Problems on Batch Reactor

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Problem-1

- Liquid A decomposes by first-order kinetics, and in a batch reactor 50% of A is converted in a 5-min run. How much would it take to reach 75% Conversion?

Solution: We have $-\ln(1 - X_A) = kt$

$-\ln(1 - 0.5) = k.5,$ k=0.1386 min^{-1}

For 75% conversion, $-\ln(1 - 0.75) = 0.1386.t$

t= 10 mins Ans.

Problem-2

The first-order reversible liquid reaction $A \leftrightarrows R$, $C_{A0}= 0.5mol/L$, $C_{R0}=0$, takes place in a batch reactor. After 8 mins, conversion of A is 33.3%, while equilibrium conversion is 66.7%. Find the rate equation.

Solution: $A \leftrightarrows R$, $C_{A0}= 0.5mol/L$, $C_{R0}=0$

$$-r_A= k_1C_A - k_2C_R \quad = k_1C_{A0}(1-X_A)- k_2 C_{R0}(1+X_A)$$

As $C_{A0} X_A = C_{R0} X_R$

$$-r_R= k_1C_A - k_2C_R \quad = k_1C_{A0}(1-X_A)- k_2 (C_{R0}+C_{A0}X_A)$$

- $C_{A0}\frac{dX_A}{dt}$ = $k_1C_{A0}(1-X_A)- k_2\,C_{A0}X_A$
- $\int_0^{X_{Af}}\frac{dX_A}{k1-X_A(k_1+k_2)} = \int_0^t dt$
- $t = -\frac{1}{(k_1+k_2)}\ ln\frac{k_1}{k1-X_A(k_1+k_2)}$
- $= -\frac{1}{k_1(1+k_2/k_1)}\ ln\frac{k_1}{1-X_A(1+k_2/k_1)}$
- $K_e = \frac{k_1}{k_2} = \frac{C_{Re}}{C_{Ae}} = \frac{C_{R0}+C_{A0}X_{Ae}}{C_{A0}(1-X_{Ae})} = \frac{X_{Ae}}{(1-X_{Ae})}$
- $\frac{k_2}{k_1} = \frac{1}{X_{Ae}} - 1 = \frac{1}{0.667} - 1$ =0.4993

- $t = -\frac{1}{k_1(1+0.4993)} \; ln\frac{k_1}{1-X_A(1+0.4993)}$
- Given at t = 8 min, X_A =0.333
- $k_1 = 0.05767, k_2 = 0.0288$

- $-r_A = 0.05767C_A - 0.0288C_R$ Answer

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Problem-3

The irreversible reaction $2H_2 + 2NO \rightarrow N_2 + H_2O$ is carried out in a constant volume reactor reactor using equimolar amounts of hydrogen and nitric oxide.
The reactor data is as follows.

P_t, mm Hg	200	240	280	320	326
$t_{1/2}$, sec	265	186	115	104	67

Find the overall order of the reaction

Solution:

$$aA + bB \rightarrow cC + dD$$

$$-r_A = -\frac{dC_A}{dt} = kC_A^a C_B^b$$

Reaction is performed with a stoichiometric ratios throughout the reaction period.

$\frac{C_B}{C_A} = \frac{b}{a}$ and $-\frac{dC_A}{dt} = kC_A^a\left(\frac{b}{a}C_A\right)^b = k\left(\frac{b}{a}\right)^b C_A^{a+b} = k'C_A^n$

