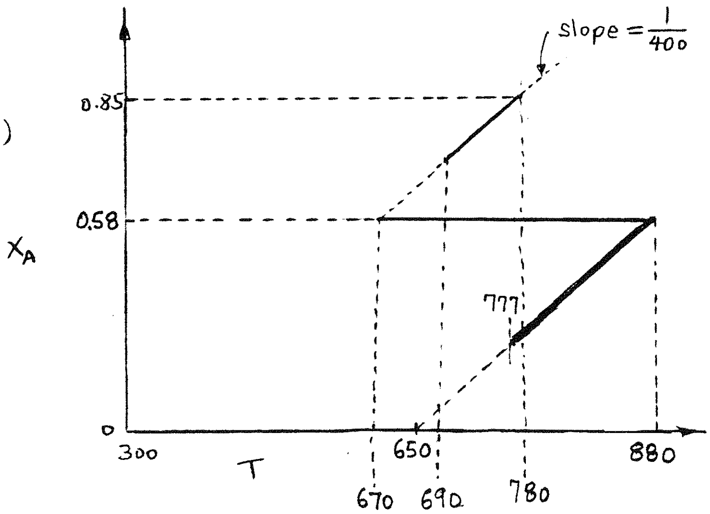
$W_2 = F_{A0} \cdot \text{area2} = (20)(17.3)$
$= \underline{346 \text{ kg}}$

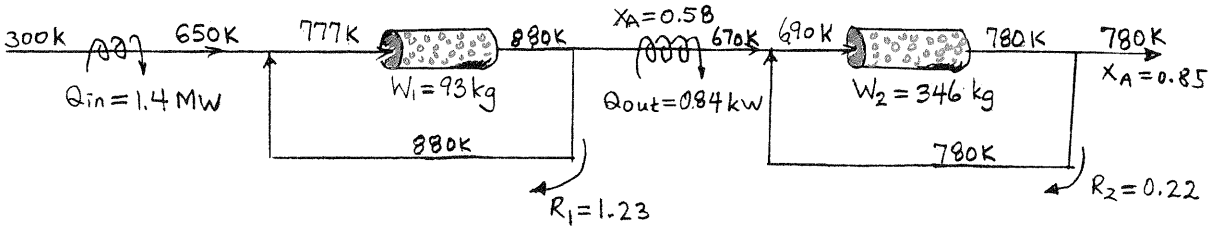
Heat duty

$Q_1 = F_{A0} C_p (\Delta T) = (20)(200)(650-300)$
$= 1.4\times10^6$ J/s (heating)

$Q_2 = F_{A0} C_p (\Delta T) = (20)(200)(670-880)$
$= -0.84\times10^6$ J/s (cooling)

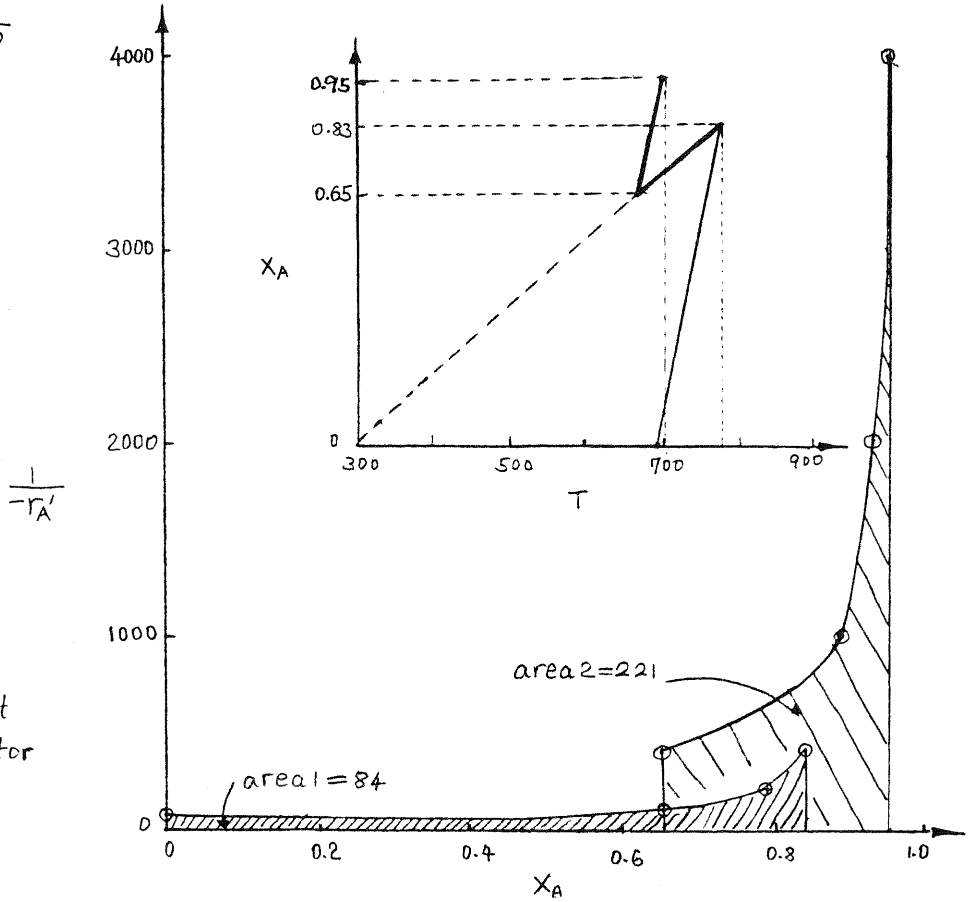
Note that this solution was obtained after a few trials.





19.21 Injection of cold feed

slope $= \frac{40\times20}{80000} = \frac{1}{100}$



Fraction of feed A that goes to the first reactor

$\frac{0.65}{0.83} = 0.7831$

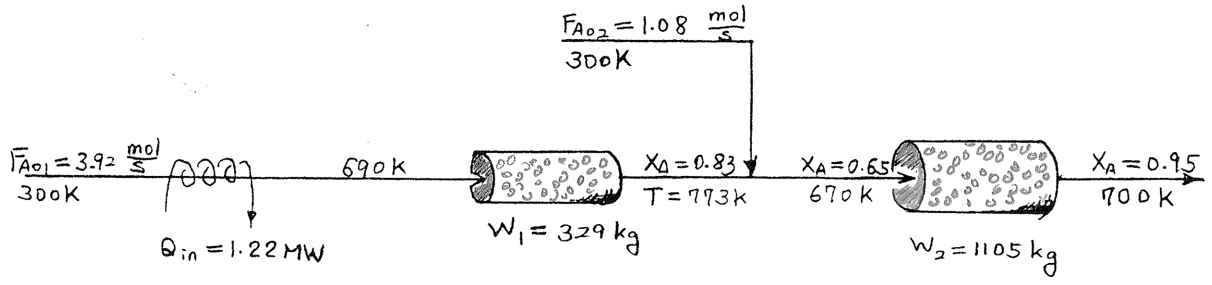
$W_1 = F_{A01}\cdot \text{area}1 = (5\times0.7831)(84) = \underline{329\text{ kg}}$

$W_2 = F_{A0}\cdot \text{area}2 = (5)(221) = \underline{1105\text{ kg}}$

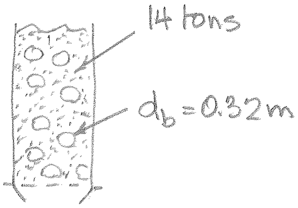
$\Big\}\ W_{total} = \underline{1434\text{ kg}}$

$Q = F_{A01}\cdot C_p\cdot(\Delta T) = (5\times0.7831)(800)(690-300) = \underline{1.22\times10^6\,J/s\text{ (heating)}}$

Note: only one heat exchanger is needed in this design.



20.1



Refer to Example 1, from which we have

$$\delta = 0.196 \qquad f_b = 0.001$$
$$\varepsilon_f = 0.6 \qquad f_c = 0.047 \Big\} \; f = 0.4$$
$$K_{bc} = 0.614\,s^{-1} \qquad f_e = 0.352$$
$$K_{ce} = 0.133\,s^{-1} \qquad H_{BFB} = 2(2.875) = 5.57\,m$$

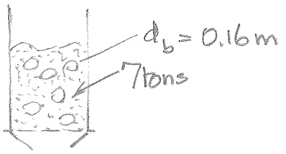
The performance expression becomes

$$\ln\frac{C_{A0}}{C_A} = \frac{[\;-\!-\!-\!-\;]}{0.4} \cdot \frac{5.57(0.4)}{0.3} = 0.0415\,(18.568) = 0.77$$

see Fig 10

$$\frac{C_A}{C_{A0}} = 0.463 \quad \text{--- or ---} \quad X_A = 53.7\% \longleftarrow$$

20.3



Solve the material balances

$$u_{br} = 0.711(g d_b)^{1/2} = 0.711(9.8 \times 0.16)^{1/2} = 0.8904\ m/s$$
$$u_b = 0.30 - 0.03 + 0.8904 = 1.16\ m/s$$
$$\delta = (0.3 - 0.03)/1.16 = 0.2327$$
$$\varepsilon_f = 1 - (1 - 0.5)(1 - 0.2327) = 0.6164$$

$$K_{bc} = 4.5\left(\frac{0.03}{0.16}\right) + 5.85\left[\frac{(20\times10^{-6})^{1/2}(9.8)^{1/4}}{(0.16)^{5/4}}\right] = 1.301\,s^{-1}$$

$$K_{ce} = 6.77\left[\frac{0.5\,(2\times10^{-5})\,1.16}{(0.16)^3}\right]^{1/2} = 0.3609\,s^{-1}$$

$$f_b = 0.001$$
$$f_c = 0.2327(0.5)\left[\frac{3\times0.03/0.5}{0.89 - 0.03/0.5} + 0.33\right] = 0.0636 \Bigg\} \; f = 0.3836$$
$$f_e = (1 - 0.6164) - 0.0636 - 0.001 = 0.3190$$

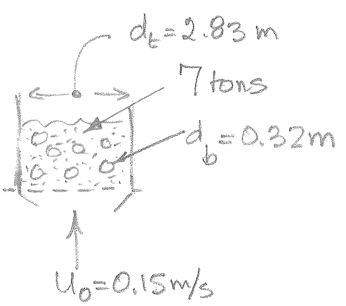
$$H_{BFB} = \frac{W}{\rho A(1-\varepsilon_f)} = \frac{7000}{2000\,\pi\,(1-0.6164)} = 2.904\ m$$

$$\ln\frac{C_{A0}}{C_A} = \left[0.001(0.8) + \cfrac{1}{\cfrac{1}{0.2327(1.301)} + \cfrac{1}{0.0636(0.8) + \cfrac{1}{\cfrac{1}{0.2327(0.3609)} + \cfrac{1}{0.3190(0.8)}}}}\right]\frac{2.904}{0.3}$$

$$= [0.0837]\,9.68 = 0.8102$$

$$\therefore\ \frac{C_A}{C_{A0}} = 0.445 \quad \text{---} \quad \text{or} \quad X_A = 55.5\% \longleftarrow$$

20.5



Solve the material balance

$$u_{br} = 0.711(9.8 \times 0.32)^{1/2} = 1.2592 \text{ m/s}$$

$$u_b = 0.15 - 0.03 + 1.2592 = 1.3792 \text{ m/s}$$

$$\delta = (0.15 - 0.03)/1.3792 = 0.087$$

$$\varepsilon_f = 1 - (1-0.5)(1-0.087) = 0.5435$$

$$K_{bc} = 4.5\left(\frac{0.03}{0.32}\right) + 5.85\left[\frac{(2\times10^{-5})^{1/2}(9.8)^{1/4}}{(0.32)^{5/4}}\right] = 0.6140 \text{ s}^{-1}$$

$$K_{ce} = 6.77\left[\frac{0.5(2\times10^{-5})1.2592}{(0.32)^3}\right]^{1/2} = 0.1327 \text{ s}^{-1}$$

$$\left.\begin{aligned} f_b &= 0.001 \\ f_c &= 0.087(0.5)\left[\frac{3(0.03)/0.5}{1.25 - 0.03/0.5} + 0.33\right] = 0.0209 \\ f_e &= (1-0.5435) - 0.0209 - 0.001 = 0.4346 \end{aligned}\right\} f = 0.4565$$

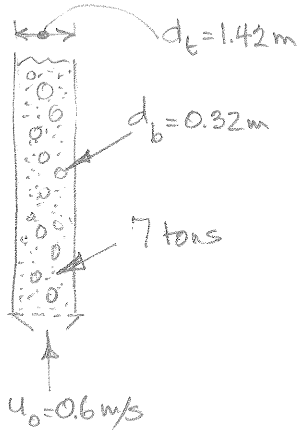
$$H_{BFB} = W/\rho A(1-\varepsilon_f) = 7000/2000(2\pi)(1-0.5435) = 1.22 \text{ m.}$$

$$\ln\frac{C_{A0}}{C_A} = \left[0.001(0.8) + \cfrac{1}{\cfrac{1}{0.087(0.614)} + \cfrac{1}{0.0209(0.8) + \cfrac{1}{\cfrac{1}{0.087(0.1327)} + \cfrac{1}{0.4346(0.8)}}}}\right]\frac{1.22}{0.15}$$

$$= [0.0263]\, 8.133 = 0.2139$$

$$\therefore \frac{C_{Af}}{C_{A0}} = 0.8074 \quad \text{--- or} \quad X_A = 19\% \longleftarrow$$

20.7



$K_{ce} = 6.78$

Again solve

$$u_{br} = 1.26 \text{ m/s}$$

$$u_b = 0.6 - 0.03 + 1.26 = 1.83 \text{ m/s}$$

$$\delta = \frac{0.6 - 0.03}{1.83} = 0.3115$$

$$\varepsilon_f = 1 - (1-0.5)(1-0.3115) = 0.6558$$

$$\left.\begin{aligned} K_{bc} &= 0.614 \text{ s}^{-1} \\ K_{ce} &= 0.133 \text{ s}^{-1} \end{aligned}\right\} \text{from Example 1}$$

20.7 continued

$$f_b = 0.001$$

$$f_c = 0.3115(1-0.5)\left[\frac{3\times 0.03/0.5}{1.26-0.03/0.5} + 0.33\right] = 0.0748 \quad \Bigg\} \; f = 0.3442$$

$$f_e = (1-0.6558) - 0.0748 - 0.001 = 0.2684$$

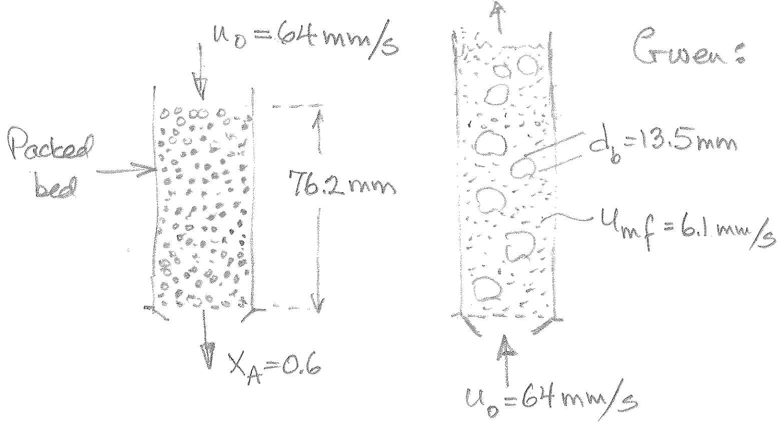
$$H_{BFB} = W/\rho A(1-\varepsilon_f) = 7000/2000(\pi/2)(1-0.6558) = 6.4735\text{ m}$$

$$\ln\frac{C_{A0}}{C_A} = \left[0.001(0.8) + \cfrac{1}{\cfrac{1}{0.3115(0.614)} + \cfrac{1}{0.0748(0.8) + \cfrac{1}{\cfrac{1}{0.3115(0.133)} + \cfrac{1}{0.2684(0.8)}}}}\right]\frac{6.4735}{0.6}$$

$$= [0.0641]\,10.7892 = 0.6914$$

$$\therefore \frac{C_A}{C_{A0}} = 0.5009 \quad \cdots \text{ or } X_A = 50\% \longleftarrow$$

20.9



Given: First order reversible rx

$X_{Ae} = 0.94$

$u_{mf} = 6.1$ mm/s

$\varepsilon_m = 0.4$

$\varepsilon_{mf} = 0.5$

$\alpha = 0.33$

$\mathcal{D} = 2\times10^{-5}\ \text{m}^2/\text{s}$

Find $X_{Af_2} = ?$

For a reversible first order reaction Eq 3.54 or Eq 5.22 gives

For plug flow: $$X_{Ae}\ln\frac{X_{Ae}}{X_{Ae}-X_{Ap}} = k'''\tau''' \quad \text{-------------} \quad (i)$$

$$\text{or } k''' = \frac{v}{V}X_{Ae}\ln\frac{X_{Ae}}{X_{Ae}-X_A} = \frac{u_0 A}{H_p A(1-\varepsilon_m)}X_{Ae}\ln\frac{X_{Ae}}{X_{Ae}-X_A}$$

$$= \frac{64}{76.2(1-0.4)}(0.94)\ln\frac{0.94}{0.94-0.60} = 1.3381\ \frac{\text{m}^3}{\text{m}^3\text{cat}\cdot\text{s}}$$

