Sheet 2

3.1

$$-r_{A_1} = -\frac{dC_A}{dt} = 0.2 \ \frac{mol}{Lit.s} \Rightarrow C_A = 1 \ \frac{mol}{lit}$$

$$-r_{A_2} = \frac{-dC_A}{dt} = ? \Rightarrow C_A = 10 \ \frac{mol}{lit}$$

في هذا السؤال كيف ان يجد ركيه اتفاعل حتى يمكن حله
- نفرضه first order

$$-r_{A_1} = k C_A^1$$

$$0.2 = k (1)^1 \Rightarrow k = 0.2$$

$$-r_{A_2} = 0.2 * 10 = 2 \ mol/lit.s$$

3.2

$$x_A = 0.5 \Rightarrow time = 5 min$$

$$x_A = 0.75 \Rightarrow time = ?$$

at first order ✓

$$-\ln(1 - x_A) = kt \Rightarrow -\ln(1-0.5) = k(5)$$

$$\therefore k = 0.1386 \ min^{-1}$$

Now for $x_A = 0.75$

$$-\ln(1 - 0.75) = 0.1386 \ (t)$$

$$\therefore t = 10 \ min$$

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Q 3.3

Repeat 3.2 for 2nd order

$$\frac{1}{C_{A_0}} \frac{X_A}{1-X_A} = kt$$

Home work

3.4

time = 10 min $\Rightarrow$ $X_A = 0.75$

time = 20 min $\Rightarrow$ $X_A = ?$

product by ½ order rate

هنا يوجد عندي كانت المرتبة $\frac{1}{2}$ لذا يجب ان نشتق

$$-r_A = k C_A^{0.5}$$

$$C_{A_0} \frac{dX_A}{dt} = k C_{A_0}^{0.5} (1-X_A)^{0.5}$$

$$C_{A_0}^{0.5} \frac{dX_A}{(1-X_A)^{0.5}} = k\,dt \qquad \text{let } \frac{k}{C_{A_0}} = k'$$

$$\int_0^{X_A} (1-X_A)^{-0.5} = k' \int_0^t dt$$

$$\frac{-(1-X_A)^{0.5}}{0.5}\Big|_0^{X_A} = k' t$$

$$2\left[-(1-X_A)^{0.5} + 1\right] = k't$$

for time = 10 $X_A = 0.75$

$$2\left[-(1-0.75)^{0.5} + 1\right] = k'(10)$$

$\therefore k = 0.1$

for time = 20 min

$$2\left[-(1-X_A)^{0.5} + 1\right] = 0.1 \times 20$$

$\Rightarrow X_A =$ [illegible]

$\therefore$ in 20 min conversion is 100%

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3.6

(3)

$C_{A_o} = 1 \frac{mol}{lit}$ $\quad t = 8 min \quad x_A = 0.8$

$t = 18 min \quad x_A = 0.9$

rate eq. ? let the reaction first order

واحد

حل آخر إذا لم يعطى وقت

$$-r_A = -\frac{dC_A}{dt} = K C_A^n$$

$$C_A^{1-n} - C_{A_o}^{1-n} = (n-1) K t$$

$$C_A = C_{A_o}(1 - x_A)$$

at 8 min $C_A = 1(1-0.8) = 0.2 \frac{mol}{lit}$

at 18 min $C_A = 1(1-0.9) = 0.1 \frac{mol}{lit}$

$$(0.2)^{1-n} - (1)^{1-n} = (n-1) K (8) \quad \text{---} (1)$$

$$(0.1)^{1-n} - (1)^{1-n} = (n-1) K (18) \quad \text{---} (2)$$

sub. eq (1) in (2)

$$\frac{(0.2)^{1-n} - (1)^{1-n}}{(n-1)(8)} = \frac{(0.1)^{1-n} - (1)^{1-n}}{(n-1)(18)} \quad * (n-1)$$

$$\frac{(0.2)^{1-n} - (1)^{1-n}}{(0.1)^{1-n} - (1)^{1-n}} = \frac{8}{18} = 0.44$$

by try and Error when $n = 1.5$ $\quad 0.57 \neq 0.44$

when $n = 2$ $\quad 0.44 \doteq 0.44$ ✓

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3.6 cont'