By integrating for n≠1 gives

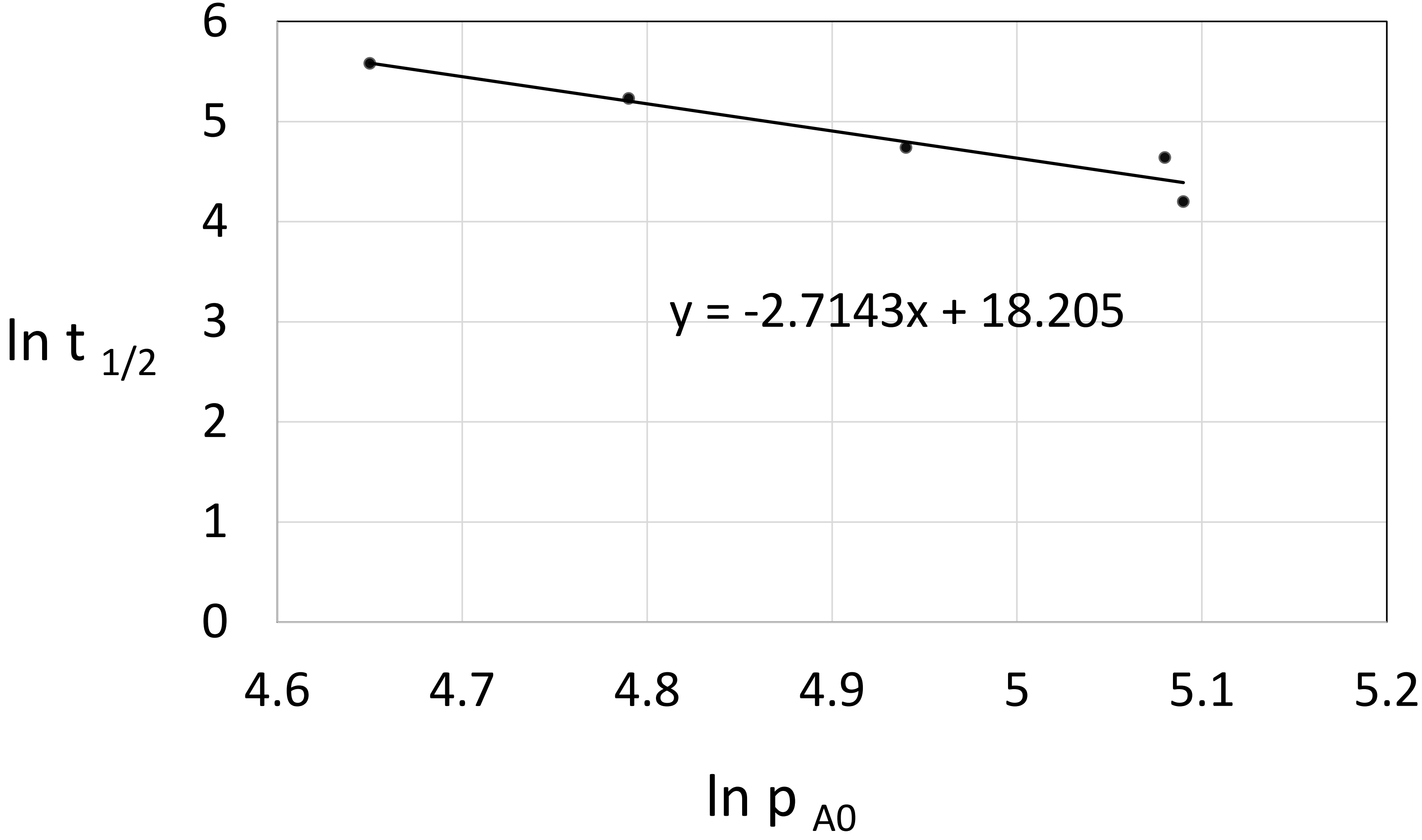
$$(C_A^{1-n} - C_{A0}^{1-n}) = k'(n-1)t$$

For half-life period: $t = \frac{1}{2}$, $C_A = \frac{C_{A0}}{2}$ and $t_{\frac{1}{2}} = \frac{0.5^{1-n}-1}{k(n-1)}\ C_{A0}^{1-n}$ (44)

$$t_{\frac{1}{2}} = \frac{2^{n-1}-1}{k'(n-1)}\ C_{A0}^{1-n}$$

- $ln(t_{1/2}) = ln\left[\frac{2^{n-1}-1}{k\prime(n-1)(RT)^{1-n}}\right] + (1-n)\ln(p_{A0})$
- As H_2 and NO are using in equimolar amounts $p_{A0} = p_T/2$

$\ln(p_{A0})$	4.65	4.79	4.94	5.08	5.09
$ln(t_{1/2})$	5.58	5.23	4.74	4.64	4.20



Slope= -2.714 = 1-n

So, n= 3.714≈ 4

Problem-4

The aqueous reaction $A \rightarrow R + S$ is carried out in a batch reactor with C_{Ao}=0.183mol/l, C_{Ro}=0 and C_{So}=55 mol/l. The reactor data is as follows:

t, min	0	36	65	100	160	∞
C_A,mol/l	0.183	0.145	0.122	0.103	0.0795	0.0494

Find a rate equation for this reaction.

