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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CONTENTS

1.1 Find the rate of reaction defined as

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

Evaluate terms

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

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

O_2 used

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

Thus the rate of reaction

$$\frac{2.0\times10^5 \text{mol } O_2/\text{day}}{10667 m^3} = 18.75 \text{ mol}/m^3 \cdot \text{day}$$
$$= 2.17\times10^{-4} \text{mol}/m^3 \cdot s$$

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

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

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

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

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

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

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

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

$$-r''' = \frac{1}{V_{cat}}\frac{dN}{dt} = \frac{1}{625}(133) = 2.13 \text{ mol}/m^3\,cat \cdot s$$

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

---

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

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

2.7a) We are given $-\frac{dp_A}{dt} = k_p p_A^2$

($-\frac{dp_A}{dt}$: atm/hr; k_p: 3.66; p_A^2: $(atm)^2$)

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

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

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

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

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

2.9 From Eq. 35 we write

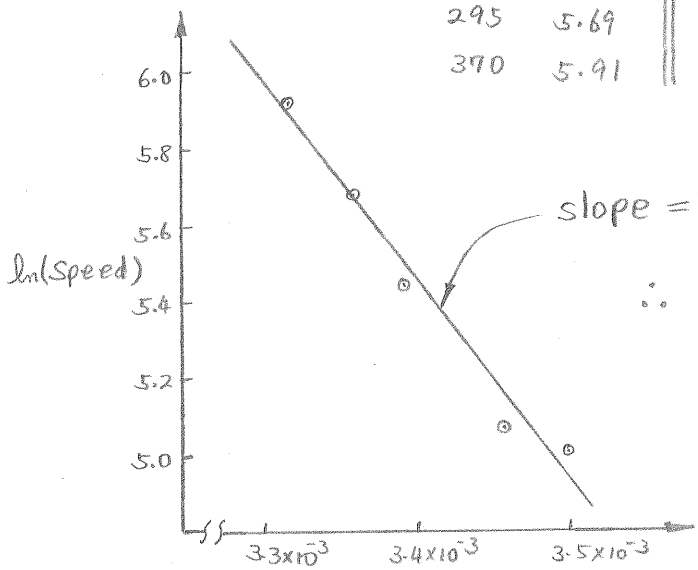
$$\frac{k_{650}}{k_{500}} = e^{-\frac{E}{R}\left(\frac{1}{T_{650}} - \frac{1}{T_{500}}\right)}$$

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

$$= 1971$$ ←

2.11

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



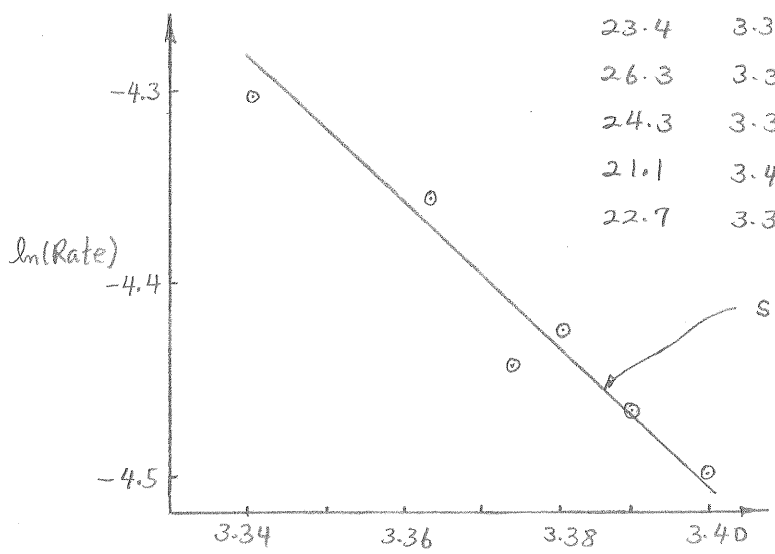
slope $= \frac{-E}{R} = -5420$

$\therefore E = (5420)(8.314) = 45062$ J

$\cong 45$ kJ

2.13

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



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

$E = (3392)(8.314)$

$= 28201$ J/mol

$= 28.2$ kJ/mol

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

$\therefore n = 1.585$ ←

↑ 3

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

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

$50 = k(2)^a(125)^b$ ---(i)

$32 = k(2)^a(64)^b$ ---(ii)

$48 = k(3)^a(64)^b$ ---(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 $2A \underset{2}{\overset{1}{\rightleftharpoons}} A + A^*$, $A^* \xrightarrow{3} R + S$ ... 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

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

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:

$$H_3PO_2 + H^+ \underset{k_2}{\overset{k_1}{\rightleftharpoons}} X^* + H^+$$
$$X^* + O_x \underset{k_4}{\overset{k_3}{\rightleftharpoons}} H_3PO_3$$

... where X^* 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

$$A + E \underset{2}{\overset{1}{\rightleftharpoons}} X \quad \text{.... (1)}$$
$$X \longrightarrow R + E \quad \text{... (2)}$$

with

$$E_0 = E + X \quad \text{... (3)}$$

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

$$dX/dt = 0 \quad \text{.. (5)}$$

2.1-23 (continued)

For M-M

From (2)

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

From (5)

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

Eliminate E with (3)

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

or

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

Eq (7) in (6) gives

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

For B-H

From (2)

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

From (5)

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

Eliminate E with (3)

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

or

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

Eq (9) in (8) gives

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

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

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

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

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

We also can find the rate constant. Thus replacing values

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

Hence the rate of disappearance of monomer is given by

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

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

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

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

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

(Continued)

After his raise we have $t=0 \cdots \$_0 = ?$; $t = 3\text{ hrs} \quad \$ = 135$ } ... from this find $\$_0$

For unchanged betting habits

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

Hence his raise is $208 - 180 \cdots$ or $\$28$

3.9 For a first order reversible reaction

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

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

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

Now from thermodynamics we know that

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

(K: equilibrium constant)

Thus $\cdots \quad k_1 = 2k_2 \quad \cdots \quad (ii)$

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

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

($-r_A$: mol/lit.min; 0.05775: min^{-1}; C_A: mol/lit; 0.028875: min^{-1}; C_R: mol/lit)

3.11 From the table of data

at $C_A = 500$ $t = 100$ min

Thus

at $t = 5$ hrs $+ 100$ min $= 400$ min

$C_A = 200 \frac{mol}{m^3}$ ... or $X_A = 0.6$ ◀

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)

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

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

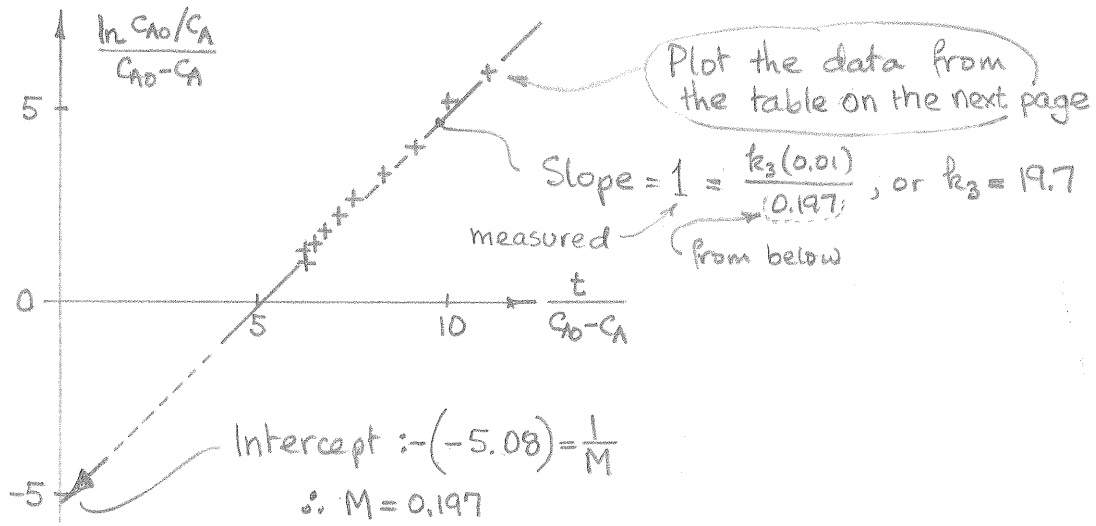
9.15 We can test the fit of the Michaelis-Menten type equation in many ways, integral or differential. We will sketch these different solutions in turn. But first let us transform the M-M equation into the following useful form

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

use this form

Integral method Integrating (i) gives

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



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

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

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

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

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

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

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

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

3.21

Given

Filled with pure A at 25°c

t° is raised to 100°c

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

$2A \rightarrow B$

Tabulate

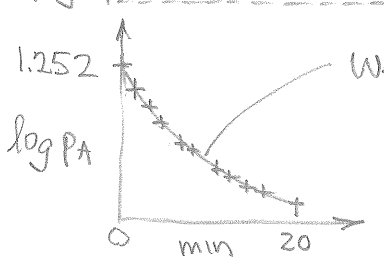
① time (min)	② π (atm)	③ p_A (atm)	④ $1/p_A$ (atm^{-1})
0	(1.252)	(1.252)	(0.800)
1	1.14	1.028	0.975
2	1.04	0.828	1.208
3	0.982	0.712	1.404
4	0.940	0.628	1.592
5	0.905	0.558	1.792
6	0.870	0.488	2.049
7	0.850	0.448	2.232
8	0.832	0.412	2.427
9	0.815	0.378	2.646
10	0.800	0.348	2.873
15	0.754	0.256	3.90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

given — calc.

Column ③ is obtained from Eq 5, or

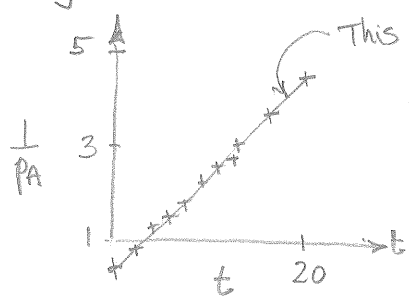
$$p_A = p_{A0} - \frac{a}{\Delta n}(\pi - \pi_0) = 1.252 - \frac{2}{(-1)}(\pi - 1.252) = 2p_A - 1.252$$

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

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

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

or $k_c = 6.3$ lit/mol min

$\therefore -r_A = 6.3 C_A^2$ mol/lit.min

lit/mol.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.