For the fluidized bed the performance equation (compare with eq (i)) is

$$X_{Ae}\ln\frac{X_{Ae}}{X_{Ae}-X_A} = \underbrace{\left[f_b k''' + \frac{}{\cdots}\right]}_{f_{total}}\underbrace{\frac{H_{BFB} f_{total}}{u_0}}_{\tau'''} \quad \cdots \quad (ii)$$

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

$$\frac{u_b}{u_e} = \frac{0.316}{0.006/0.5} = 26.3 \text{ --- yes it is a vigorously fluidized bed}$$

$$\delta = (0.064 - 0.0061)/0.3165 = 0.1829$$

$$\varepsilon_f = 1 - (1-0.5)(1-0.1829) = 0.5915$$

$$K_{bc} = 4.5\left(\frac{0.0061}{0.0135}\right) + 5.85\left[\frac{(2\times10^{-5})^{1/2}(9.8)^{1/4}}{(0.0135)^{5/4}}\right] = 2.0333 + 10.0589 = 12.0922 \text{ s}^{-1}$$

$$K_{ce} = 6.77\left[\frac{0.5(2\times10^{-5})0.3165}{(0.0135)^3}\right]^{1/2} = 7.6785 \text{ s}^{-1}$$

$$\left.\begin{aligned} f_b &= 0.001 \\ f_c &= 0.1829(1-0.5)\left[\frac{3(0.0061)/0.5}{0.2568 - 3(0.0061)/0.5} + 0.33\right] = 0.2393 \\ f_e &= (1-0.5915) - 0.2393 - 0.001 = 0.1682 \end{aligned}\right\} f = 0.4085$$

$$H_{BFB} = H_{fixed}\left(\frac{1-\varepsilon_m}{1-\varepsilon_{mf}}\right)\frac{1}{1-\delta} = (0.0762)\left(\frac{1-0.4}{1-0.5}\right)\frac{1}{1-0.1829} = 0.1119 \text{ m}$$

Now replace values into Eq (ii)

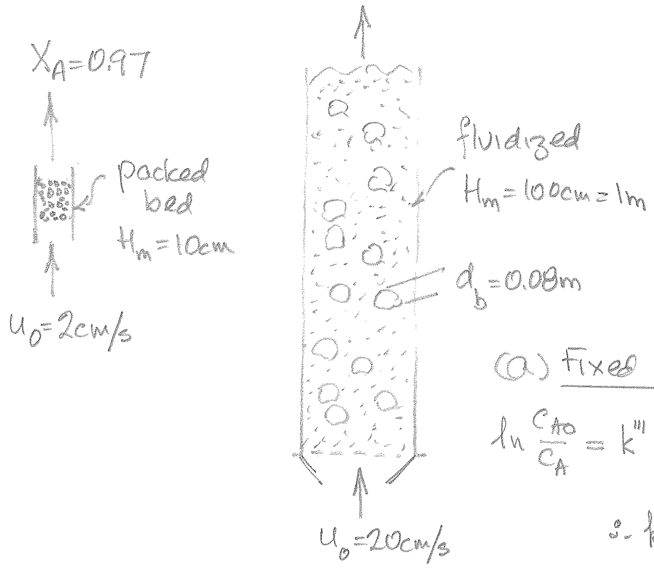
$$X_{Ae} \ln \frac{X_{Ae}}{X_{Ae} - X_A} = \left[0.001(1.3383) + \frac{1}{\dfrac{1}{0.1829(12.0922)} + \dfrac{1}{0.2393(1.3381) + \dfrac{1}{\dfrac{1}{0.1829(7.6785)} + \dfrac{1}{0.1682(1.3381)}}}}\right]\frac{0.1119}{0.064}$$

$$\ln \frac{0.94}{0.94 - X_A} = \left[0.4185\right] 1.7484 \left(\frac{1}{0.94}\right) = 0.7784$$

$$\therefore \quad \frac{X_{Ae}}{X_{Ae} - X_A} = 2.1780 \quad \text{or} \quad X_A = 0.5084 \longleftarrow$$

Note. Compare this calculated X_A value with that found experimentally, as shown in fig 3, pg 520 of Mathis & Watsons paper.

20.11



$\varepsilon_m=\varepsilon_{mf}=0.5$
$\mathcal{D}=3\times10^{-5}\ m^2/s$
$u_{mf}=0.032\ m/s$
$\alpha=0.34$

(a) Fixed bed experiment

$$\ln\frac{C_{A0}}{C_A}=k'''\frac{V_s}{v}=k'''\frac{H_mA(1-\varepsilon_m)}{u_0A}=k'''\frac{0.1(1-0.5)}{0.02}$$

$$\therefore k'''=\frac{0.02}{0.1(1-0.5)}\ln\frac{100}{3}=1.4026\ m^3/m^3cat\cdot s \longleftarrow (a)$$

(b) Fluidized bed

$u_{br}=0.711(9.8\times0.08)^{1/2}=0.6295\ m/s$

$u_b=0.2-0.032+0.6295=0.7975\ m/s$

$\delta=(0.2-0.032)/0.7975=0.2107$

$\varepsilon_f=1-(1-0.5)(1-0.2107)=0.6053$

$$K_{bc}=4.5\left(\frac{0.032}{0.08}\right)+5.85\left[\frac{(3\times10^{-5})^{1/2}(9.8)^{1/4}}{(0.08)^{5/4}}\right]=3.1325\ s^{-1}$$

$$K_{ce}=6.77\left[\frac{0.5(3\times10^{-5})0.6295}{(0.08)^3}\right]^{1/2}=0.9194\ s^{-1}$$

$$\left.\begin{array}{l} f_b=0.001 \\ f_c=0.2107(1-0.5)\left[\dfrac{3(0.032)/0.5}{0.7975-0.032/0.5}+0.34\right]=0.0634 \end{array}\right\} f=0.3947$$

$f_e=(1-0.6053)-0.0634-0.001=0.3303$

$$H_{BFB}=\frac{H_m(1-\varepsilon_m)}{1-\varepsilon_f}=\frac{1.0(0.5)}{1-0.6053}=1.2668\ m$$

$$\ln\frac{C_{A0}}{C_A}=\left[0.001(1.4026)+\cfrac{1}{\cfrac{1}{0.2107(3.1325)}+\cfrac{1}{0.0634(1.4026)+\cfrac{1}{\cfrac{1}{0.9194(0.2107)}+\cfrac{1}{0.3303(1.4026)}}}}\right]\frac{1.27}{0.2}$$

$$=\left[0.1695\right]6.334=1.0736$$

$$\therefore \frac{C_A}{C_{A0}}=0.3418 \quad \text{--- or} \quad X_A=34\% \longleftarrow (b)$$

(c) Big fixed bed

$$\frac{C_A}{C_{A0}}=e^{-k'''H_ff}=e^{-1.4026(1.27)0.3947}=0.03 \quad \text{--- or} \quad X_A=97\% \longleftarrow (c)$$

21.1 Let us start by guessing the simplest rate form.

$$\left.\begin{aligned} -r_A' &= k' C_A a \\ -\frac{da}{dt} &= k_d a \end{aligned}\right\} \cdots$$ 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

$$\left(\frac{C_{A0}}{C_A} - 1\right) = k'\tau' e^{-k_d t}$$

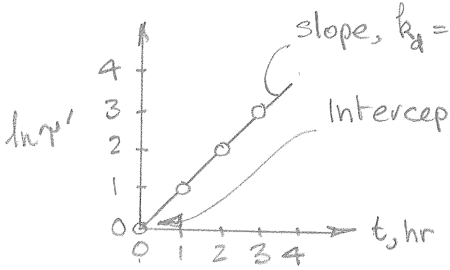
or

$$\underbrace{\ln \tau'}_{y} = \underbrace{\ln\left[\left(\frac{C_{A0}}{C_A} - 1\right)\frac{1}{k'}\right]}_{a} + \underbrace{k_d t}_{bx}$$

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



slope, $k_d = 1$

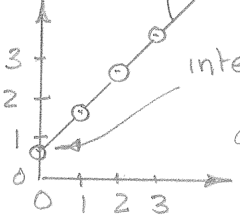
Intercept $= 0 = \ln\left[\left(\frac{C_{A0}}{C_A} - 1\right)\frac{1}{k'}\right]$

$\therefore k' = \left(\frac{2}{1} - 1\right) = 1$

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

Run 2



slope, $k_d = 1$

intercept $= 0.693 = \ln\left[\left(\frac{C_{A0}}{C_A} - 1\right)\frac{1}{k'}\right]$

again we find $k' = 1$

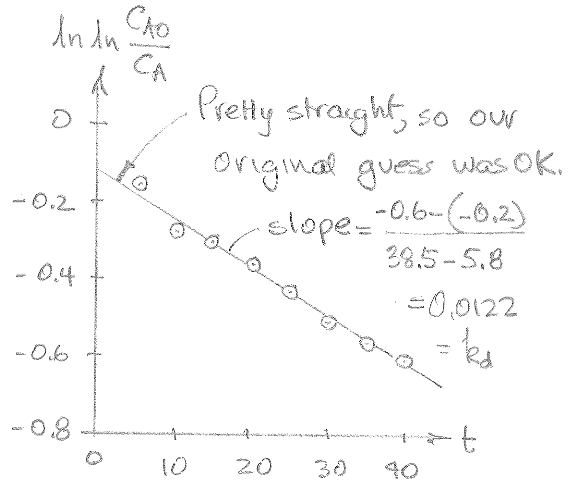
For both runs we find

$$\left.\begin{aligned} -r_A &= C_A a, \ \mathrm{mol/gm\cdot min} \\ -\frac{da}{dt} &= a, \ \mathrm{hr}^{-1} \end{aligned}\right\} \longleftarrow$$

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

$$\ln \ln \frac{C_{A0}}{C_A} = \ln(k'\tau') - k_d t$$

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	−0.3093
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



Pretty straight, so our original guess was OK.

$$\text{slope} = \frac{-0.6-(-0.2)}{38.5-5.8} = 0.0122 = k_d$$

$$\therefore\ -\frac{da}{dt} = 0.0122\, a,\ \text{hr}^{-1}$$

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

$$-\frac{dC_A}{dt} = \frac{kW}{V}(C_A - C_{Ae})\, a = k''a\,(C_A - C_{Ae}) \qquad \text{---(i)}$$

$$-\frac{da}{dt} = k_d\, a \qquad \text{---(ii)}$$

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

$$\ln \frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}} = \frac{k''}{k_d}\left(1 - e^{-k_d t}\right) \qquad \text{---(iii)}$$

21.5
continued

Now at $t=\infty$ this expression reduces to

$$\ln \frac{C_{A0}-C_{Ae}}{C_{A\infty}-C_{Ae}} = \frac{k''}{k_d} \qquad \text{--- (iv)}$$

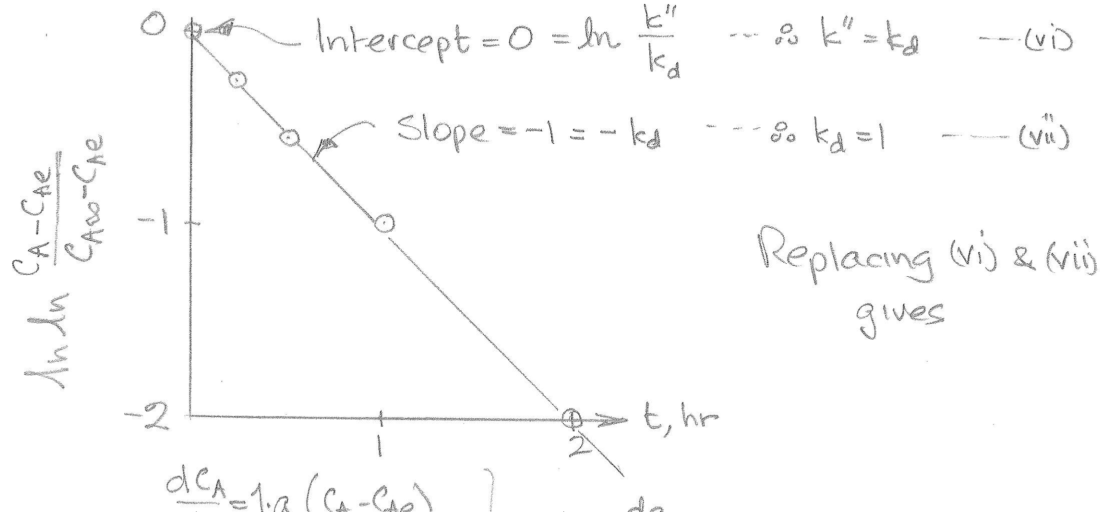
and on combining (iii) and (iv), rearranging and taking logs we obtain finally, for the batch-batch system

$$\boxed{\ln\ln \frac{C_A-C_{Ae}}{C_{A\infty}-C_{Ae}} = \ln\frac{k''}{k_d} - k_d t} \qquad \text{-- (v)}$$

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	$0.5/0.184=2.717$	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



Intercept $= 0 = \ln\frac{k''}{k_d}$ $\quad\cdots\therefore\ k''=k_d$ --(vi)

Slope $= -1 = -k_d$ $\quad\cdots\therefore\ k_d=1$ --(vii)

Replacing (vi) & (vii) in (v) gives

$$\left.\begin{array}{l} \dfrac{dC_A}{dt} = 1\cdot a\,(C_A-C_{Ae}) \\ \underset{\text{mol/gm.hr}}{-r_A'} = 1\cdot \underset{\text{lit fluid/gm cat}}{\dfrac{V}{W}}\, a\,(C_A-C_{Ae}) \end{array}\right\} \text{ with } -\underset{\text{hr}^{-1}}{\dfrac{da}{dt}} = a \longleftarrow$$

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 <u>absence of pore diffusion resistance</u> Eq 48 gives

$$\frac{k_1' a}{T_1^2} = \frac{k_2' a}{T_2} = \text{constant, for all } T_1 \ \& \ T_2$$

or

$$\frac{a_2}{a_1} = \frac{T_2^2}{T_1^2} \cdot \frac{k_1'}{k_2'} = \frac{T_2^2}{T_1^2} \frac{k_0' \exp(-7200/T_1)}{k_0' \exp(-7200/T_2)}$$

$$= \left(\frac{800}{600}\right)^2 \exp\left[-7200\left(\frac{1}{600} - \frac{1}{800}\right)\right] = \left(\frac{800}{600}\right)^2 (0.0498) = 0.0885$$

So at the end of the run $\qquad a_2 = 8.85\% \longleftarrow$

In the <u>presence of strong pore resistance</u> Eq 50 gives

$$\frac{k_1' a}{T_1^3} = \frac{k_2' a}{T_2^3}$$

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

$$a_2 = 11.8\% \longleftarrow$$

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 <u>strong diffusion regime</u> Eq 43 gives

$$\ln \frac{C_{A0}}{C_A} = \frac{k'\tau'}{M_T} \exp\left(-\frac{k_d t}{2}\right)$$

Taking logs

$$\ln \ln \frac{C_{A0}}{C_A} = \ln\left(\frac{k'\tau'}{M_T}\right) - \frac{k_d t}{2} \quad \text{- - - - - - - - - (i)}$$

at $t=0$: $\quad \ln \ln \frac{100}{12} = \ln\left(\frac{k'\tau'}{M_T}\right) - 0$

at $t=250$: $\quad \ln \ln \frac{100}{36} = \ln\left(\frac{k'\tau'}{M_T}\right) - \frac{k_d}{2}(250)$

$\Big\}$ ... combining gives $k_d = 0.004199$

In the <u>diffusion resistance free regime</u> Eq 42 gives

$$\ln \frac{C_{A0}}{C_A} = \frac{k'\tau'}{M_T} \exp(-k_d t)$$

Again taking logs gives

$$\ln \ln \frac{C_{A0}}{C_A} = \ln\left(\frac{k'\tau'}{M_T}\right) - k_d t \quad \text{- - - - - - - - - - - (ii)}$$

Replacing values gives

at $t=0$: $\quad \ln \ln \frac{100}{12} = \ln\left(\frac{k'\tau'}{M_T}\right) - 0.$

at the end of the run when $X_A = 64\%$, but time is unknown

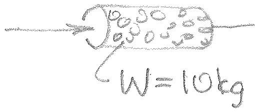
$$\ln \ln \frac{100}{36} = \ln\left(\frac{k'\tau'}{M_T}\right) - 0.004199\, t$$

Combining equations gives

$$0.004199\, t = \ln\ln\frac{100}{12} - \ln\ln\frac{100}{36} \quad \cdots \therefore\ t = 125 \text{ days}$$

the catalyst is killed more rapidly in the diffusion-free regime

21.11 Given: $v = 100\ \text{lit/min}$, $700^\circ C$, $8\ \text{atm}$ $\longrightarrow$



Run until $a = 0.1\, a_{t=0}$

$-r_A' = 0.030\, C_A a, \ \frac{\text{mol}}{\text{gm}\cdot\text{min}}$

$-\frac{da}{dt} = 3a^3, \ \text{day}^{-1}$

Find (a) t, (b) $\bar{X}_A$

Focus on catalyst activity

For the decaying catalyst we have: ... $-\overset{\text{day}^{-1}}{\frac{da}{dt}} = 3a^3$