Solution: $-r_A = k_1C_A - k_2C_RC_S = k_1C_{A0}(1-X_A) - k_2(C_{A0}X_A)(C_{S0}+C_{A0}X_A)$

As $C_R = C_{A0}X_A$ and $C_S = C_{S0}+C_{A0}X_A$

At equilibrium, $C_{Ae} = C_{A0}(1-X_{Ae})$, $C_{Re} = C_{A0}X_{Ae}$ and $C_{Se} = C_{S0}+C_{A0}X_{Ae}$

- X_{ae}= (C_{A0}- C_{Ae})/C_{A0}= (0.1823-0.0494)/0.1823 = 0.73

C_{Re}= $C_{A0}X_{Ae}$ =0.1823×0.73=0.1331

and C_{Se} = C_{S0} +$C_{A0}X_{Ae}$= 55+0.1823×0.73 =55.1331

At equilibrium, -r_A= 0

$$\frac{k_1}{k_2} = \frac{C_{Re}C_{Se}}{C_{Ae}} = \frac{0.1331 \times 55.1331}{0.0494} = 149.06$$

$$k_1 = 149.06\, k_2$$

$$C_{A0}\frac{dX_A}{dt} = k_1 C_{A0}(1 - X_A) - k_2(C_{A0}X_A)(C_{S0} + C_{A0}X_A)$$

Neglecting higher power of X_A

$$\frac{dX_A}{dt} = k_1(1 - X_A) - k_2X_A(C_{S0} + C_{A0}X_A)$$

$$\frac{dX_A}{dt} = 149.06k_2 - 204.06\ k_2X_A$$

$$\int_0^{X_A} \frac{dX_A}{149.06 - 204.06\ \mathrm{X_A}} = k_2 \int_0^t dt$$

$ln\left[\frac{149-204\ \mathrm{X_A}}{149}\right] = -204k_2t$ At t=36 min, X_A= 0.203

$k_2 = 4.45\ \times 10^{-5}$lit/mol.min and $k_1 = 6.6 \times 10^{-3}$/min

$-r_A = 6.6 \times 10^{-3} C_A - 4.45\ \times 10^{-5} C_R C_S$ Ans.

Problem-5

A zero-order homogeneous gas reaction A$\rightarrow$ rR proceeds in a constant volume bomb, with 20% inerts , and the pressure rises from 1 to 1.3 atm in 2 min. If the same reaction takes place in a constant pressure batch reactor, what is the fractional volume change in 4-min if feed is at 3 atm and consists of 40% inerts ?

Solution: A$\rightarrow$ rR is zero order reaction

0.8moles A + 0.2 moles inerts = 0.8 r moles R and 0.2 moles inerts

For constant volume reactor, pressure rises, Δn = r-1, a=1

- $-r_A = \frac{dC_A}{dt} = k, -r_A = \frac{dp_A}{RTdt} = k$

$$-\frac{1}{RT}\int_{p_{A0}}^{p_A} dp_A = kt\ , -\frac{1}{RT}(p_A - p_{A0}) = kt$$

$$-\frac{1}{RT}(p_A - p_{A0}) = kt$$

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

$$-\frac{a}{\Delta nRT}(\pi - \pi_0) = kt$$

$-\frac{a}{(r-1)RT}(\pi - \pi_0) = kt$ or, $-\frac{1}{(r-1)RT}(1.3 - 1) = k.2$

$$\frac{0.15}{(r-1)RT} = k$$

Constant pressure batch is variable volume reactor

Design equation is $t = C_{A0}\int_0^{X_A}\frac{dX_A}{(1+\varepsilon_A X_A)(-r_A)}$

$$C_{A0}\int_0^{X_A}\frac{dX_A}{(1+\varepsilon_A X_A)} = \mathrm{kt}$$ As $(-r_A) = k$

$$\frac{C_{A0}}{\epsilon_A}\ln(1+\epsilon_A X_A) = kt$$

$$\frac{C_{A0}}{\epsilon_A}\ln\frac{V}{V_0} = kt$$

Stoichiometry:

0.6A +0.4 inerts $\rightarrow$ 0.6r R +0.4 inerts

$$\epsilon_A = \frac{0.6(r-1)}{1}$$

$$p_{A0} = 0.6\times\pi = 0.6\times 3 = 1.8\,atm$$

$$C_{A0} = \frac{1.8}{RT}$$

$$\frac{1.8}{RT0.6(r-1)} \quad ln\frac{V}{V_0} = kt = \frac{0.15}{(r-1)RT} \times 4$$

$$ln\frac{V}{V_0} = \frac{0.15}{3} \times 4 = 0.2$$

$$\frac{V}{V_0} = 1.221$$

Fractional volume change $= \frac{\Delta V}{V_0} = 0.221\ Ans$