Sub $n=2$ in eq 2

$$(0.2)^{1-2} - (1)^{1-2} = (2-1)\,K\,(8)$$

$$\frac{5-1}{8} = K \Rightarrow K = 0.5 \ \frac{lit}{mol \cdot min}$$

$$-r_A = \left[0.5 \ \frac{lit}{mol.min}\right] C_A^2$$

3.9

First order $A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} R$ $C_{A0} = 0.5$ 8min

$C_{R0} = 0$

$M = \frac{C_{R0}}{C_{A0}} = 0$

$X_{Ae} = 0.667 \Rightarrow X_A = 0.333$

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

$$-\ln\left(1 - \frac{0.333}{0.667}\right) = \frac{0+1}{0+0.667} k_1 (8)$$

$$0.69 = 11.99\, k_1 \Rightarrow k_1 = 0.05754$$

$$\frac{k_1}{k_2} = \frac{M + X_{Ae}}{1 - X_{Ae}}$$

$$\frac{0.05754}{k_2} = \frac{0.667}{0.333} \Rightarrow k_2 = 0.02872$$

$$-r_A = 0.05754\, C_A - 0.02872\, C_R$$

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3.10

Home work

5

3.11

$C_{A0} = 500$

form data $C_A = 500 \Rightarrow$ time $= 100$ min

C_A at $(5\text{hr} + 100\text{min}) = 200 \frac{mol}{m^3}$ (300 min)

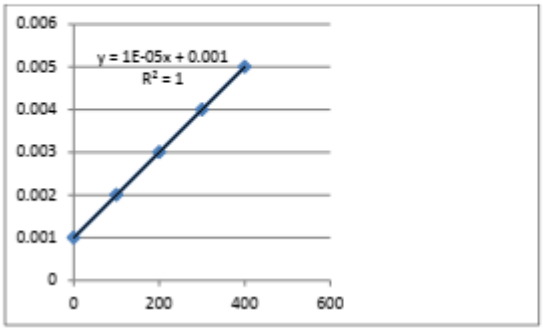
$X_A = 1 - \frac{C_A}{C_{A0}}$

$= 1 - \frac{200}{500} = 0.6$

3.12

From the table of data,

$\frac{1}{Ca} \rightarrow t$ *is straight line,* Reaction is second order.



Ca	t	1/ca
1000	0	0.001
500	100	0.002
333	200	0.003003
250	300	0.004
200	400	0.005

3.13

C_{Rmax}

t_{max}

$k = 1 * 10^{-5}\ (mol/l)^{-1}(min)^{-1}$

$\frac{1}{Ca} = \frac{1}{Cao} + kt$

$t = 5*60 = 300$ min

$C_{ao} = 500\ mol/m^3$

$\frac{1}{Ca} = 0.003 + \frac{1}{500}$

$C_a = 200\ mol/m^3$

$X_a = \frac{Cao - Ca}{Cao} = \frac{500-200}{500} = 0.6$

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3.18

$C_{e0} = 0.001 \frac{mol}{lit}$

$C_{A0} = 10 \frac{mol}{lit}$

$$-r_A = -\frac{dC_A}{dt} = \frac{200\, C_{e0} C_A}{2 + C_A}$$

what time for $C_A = 0.025$ mol/lit

(6)

$$-\int_{C_{A0}}^{C_A} dC_A \left(\frac{2 + C_A}{C_A}\right) = 200\, C_{e0}\, t$$

$$-\left[2 \ln C_A \Big|_{C_{A0}}^{C_A} + C_A \Big|_{C_{A0}}^{C_A}\right] = 200\, C_{e0}\, t$$

$$-\left[2 \ln \frac{C_A}{C_{A0}} + C_A - C_{A0}\right] = 200\, C_{e0}\, t$$

when $C_A = 0.025 \Rightarrow t = 109.79$ min

3.17

for 1st order $x_A = ?$ after 1 day

$$-\ln \frac{C_A}{C_{A0}} = kt$$

$\frac{C_A}{C_{A0}}$ at $t_{1/2} = 0.5$

$0.6931 = k\,(76\ min) \Rightarrow k = 9.12 \times 10^{-3}\ min^{-1}$

after 1 day (24 hr * 60 min)