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: $t = 16.5$ 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

$$\tau' = -\int_{C_{A0}}^{C_A} \frac{dC_A}{k C_A a} = \frac{1}{\underset{\uparrow}{k}a} \ln \frac{C_{A0}}{C_A}$$

$0.03\ \frac{\text{lit}}{\text{gm}\cdot\text{min}}$

$$\tau' = \frac{W C_{A0}}{F_{A0}} = \frac{W}{v} = \frac{10\ \text{kg}}{100\ \text{lit/min}} = 100\ \frac{\text{gm}\cdot\text{min}}{\text{lit}}$$

hence the reactor output is related to catalyst activity by the expression: $\frac{C_A}{C_{A0}} = e^{-3a}$ ... (ii)

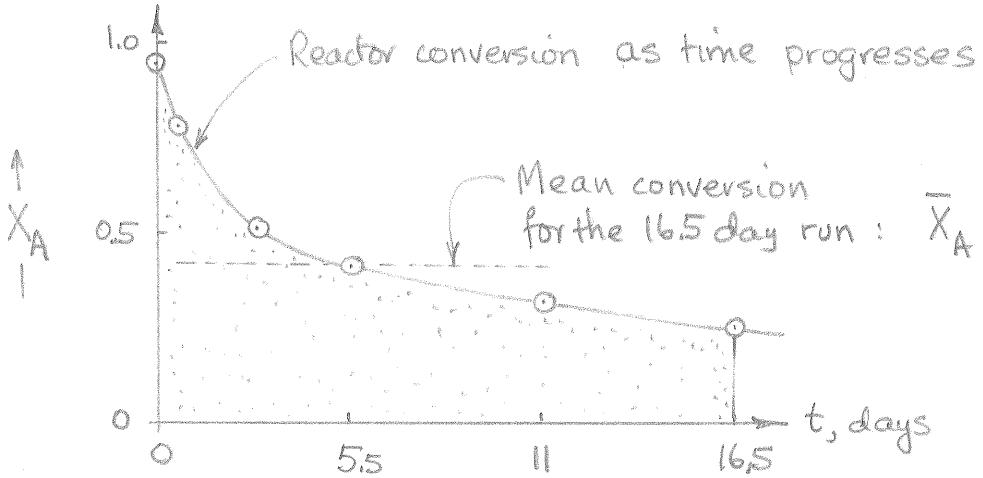
Now the mean conversion is the time average $C_{A,\text{out}}$ over the 16.5 days, or ... $$\frac{\bar{C}_A}{C_{A0}} = \frac{\int_{\text{beginning}}^{\text{end of run}} \left(C_A/C_{A0}\right)_{\text{any time}} dt}{t_{\text{run}}}$$

21.11 continued Replacing (i) & (ii) in the above expression gives

$$\frac{\bar{C}_A}{C_{A0}} = \frac{1}{16.5}\int_0^{16.5\,\text{days}} e^{-3a}\,dt = \frac{1}{16.5}\int_0^{16.5} e^{-3\sqrt{1/1+6t}}\,dt \quad \text{--- (iii)}$$

Evaluate this integral by tabulation & graphical integration. Thus

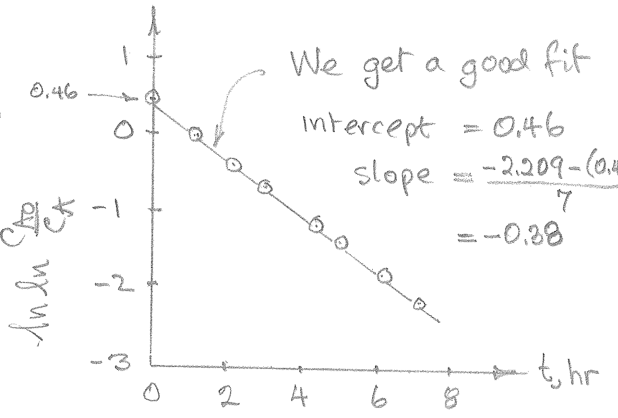
t	a	$e^{-3\sqrt{1/1+6t}}$	$X_A = 1 - C_A/C_{A0}$
0	1	0.05	0.95
0.5		0.223	0.78
2.75		0.488	0.51
5.5		0.598	0.4
11		0.693	0.31
16.5	0.1	0.74	0.26



$\bar{X}_A = 40\sim42\%$ ← b)

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	$7.8\times10^{-3}\cong0$
2	0.510	2.041	−0.338
3	0.397	1.658	−0.6815
4.25	0.255	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



We get a good fit

intercept = 0.46

$$\text{slope} = \frac{-2.209-(0.46)}{7} = -0.38$$

21.13 continued Equation 30 and Fig 5 give

$$\ln\ln\frac{C_{A0}}{C_A} = \underbrace{\ln(k'\tau')}_{0.46} - \underset{0.38}{k_d}\, t$$

Solving for k':

$$\underset{4100\ \mathrm{kg\cdot s/m^3}}{k'\tau'} = e^{-0.46} = 1.584 \qquad \therefore\ k' = 3.86\times10^{-4}\ \mathrm{m^3/kg\cdot s}$$

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

$$(M_{Td})_{t=0} = M_T = \frac{7.2\times10^{-5}}{6}\sqrt{\frac{(3.86\times10^{-4})(630)}{5\times10^{-10}}} = 0.264$$

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

$$\left.\begin{aligned} -r_A' &= \left(3.86\times10^{-4}\ \frac{\mathrm{m^3}}{\mathrm{kg\cdot s}}\right) C_A\, a \\ -\frac{da}{dt} &= (0.38\ \mathrm{hr^{-1}})\, a \end{aligned}\right\} M_T < 0.4 \longleftarrow$$

<u>Note</u> 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.

$$\therefore\ \frac{k'\tau'}{M_T} = e^{0.46} = 1.584, \quad \text{or} \quad \frac{k'\tau'\mathcal{D}^{1/2}}{L(k'\rho_s)^{1/2}} = 1.584 \quad \text{--- thus} \quad k' = 2.7\times10^{-5}$$

Evaluate M_T

$$M_T = \frac{7.2\times10^{-5}}{6}\sqrt{\frac{(2.7\times10^{-5})(630)}{5\times10^{-10}}} = 7\times10^{-2}$$

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

---

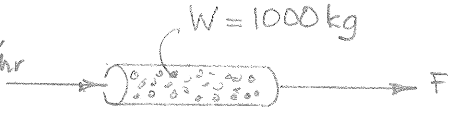
21.15

Given $-r_A' = k' C_A^2 a = 0.2 C_A^2 a$, 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

$F_{A0} = 5000$ mol/hr
730K
3atm



Find $\left\{ \begin{array}{l} X_{A,\text{start}} \\ X_{A,\text{end}} \cdots \text{after 12 days} \\ \bar{X}_A \text{ for the 12 days} \end{array} \right.$

$C_{A0} = p_{A0}/RT = 3(101325)/8.314(730) = 50 \frac{\text{mol}}{\text{m}^3}$

a) $-\frac{da}{dt} = \left(0.01 \frac{\text{m}^3}{\text{mol.day}}\right)\left(50 \frac{\text{mol}}{\text{m}^3}\right) a = 0.5 a$, day^{-1} ⟵ (a)

$\tau' = \frac{W C_{A0}}{F_{A0}} = \frac{(1000\text{kg})(50 \text{ mol/m}^3)}{5000 \text{ mol/hr}} = 10$ kg/m³·hr ⟵ (a)

at any time

$$\underset{10}{\tau'} = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} = \int_{C_A}^{C_{A0}} \frac{dC_A}{k' a C_A^2} = \frac{1}{k'a}\left[\frac{1}{C_A} - \frac{1}{C_{A0}}\right] = \frac{1}{k' a C_{A0}}\left[\frac{C_{A0}}{C_A} - 1\right]$$

$\therefore k' a C_{A0} \tau' = \frac{C_{A0}}{C_A} - 1 \quad \cdots \text{or} \quad \frac{C_A}{C_{A0}} = \frac{1}{1 + 0.2a(50)10} = \frac{1}{1+100a}$ ⟵ (a)

(b) At the start $a = e^{-0.5t} = e^0 = 1$

$\therefore \frac{C_A}{C_{A0}} = \frac{1}{1+100} \cong \frac{1}{100} \quad \cdots \text{or} \quad X_{A,\text{start}} = 99\%$ ⟵ (b)

(c) After 12 days $a = e^{-0.5(12)} = \frac{1}{400}$

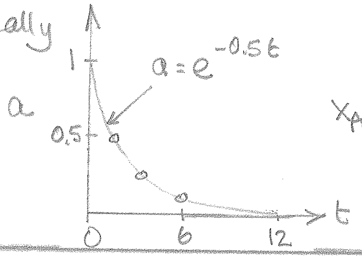
$\therefore \frac{C_A}{C_{A0}} = \frac{1}{1 + 100/400} = 0.8 \quad \cdots \text{or} \quad X_{A,\text{end}} = 20\%$ ⟵ (c)

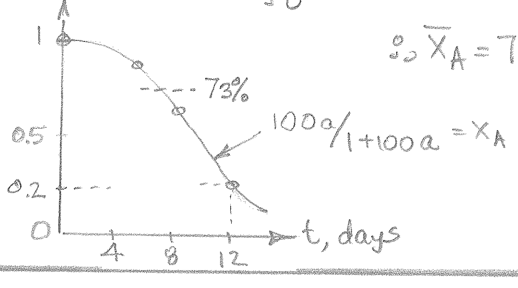
(d) Find $\bar{X}_A$: $\frac{\bar{C}_A}{C_{A0}} = \frac{1}{t_{run}} \int_0^{t_{run}} \frac{C_A}{C_{A0}} dt = \frac{1}{12} \int_0^{12} \frac{dt}{1 + 100 e^{-0.5t}}$

$$= \frac{1}{12}\left[t + 2\ln\left(1 + 100e^{-0.5t}\right)\right]_0^{12} = 0.27$$

$\therefore \bar{X}_A = 73\%$ ⟵ (d)

Graphically





22.1 First let us see if either extreme with its simplifications apply

$$\left.\begin{array}{l} C_A^* = \dfrac{p_A}{H_A} = \dfrac{1013250}{86000} = 11.78 \quad \text{constant throughout} \\ \text{At inlet} \quad C_{B0} = 400 \text{ mol/m}^3 \\ \text{guess } X_B \leq 90\% \quad C_B = 40 \text{ mol/m}^3 \end{array}\right\}$$

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

$$a_c = \frac{6f_s}{d_p} = \frac{6(0.58)}{5\times10^{-3}} = 696 \text{ m}^2/\text{m}^3$$

$$\therefore k_c a_c = (3.86\times10^{-5})(696) = 0.0269 \text{ s}^{-1}$$

$$M_T = L\sqrt{\frac{k'\rho_s}{\mathcal{D}}} = \frac{5\times10^{-3}}{6}\sqrt{\frac{(1.77\times10^{-5})(1800)}{4.16\times10^{-10}}} = 7.3 \quad \dots \therefore \mathcal{E} = 0.13$$

Now to the rate equation

$$-r_A'''' = \frac{1}{\frac{1}{86000(10^{-4})} + \frac{1}{0.02} + \frac{1}{0.0269} + \frac{1}{(1.77\times10^{-5})(1800)(0.13)(0.58)}} \cdot \frac{1013250}{86000}$$

$$= \frac{1}{\underbrace{0.116}_{\text{negligible}} + 50 + 37.17 + \underbrace{416.3}_{\text{main resistance}}} \cdot \frac{1013250}{86000} = 0.0234$$

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

$$F_{A0}X_A = \underbrace{F_{B0}}_{F_{B0} = v_l C_{B0} = (2\times10^{-4})(400) = 0.08 \text{ mol/s.}} X_B = (-r_A'''')V_r$$

$$\therefore X_B = \frac{(-r_A'''')V_r}{F_{B0}} = \frac{(0.0234)(5\times0.1)}{0.08} = 0.146 \cong \underline{15\%}$$

this is < 90%, so it satisfies our assumption

22.3 This reaction is in mixed flow, so evaluate terms

$$a_c = \frac{6f_s}{d_p} = \frac{6(0.0056)}{10^{-5}} = 3360\ \frac{m^2}{m^3}, \qquad k_{Ac}a_c = 10^{-3}(3360) = 3.36\ s^{-1}$$

$$C_A = \frac{p_A}{H_A} = \frac{200(101325}{2.776\times10^5} = 73\ \frac{mol}{m^3} \cdots \text{stays constant}$$

$$C_B = 2000\ \frac{mol}{m^3}$$

$\Big\}$ in any case $C_B \gg C_A$

So consider this to be a 1st order reaction with respect to A, or

$$-r_A = (5.96\times10^{-6} C_A^{-0.4} C_{Bf}) C_A$$

$$M_T = \frac{d_p}{6}\sqrt{\frac{n+1}{2}\cdot\frac{k' C_A^{-0.4} C_{Bf}}{\mathcal{D}}} = \frac{10^{-5}}{6}\sqrt{\frac{1.6}{2}\cdot\frac{(5.97\times10^{-6})(73)^{-0.4} C_{Bf}\times 8900}{2\times10^{-9}}}$$

$$= 0.003258\, C_B^{1/2}, \quad \text{even at } C_B = 2000,\ M_T < 1 \ \therefore\ \mathcal{E}_A = 1$$

Now to the rate

$$r_A'''' = \frac{1}{\frac{1}{0.05} + \frac{1}{3.36} + \frac{1}{(5.96\times10^{-6})73^{-0.4} C_{Bf}(1)(0.0056)8900}} \cdot \frac{101325\times200}{2.776\times10^5}$$

main resistance

$$= \frac{73}{20.2976 + 1872.6/C_B}$$

Now make a material balance $\underbrace{F_{A0}}_{\text{not useful}} X_A = \underbrace{F_{B0} X_B}_{v_\ell (C_{B0} - C_B) \cdots \text{useful.}} = (-r_A'''')V_{reactor}$

$$\therefore\ 10^{-2}(2000 - C_B) = \frac{73}{(20.2976 + 1827.6/C_B)}\cdot 2 \quad \cdots \text{or}\quad 2000 - C_B = \frac{14600}{(20.9276 + 18728.6/C_B)}$$

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 ← ok

$\therefore C_B = 1550\ mol/m^3$

and $X_B = 1 - \frac{1550}{2000} = 22.5\%$ ←

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

$$C_A = \frac{p_A}{H_A} = \frac{101325}{28500} = \overset{\text{constant}}{3.555} \text{ mol/m}^3$$

At start: $C_{B0} = 1097 \text{ mol/m}^3$

At end of run $C_{Bf} = 109.7 \text{ mol/m}^3$

Comparing we see that $C_B \gg C_A$ throughout the run.