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

Replacing in Eq 33a gives

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

or

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

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

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

(a) We could first transform at 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 $t=\infty$ there is still some unreacted p_A. So the rate equation we will test is

$$A \underset{2}{\overset{1}{\rightleftharpoons}} R, \quad \frac{dC_A}{dt} = k_1 C_A - k_2 C_R \quad \text{---(53)}$$

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)

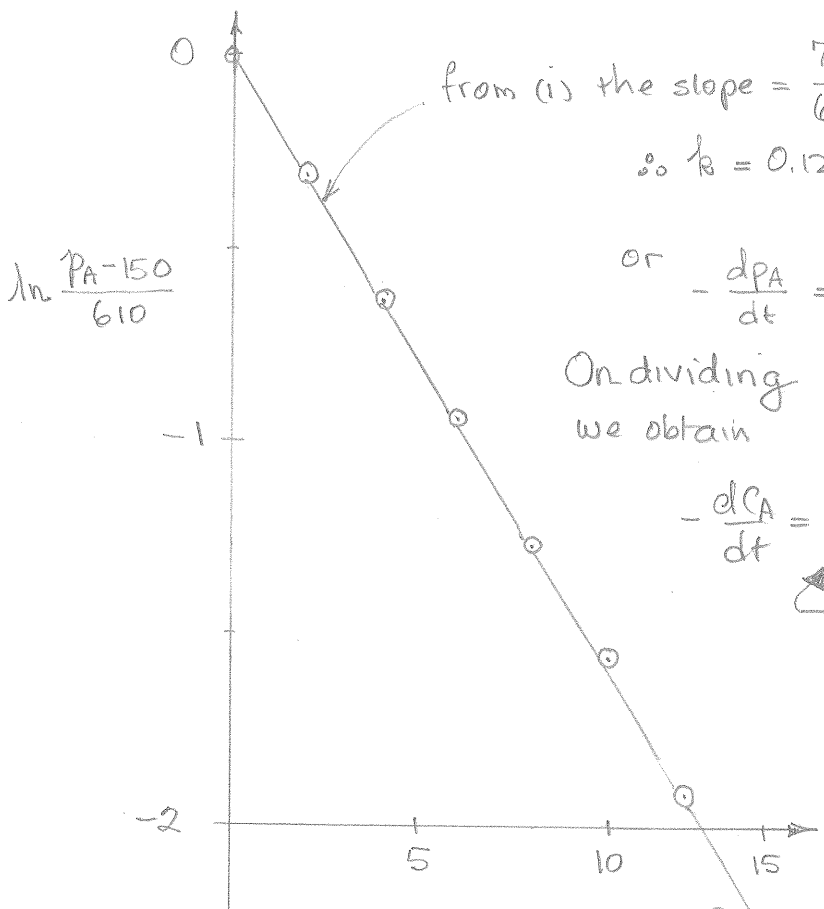
In pressure units this integrated expression becomes

$$\ln \frac{P_A - P_{Ae}}{P_{A0} - P_{Ae}} = \frac{k_1 t}{(P_{A0} - P_{Ae})/P_{A0}} \qquad \text{---(i)}$$

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	-1.5951
12	240	90/610	-1.9136
14	215	65/610	-2.2391
∞	150	0	-∞

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



from (i) the slope $= \frac{760}{610} k_1 = \frac{12}{12.4}$

$\therefore k_1 = 0.1295\ min^{-1}$

or $-\frac{dP_A}{dt} = (0.1295\ min^{-1}) P_A$

On dividing both sides by RT we obtain

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

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

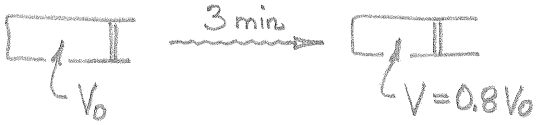
3.27 Since we are told that the reaction is elementary the stoichiometric equation shows that the reaction is 2nd order. So for a small relative concentration change we can write

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

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

$$\therefore -r_{NH_2\text{-}CO\text{-}NH_2} = (6.6 \times 10^{-5}) C^2_{NH_2\text{-}CO\text{-}NH_2}, \frac{\text{mol}}{\text{lit·hr}}$$ ⟵

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

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

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

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

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

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

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

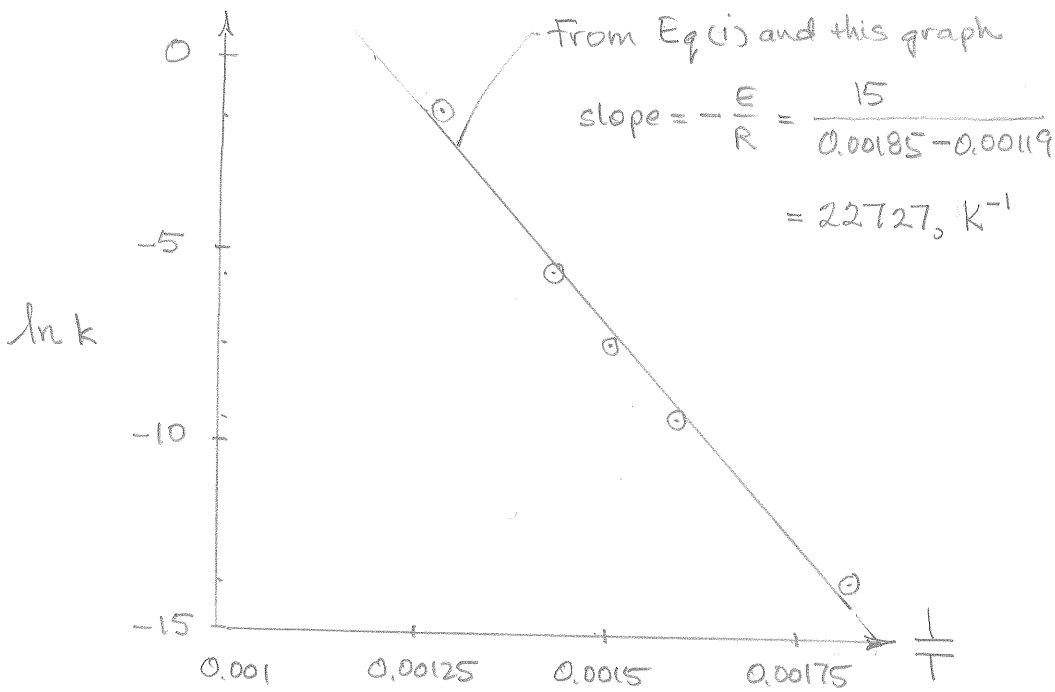
So to find the value of the rate constant, or k_0 and E/R, we must plot $\ln k$ vs $1/T$. The slope gives E/R and the intercept gives k_0. Let us follow this procedure

4.31 (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	0.000588	−7.4388
356	629	0.001590	80.9×10^{-6}	−9.4223
273	546	0.001832	0.942×10^{-6}	−13.8753

Next plot as shown below



From Eq (i) and this graph

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

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

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

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

4.1

gas

$A + B \rightarrow R + S$

$C_{AO} = 100$, $C_{BO} = 100$ → $X_A = 0.8$

$\varepsilon_A = 0$, $\varepsilon_B = 0$

$X_B = 0.8$

$C_A = 0.2$

$C_B = 0.2$

4.3

gas

$A + B \rightarrow R$

$C_{AO} = 200$, $C_{BO} = 100$ → $C_A = 50$

Take 300 moles of feed gas. Consider A

at $X_A = 0$ $\quad V = 200A + 100B + 0R = 300$

at $X_A = 1$ $\quad V = 0A - 100B + 200R = 100$

$$\varepsilon_A = \frac{100 - 300}{300} = -\frac{2}{3}$$

Now consider B

at $X_B = 0$ $\quad V = 300$

at $X_B = 1$ $\quad V = 100A + 0B + 100R = 200$

$$\varepsilon_B = \frac{200 - 300}{300} = -\frac{1}{3}$$

∴ from Eq. 5

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

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

4.5

gas

$A + B \rightarrow 2R$

$C_{AO} = 100$, $C_{BO} = 200$, $T_0 = 400\,K$, $\Pi_0 = 4\,atm$ → $C_A = 20$, $T = 300\,K$, $\Pi = 3\,atm$

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

4.5 (continued)

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

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

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

4.7

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

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

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

↑ 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

$$dt = \frac{dV}{v}$$
$$dV = \frac{F_{A0}\, dX_A}{(-r_A)}$$

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

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

$\frac{v}{v_0}$: changes with conversion

$(1+\varepsilon_A X_A)$: 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
$\upsilon = 400$ lit/min
$X_A = 0.999$
$V = ?$

$A + B \rightarrow R$
$-r_A = 200 C_A C_B$ mol/lit·min

For a 2nd order reaction, Eq 3.14 gives

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

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

Replacing all values

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

or $\tau = 0.31$ min

Therefore $V = \tau\upsilon = (0.31)(400) = 124$ lit ◄

5.7 First find the rate constant: $k = \ln 2 / t_{\frac{1}{2}} = \ln 2 / 5.2 = 0.1333$ 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,

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

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

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

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

5.11

$C_{A0} = 2$ mol/lit, $\upsilon = 25$ lit/min → (V = ?) → $X_A = 0.95$

$$-r_A = \frac{0.1 C_A}{1+0.5 C_A} \quad \text{mol/lit·min}$$

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

Then for mixed flow

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

5.13

$F_{A0} = 10$ mol/hr

2/3 phos – 1/3 inerts

→ $X_A = 0.75$

$T = 649°C$

$\Pi = 11.4$ atm

$V = ?$

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

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

For a 1st order reaction

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

Evaluate terms

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

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

$F_{A0} = 10$ mol/hr

$\varepsilon_A = 0.5$ ←

$4A \rightarrow 7R$

reactants: $40 \rightarrow 70$

inerts: $20 \rightarrow 20$

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

Replacing in (i) gives

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

5.15

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

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

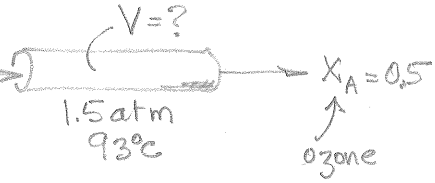
$$X_A = \frac{C_{A0}-C_A}{C_{A0}+\varepsilon_A C_A} = \frac{1-0.5}{1+(-0.5)(0.5)} = \frac{2}{3}$$

So for mixed flow

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

5.17

20% oxone (A)
80% air
$\upsilon = 1$ 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