$$-\ln(1 - x_A) = kt$$

$$-\ln(1 - x_A) = 9.12 \times 10^{-3}\ min^{-1} * (24 \times 6)\ min$$

$$1 - x_A = 1.979 \times 10^{-6}$$

$\therefore x_A = 0.9999$

$\Rightarrow$ conversion after 1 day is 99.99 %

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3.19

Home work

ايجاد الاشتقاق عند X_A ثم حساب rate

3.20

Home work

$$-\frac{dC_A}{dt} = KC_A^2$$

اشتق مرتين

3.22

Home work

$X_A = ?$

3.23 $C_{A0} = 1$ mol/lit

$t = 1$ hour $\Rightarrow X_A = 0.75$

$t = 2$ hour $\Rightarrow X_A = 1$

find eq. rate

$n = ?$ $K = ?$

let nth order

$$C_A^{1-n} - C_{A0}^{1-n} = (n-1)Kt$$

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

at $X_A = 0.75$ $C_A = 0.25$

$X_A = 1$ $C_A = 0$

at 1 hour

$$0.25^{1-n} - 1^{1-n} = (n-1)K(1) \quad \text{---} (1)$$

at 2 hour $0^{(1-n)} - 1^{(1-n)} = (n-1)K(2)$ --- (2)

sub (2) in (1)

$$\frac{0.25^{1-n} - 1^{1-n}}{1(n-1)} = \frac{-1^{1-n}}{2(n-1)} \quad * (n-1)$$

$$n = \frac{1}{2}$$

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3.23 dat

sub $n=\frac{1}{2}$ in eq (1) or (2)

$$-1^{0.5} = -0.5\,(K)(2) \Rightarrow K = 1\ \frac{mol^{1/2}}{lit^{1/2}.hr}$$

$$\therefore -r_A = \left[1\ \frac{mol^{1/2}}{lit^{1/2}.s}\right] C_A^{1/2}$$

3.24 the reaction is Homogeneous Catalyzed

time = ? for $C_{A0} = 10\ \frac{mol}{lit}$ → $C_A = 2\ \frac{mol}{lit}$

$$-r_A = k_1 C_A + k_2 C_c C_A$$

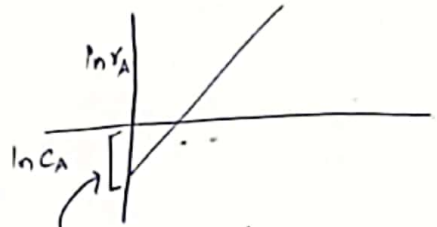
$$-r_A = C_A(k_1 + k_2 C_c)$$

$$-r_A = C_A\, k_{obs} \quad \text{to be } \vec{1^{st}}$$

$$\ln(r_A) = \ln C_A + \ln k_{obs}$$

$$y \quad mx + \text{inter.}$$

$\ln r_A$	$\ln C_A$
-2.8134	0
-2.30	0.6931
-1.39	1.39
0	1.79



$$-2.85219 = \ln k_{obs} \Rightarrow k_{obs} = 0.05949$$

$$-\frac{dC_A}{dt} = (0.05949)\,C_A$$

$$\therefore -\ln\frac{C_A}{C_{A0}} = (0.05949)\,t$$

$$\therefore t = 27.1\ hr$$

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3.29

$$2A \rightarrow B$$

0.8	0.4	starting with 80% A
0.2	0.2	inert
1	0.6	

$$\varepsilon_A = \frac{0.6 - 1}{1} = -0.4$$

let $V_0 = 1$

V decreases by 20% in 3 min

$\Rightarrow V = 0.8 V_0$

first order variable volume

$$-\ln\left[1 - \frac{\Delta V}{\varepsilon_A V_0}\right] = kt \qquad \Delta V = V - V_0 = 0.8 - 1 = -0.2$$

$$-\ln\left[1 - \frac{-0.2}{-0.4}\right] = k(3)$$

$$0.693 = k\,(3\ \text{min}) \Rightarrow k = 0.231\ \text{min}^{-1}$$

3.30

Homework

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