Use the equations for the $C_B \gg C_A$ extreme

$$a_c = \frac{6 f_s}{d_p} = \frac{6(0.25)}{3\times10^{-4}} = 5000 \frac{\text{m}^2}{\text{m}^3}$$

$$k_{Ac} a_c = 10^{-5}(5000) = 0.05 \text{ s}^{-1}$$

$$M_T = L\sqrt{\frac{k' \rho_s}{\mathcal{D}}} = \frac{3\times10^{-4}}{6}\sqrt{\frac{0.05(750)}{8.35\times10^{-10}}} = 10.6 \qquad \therefore \mathcal{E} = \frac{1}{10.6} = 0.0944$$

We are now ready to write the rate expression

$$-r_A'''' = \frac{1}{\frac{1}{0.04} + \frac{1}{0.05} + \frac{1}{0.05(750)(0.0944)(0.25)}} \cdot \frac{101325}{28500}$$

$$= \frac{1}{25 + 20 + 1.13}(3.555) = 0.0771 \text{ mol A/m}^3 \text{ reactor} \cdot \text{s}$$

Finally go to the material balance. Writing it for A

$$\underbrace{F_{A0} X_A}_{\text{useless}} = \underbrace{\frac{V_l}{b}\left(-\frac{dC_B}{dt}\right) = (-r_A'''')V_r}_{\text{use these terms to integrate}}$$

$$t = \frac{V_l (C_{B0} - C_B)}{b V_r (-r_A'''')} = \frac{0.65(1097 - 109.7)}{2/3\,(1)(0.0771)} = 12{,}485 \text{ s}$$

$$= 3 \text{ hr } 28 \text{ min}$$

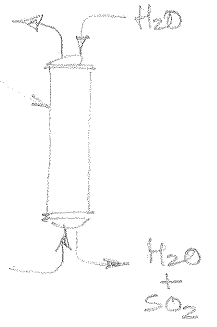
22.7 **Preliminary** $SO_2 + \frac{1}{2}O_2 \longrightarrow \cdots$

$A + \frac{1}{2}B \longrightarrow \cdots$

$-r_A' = 0.01553\, C_B$, mol/kg·s

$-r_B' = -\frac{1}{2} r_A' = 0.007765\, C_B$, mol/kg·s

$V_2 = 0.2\ m^3$



$p_A = 0.002(101325)$ Pa

$p_B = 0.21(101325)$ Pa

$\pi = 1$ atm

$v_0 = 0.01\ m^3/s$

In terms of concentrations

$$C_{A\,in} = \frac{p_A}{H_A} = \frac{0.002(101325)}{380000} = 5.333 \times 10^{-4}\ mol/m^3$$

$$C_{B\,in} = \frac{p_B}{H_B} = \frac{0.21(101325)}{78000} = 2446 \times 10^{-4}\ mol/m^3$$

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 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

$$-r'_{A\,inlet} = k' C_A^0 C_B^1 = \left(k' \frac{C_B}{C_A}\right) C_A = \left(k' \frac{p_B}{p_A} \cdot \frac{H_A}{H_B}\right)$$

$$= \left(0.01553 \frac{21}{0.2} \frac{380000}{87000}\right) C_A = \underset{\nwarrow\, m^3/kg \cdot s}{7.122}\, C_A \ mol/kg{\cdot}s$$

Now the overall rate in the tower is

$$-r_A'''' = \frac{1}{\frac{1}{(k_i a_i)_{l+g}} + \frac{1}{k_{Ac} a_c} + \frac{1}{k' \rho_s \varepsilon_A f_c}} \cdot \frac{p_A}{H_A} \qquad \text{--- (i)}$$

Evaluate terms

22.7
continued

$$(k_i a_i)_{l+g} = 0.01\ s^{-1}$$

$$a_c = \frac{6 f_s}{d_p} = \frac{6(0.6)}{0.005} = 720\ m^2/m^3$$

$$k_c = 4\times10^{-5}\ m/s$$

$$M_T = \frac{d_p}{6}\sqrt{\frac{k' \rho_s}{\mathcal{D}}} = \frac{0.005}{6}\sqrt{\frac{7.122(850)}{5.35\times10^{-10}}} = 2803$$

$$\mathcal{E} = 357\times10^{-6}$$ --- strong pore diffusion resistance

Replace in (i)

$$-r_A'''' = \frac{1}{\frac{1}{\underset{\uparrow s^{-1}}{0.01}} + \frac{1}{\underset{\uparrow m/s}{4\times10^{5}}\underset{\uparrow m^2/m^3}{(720)}} + \frac{1}{\underset{\uparrow m^3/kg\cdot s}{7.122}\underset{\uparrow kg/m^3 solid}{(850)}\underset{\uparrow (-)}{(357\times10^{-6})}\underset{\uparrow m^3 solid/m^3}{(0.6)}}}\ \overset{C_A}{\overbrace{\frac{0.002(101325)}{380000}}}$$

$$= \frac{1}{100+34.7+0.77}C_A$$

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

$$\frac{V_r}{v_0} = \frac{0.2m^3}{0.01m^3/s} = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A''''} = \int_{C_A}^{C_{A0}} \frac{dC_A}{0.0074C_A} = \frac{1}{0.0074}\ln\frac{C_{A0}}{C_A}$$

$$\therefore \frac{C_A}{C_{A0}} = e^{-V_r(0.0074)/v_0} = e^{-0.2(0.0074)/0.01} = 0.862$$

$\therefore$ the conversion of SO_2 $X_{SO_2} = X_A = 14\%$ ◄

23.1

$$M_H = \sqrt{\frac{\mathcal{D} k C_B}{k_{Al}^2}} = \sqrt{\frac{10^{-6}(10)(10^2)}{1^2}} = 3.16 \times 10^{-2} \quad \therefore E = 1$$

$$-r_A'''' = \frac{p_A}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_Bf_l}} = \frac{10^2}{\frac{1}{0.1} + \underset{\uparrow\, 50\%}{\frac{10^5}{10^2(1)}} + \underset{\uparrow\, 50\%}{\frac{10^5}{10(10^2)0.1}}} = 0.05 \ \frac{\text{mol}}{\text{hr}\cdot\text{m}^3\,\text{reac.}}$$

(a) Reaction rate = 0.05 mol/hr·m³ reactor ◄ a)

(b) Resistance: 50% liquid film, 50% main body
Reaction zone: main body of liquid
Behavior in liquid film: physical transport } ◄ b)

23.3

$$M_H = \sqrt{\frac{\mathcal{D} k C_B}{k_{Al}}} = \sqrt{\frac{10^{-6}(10)(10^2)}{1}} = 3.16 \times 10^{-2} \quad \therefore E = 1$$

$$-r_A'''' = \frac{p_A}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_Bf_l}} = \frac{10^2}{\underset{\uparrow\, 33\%}{\frac{1}{0.1}} + \underset{\uparrow\, 33\%}{\frac{10^3}{10^2(1)}} + \underset{\uparrow\, 33\%}{\frac{10^3}{10(10^2)(10^{-1})}}} = 3.33$$

(a) Reaction rate = 3.33 $\frac{\text{mol}}{\text{hr}\cdot\text{m}^3\,\text{reactor}}$ ◄ 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
Behavior in liquid film: physical transport } ◄ b)

23.5

$$M_H = \sqrt{\frac{\mathcal{D} k C_B}{k_{Al}}} = \sqrt{\frac{10^{-6}(10^{-2})10^2}{1}} = 10^{-3} \quad \cdots \quad \therefore E = 1$$

$$-r_A''' = \frac{p_A}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_Bf_l}} = \frac{10^2}{\underset{\uparrow\, 50\%}{\frac{1}{0.1}} + \frac{H_A}{10^2(1)} + \underset{\uparrow\, 50\%}{\frac{H_A}{10^{-2}(10^2)0.1}}} = 5$$

(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
Behavior of liquid film: physical transport } ◄ b)

23.7 Make one change in Example 1

$$C_B = 100 \Longrightarrow C_B = 1$$

First evaluate M_H and E_i and from this find E

$$M_H = \sqrt{\frac{\mathscr{D} k C_B}{k_{Al}}} = \sqrt{\frac{10^{-6}(10^6)1}{1}} = 1$$

$$E_i = 1 + \frac{1(1)10^5}{2(5\times10^3} = 1 + 50 = 51$$

Since $E_i > 5 M_H$ Fig 4 shows that we have a pseudo-1st order reaction in the film and

$$E = M_H = 1$$

Now to the rate expression

$$-r_A'''' = \frac{p_A}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_B^2 f_l}} = \frac{3\times10^5}{\frac{1}{0.01} + \frac{10^5}{20(1)} + \frac{10^5}{10^6(1^2)0.98}}$$

$$= \frac{5\times10^3}{100+\underset{\uparrow}{5000}+0.1} = \frac{5000}{5001} \simeq 1 \text{ mol/hr}\cdot\text{m}^3 \text{ of reactor}$$

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

23.9 (a) Find $-r_A''''$ with reaction

$$M_H = \sqrt{\frac{\mathscr{D} k C_B}{k_{Al}}} = \infty \quad \text{... because } k = \infty$$

$$E_i = 1 + \frac{\mathscr{D}_B C_B H_A}{\mathscr{D}_A p_{Ai}} = 1 + 0.64\,\frac{250(10^{-4})}{0.02\ 10^{-3}} = 1 + 800 = 801$$

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

$$-r_A'''' = \frac{p_A}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_Bf_l}} = \frac{p_A}{\frac{1}{60} + \frac{10^{-4}}{0.03(801)} + 0} = \frac{0.02}{16.7\times10^{-3} + 4\times10^{-6}}$$

99.97% of the resistance. this verfies our assumption

$$\left.\begin{array}{l} -r_A'''' = k_{Ag}a\,p_A = 60(0.02) = 1.2\ \text{mol/m}^3\cdot\text{s} \\ \text{Gas film controls} \end{array}\right\} \longleftarrow$$

(b) Straight absorption

$$-r_A'''' = \frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}a}}(p_A - 0) = \frac{p_A}{\frac{1}{60} + \frac{10^{-4}}{0.03}} = \frac{p_A}{16.67\times10^{-3} + 3.3\times10^{-3}}$$

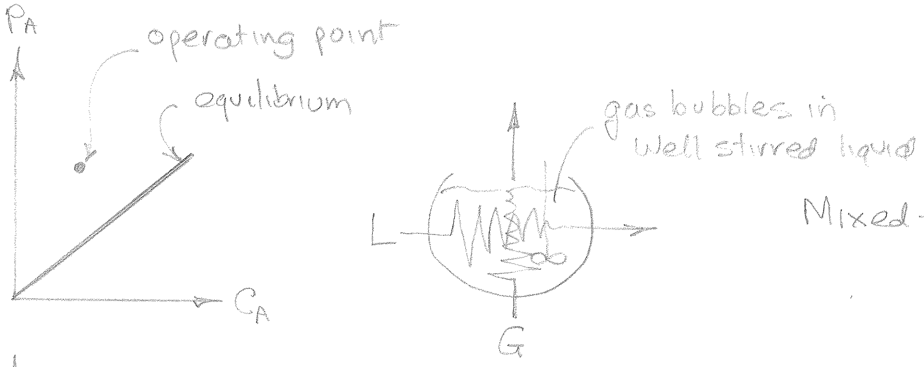
83% in gas phase

$$= 50\,p_A = 50(0.02) = 1\ \text{mol/m}^3\cdot\text{s}$$

$\therefore$ the rate is raised by 20% by adding MEA $\longleftarrow$

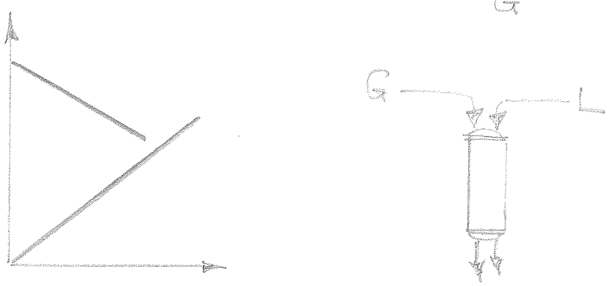
24.1

(a)



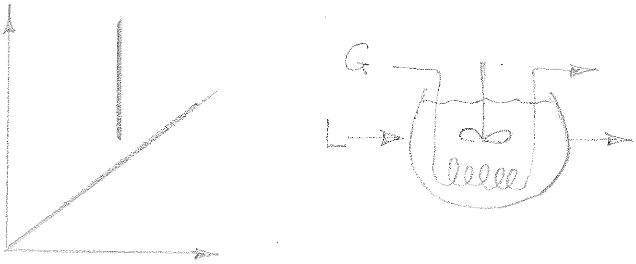
Mixed-mixed

(b)



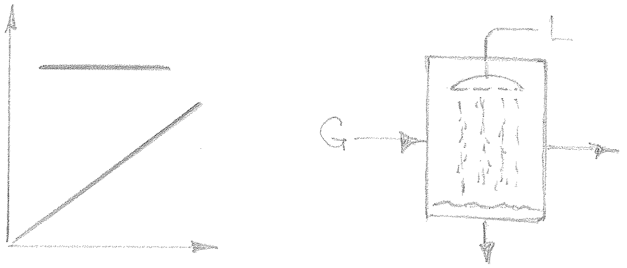
Cocurrent plug flow

(c)



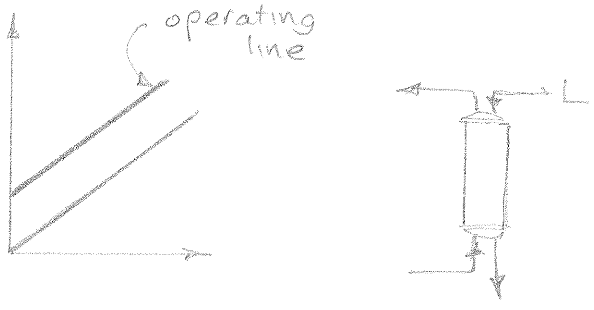
Plug-gas mixed-liquid

(d)



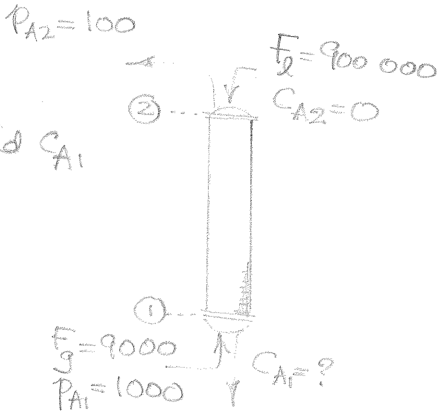
Mixed-gas plug-liquid

(e)



Countercurrent plug flow

24.3 Straight mass transfer   Counter current $H_A = 18$



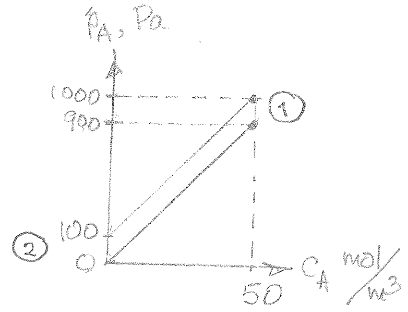
By material balance between ① & ② we find C_{A1}

$$\frac{90000}{10^5}(1000-100) = \frac{900\,000}{55\,556}(C_{A1}-0)$$

or $C_{A1} = 50 \text{ mol/m}^3$

At equilibrium $p_A^* = H_A C_A$ -- or $\overset{\text{at } C_{A1}}{p_{A1}^*} = 18 \times 50 = 900$

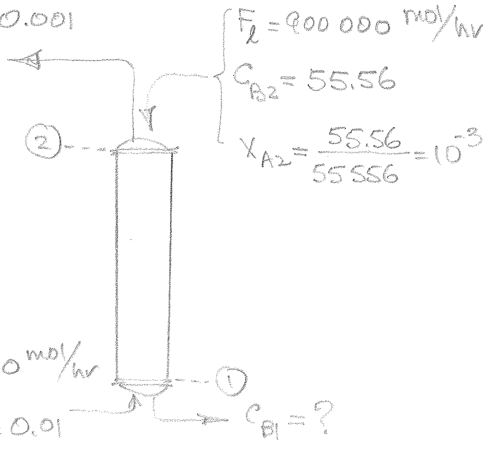
Now draw the p_A vs C_A diagram. We see that the operating & equilibrium lines are parallel. Thus the rate of transfer is the same everywhere. So we find



$$-r_A'''' = \frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}a}}(p_A - p_A^*) = \frac{1}{\frac{1}{0.36} + \frac{18}{72}}(1000-900) = 33$$

$$\therefore V_r = \frac{F_g}{\pi}\int_{1000}^{100} \frac{dp_A}{-r_A''''} = \frac{90\,000}{10^5}\,\frac{(1000-100)}{33} = 24.5 \text{ m}^3 \longleftarrow$$

24.5 By material balance find C_{B1} (see diagram on right)



$$F_g(Y_{A1} - Y_{A2}) = F_l(X_{A2} - X_{A1})$$

or

$$90000\left(\frac{0.01}{0.99} - \frac{0.001}{0.999}\right) = 900\,000\,(0.001 - X_{B1})$$

or $C_{B1} = 5 \text{ mol/m}^3$

We need to evaluate E_i & M_H to find the rate

$$\left.\begin{aligned} E_i &= 1 + \frac{\mathcal{D}_B C_B}{b\,\mathcal{D}_A C_A} = 1 + \frac{C_B}{C_A} = 1 + \frac{C_B H_A}{p_{Ai}} = 1 + \frac{10^5 C_B}{p_{Ai}} \\ M_H &= \sqrt{\frac{\mathcal{D}_A k C_B}{k_{Al}^2}} = \infty \end{aligned}\right\}$$

Since $E_i \ll M_H$ Fig 23.4 shows that $E = E_i$

24.5 continued Now determine the rate at top, bottom and intermediate point

<u>At top,</u> ②

$$E_i = 1 + \frac{55.56\times10^5}{100} = 5.556\times10^4$$

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 $E = E_i = 5.556\times10^4$. Now to the rate

$$-r_A'''' = \frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{k C_B f_l}} \cdot p_A = \frac{1}{\underset{<99\%}{\frac{1}{0.36}} + \underset{<1\%\text{ of resistance}}{\frac{10^5}{72(5.556\times10^4)}} + \frac{10^5}{\infty}} \cdot p_A = 0.36\, p_A$$

<u>At bottom,</u> ①

$$E_i = 1 + \frac{55.56\times10^5}{100} = 501$$

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 guessed

Try again

Guess $p_{Ai} = 500$, 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 $p_{Ai} = 100$, or 10% resistance in the gas film. Then $E_i = 5001$ &

$$-r_A'''' = \frac{1}{1/0.36 + 1/3.6}\, p_A = 0.33\, p_A$$

91% of resistance in gas film — close enough

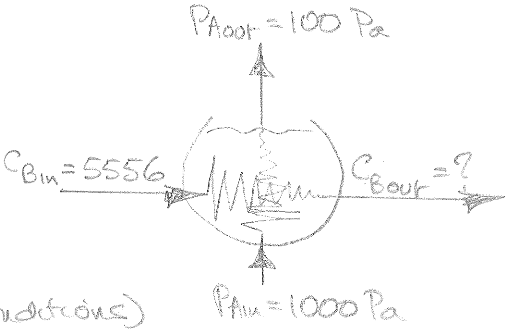
$$\text{So } (-r_A'''')_{mean} = \frac{0.36 + 0.33}{2} = 0.345\, p_A$$

