Universiti Malaysia PAHANG
Engineering • Technology • Creativity

Chemical Reaction Engineering I

Mind Map 1

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Rate Analysis methods

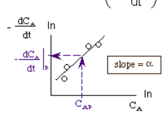
Batch Reactor Data

Taking the natural log of $\left[-\frac{dC_A}{dt} = kC_A^{\alpha}\right]$

$$\ln\left(-\frac{dC_A}{dt}\right) = \ln k + \alpha \ln C_A$$

The reaction order can be found from a ln-ln plot of:

$$\left(-\frac{dC_A}{dt}\right) \text{ vs } C_A$$



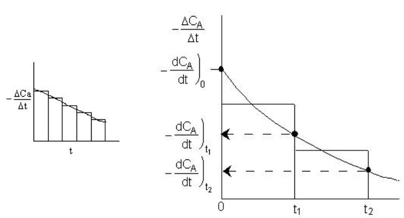
$$k = \frac{-\left.\frac{dC_A}{dt}\right|_P}{C_{AP}^{\alpha}}$$

Methods of Initial Rates

Method of Half-Lives

Differential Method

1. Graphical Method

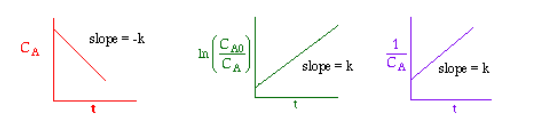


2.Numerical Method

3.Polynomial Fit (polymath)

Integral Method

Zero Order	First Order	Second Order
Zero order, $\alpha = 0$	First order $\alpha = 1$	Second order $\alpha = 2$



Zero Order	First Order	Second Order
$\frac{dC_A}{dt} = r_A = -k$	$\frac{dC_A}{dt} = r_A = -kC_A$	$\frac{dC_A}{dt} = r_A = -kC_A^2$
at $t = 0,\ C_A = C_{A0}$	at $t = 0,\ C_A = C_{A0}$	at $t = 0,\ C_A = C_{A0}$
$\Rightarrow C_A = C_{A0} - kt$	$\Rightarrow \ln\left(\frac{C_{A0}}{C_A}\right) = kt$	$\Rightarrow \frac{1}{C_A} - \frac{1}{C_{A0}} = kt$

If the data do not fall on a straight line for α=0,1, or 2 such as α=2;

Graphical Method (exercise) – Test 20142015

The liquid-phase isomerization reaction of maleic acid to form fumaric acid takes place in an ideal batch reactor at 180°C

$$Cis\text{-}HO_2CCH{=}CHCO_2H \rightarrow Trans\text{-}HO_2CCH{=}CHCO_2H$$

Maleic Acid → Fumaric Acid

The concentration-time data for maleic acid was obtained as follows:-

C_A (mol.dm^{-3})	1.0	0.95	0.816	0.707	0.5	0.37
t (hr)	0	0.278	1.389	2.78	8.33	16.66

a) Determine the rate law and its parameters with the right unit. (ans: order=2.8)
b) Demonstrate how a flow reactor can be used to determine the rate law
c) Explain how the volume of the batch reactor can be determined.

Numerical Method (exercise)- Test Sem 1 20162017

The irreversible liquid phase isomerization of tetrahydrocyclopentadiene (A) into adamantane (B) was carried out in a batch reactor and simplified as

$$A \rightarrow B$$

The concentration-time data were obtained as in Table 1.

t (min)	0	10	20	30
C_A (mol/dm^3)	1	0.6	0.4	0.3

a) Develop the rate law of the isomerization reaction using the data given.

b) If the reaction is an elementary reaction, design the batch reactor that could consume 90 % of 1 mol/dm^3 tetrahydrocyclopentadiene. (k=0.053 min^{-1})

Authors Information

Credit to the authors:
Dr Mohd Sabri Mahmud, Assoc Prof Dr Maksudur Rahman Khan, Madam Hamidah Abdullah