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

Evaluate terms

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

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

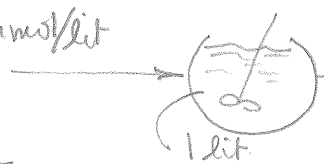
Replacing in (i) gives

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

$$= 2.125 \text{ lit} = 2.1 \text{ m}^3$$

5.19

$C_{A0} = 120$ mmol/lit
3 atm
30°C
various υ_0



$A \rightarrow 3R$

Find a rate equation

For each run

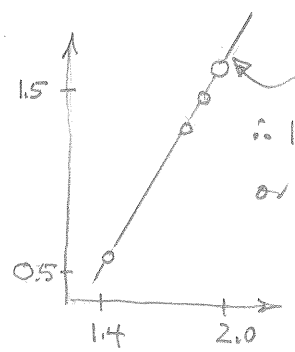
$$-r_A = \frac{C_{A0}X_A\upsilon_0}{V} = \frac{C_{A0}(C_{A0}-C_A)\upsilon_0}{(C_{A0}+\varepsilon_A C_A)V} = \frac{120(120-C_A)\upsilon_0}{(120+2C_A)}$$

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

Now tabulate

υ_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



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

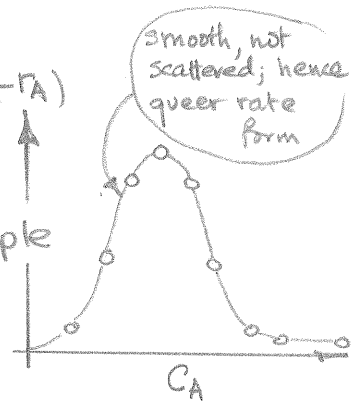
or $0.5563 = \log k + 2(1.477)$

$\therefore k = 0.004$

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

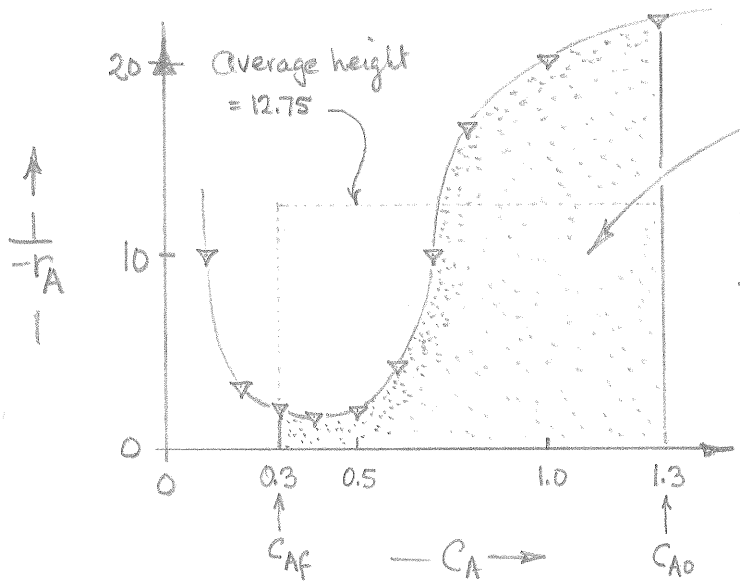
5.21 The approach which probably first comes to mind is to find a rate equation to represent the data, first order, second, etc., and then integrate it to give the time; thus

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



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

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

or

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

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

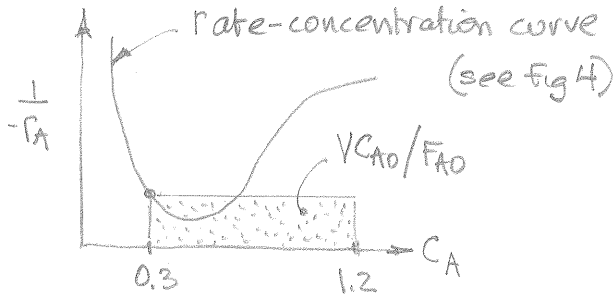
$C_{A0} = 1.2$ mol/lit
$F_{A0} = 1000$ mol/hr → ⊙ → $X_A = 0.75$

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,

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

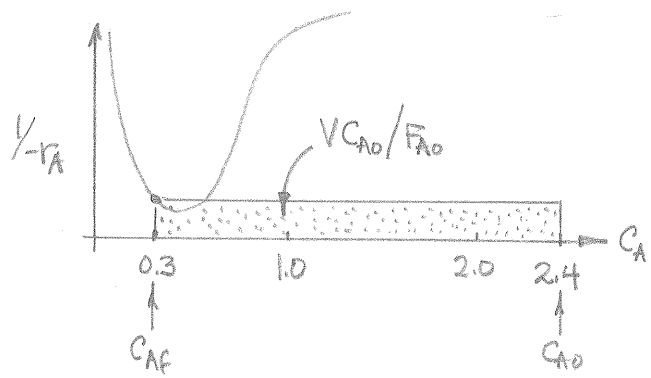


$$= \frac{1000\ \frac{\text{mol}}{\text{hr}}}{1.2\ \frac{\text{mol}}{\text{lit}}} \cdot \frac{\left(1.2 - 0.3\ \frac{\text{mol}}{\text{lit}}\right)}{\left(0.5\ \frac{\text{mol}}{\text{lit}\cdot\text{min}}\right)} \cdot \frac{1\text{ hr}}{60\text{ min}} = 25\text{ lit} \quad \text{a)}$$

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

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

or $V = 50$ lit. b)



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

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

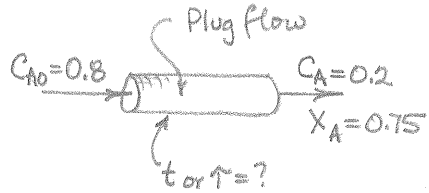
$$= \frac{1000}{2.4} \cdot \frac{(2.4 - 0.3)}{0.5} \cdot \frac{1}{60}$$

or $V = 29.167$ lit 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	2000

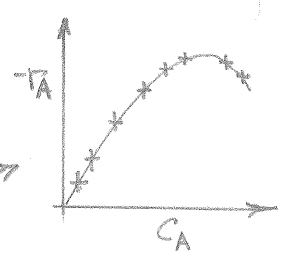
Holding time for plug flow.

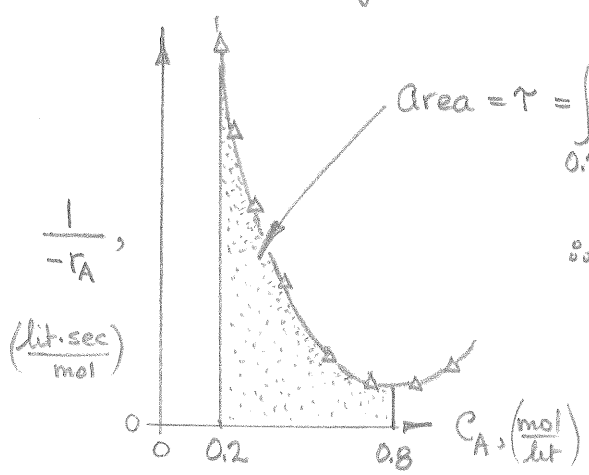


We may solve this by using conversions as suggested in the text. However since $\varepsilon_A = 0$ the use of concentrations poses no problems. Let us use this. Then the performance expression is Eq. 19, or

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

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.





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

∴ for a plug flow reactor

$\tau = t = 300$ sec ←

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

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

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

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

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

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

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

Let us see if this is Imbibit's volume. With his density being 62.4 #/ft³

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

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

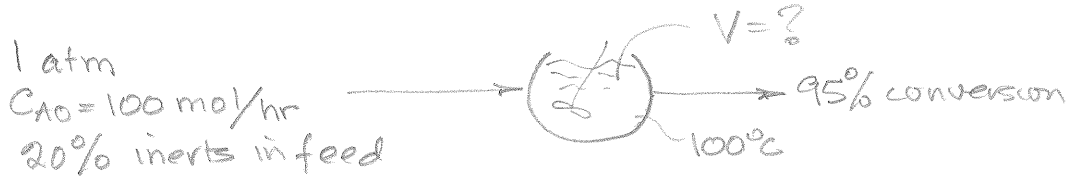
b) Why did Watson never come up with this explanation? Because smoking near 99% alcohol was not really cool.

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 $2A \rightarrow R + S$

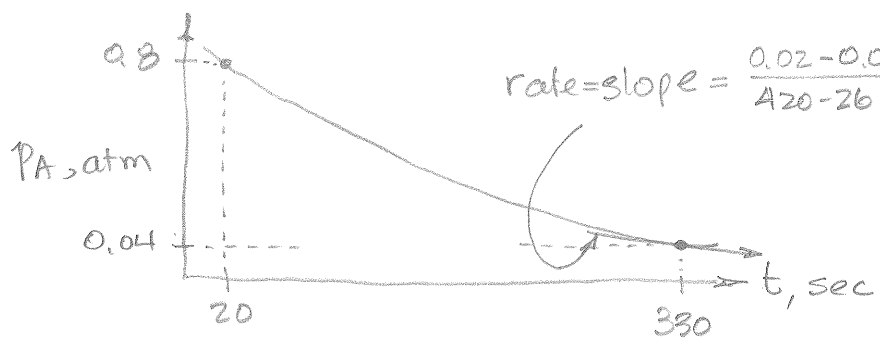


$\therefore \dot{n}_{feed} = 100\left(\frac{100}{80}\right) = 125$ mol/hr

$P_{A0} = 0.8$ 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



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

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

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

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

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

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

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 $$C_{A2} = 0.25 \text{ mol/lit.}$$ ◀

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 ◀

6.5

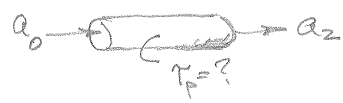
$\therefore \bar{t}_i = 2$ weeks $= 20160$ min

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

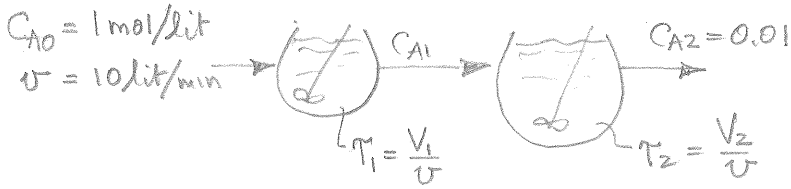
For plug flow



$$\frac{a_2}{a_0} = 1.0017 \times 10^{-6} = e^{-k\tau_p} = e^{-0.0495\,\tau_p}$$

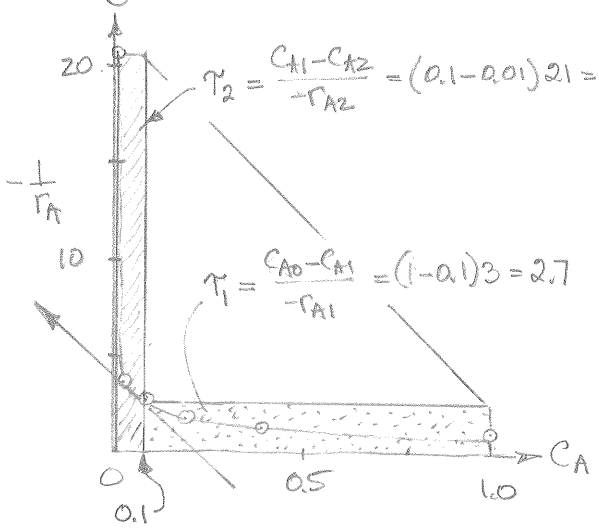
$$\tau_p = \frac{\ln(1.0017 \times 10^{-6})}{-0.0495} = 279 \text{ min} = 4.65 \text{ hr}$$ ◀ (instead of 2 weeks for the MFR)