Hence

$$V = \frac{F_g}{\pi}\int \frac{dp_A}{-r_{A,mean}''''} = \frac{90000}{10^5}\int_{10^2}^{10^3} \frac{dp_A}{0.345\, p_A} = \frac{90000}{34500}\ln\frac{10}{1} = 6\ m^3$$

Gas film resistance is 91% of total, 9% is from liquid ←

24.7 First determine C_{Bout} -- see sketch at right



$$F_g\left(Y_{out} - Y_{in}\right) = F_\ell\left(X_{in} - X_{out}\right)$$

or

$$90000\left(\frac{0.01}{0.99} - \frac{0.001}{0.999}\right) = 9000\left(\frac{5556}{55556} - \frac{C_{Bout}}{55556}\right)$$

$$\therefore C_{Bout} = 500 \text{ mol/m}^3$$

Next determine the rate (note, at the exit conditions)

$$M_H = \sqrt{\frac{\mathscr{D} k C_B}{k_{A\ell}}} = \sqrt{\frac{3.6\times10^{-6}(2.6\times10^5)500}{0.72^2}} = 30$$

$$E_i = 1 + \frac{C_B H_A}{p_{Ai}} = 1 + \frac{500(10^5)}{\underset{\text{or lower}}{100}} = 5\times10^5, \text{ or higher}$$

Since $E_i \gg M_H$, Fig 23.4 shows that $E = M_H = 30$

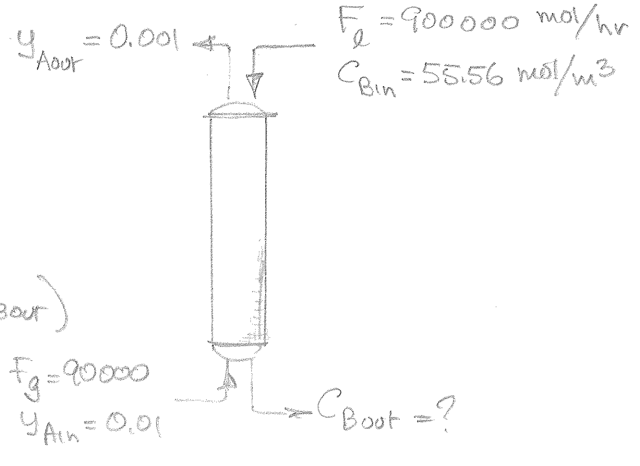
$$-r_A'''' = \frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{A\ell}aE} + \frac{H_A}{kC_Bf_\ell}} \cdot p_A = \frac{1}{\frac{1}{0.72} + \frac{10^5}{144(30)} + \frac{10^5}{2.6\times10^5(500)(0.9)}} \cdot p_A$$

$$= \frac{1}{\underbrace{1.389}_{5.7\% \text{ of the resistance}} + \underbrace{23.15}_{94\% \text{ of the resistance}} + 0} = 0.041\ p_A$$

$$\therefore\quad V_r = \frac{F_g}{\pi}\frac{\Delta p_A}{(-r_A'''')} = \frac{90000(1000-100)}{10^5(0.041)100} = 197.6 \text{ m}^3$$

Liquid film contributes 94.3% of the resistance

24.9 First determine C_{Bout} by a material balance



$$F_g\left(Y_{Ain} - Y_{Aout}\right) = F_\ell\left(X_{Bout} - X_{Bin}\right)$$

or

$$90000\left(\frac{0.01}{0.99} - \frac{0.001}{0.999}\right) = \frac{900000}{55556}\left(55.56 - C_{Bout}\right)$$

From which

$$C_B = 5 \text{ mol/m}^3$$

24.9 continued

At top
$$M_H = \sqrt{\frac{\mathscr{D} k C_B}{k_{Al}}} = \sqrt{\frac{3.6\times10^{-6}(2.6\times10^{7})55.56}{0.72^2}} = 100$$

$$E_i = 1 + \frac{55.56(10^5)}{100} = 55561 \gg M_H \quad \cdots \therefore E = M_H = 100$$

$$-r_A'''' = \frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_Bf_l}} \cdot p_A = \frac{1}{\frac{1}{0.36} + \underset{\uparrow}{\frac{10^5}{72(100)}} + \frac{10^5}{2.6\times10^7(55.56)(0.9)}} \cdot 10^2 = 6$$

liquid film = 83% of total resistance

At bottom
$$M_H = \sqrt{\frac{3.6\times10^{-6}(2.6\times10^{7})5}{(0.72)^2}} = 30$$

$$E_i = 1 + \frac{5(10^5)}{1000} = 501 \gg M_H \quad \cdots \therefore E = M_H = 30$$

$$-r_A'''' = \frac{1}{\frac{1}{0.36} + \underset{\uparrow}{\frac{10^5}{72(30)}} + \frac{10^5}{2.6\times10^7(5)0.9}} \cdot 10^3 = 20.4$$

liquid film = 94%

Near the middle where $C_B = 30.56$. A mat. balance then gives $\left\{ \begin{array}{l} p_A = 547\ \text{Pa} \\ Y_A = 0.0055 \end{array} \right.$

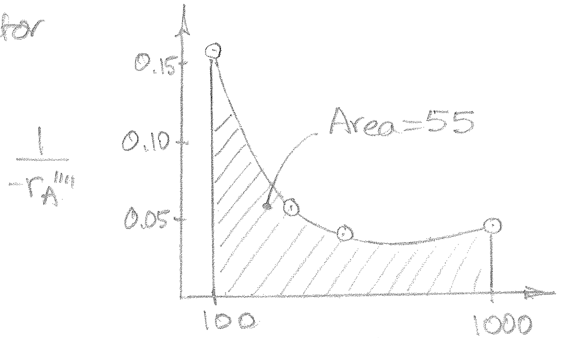
$$\left. \begin{array}{l} M_H = \sqrt{\dfrac{3.6\times10^{-6}(2.6\times10^{7})30.56}{(0.72)^2}} = 74 \\ E_i = \text{large} \end{array} \right\} \therefore E = M_H = 74$$

and
$$-r_A'''' = 25.4$$

About 1/4 from the top where $p_A = 300\ \text{Pa}$ & $C_B = 44.4$ we find
$M_H = 89.5$, E_i = very large, so $E = M_H = 89.5$ & $-r_A'''' = 16.4$

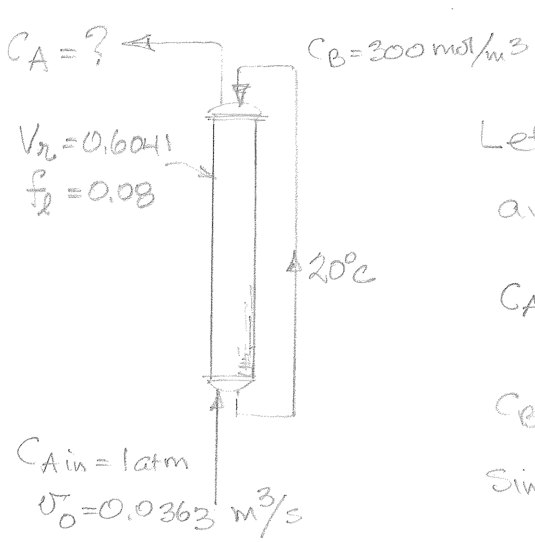
So now to the performance of the reactor

	p_A	$-r_A''''$	$1/-r_A''''$
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



$$\left. \begin{array}{l} V_r = \dfrac{F_g}{\pi} \displaystyle\int \dfrac{dp_A}{-r_A''''} = \dfrac{90000}{10^5}(\text{area}) = \dfrac{90000}{10^5}(55) = 49.5\ \text{m}^3 \\ \text{Liquid film resistance dominates, } 83 \sim 94\% \end{array} \right\}$$

24.11



Let us start by evaluating C_A & C_B, and then the rate

$$C_{A\,in} = \frac{p_{A\,in}}{H_A} = \frac{101325}{3500} = 28.95\ \text{mol/m}^3$$

$C_{B\,in} = 300\ \text{mol/m}^3$

Since $C_B \gg C_A$ we have an excess of B so we can take $C_B \cong \text{constant} = 300$

Now to the rate of rx

$$M_H = \sqrt{\frac{1.4\times10^{-9}(0.433)300}{0.25/120}} = 2.05$$

$$E_i = 1 + \frac{300(3500)}{101325} = 11.36$$

since $E_i > 5 M_H$ we have $E = M_H = 2.05$

so

$$-r_A'''' = \frac{1}{0 + \frac{3500}{0.025(2.05)} + \frac{3500}{0.433(300)0.08}} \cdot p_A$$

$$= \frac{p_A}{0 + 68292 + 337} = 1.457\times10^{-5}\, p_A = 1.4764$$

99.5% of the resistance

pure CO_2 at 1 atm,
$\therefore p_A = \text{constant}$, and $r_A'''' = \text{const}$

From Eq 15

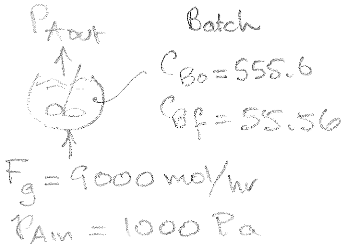
$$\frac{V_r}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A''''} = \frac{X_A}{-r_A''''}$$

because $-r_A'''' = \text{constant}$

$$\text{so}\quad X_A = \frac{V_r}{F_{A0}}(-r_A'''') = \frac{0.6041}{1.05}(1.48) = 0.8515 = 85\%$$

$F_{A0} = v_0 C_{A0} = 0.0363(28.95) = 1.05$

24.13 Here we have a batch agitated tank $\underset{\sim\sim\sim}{k = 2.6\times10^5}$ $\underset{\sim\sim\sim}{H_A = 10^5}$



At the beginning $C_B = 555.6$

$$\left.\begin{aligned} M_H &= \frac{\sqrt{3.6\times10^{-6}(2.6\times10^5)555.6}}{144/100} = 15.84 \\ E_i &= 1 + \frac{555.6(10^5)}{\underset{\nwarrow}{10^3}} = 55561 \end{aligned}\right\}$$

guess this or something smaller
whatever we guess makes
no difference

Now $M_H \ll E_i$ so $E = M_H = 15.84$.

Next, since $E = M_H$ and $p_A \ll \pi$ we can use the shortcut just above Eq 19 to evaluate the rate. So

$$-r_A'''' = \frac{1}{\frac{\pi V_r}{F_g} + \frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_B f_l}} \cdot p_{A\,in}$$

$$= \frac{1}{\frac{10^5(1.62/0.9)}{9000} + \frac{1}{0.72} + \frac{10^5}{144(15.84)} + \frac{10^5}{2.6\times10^5(555.6)0.9}} \cdot p_A$$

$$= \frac{1}{20 + 1.3889 + 43.8417 + 0.0008} \cdot 1000 = 15.33$$

main resistances — negligible

or $\dfrac{1}{-r_A''''} = 0.06523$

At the end of the run $C_B = 55.56$

$$\left.\begin{aligned} M_H &= 5.01 \\ E_i &= 1 + \frac{55.6(10^5)}{10^3} = 5561 \end{aligned}\right\}$$ $E = M_H$ and again use the shortcut

$$-r_A'''' = \frac{1}{20 + 1.3889 + \underbrace{10^5/144(5.01)}_{138.61} + \sim 0} \cdot 1000 = 6.25$$

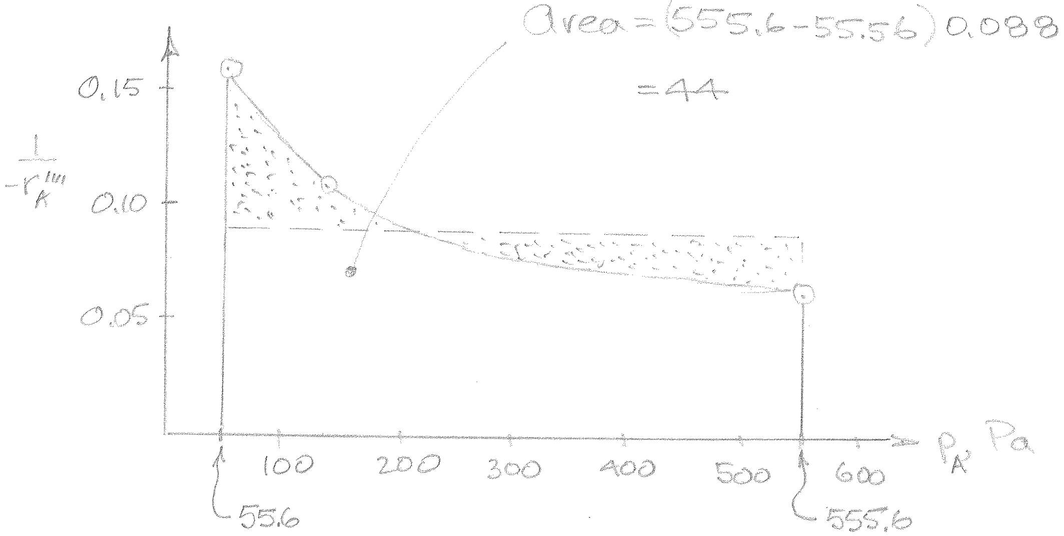
$\therefore \dfrac{1}{-r_A''''} = 0.16$

24.13 continued <u>At some intermediate conditon</u>, say at $C_B = \frac{555.6}{4} = 138.9$

$$\left.\begin{array}{l} M_H = \frac{15.84}{2} = 7.92 \\ E_i = 55561/_4 = 13890 \end{array}\right\} E = M_H = 7.92$$

$$\therefore \quad -r_A'''' = \frac{1}{20 + 1.3889 + \frac{10^5}{144(7.92)}^{+\sim 0}} \cdot 1000 = 9.168$$

$$\text{and} \quad \frac{1}{-r_A''''} = 0.109$$


Area = (555.6 − 55.56) 0.088
= 44

The length of time that we have to bubble gas through the liquid is

$$t = \frac{f_\ell}{b}\int \frac{dC_B}{-r_A''''} = f_\ell\,(\text{area}) = 0.9(44) = 39.6\text{ hr}$$

$b = 1$

The minimum time needed if all the A reacts with B is

$$t_{min} = \frac{V_\ell\,(C_{B0} - C_{Bf})}{F_g\,(p_A/(\pi - p_A))} = \frac{1.62\,(555.6 - 55.56)}{9000\,(1000/99000)} = 8.91\text{ hr} \longleftarrow a)$$

$$\therefore \text{ Efficiency of use of A} = \frac{8.91}{39.6} = 22.5\% \longleftarrow b)$$

24.15 Here we have a batch agitated tank with $\underline{k = 2.6\times10^3}$, $\underline{H_A = 10^5}$

<u>At the beginning</u> $C_B = 555.6\ \text{mol/m}^3$

$$\left.\begin{aligned} M_H &= \frac{\sqrt{2.6\times10^3(3.6\times10^{-6})555.6}}{144/100} = 1.584 \\ E_i &= 1 + \frac{555.6(10^5)}{\underset{\text{guess}}{10^3}} = 55561 \end{aligned}\right\} E = M_H = 1.584$$

Use the shortcut formula just above Eq 19, thus

$$-r_A'''' = \frac{1}{\frac{V_r\pi}{F_g} + \frac{1}{k_{Ag}a} + \frac{H_A}{k_{Al}aE} + \frac{H_A}{kC_Bf_l}}\cdot p_{Ain}$$

$$= \frac{1}{\frac{(1.62/0.9)10^5}{9000} + \frac{1}{0.72} + \frac{10^5}{144(1.584)} + \frac{10^5}{2.6\times10^3(555.6)0.9}}\cdot 1000$$

$$= \frac{1}{20 + 1.3889 + 438.4 + \sim0}\cdot 1000 = 2.175$$

$$\therefore \frac{1}{-r_A''''} = 0.460$$

<u>At the end of the run</u> $C_B = 55.56$

$$\left.\begin{aligned} M_H &= 1.584/\sqrt{10} = 0.5 \\ E_i &= 1 + \frac{55.56(10^5)}{\underset{\text{or smaller}}{10^3}} = \text{big or bigger} \end{aligned}\right\} \therefore E = M_H = 0.5$$

Shortcut →

$$-r_A'''' = \frac{1}{20 + 1.3889 + \underbrace{438.9(\sqrt{10})}_{1388} + \sim0}\cdot 1000 = 0.7096$$

$$\therefore \frac{1}{-r_A''''} = 1.41$$

24.15 continued

At some intermediate condition, say $C_B = 555.6/4 = 138.9$

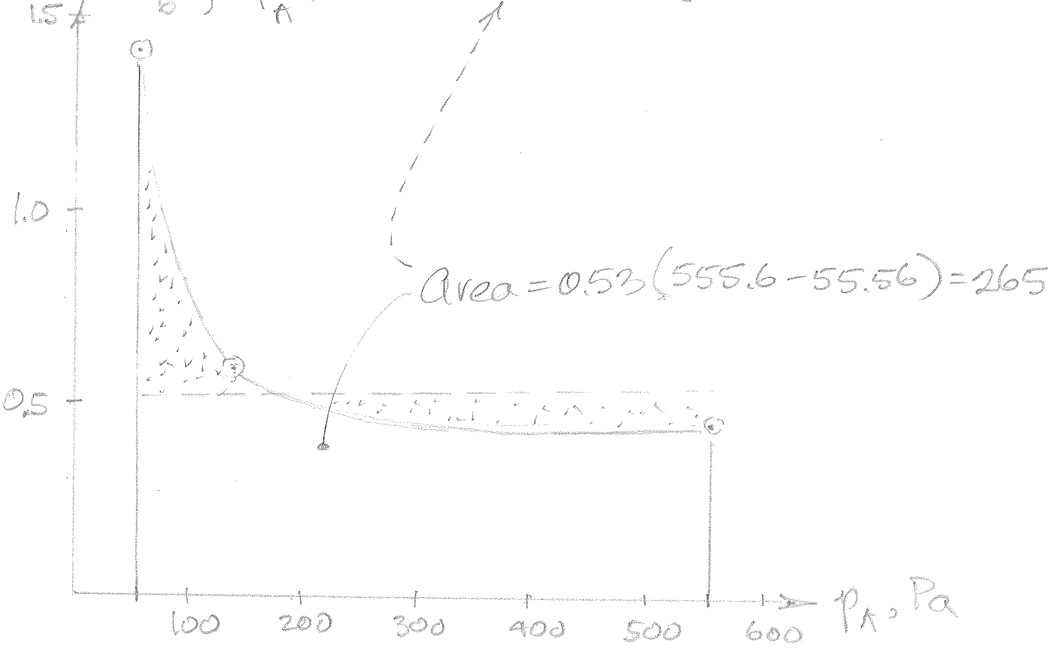
$$\left.\begin{array}{l} M_H = 1.584/4 = 0.792 \\ E_i = 1 + \frac{555.6(10^5)}{10^3} = \text{big} \end{array}\right\} E = 1 + \frac{M_H^2}{3} = 1.2$$

$$\therefore\ -r_A'''' = \frac{1}{20 + 1.3889 + \underbrace{10^5/144(1.2)}_{\text{main resistance}}} \cdot 1000 = 1.666$$

$$\therefore\ \frac{1}{-r_A} = 0.600$$

The length of time needed to bubble gas through the reactor is

$$t = \frac{f_l}{b}\int \frac{dC_B}{-r_A''''} = f_l\,(\text{area}) = 0.9(265) = 238.5\,\text{hr} \longleftarrow (a)$$



$$t_{min} = \frac{V_l(C_{B0} - C_{Bf})}{F_g\,(p_{Am}/(\pi - p_{Am}))} = \frac{1.62(555.6 - 55.56)}{9000(1000/99000)} = 8.91\,\text{hr}$$

$$\therefore\ \text{Efficiency of use of A} = \frac{8.91}{238.5} = 3.7\% \longleftarrow (b)$$

25.1 Test the 3 possible shrinking-core mechanisms to see which is consistent with the following reported data

$$\left.\begin{aligned} X_B &= 0.875 \quad \text{at} \quad t = 1\,\text{hr} \\ X_B &= 1.000 \quad \text{at} \quad t (= \tau) = 2\,\text{hr} \end{aligned}\right\} \cdots \text{or } X_B = 7/8 \text{ at } \frac{t}{\tau} = 0.5$$

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: $0.5 \overset{?}{=} 0.875$ ... 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 $0.5 \overset{?}{=} 1 - 3(1/8)^{2/3} + 2(1/8) = 0.5$ ... 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: $0.5 \overset{?}{=} 1 - (1/8)^{1/3}$ ... 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.

25.3 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

$$\frac{t}{\tau} = 1-(1-X_B)^{1/3} \quad \cdots \text{ where } \tau = \frac{\rho_B R_o}{b\, k_s C_{Ag}}$$

but $\rho_B = \dfrac{2.2\,\text{gm/cm}^3}{12\,\text{gm/mol}} = 0.183\ \text{mol/cm}^3$

$$C_{Ag} = \frac{1\,\text{mol}}{22400\,\text{cm}^3}\cdot\frac{273}{273+900}\cdot 0.08 = 8.30\times10^{-7}\ \text{mol/cm}^3$$

for the reaction $C + O_2 \longrightarrow CO_2 \quad \cdots \quad b = 1$

Replacing these quantities in the τ expression gives

$$\tau = \frac{(0.183)(0.5)}{(1)(20)(8.3\times10^{-7})} = 5510\ \text{sec} = 1.53\ \text{hr} \longleftarrow$$

25.5 Let 1 refer to particles of size R
2 " " " " " 2R } then $\tau_2 = 3\tau_1$ ----(o)

Now $\tau_1 = \tau_{1ash} + \tau_{1rxn}$ -----(i)

$\tau_2 = \tau_{2ash} + \tau_{2rxn}$ -----(ii)

But $\tau_{2ash} = 4\tau_{1ash}$ ---------(iii)

$\tau_{2rxn} = 2\tau_{1rxn}$ -------(iv)

So (iii) & (iv) & (o) in (ii) gives $3\tau_1 = 4\tau_{1ash} + 2\tau_{1rxn}$ -----(v)

From (i) and (v) we find $\tau_{1ash} = \tau_{1rxn}$

∴ the % contribution of ash diffusion for R = 50% ←

25·7

guess ash diffusion controls ← guess reaction controls

d_t	X_B	t	$\frac{R^2}{t}\left[1-3(1-X_B)^{2/3}+2(1-X_B)\right]$	$\frac{R}{t}\left[1-(1-X_B)^{1/3}\right]$
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

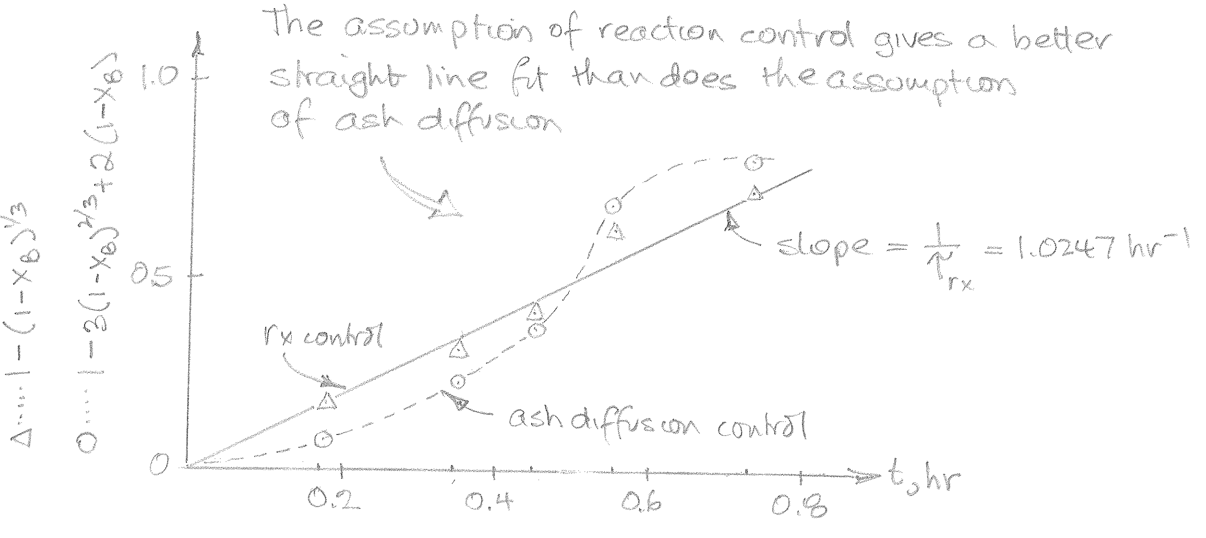
d_t	X_B	t	$\frac{R^2}{t}\left[1-3(1-X_B)^{2/3}+2(1-X_B)\right]$	$\frac{R}{t}\left[1-(1-X_B)^{1/3}\right]$
1	1	200	1.25×10^{-3} ←	2.5×10^{-3}
1.5	1	450	1.25×10^{-3} ←	1.67×10^{-3}

same

∴ ash diffusion controls ◄——

25·11 Plot assuming that reaction, and then ash diffusion controls

t, hr	0.180	0.347	0.453	0.567	0.733
X_B	0.45	0.68	0.80	0.95	0.98
$1-(1-X_B)^{1/3}$	0.1807	0.3160	0.4152	0.6316	0.7286
$1-3(1-X_B)^{2/3}+2(1-X_B)$	0.0861	0.2365	0.3740	0.6928	0.8190


The assumption of reaction control gives a better straight line fit than does the assumption of ash diffusion

From the above plot $\frac{t}{\tau_{rx}} = 1-(1-X_B)^{1/3}$

$\tau_{rx} = \tau = 0.98$ hr ◄——

26.1 For plug flow, SCM/ash diffusion control, in the original reactor

$$\frac{t_p}{\tau} = 1-3(1-X_B)^{2/3}+2(1-X_B) = 1-3(1-0.8)^{2/3}+2(1-0.8) = 0.374$$

Now double t_p. Then the conversion X_B' is

$$\frac{2t_p}{\tau} = 2(0.374) = 1-3(1-X_B')^{2/3}+2(1-X_B')$$

or $X_B' = 96.5\% \longleftarrow$

26.3 For plug flow SCM/reaction control $\tau \propto R$, therefore

$\tau_{4mm} = 4\,hr$ (given)
$\tau_{2mm} = 2\,hr$ (calculated)
$\tau_{1mm} = 1\,hr$ (calculated)

So for 100% conversion the residence time must be longer than τ_{4mm}. Therefore $\tau_{reactor} = 4\,hr$ or more $\longleftarrow$

26.5 We are given that: $W_1 = W_2$, $C_{A0,1} = C_{A0,2}$, $\bar{t}_1 = \bar{t}_2$, $F_{A0,1} = F_{A0,2}$

∴ we end up with the same conversion. $\longleftarrow$

Note: Size of reactor is unimportant, weight of solids is

26.7 Following the procedure of Example 3 we have ..

$$\bar{t} = 10\,min \begin{cases} \tau(50\mu m) = 2.5\,min \\ \tau(100\mu m) = 10\,min \\ \tau(200\mu m) = 40\,min \end{cases}$$ from equ 25.37 for ash diff

So from Eq 11

$$1-\bar{\bar{X}}_B = \left[\frac{1}{5}\left(\frac{2.5}{10}\right) - \frac{19}{420}\left(\frac{2.5}{10}\right)^2 + \right]\frac{3}{10} + \left[\frac{1}{5}\left(\frac{10}{10}\right) - \frac{19}{420}\left(\frac{10}{10}\right)^2 + \frac{41}{4620}\left(\frac{10^3}{10^3}\right)^3 + \cdots\right]\frac{4}{10}$$

$$+\left[\frac{1}{5}\left(\frac{40}{10}\right) - \frac{19}{420}\left(\frac{40}{10}\right)^2 + \frac{41}{4620}\left(\frac{40}{10}\right)^3 - 0.00149\left(\frac{40}{10}\right)^4 + \cdots\right]\frac{3}{10}$$

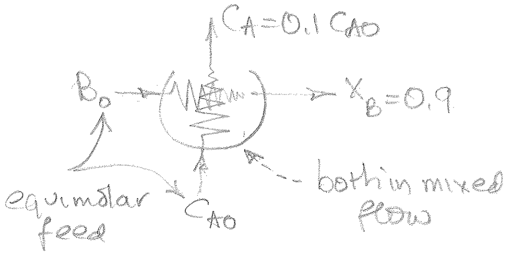
converges too slowly, so use Fig. 4. This gives $1-\bar{X}_B = 0.35$

$$= 0.0141 + 0.0654 + 0.105 = 0.1845$$

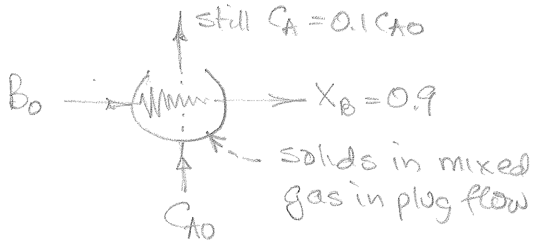
∴ the conversion for ash resistance control is $\bar{\bar{X}}_B = 81.5\%$

(for reaction control Example 3 gives $\bar{\bar{X}}_B = 77.8\%$) $\longleftarrow$

26.9 In Example 4 we have:



Here we have:



Here $\bar{C}_A = \frac{C_{A0}-C_{Af}}{\ln C_{A0}/C_{Af}} = \frac{C_{A0}-0.1C_{A0}}{\ln C_{A0}/0.1C_{A0}} = \frac{0.9}{\ln 10} = 0.39$ ← instead of 0.1, as in Example 4

∴ Wt of solids needed $= \frac{23\text{ tons}}{3.9}$

$= 5.88$ tons ←

26.11 For SCM/reaction control, $1-X_B=(1-t/\tau)^3$

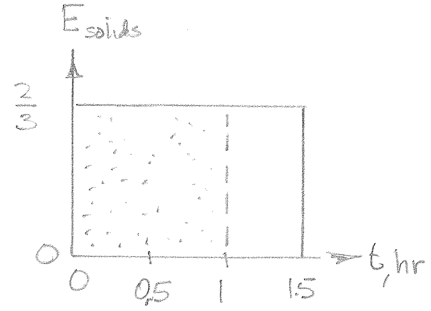
So from Eq 16, with $\tau = 1$ hr,

$$1-\bar{X}_B = \int_0^\tau (1-X_B)_{part}\, E_{solids}\, dt$$

$$= \int_0^\tau \left(1-\frac{t}{\tau}\right)^3 \frac{2}{3}\, dt$$

$$= \frac{2}{3}\int_0^1 (1-t)^3 dt = \frac{2}{3}\cdot\frac{1}{4} = \frac{1}{6}$$

∴ $\bar{X}_B = 83.3\%$ ←



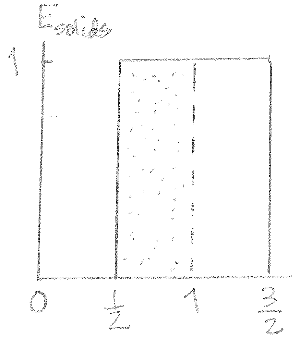
26.13 For SCM/reaction control, $1-X_B=(1-t/\tau)^3$

So from Eq 16, with $\tau=1$

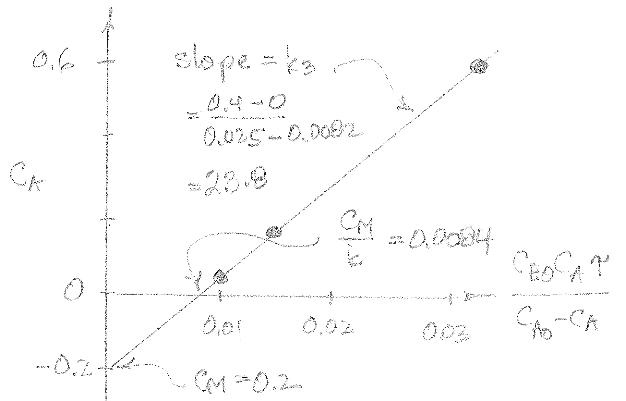
$$1-X_B = \int_{1/2}^{1.0} (1-t)^3 (1)\, dt$$

$$= -\frac{(1-t)^4}{4}\Bigg|_{\frac{1}{2}}^{1} (1) = \left[\frac{1}{64}-0\right] = 0.0156$$

∴ $\bar{X}_B = 98.44\%$ ←



27.1



For mixed flow & Monod kinetics Eq 8 gives

$$\underbrace{C_A}_{y} = \underbrace{-C_M}_{a} + \underbrace{k_3}_{b}\underbrace{\left(\frac{C_{E0}C_A\tau}{C_{A0}-C_A}\right)}_{x}$$

Plotting gives (see Fig. 6)

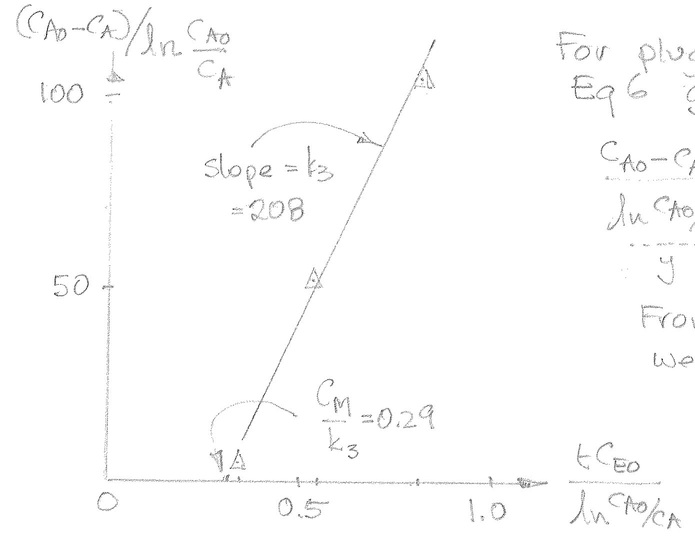
$$-r_A = \frac{23.8\, C_A C_{E0}}{0.2+C_A}, \ \text{mol/lit·hr}$$