6.7



$$-r_A = \frac{C_A}{0.2 + C_A^2} \frac{\text{mol}}{\text{lit} \cdot \text{min}}$$

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



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

$$\therefore V_1 = \tau_1 \upsilon = 2.7(10) = 27 \text{ lit}$$
$$V_2 = \tau_2 \upsilon = 1.9(10) = 19 \text{ lit}$$

6.9 With recycle for a first order reaction we have

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

Without recycle (plug flow)

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

Therefore

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

no recycle is better

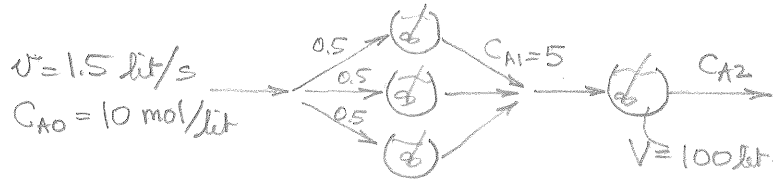
6.11 For this autocatalytic reaction the maximum rate occurs where $C_A = C_R$. Thus operate at $C_A = 5$, if possible. Here

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

So for mixed flow

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

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



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

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

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

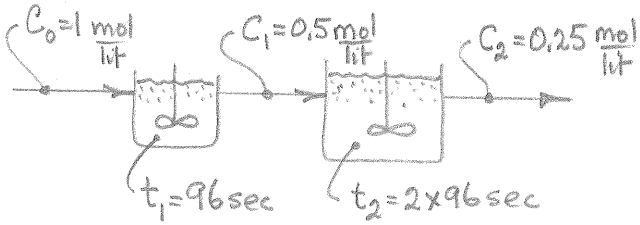
$$-\frac{dC}{dt} = kC \quad \text{--- or ---} \quad \ln\frac{C_0}{C} = kt \quad \text{--- or ---} \quad \ln 2 = k(20\,hrs) \quad \text{--- or ---} \quad k = \frac{\ln 2}{20\,hr}$$

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

$$\frac{C_{out}}{C_0} = \frac{1}{(1 + k\tau_i)^2} = \frac{1}{\left(1 + \frac{\ln 2}{20}(40)\right)^2} = \frac{1}{(1 + 20\ln 2)^2} = 0.00453$$

∴ 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.

For 1st reactor: $\tau_1 = \frac{C_0 - C_1}{k C_1^n}$

For 2nd reactor: $\tau_2 = \frac{C_1 - C_2}{k C_2^n}$

combining ... $\frac{\tau_1}{\tau_2} = \frac{C_0 - C_1}{C_1 - C_2} \left(\frac{C_2}{C_1}\right)^n$

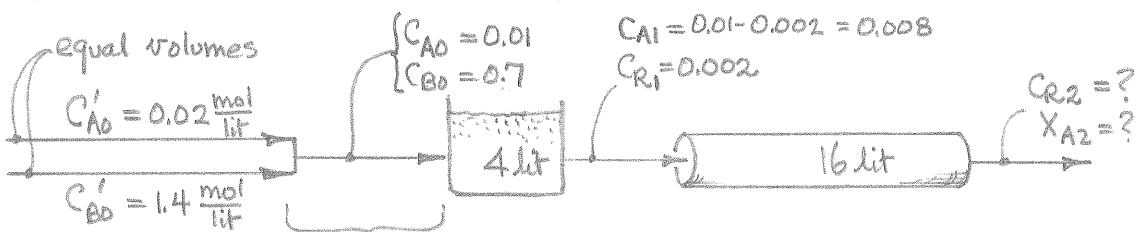
$$\therefore n = \frac{\log \frac{\tau_1}{\tau_2} + \log \frac{C_1 - C_2}{C_0 - C_1}}{\log \frac{C_2}{C_1}} = \frac{\log \frac{1}{2} + \log \frac{1}{2}}{\log \frac{1}{2}} = 2$$

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

Hence the rate

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

6.17



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

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

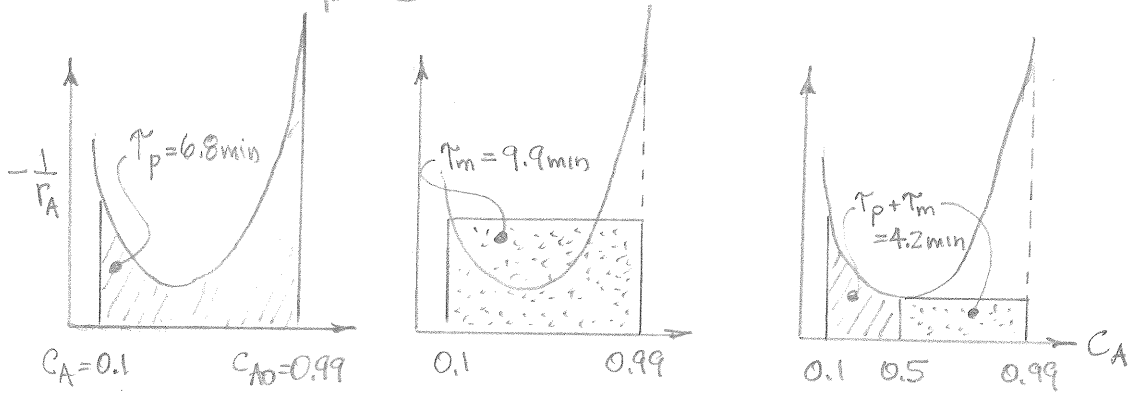
For the reactor: $k\tau_p = 4(k\tau_m) = 4\left(\frac{1}{4}\right) = \int_{0.008}^{C_{A2}} \frac{dC_A}{C_A} = \ln \frac{0.008}{C_{A2}}$ ... or $C_{A2} = 0.00293$

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

6.19 Let us solve by using the graphical procedure, and let's use concentrations, not conversions. First prepare the $-r_A$ 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 ◀——— a)

$\tau_m = 9.9$ min ◀——— b)

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

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

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

$C_{A0} = 10$ → [ ] → C_{A1}

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

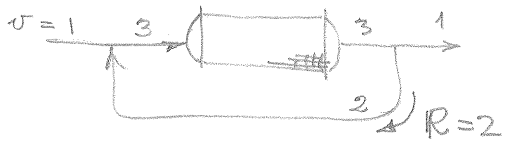
With recycle

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

6.21 (continued)

Combining (i) & (ii) gives

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



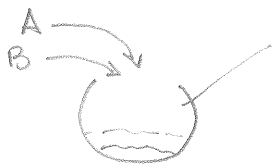
Solving for C_{Af} gives

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

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

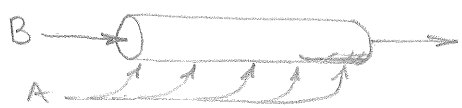
7.3 For $A + B \rightarrow R$, $2A \rightarrow S$, $2B \rightarrow T$ — for A use low C_A, for B use low C_B

Thus



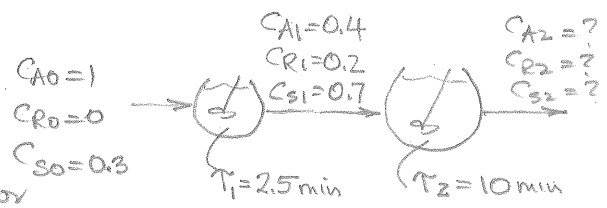
drip A and B in slowly
keep X_A high
keep X_B high
Don't have an excess of either A or B

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



7.7 Given

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



For mixed flow in the first reactor

$$\tau_1 = \frac{C_{R1} - C_{R0}}{k_1 C_{A1}^2} \quad \therefore k_1 = \frac{0.2 - 0}{2.5(0.4)^2} = 0.5$$

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

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

Also

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

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

7.9

$C_{A0}=40$ → [ ] → $X_A=0.9$

$C_R, C_S, \tau = ?$

$A \xrightarrow{1} R \quad r_R = k_1 C_A^2 \quad k_1 = 0.4 \ m^3/mol.min$

$A \xrightarrow{2} S \quad r_S = k_2 C_A \quad k_2 = 2 \ min^{-1}$

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

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

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

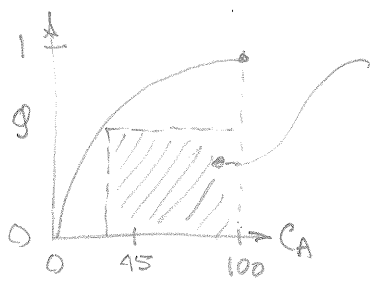
$\therefore$ $C_A = 4$, $C_S = 8$, $C_R = 28$ ◄

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

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

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

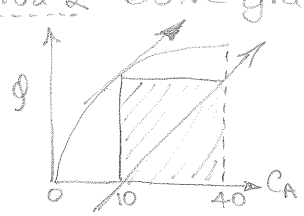
Method 1 Solve analytically

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

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

$C_R = 20$, $C_S = 10$ ◄

Method 2 Solve graphically by maximizing the shaded rectangle

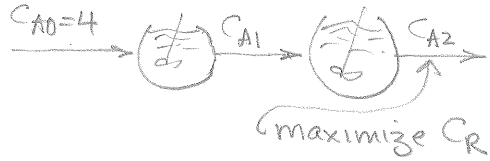


For τ: $\tau = \frac{C_{A0} - C_{Af}}{-r_A} = \frac{C_{A0} - C_{Af}}{0.4C_{Af}^2 + 2C_A} = \frac{40-10}{0.4(10)^2 + 2(10)}$