Tabulate

C_{E0}	C_{A0}	C_A	v	$\tau = V/v$	$C_{E0}C_A\tau/(C_{A0}-C_A)$
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	0.0333

given data calculated

27.3



For plug flow & Monod kinetics Eq 6 gives

$$\underbrace{\frac{C_{A0}-C_A}{\ln C_{A0}/C_A}}_{y} = \underbrace{-C_M}_{a} + \underbrace{k_3\frac{C_{E0}t}{\ln C_{A0}/C_A}}_{bx}$$

From the plot & table below we find

$$-r_A = \frac{208\, C_A C_{E0}}{60.3+C_A}, \ \text{mol/m}^3\text{·hr}$$

Tabulate

C_{E0}	C_{A0}	C_A	t	$(C_{A0}-C_A)/\ln\frac{C_{A0}}{C_A}$	$tC_{E0}/\ln\frac{C_{A0}}{C_A}$
3	400	10	1	105.7	0.81
2	200	5	1	52.9	0.54
1	20	1	1	6.34	0.33

given data calculated

27.5

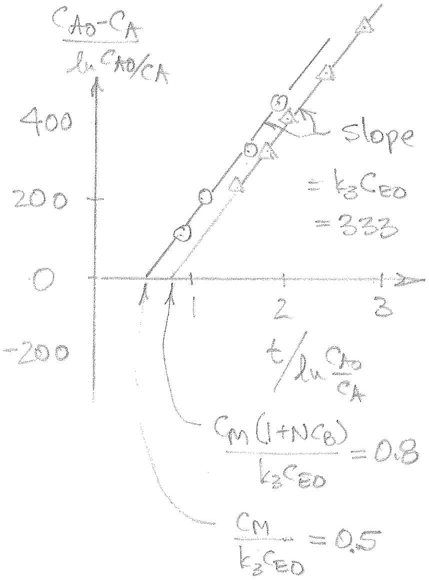
Run 1 $\begin{cases} C_{A0} = 600 \text{ mol/m}^3 \\ C_{E0} = 8 \text{ gm/m}^3 \\ C_{B0} = 0 \end{cases}$

Run 2 $\begin{cases} C_{A0} = 800 \text{ mol/m}^3 \\ C_{E0} = 8 \text{ gm/m}^3 \\ C_{B0} = C_B = 100 \text{ mol/m}^3 \end{cases}$

t	C_A	$\frac{C_{A0}-C_A}{\ln C_{A0}/C_A}$	$\frac{t}{\ln C_{A0}/C_A}$
0	600		
1	350	464	1.9
2	160	333	1.5
3	40	207	1.1
4	10	144	0.97

t	C_A	$\frac{C_{A0}-C_A}{\ln C_{A0}/C_A}$	$\frac{t}{\ln C_{A0}/C_A}$
0	800	—	—
1	560	673	2.8
2	340	538	2.3
3	180	416	2.0
4	80	313	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 $= k_3C_{E0} = 333$

$\therefore k_3 = 333/8 = 41.63$

intercept $= \frac{C_M}{k_3C_{E0}} = 0.5$

$\therefore C_M = 0.5(333) = 167$

Thus the rate equation is

$$+r_R = \frac{41.63\, C_{E0}C_A}{C_A+167} = \frac{333\, C_A}{167\, C_A}$$ ◄ with no inhibition

Run #2 Parallel slopes means competitive inhibition. From run #1

$C_{E0} = 8, \quad k_3 = 41.63, \quad C_M = 167$

intercept $= \frac{C_M(1+NC_B)}{k_3C_{E0}} = \frac{167(1+N\times 100)}{333} = 0.8 \quad \therefore N = 0.006$

The rate equation is

$$r_R = \frac{k_3C_{E0}C_A}{C_M+C_A+NC_BC_M} = \frac{41.63\, C_{E0}C_A}{167+C_A+C_B} = \frac{333C_A}{267+C_A}$$ ◄ with competitive inhibition

---

27.7 Cellulose $\xrightarrow{\text{cellulase}}$ sugar, Monod kinetics, mixed flow

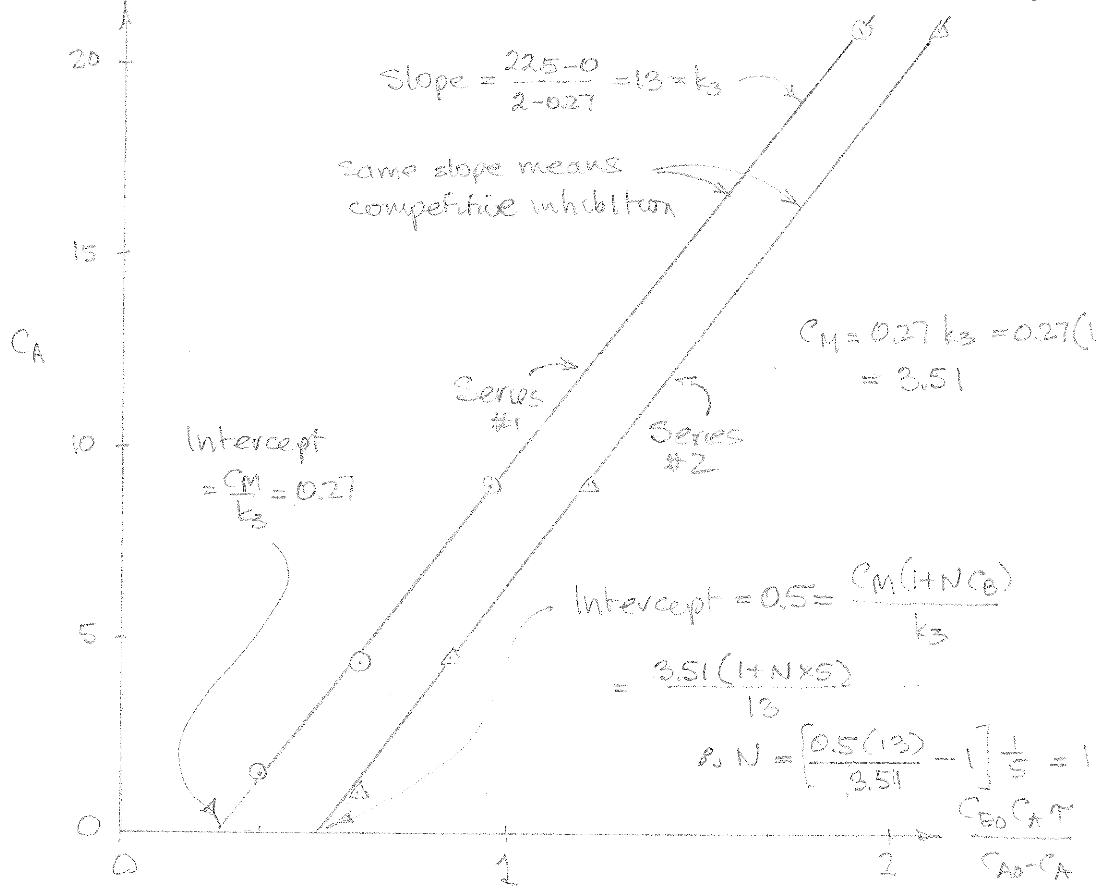
Series 1 has no inhibitor, series 2 has $C_B = 5\ \frac{kg}{m^3}$. To see which form of inhibition applies, if any, try to fit Eq 11 or 15 in Fig 9.

C_{A0}	C_A	τ	$C_{E0}C_A\tau/(C_{A0}-C_A)$
25	1.5	587	0.3747
25	4.5	279	0.6124
25	9	171	0.9616
25	21	36	1.890

Series #1 : without B

C_{A0}	C_A	τ	$C_{E0}C_A\tau/(C_{A0}-C_A)$
25	1.5	940	0.6
25	4.5	387	0.85
25	9	213	1.2
25	21	40	2.1

Series #2 : with $C_B = 5\ kg/m^3$



$$\text{Slope} = \frac{22.5-0}{2-0.27} = 13 = k_3$$

$$\text{Intercept} = \frac{C_M}{k_3} = 0.27$$

$$C_M = 0.27\,k_3 = 0.27(13) = 3.51$$

$$\text{Intercept} = 0.5 = \frac{C_M(1+NC_B)}{k_3} = \frac{3.51(1+N\times 5)}{13}$$

$$\text{so } N = \left[\frac{0.5(13)}{3.51} - 1\right]\frac{1}{5} = 1.1$$

From the plot

$$\text{With no inhibition: } r_R = \frac{k_3 C_{E0} C_A}{C_M + C_A} = \frac{65\,C_A}{3.51 + C_A}$$

$$\text{With inhibition (competitive): } r_R = \frac{k_3 C_{E0} C_A}{C_M(1+NC_B) + C_A} = \frac{65\,C_A}{3.51(1+N\times 1.1) + C_A} = \frac{65\,C_A}{26.7 + C_A}$$

27.9 For M·M kinetics the reaction rate is

1st order with respect to E
between 0 & 1st order with respect to A

So 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.
So looking at the 6 contacting patterns we see that

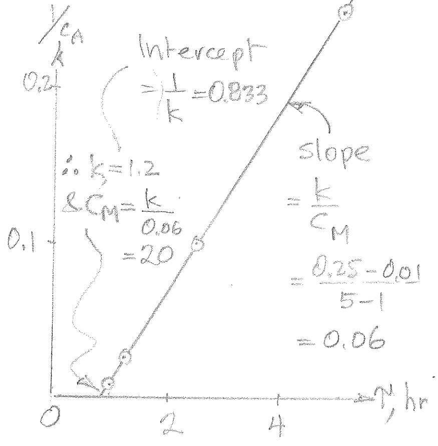
a.)
c)
d)
e)
} are not as good, while b) f) } are the best ←

29.1 For mixed flow & Monod kinetics Eq 8 gives us

$$\frac{1}{C_A} = \frac{k}{C_M}\tau_m - \frac{1}{C_M} \quad \text{or} \quad C_A = \frac{C_M}{k\tau - 1}$$

Test graphically

v	C_{A0}	C_A	C_C	$\textcircled{C/A} = \frac{C_C}{C_{A0}-C_A}$	$\tau = \frac{V}{v} = \frac{1}{v}$	$\frac{1}{C_A}$
0.2	160	4	15.6	0.1	5	0.25
0.4	160	10	15	0.1	2.5	0.1
0.8	160	40	12	0.1	1.25	0.025
1.0	160	100	6	0.1	1	0.01



$$-r_A = \frac{1.2\,C_A C_C}{20 + C_A}, \ \frac{\text{mg}}{\text{lit}\cdot\text{hr}} \longleftarrow$$

29.3 For mixed flow see Eq 8

C_{A0}	v	V	τ	$k\tau$	$C_A = C_M/(k\tau-1) = 2/(k\tau-1)$
6	1	1	1	1.2	10

Because $C_A > C_{A0}$ ...

we have washout ⟵ impossible data

29.5 Our reaction is

$$r_C = \frac{1.2\,C_A C_C}{2 + C_A}, \quad \text{with } \textcircled{C/A} = 0.1$$

For optimum operations

$$N = \sqrt{1 + \frac{C_A}{C_M}} = \sqrt{1 + \frac{6}{2}} = 2$$

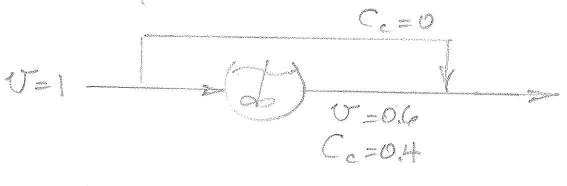
$$k\tau_{opt} = N/(N-1) = 2/1 = 2$$

$$\therefore \tau_{opt} = \frac{2}{1.2} = 1.67$$

Now for $V = 1\,m^3$ if all feed goes through the reactor

$$\tau = \frac{V}{v} = \frac{1}{1} = 1 < \tau_{opt} \text{ ... so bypass some feed}$$

and $v_{opt} = \frac{V}{\tau_{opt}} = \frac{1}{1.67} = 0.6$ so



$$\therefore C_{C_{exit}} = 0.4 \times 0.6 + 0 = 0.24 \ \text{gm}/\text{m}^3 \longleftarrow$$

29.7 We are given: $A \xrightarrow{C} R + C$, $r_C = \frac{k C_A C_C}{C_A + C_M} = \frac{2 C_A C_C}{C_A + 1}$ & $\boxed{C/A} = 0.5$

For optimum operations with a single MFR ($C_{A0} = 3$, $C_{C0} = 0$, $v = \frac{1}{3}$)

$$N = \sqrt{1 + \frac{C_{A0}}{C_M}} = \sqrt{1 + \frac{3}{1}} = 2$$

$$k\tau_{opt} = \frac{N}{N-1} = \frac{2}{1} = 2, \quad \therefore \tau_{opt} = 1$$

$$C_{A0pt} = \frac{C_{A0}}{N+1} = \frac{3}{2+1} = 1, \quad \therefore C_{C,opt} = \boxed{C/A}(C_{A0} - C_A) = 0.5(3-1) = 1$$

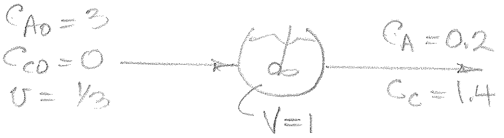
$$\tau_{washout} = N^2/N^2-1 = 4/4-1 = \frac{4}{3}$$

Thus with $v = \frac{1}{3}$, $\tau = \frac{V}{v} = 3$ ... we are beyond the optimum τ

Hence $\tau_M = \frac{1}{k}\frac{C_M + C_A}{C_A} = \frac{1}{2}\frac{C_A + 1}{C_A} = 3$ ... or $C_{Aout} = 0.2$

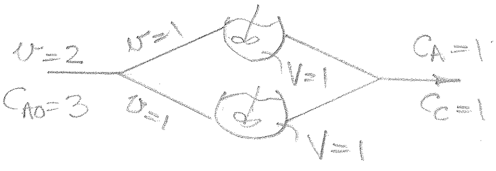
and $C_{C,out} = \boxed{C/A}(C_{A0} - C_{Aout}) = 0.5(3 - 0.2) = 1.4$

Thus



29.9 From the previous problems (see above) we know that $\tau_{opt} = 1$

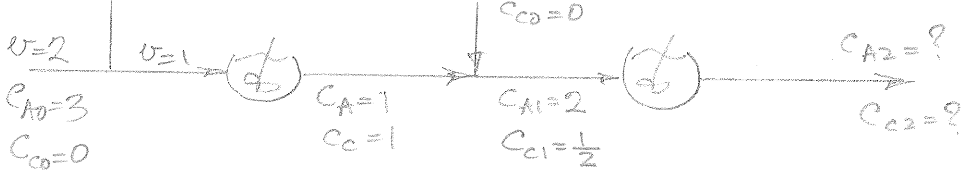
So the best arrangement is



$\tau = \frac{1}{k} \cdot \frac{C_A + C_M}{C_A} = \frac{1}{2}\frac{C_A + 1}{C_A}$ ...

or $\left.\begin{matrix} C_A = 1 \\ C_C = 1 \end{matrix}\right\}$

Alternative solution I wonder whether the scheme below is equally good, or maybe better



Let us check this

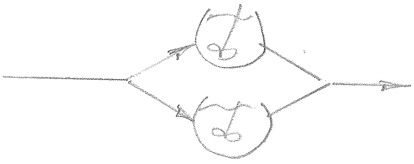
29.9 (continued) For the second reactor, from Eq 12

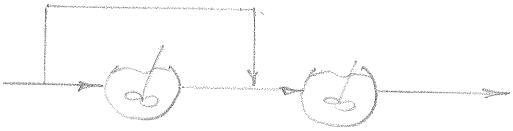
$$k\tau_m = \frac{(C_{A1}-C_{A2})(C_{A2}+C_{M})}{(A/C)C_{C1}C_{A2}+(C_{A1}-C_{A2})C_{A2}} = \frac{(2-C_{A2})(C_{A2}+1)}{2(0.5)C_{A2}+(2-C_{A2})C_{A2}}$$

or $3C_{A2}-C_{A2}^2 = 2+C_{A2}-C_{A2}^2$

or $C_{A2} = 1$
$C_{C2} = (C/A)(C_{A1}-C_{A2})+C_{C1} = 0.5+0.5 = 1$ } same as for the first arrangement

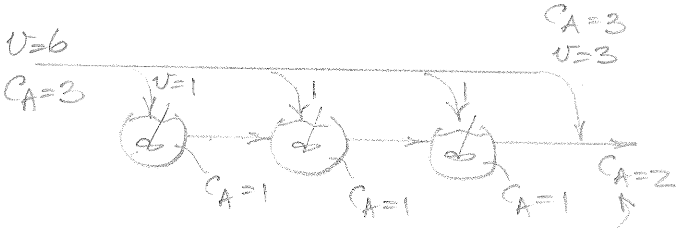
∴ both are equally good

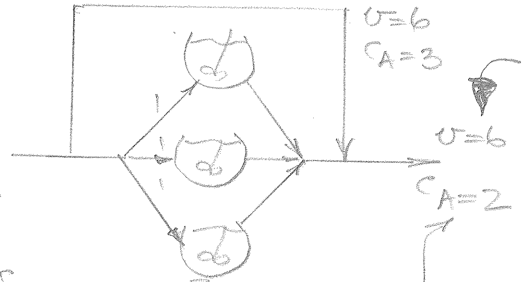




29.11 From the previous problems we have $\tau_{opt}=1$ and $C_{Aopt}=1$

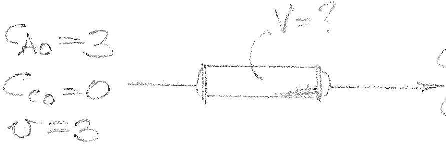
So for $v=6$
$V_{total}=3$ } we have the following good designs





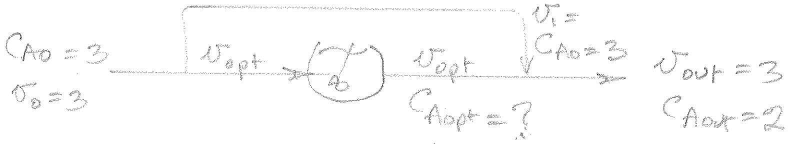
$C_{A2} = \left[3(3)+3(1)\right]\frac{1}{6} = 2$

29.13 Here we have a PFR and we want the minimum volume

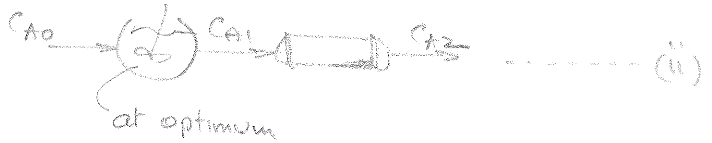


$C_C=0.5$
$C_{Aout}=? = C_{A0}-\frac{(C_C-C_{C0})}{(C/A)} = 3-0.5/0.5 = 2$

Now recall that if $C_{Aout} > C_{A,opt}$ use bypass with the reactor at C_{opt}



29.13 (continued) On the other hand if $C_{Aout} < C_{Aopt}$ then the best is to use



Here we want the design of (i), not (ii). So the size of the MFR should be such that

$$\tau_{opt} = 1 \quad \text{and} \quad C_{A2} = 1 .$$

Now evaluate the flows v_1 and v_{opt}

$$v_1 + v_{opt} = 3$$

$$v_1 C_{A0} + v_{opt} \times C_{Aopt} = C_{Aout} v_{out}$$

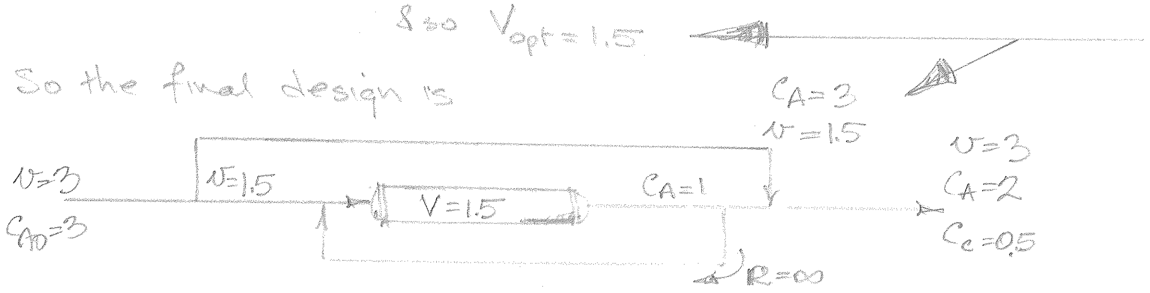
or $v_1 3 + (3 - v_1) 1 = 2(3)$ --- solve

or $v_1 = 1.5$

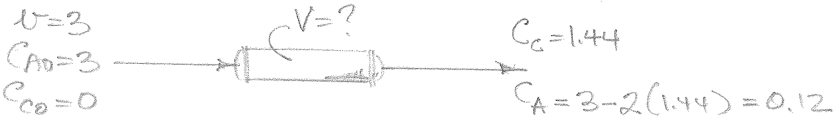
$v_{opt} = 1.5$

& so $V_{opt} = 1.5$

So the final design is



29.15 Given



Find the optimum

$$N = \sqrt{1 + \frac{C_{A0}}{C_M}} = \sqrt{1 + \frac{3}{1}} = 2 \qquad \frac{C_c}{C_{cmax}} = \frac{N}{N+1} = \frac{2}{2+1} \quad \therefore \quad \begin{matrix} C_{c,opt} = 1 \\ C_{A,opt} = 1 \end{matrix}$$

So use mixed flow up to $C_c = 1$ then use plug flow. So for mixed flow

$$k\tau = \frac{C_M + C_A}{C_A} = \frac{1+1}{1} = 2 \quad \text{or} \quad V_m = \frac{2v}{k} = \frac{2 \times 3}{2} = 3$$

29.15 (continued) For the rest of the reactor use plug flow

$$k\tau = \left(\frac{C_M}{C_{A0}+\boxed{A/C}\,C_{C0}}+1\right)\ln\frac{C_C}{C_{C0}} - \left(\frac{C_M}{C_{A0}+\boxed{A/C}\,C_{C0}}\right)\ln\frac{C_A}{C_{A0}}$$

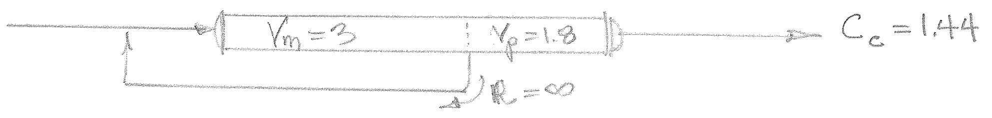
replacing values gives

$$2\left(\frac{V_p}{v}\right) = \left(\frac{1}{1+2\times1}+1\right)\ln\frac{1.44}{1} - \left(\frac{1}{1+2\times1}\right)\ln\frac{0.12}{1} = 1.1929$$

so

$$V_p = 3\times\frac{1.1929}{2} = 1.8$$

and $V_{total} = 3+1.8 = 4.8$

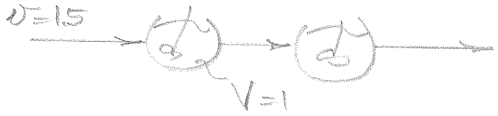


29.17 Reactor contacting patterns a), d), and f) can never be optimum. I can always do better

Patterns b), c) and e) could under certain conditions be optimum.

29.19 Calculate the conversion from the three flow patterns of Fig P19

Pattern (a)



$\therefore \tau = \frac{V}{v} = \frac{1}{1.5} = \frac{2}{3}$

Determine $N = \sqrt{\frac{C_{A0}}{C_M}+1} = \sqrt{\frac{3}{1}+1} = 2$

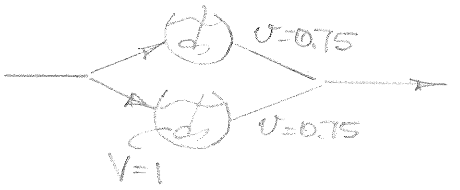
Then $k\tau_{washout} = N^2/N^2-1 = 4/4-1 = 4/3$

$$\therefore \tau_{washout} = \frac{4}{3}\left(\frac{1}{2}\right) = \frac{2}{3}$$

But this is the τ value for this arrangement. So we have washout and no reaction with pattern (a)

29.19
(continued)

Pattern (b)



$v = 1.5 \quad \therefore \tau = \frac{V}{v} = 1.33$

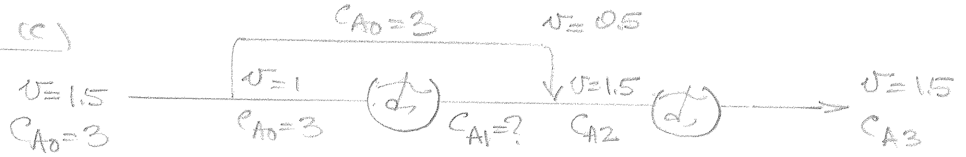
For each mixed flow unit

$$C_{A\,out} = \frac{C_M}{k\tau - 1} = \frac{1}{2\left(\frac{4}{3}\right) - 1} = 0.6 \longleftarrow \text{pretty good}$$

↑ this is not bad

Let us try the third pattern

Pattern (c)



For reactor 1 (at the optimum) $\tau = 1$

by material balance

$$C_{A1} = \frac{C_M}{k\tau - 1} = \frac{1}{2(1) - 1} = 1 \quad \therefore C_{A2} = \frac{3(0.5) + 1(1)}{1.5} = \frac{5}{3}$$

$$\therefore C_{C1} = 2 \quad C_{C2} = \frac{2(1) + 0}{1.5} = \frac{4}{3}$$

For reactor 2 (not at optimum) $\tau = \frac{V}{v} = \frac{2}{3}$

Then from Eq 12

$$k\tau = \frac{(C_{A2} - C_{A3})(C_{A2} + C_M)}{\enclose{circle}{A/C}\, C_{C2} C_{A3} + C_{A3}(C_{A2} - C_{A3}}$$

$$2\left(\frac{2}{3}\right) = \frac{(5/3 - C_A)(5/3 + 1)}{4/3\, C_A + C_A(5/3 - C_A)}$$

or

$$12C_A - 4C_A^2 = -3C_A^2 + 2C_A + 5$$

or

$$C_{A\,out} = 5 - \sqrt{20} = 0.528 \longleftarrow \text{this is best}$$

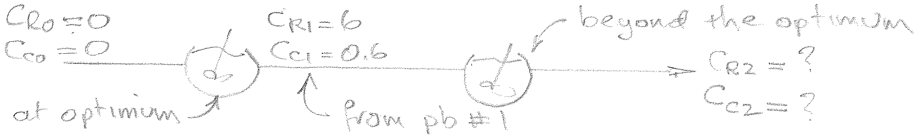
30.1 For a MFR, $n=1$, the best way to run the reaction is at $k\tau = 2$ where $C_{R\,opt} = C_R^*/2 = 12/2 = 6$ -- see after Eq 11.

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

$C_C = \enclose{circle}{C/R}\, C_R = \enclose{circle}{C/A}\enclose{circle}{A/R}\, C_R = 0.01(10)6 = 0.6$

30.3 For each tank $k\tau = 2$, so put them in series



For the second reactor, from Eq 9

$$2 = k\tau = \frac{C_{R2} - C_{R1}}{\left(1 - C_{R2}/C_R^*\right)\left(C_{R2} - C_{R1} + \enclose{circle}{R/C}\, C_{C1}\right)} = \frac{C_{R2} - 6}{\left(1 - C_{R2}/12\right)\left(C_{R2} - 6 + 6\right)}$$

$\therefore C_{R2} = 9.7$ $\quad C_{C2} = \enclose{circle}{C/A} / \enclose{circle}{R/A}\, C_{R2} = (0.01/0.1)9.7 = 0.97$

30.5 From the above problems $C_R = 6$ represents the optimum

Therefore $k\tau_{opt} = 2$

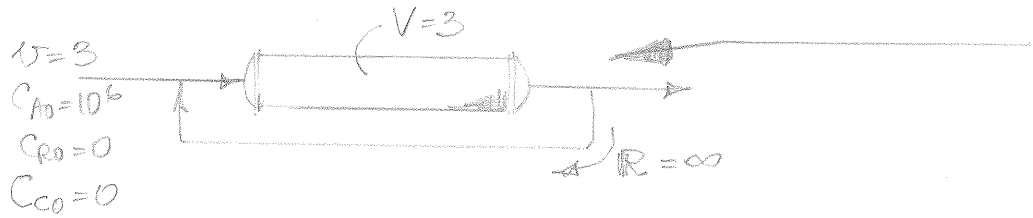
or $\tau_{opt} = 1 = \dfrac{V}{v}$

Since $v = 3$ (given) we want

$V = 3$, and mixed flow

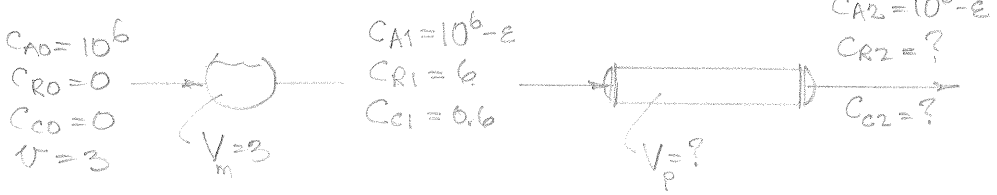
Note: with $R = \infty$ you get mixed flow.

Thus



30.7 The optimum is where $C_R = C_R^*/2 = 6$, and $k\tau = 2$

But with $k=2$ this means that $\tau = V/v = 1$. So for $v=3$ our mixed flow region should have a volume $V_m = 3$, the rest should be in plug flow. Thus we want



From earlier problems the composition after the mixed flow regions are as shown above.

For the plug flow section Eq 5 gives

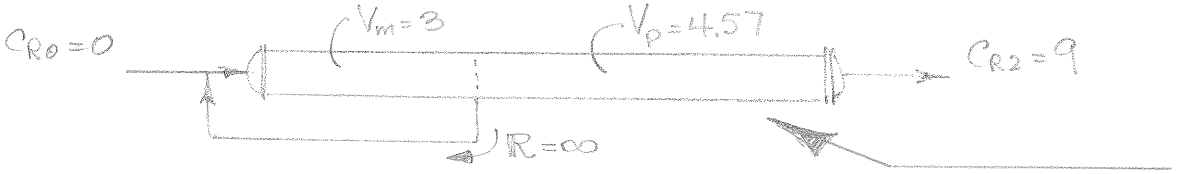
$$k\tau_p = k\frac{V_p}{v} = \frac{C_R^*}{C_R^* - C_{R1} + (R/C)C_{C1}} \ln \frac{\left[C_{C1} + (C/R)(C_{R2} - C_{R1})\right](C_R^* - C_{R1})}{C_{C1}(C_R^* - C_{R2})}$$

With $(R/C) = (R/A)/(C/A) = 0.1/0.01 = 10$, replacing all values in the above gives

$$2\left(\frac{V_p}{3}\right) = \frac{12}{12 - 6 + 10(0.6)} \ln \frac{\left[6 + 0.1(9-6)\right](12-6)}{0.6\,(12-9)}$$

$$V_p = \frac{3}{2} \ln \frac{6.3\,(6)}{0.6\,(3)} = 4.57$$

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 $k = \sqrt{3}$, $\therefore \tau_{m,opt} = 1.73/\sqrt{3} = 1$ ...

Or $v = \tau V = 1 \times 30 = 30\ m^3/hr$.

$$\therefore C_{R\max} = \frac{C_R^*}{n+1} = \frac{0.12}{0.5+1} = 0.08\ \frac{kg\ alc}{kg\ sol^n} \times \frac{1000\ kg}{m^3}$$

$\therefore$ production rate is $80 \times 30 = 2400\ \frac{kg\ alc}{hr}$ ◀

30.11 Try first order poisoning and see if this fits the facts. So from Eq 10 we have

$$\text{for run \#1} \quad k\tau_1 = \frac{90}{90-54}$$

$$\text{for run \#2} \quad k\tau_2 = \frac{90}{90-75}$$

Taking ratios

$$\frac{\tau_1}{\tau_2} = \frac{15}{36} = 0.4167 \quad \cdots \text{ if poisoning follows } n=1 \text{ kinetics}$$

But actually

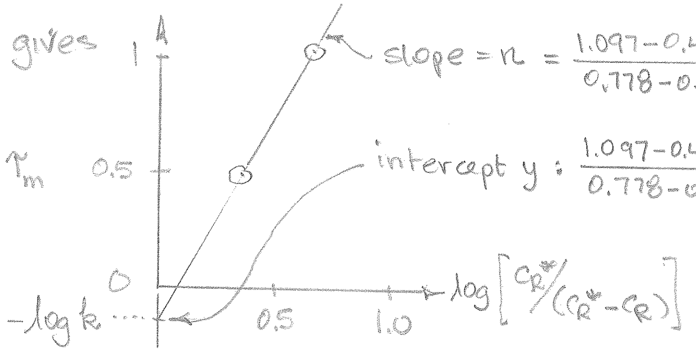
$$\frac{\tau_1}{\tau_2} = \frac{3.125}{12.5} = 0.25$$

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	$\log \tau_m$	$C_R^*/(C_R^*-C_R)$	$\log\left(C_R^*/(C_R^*-C_R)\right)$
3.125	54	0.495	2.5	0.398
12.5	75	1.097	6	0.778

Plotting gives



$$\text{slope} = n = \frac{1.097-0.495}{0.778-0.398} = 1.584$$

$$\text{intercept } y: \frac{1.097-0.495}{0.778-0.398} = \frac{0.495-y}{0.398}$$

$$\therefore y = -0.136$$

$$k = 10^{0.136} = 1.366$$

Thus the rate equation is

$$r_R = 1.366\left(1-\frac{C_R}{90}\right)^{1.584} C_c$$

Now to the optimum

$$v_{opt} = kV\left(\frac{n}{n+1}\right)^n = 1.366(50)\left(\frac{1.584}{2.584}\right)^{1.584} = 31.46 \text{ books/hr}$$

Maximum production rate

$$F_{R\,max} = (C_R v)_{opt} = \frac{kVC_R^* n^n}{(n+1)^{n+1}} = \frac{1.366(50)90(1.584)^{1.584}}{(2.584)^{2.584}}$$

$$= 1095 \,\mu m/hr \longleftarrow$$