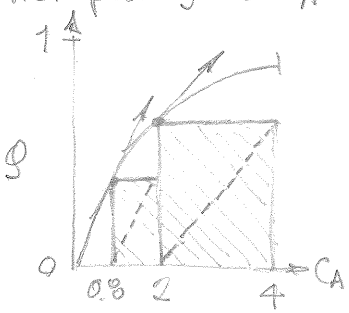
$= \frac{30}{60} = \frac{1}{2}$ min ◄

7.13

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



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

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

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

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

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

and

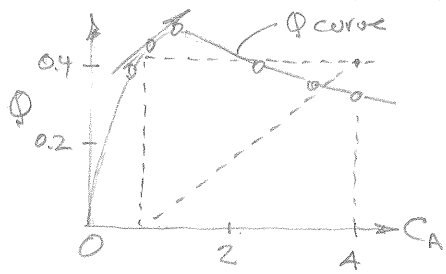
$$C_{R1} = \varphi \cdot \Delta C_A = \frac{C_{A1}}{C_{A1}+1}(C_{A0}-C_{A1}) = \frac{2}{2+1}(4-2) = 1.33$$

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

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

7.15

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



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

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

(graphical integration)

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

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

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

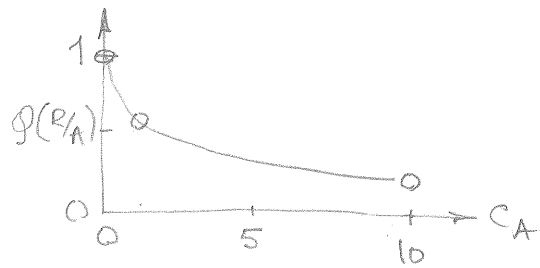
$$\varphi \text{ (at } C_A = \tfrac{2}{3}) = 2\left(\tfrac{2}{3}\right)\Big/\left(1+\tfrac{2}{3}\right)^2 = \frac{12}{25}$$

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

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

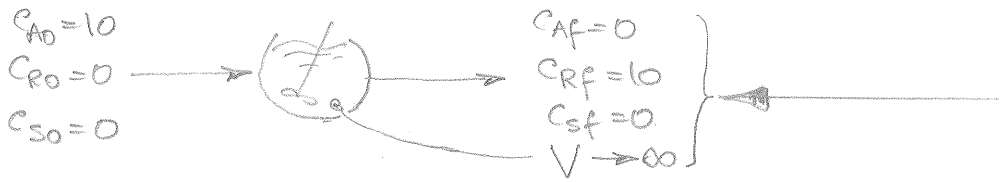
$$\varphi(P/A) = \frac{16C_A^{1/2}}{16C_A^{1/2} + 12C_A + C_A^2}$$

C_A	$\varphi(P/A)$
10	0.185
1	0.55
0	1.0



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

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

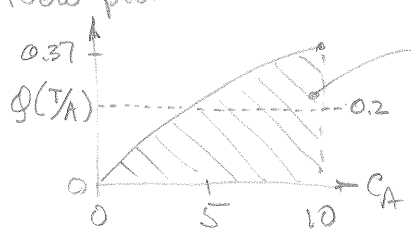


7.19 First find the φ vs C_A curve, then decide which reactor type to use

$$\varphi(T/A) = \frac{C_A^2}{16C_A^{1/2} + 12C_A + C_A^2} \qquad \frac{1}{-r_A} = \frac{1}{16C_A^{1/2} + 12C_A + C_A^2}$$

C_A	$\varphi(T/A)$	$\frac{1}{-r_A}$
10	0.37	0.0037
9	0.34	0.0042
4	0.167	0.0104
1	0.03	0.03
0.1		0.16

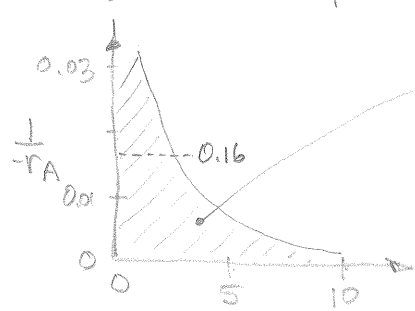
Now plot



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

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

Next, to find τ plot $-1/r_A$ vs C_A

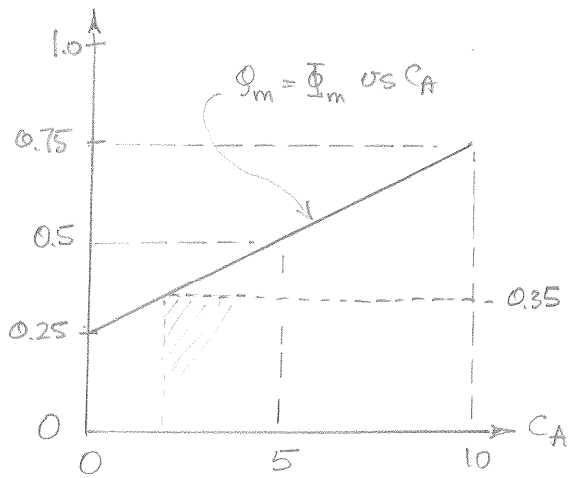


$$\tau = \int_{10}^{0} \frac{dC_A}{-r_A} = 0.016(10) = 0.16 \text{ min}$$

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

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

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 $C_{A0} = 100$

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

7.23

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

$C_A = 3$ mol/m^3
$C_B = 3$ mol/m^3

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

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

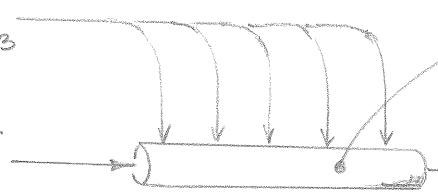
$\therefore C_R = \varphi(R/A)(-\Delta C_A) = \frac{1}{3}(30-3) = 9$ mol/m^3 $\therefore R/S = 1/2$

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

7.25

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

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



C_B everywhere $= C_{Bf} = 3$ mol/m^3

$C_A = 3$ mol/m^3

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

7.25 (continued)

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

($C_B = 3$)

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

($C_B = 3$)

So $$\frac{C_{Rf}}{C_{Sf}} = \frac{18.68}{8.32} \simeq 2.25$$

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

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

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

$$-\frac{dF}{dt} = kB$$
$$-\frac{dB}{dt} = kF$$

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

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

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 (i) gives

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

1.27 (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

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

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

Thus the British should fight ½ the French fleet in each battle.

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

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

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

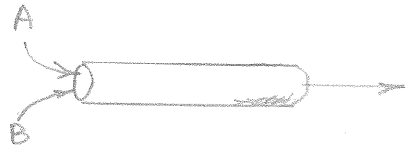
Comment Equation (i) represents the SQUARE FIREPOWER LAW. This says that the strength of a force is proportional to the square of its firepower, and it applies to battles with cooperative action. Thus 4 toughs working together as a team can take on 16 others --- one at a time.

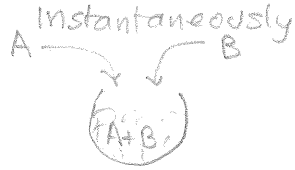
The British war office had a couple of mathematicians on their staff who in essence did the above calculation. The French military probably were more "practical", and didn't spend money on "useless" activities.

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.

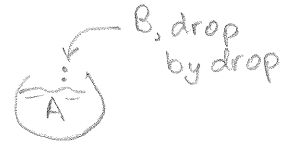
8.1

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 $A \nearrow R$ ... $r_R = k_1 C_A$, $A \searrow S$ ... $r_S = k_2 C_A$ } Then for mixed flow

$$\tau = \frac{C_R - C_{R0}}{k_1 C_A}, \quad \tau = \frac{C_S - C_{S0}}{k_2 C_A} \Bigg\} \text{ dividing gives } \frac{C_R}{C_S} = \frac{k_1}{k_2} = \text{constant}$$

This agrees with the observed so we conclude that

$A \nearrow R$ ... $r_R = k_1 C_A$, $A \searrow S$ ... $r_S = k_2 C_A$ } $k_1 = 1.5\, k_2$

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

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

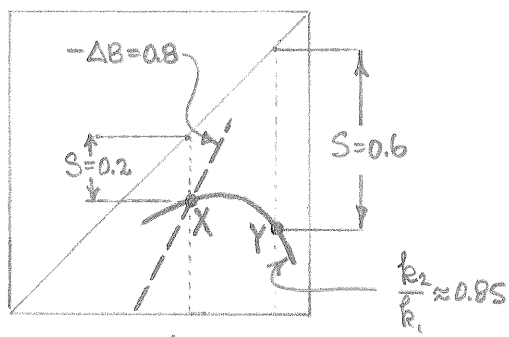
8.7 a) At the start $\begin{cases} A_0 = 1 \\ B_0 = 3 \end{cases}$

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

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

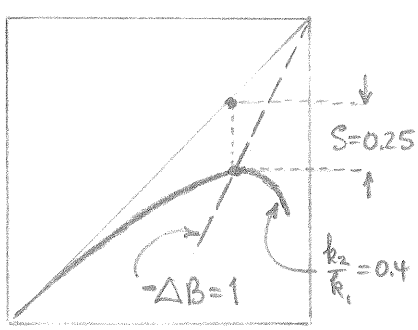
At this point $k_2/k_1 = 0.85$

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



b) Nothing ← b)

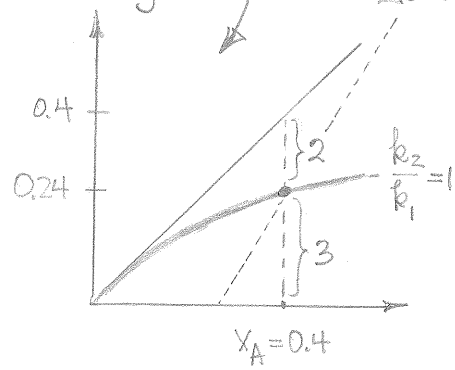
c)



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.

$\therefore k_2/k_1 \leq 0.4$ ← c)

8.9 From Fig. 14



Thus

given → $\frac{C_A}{C_{AO}} = 0.6$

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

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

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

} $\frac{k_2}{k_1}=1$ ←

8.11 Evaluate k_1 and k_2 at various pH.

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

From this table:

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

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

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

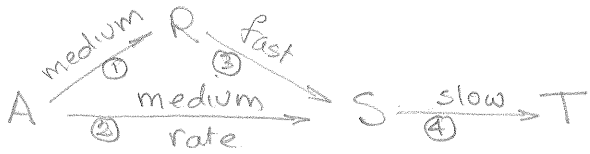
$C_A=0$ $C_R=20$ $C_S=20$ $C_T=20$ and $C_U=40$ ← a)

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

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

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

8.15 Our reaction scheme is



Combining gives

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

thus

$$A \xrightarrow[k_{123}]{0.4} S \xrightarrow[k_4]{0.004} T \quad \cdots \text{or} \quad \frac{k_{123}}{k_4} = 100$$

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

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

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

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

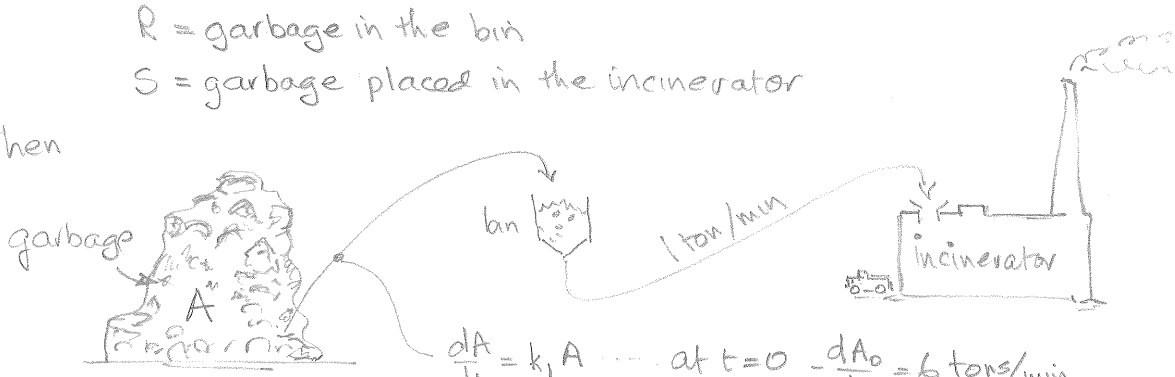
Let A = garbage still to be collected

$A_0 = 1440$ tons

R = garbage in the bin

S = garbage placed in the incinerator

Then



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

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

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

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

8.17 (continued)

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

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

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

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

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

or

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

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

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

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

The time, from Eq. (ii)

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

or 1.20 pm ◄— c)

(b) Max contents of the bin

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

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

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

or

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

Solve by trial & error

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

↑ 5.56 am ◄— d)

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

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

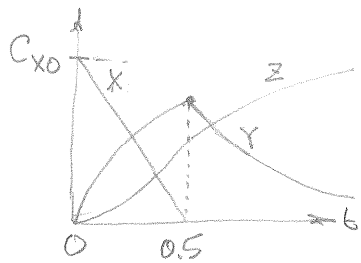
8.19 Let us follow the text. From Eq 22

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

we are given

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

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



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

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

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

$$\frac{C_Y}{C_{X0}} = \frac{1}{K}\left(e^{+K-k_2 t} - e^{-k_2 t}\right)$$

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

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

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

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

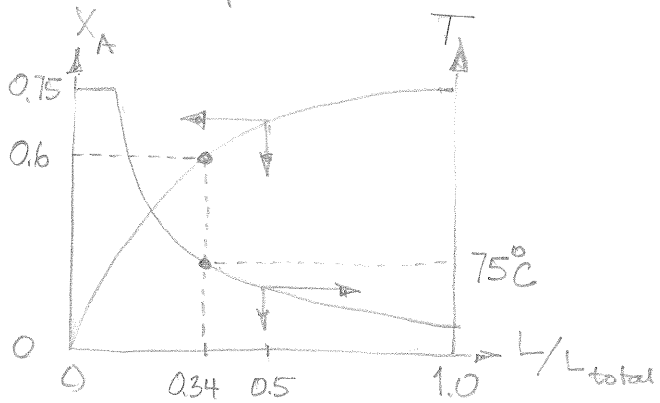
or $C_{Rmax} = 0.444\ mol/lit$

From Eq. 50

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

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

9.1 Figure E4c presents the solution to this problem



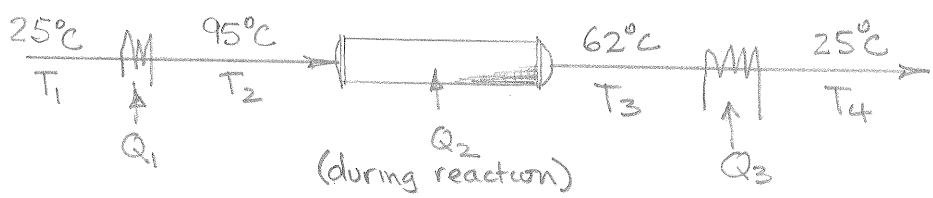
From Fig. E4c we find $\tau_{X_A=0.6} = 0.34\,\tau_{X_A=0.8}$

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

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

Also $T_{exit} = 75°C \longleftarrow$

9.3 From Fig E4a we find



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

So the heat added to the flowing stream is

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

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

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

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

(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

$$\frac{\tau}{C_{A0}} = \frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A} = \begin{pmatrix}\text{area under the} \\ -1/r_A \text{ vs } X_A \text{ curve}\end{pmatrix} \qquad \text{---- (i)}$$

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

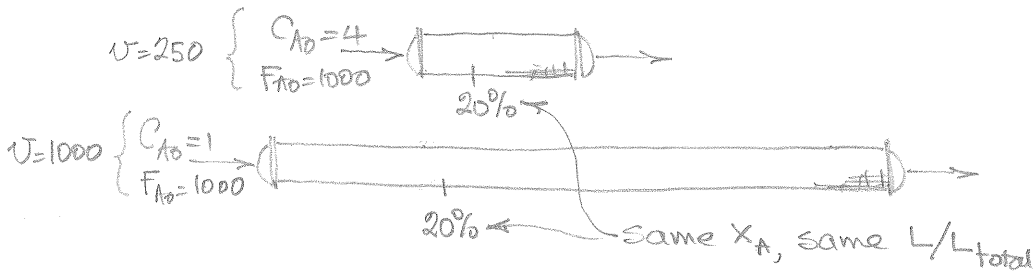
Also, from Eq (i)

$$V = F_{A0}(\text{area}) = 1000(1.62) = 1620 \text{ lit} = 1.62 \text{ m}^3 \longleftarrow \text{a)}$$

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)



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

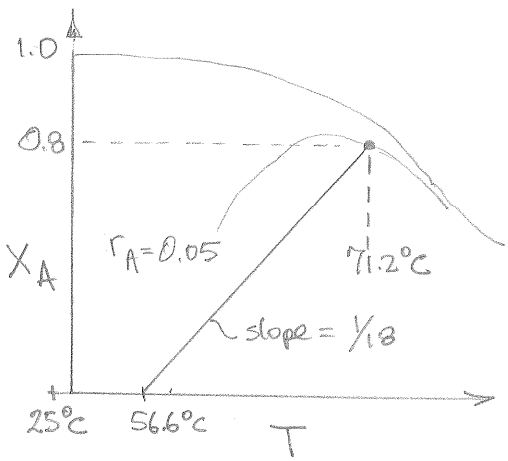
Here $C_p = 1000 \text{ cal/mol A}$

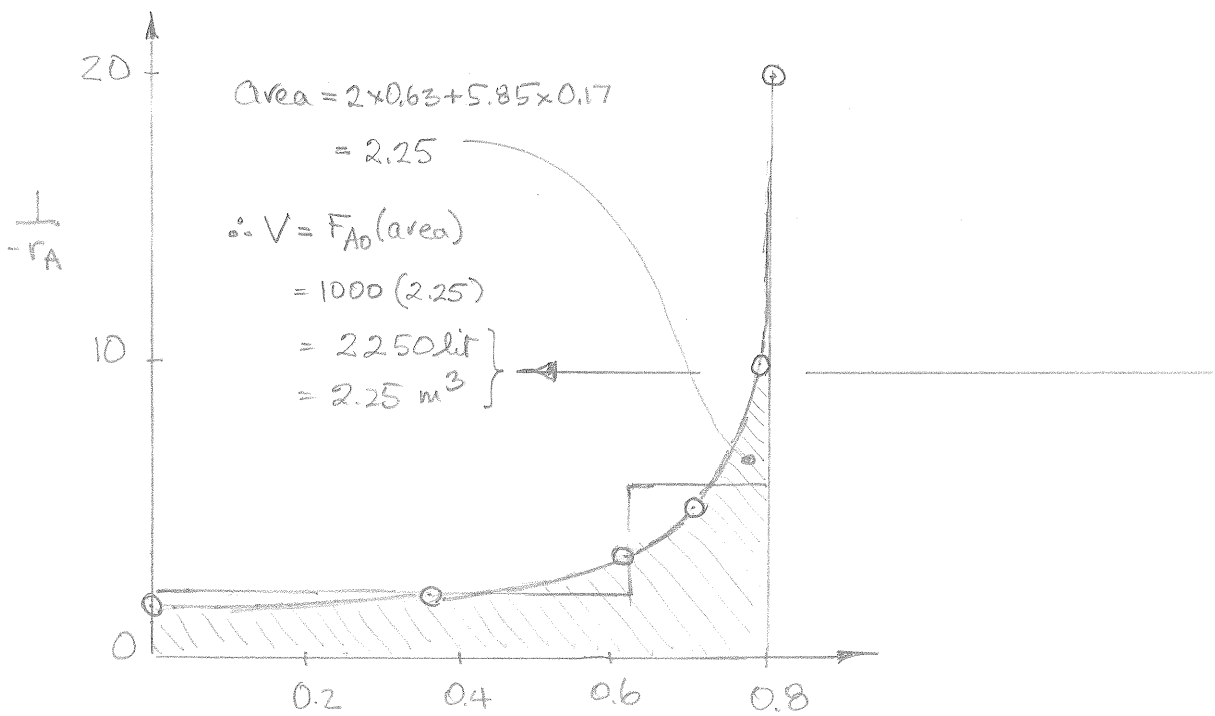
Therefore the slope of the adiabatic

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

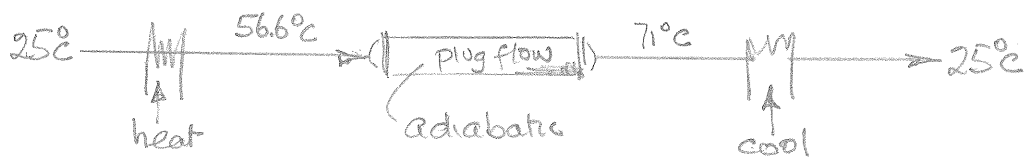
Next, from Fig E3 directly we get

X_A	$-r_A$	$-1/r_A$
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





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

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

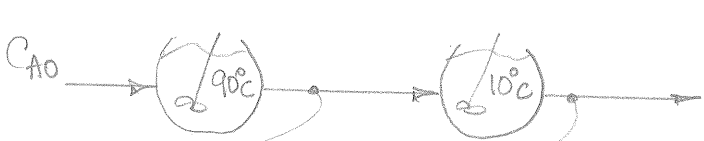
$$= 11.9 \sim 12.7 \text{ m}^3 \leftarrow$$

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

	10°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



fraction which forms R

$$\frac{C_R}{C_P + C_T} = \frac{66.31}{66.31 + 163.83} = 0.288 \qquad \frac{C_S}{C_S + C_U} = \frac{15.4}{15.4 + 3.84} = 0.800$$

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

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

$E_1 > E_2$ and $E_1 > E_3$ ◄ a)

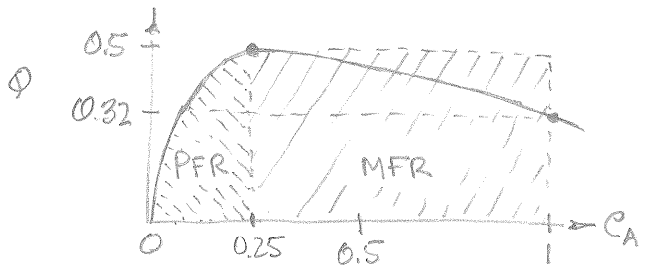
b) We should have a falling temperature when

$E_1 > E_3$ and $E_1 < E_2$ ◄ b)

10.7 From Example 1

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

The φ vs C_A curve is



so use MFR followed by PFR

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

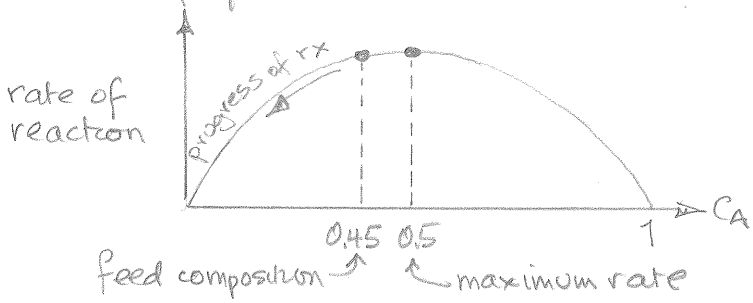
For PFR: $C_{Sp} = \int \varphi\, dC_A = \int \dfrac{8C_A dC_A}{1 + 8C_A + 16C_A^2} = 8\int_0^{0.25} \dfrac{C_A}{(1+4C_A)^2}\, dC_A$

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

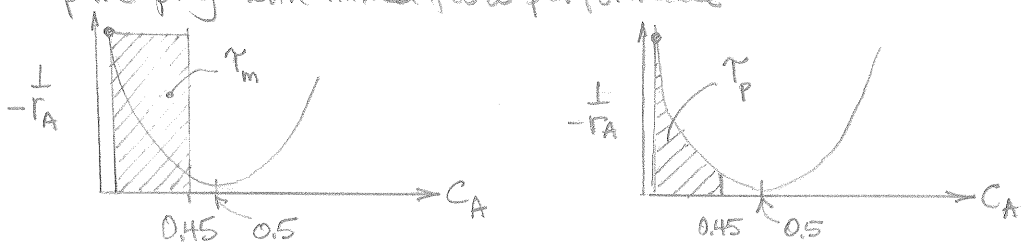
So $C_{Sp} = \left[\dfrac{1}{16}\cdot\dfrac{1}{1+4x} + \dfrac{1}{16}\ln(1+4x)\right]_0^{0.25} = \dfrac{1}{2}\left[\dfrac{1}{2} + \ln 2 - 1\right] = 0.0966$

$\therefore C_{Stotal} = C_{Sm} + C_{Sp} = 0.375 + 0.0966 = 0.4716$ ◄

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

$C_{AO} = 6$
$C_{RO} = 0.6$
$C_{TO} = 0$

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

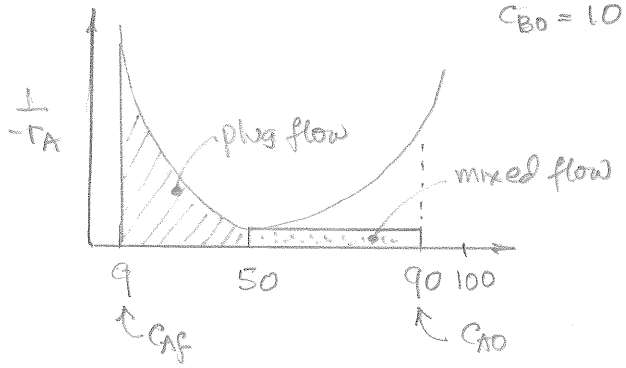
(a) So to maximize C_R/C_T do not react at all } ← a)
The design of Fig P11 is no good }

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

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

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

10.13 $A + B \longrightarrow B + B \qquad -r_A = kC_AC_B$ $\qquad C_{A0} = 90 \qquad C_{Af} = 9$ $\qquad C_{B0} = 10 \qquad C_{Bf} = 91$



Use a MFR followed by a PFR ⟵

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

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

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

$\therefore k_2/k_1 = 0.3322$

From Fig 8.13 or Eqs 8.8 & 8.9 $\qquad \frac{C_{R\max}}{C_{A0}} = 0.58$ ⟵

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

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

then
$A + B \longrightarrow R \qquad k_2/k_1 = 0.1$
$A + 4.5\,B \longrightarrow S$
$R + 3.5\,B \longrightarrow S \qquad k_3/k_1 = 0.25$

Rewrite the rates

From the Denbigh reaction set, eq 49 gives

$$\frac{C_{R,max}}{C_{A0}} = \frac{k_1}{k_{12}}\left(\frac{k_{12}}{k_3}\right)^{k_3/(k_3 - k_{12})} = \frac{1.0}{1.1}\left(\frac{1.1}{2.5}\right)^{2.5/(2.5-1.1)} = 0.588$$ ⟵

Use plug flow ⟵

10.19 Given $k_1 = k_2 = 2\times10^{13}\exp(-159000/RT)$; $k_3 = 8.15\times10^{17}\exp(-209000/RT)$; $k_4 = 2.1\times10^{5}\exp(-83600/RT)$

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

At 1200K

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

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

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

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

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

Now find C_{Rmax} from Eq 8.8

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

and

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

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

Do not recycle or bypass

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

$$\frac{C_R}{C_{A0}} = \frac{k_5}{k_6-k_5}\left[e^{-k_1t} - e^{-k_2t}\right] = (-1)\left[0-0.9762\right] = 0.9762$$

11.1 a) Check to see if the results are consistent

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

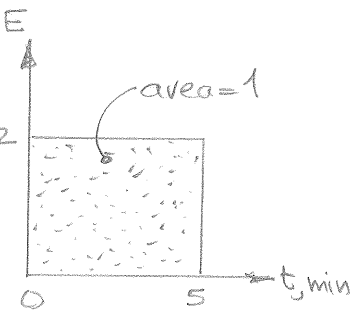
From the graph: $\text{area} = (0.05\ \text{mol/lit})(5\ \text{min}) = 0.25\ \text{mol}\cdot\text{min/lit}$ } check

So the results are consistent ← a)

b) Mean $\bar{t} = V/v$ or $V = \bar{t}\,v = 2.5 \times 4 = 10$ lit (by inspection) ← 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: $\bar{t} = V/v = 60/4 = 15$ sec

But from the experimental curve: compare

$\bar{t} = \frac{1}{3}(18\times1 + 21\times2) = 20$ 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: $\bar{t} = \frac{\Sigma tC}{\Sigma C} = \frac{30(15\cdot\frac{h}{2}) + 65(90\cdot\frac{h}{2})}{105\cdot\frac{h}{2}} = 60$ days

Area under the curve: $A = \frac{(120-20)}{2}\cdot10^{-6} = 52.5\ \frac{\text{unit}\cdot\text{days}}{m^3}$

From the material balance

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

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

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

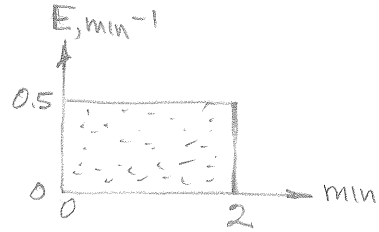
$V = (\bar{t})v = 60\ \text{days}\left(6000\ \frac{m^3}{s}\right)\left(\frac{3600\times24\ s}{\text{day}}\right) =$

$= 3.11\times10^{10}\ m^3$ ← b)

11.7 Calculate the conversion for

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

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



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 $$\left(-\tfrac{1}{2}\right)(2)(1)t = \left(\frac{C_A}{C_{A0}}\right)^{1/2} - 1$$

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

} for a batch of material

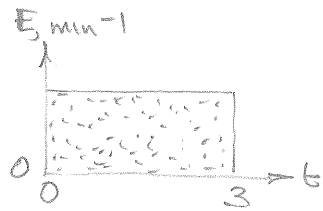
$$\therefore \frac{C}{C_0} = \int_0^2 (1-t)^2 \left(\tfrac{1}{2}\right) dt = \frac{0.5}{3}(1-t)^3\Big|_2^0 = \frac{1}{6}(1+1) = \frac{1}{3}$$

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

11.9 Calculate the conversion for

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

$-r_A = 3$ mol/lit·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 ....

$$\frac{C_A}{C_{A0}} = 1 - \frac{kt}{C_{A0}} \quad \text{for } t < \frac{C_{A0}}{k} = \frac{6}{3} = 2$$

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

} replace into above

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

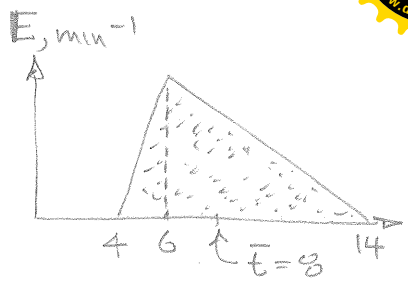
$$= \frac{1}{6}\,\frac{(2-t)^2}{2}\Big|_2^0 = \frac{1}{6}\left[\frac{2^2}{2} - 0\right] = \frac{1}{3}$$

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

11.11 Calculate the conversion for

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

$-r_A = 0.03$ mol/lit·min ← 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

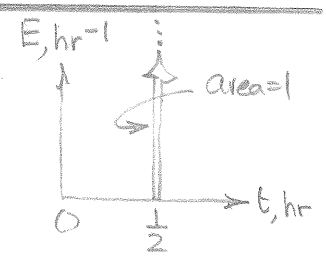
Here nothing leaves the reactor before 4 min, so everything has reacted

$C_{Af} = 0, \quad X_{Af} = 1$ ◀

11.13 For the solid particles

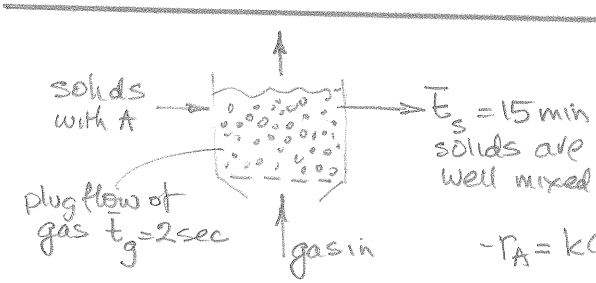
$$\overline{1-X} = \int (1-X)\, E\, dt = \int_0^1 \left(1 - \frac{t}{1}\right)^3 \delta(t - t_0)\, dt \quad (1 = 1 \text{ hr})$$

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

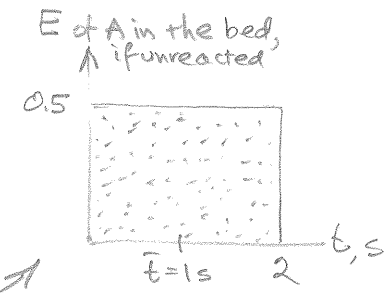


$\therefore \overline{X} = 1 - 0.125 = 0.875$ ◀

11.15



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



Conversion of A

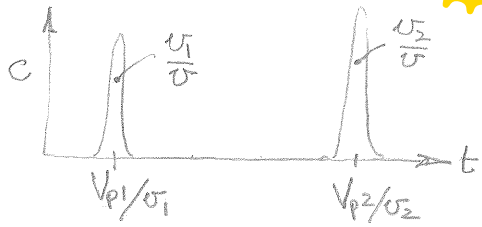
A is released uniformly by solids, so

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

$\therefore X_A = 0.5677$ ◀

↑ 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 $\upsilon = 1 m^3/s$ we have

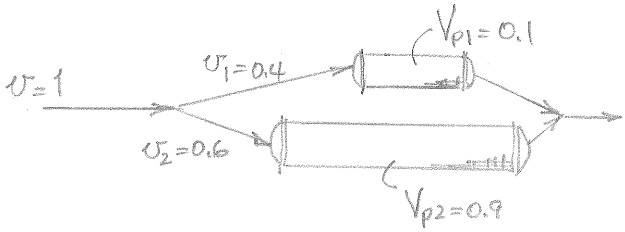


$$\upsilon_1 = \frac{16}{16+24} = 0.4\ m^3/min$$

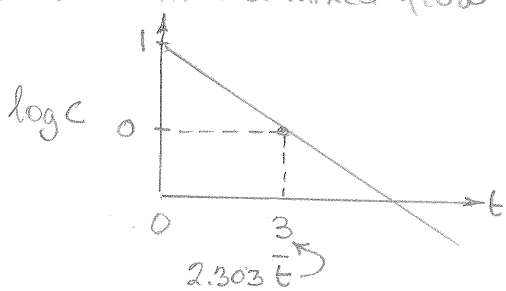
$$\upsilon_2 = \frac{24}{16+24} = 0.6\ m^3/min$$

$$V_{p1} = \bar{t}_1 \upsilon_1 = (0.25)(0.4) = 0.1\ m^3$$

$$V_{p2} = \bar{t}_2 \upsilon_2 = (1.5)(0.6) = 0.9\ m^3$$



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

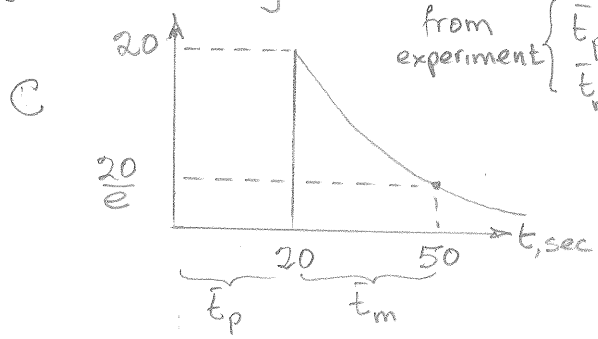
But we know that

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

(or less if there is dead space)

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

12.5 Again look at Fig 1

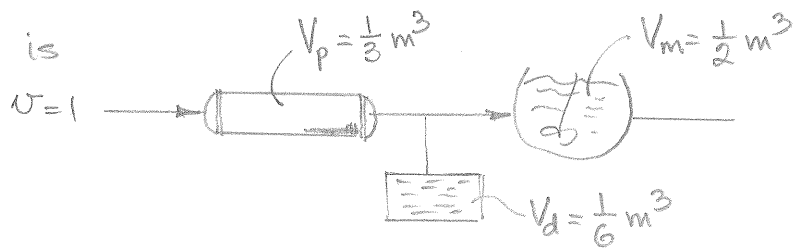


from experiment { $\bar{t}_p = 20$, $\bar{t}_m = 30$ } $\Rightarrow \bar{t}_{active} = 50\ s$

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

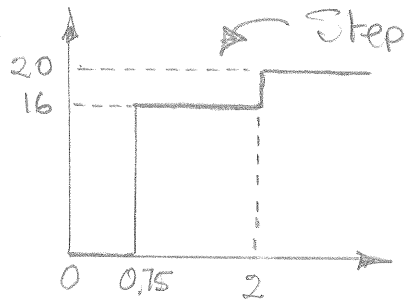
$\therefore \bar{t}_{dead} = 10\ s$

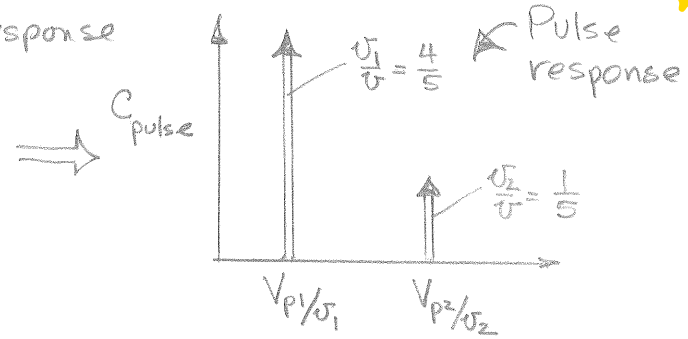
Thus our model is



12.7

Given





From the pulse response curve

$v_1 = \frac{4}{5}v = 0.8$

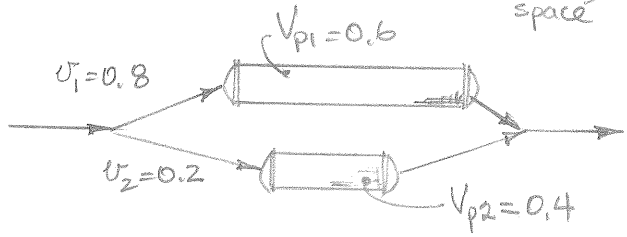
$v_2 = \frac{1}{5}v = 0.2$

$V_{p1} = v_1(0.75) = 0.8(0.75) = 0.6$

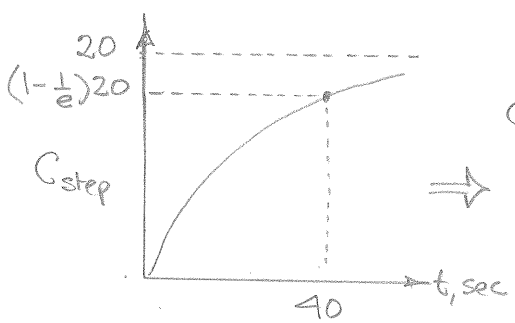
$V_{p2} = v_2(2) = 0.2(2) = 0.4$

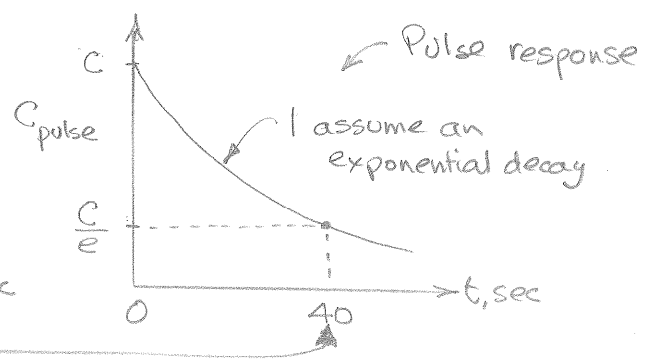
note: no dead space

So the flow model is



12.9



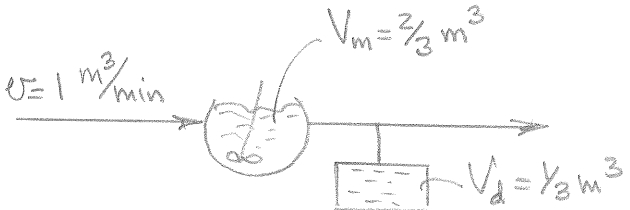


For mixed flow alone this should be 60sec. However, this curve comes out early, meaning dead spaces are present. This tracer curve shows that $\bar{t} = 40$ sec, thus

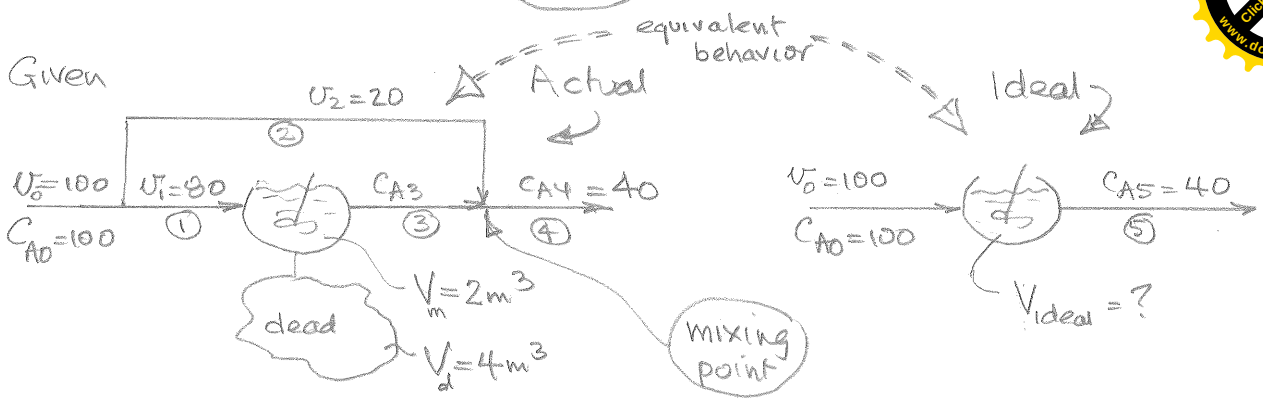
$V_m = 2/3\ m^3$

$V_d = 1/3\ m^3$

and our flow model is



11.11 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 2nd order reaction

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

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

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

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

or

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