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Universiti Malaysia PAHANG
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Process Chem and Pharmaceutical Engineering 1

Chemical Reaction Part 1

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Chapter Description

- **Aims**
  - Define reaction rate and the factors affecting the rate

- **Expected Outcomes**
  - Define reaction rate and the factors affecting the rate
  - Construct mass and mole balances for different types of process corresponding to the stoichiometry and conversion
  - Factors affecting reaction rate

- References
  - Chemistry, A molecular Approach, Nivaldo J. Tro, Pearson, 4th Edition, 2017

Chemical Kinetics

- Chemical reaction: speeds or rates
- Kinetic = movement/change
- Reaction rate: Change of concentration of a reactant or a product with time (i.e, M/s)
- $aA + bB \rightarrow cC + dD$
- The reactant is consumed while product is formed

$$Rate = -\frac{1}{a}.\frac{\Delta[A]}{\Delta t} = -\frac{1}{b}.\frac{\Delta[B]}{\Delta t} = \frac{1}{c}.\frac{\Delta[C]}{\Delta t} = \frac{1}{d}.\frac{\Delta[D]}{\Delta t}$$

$$H_2(g) + I_2(g) \rightarrow 2HI(g)$$

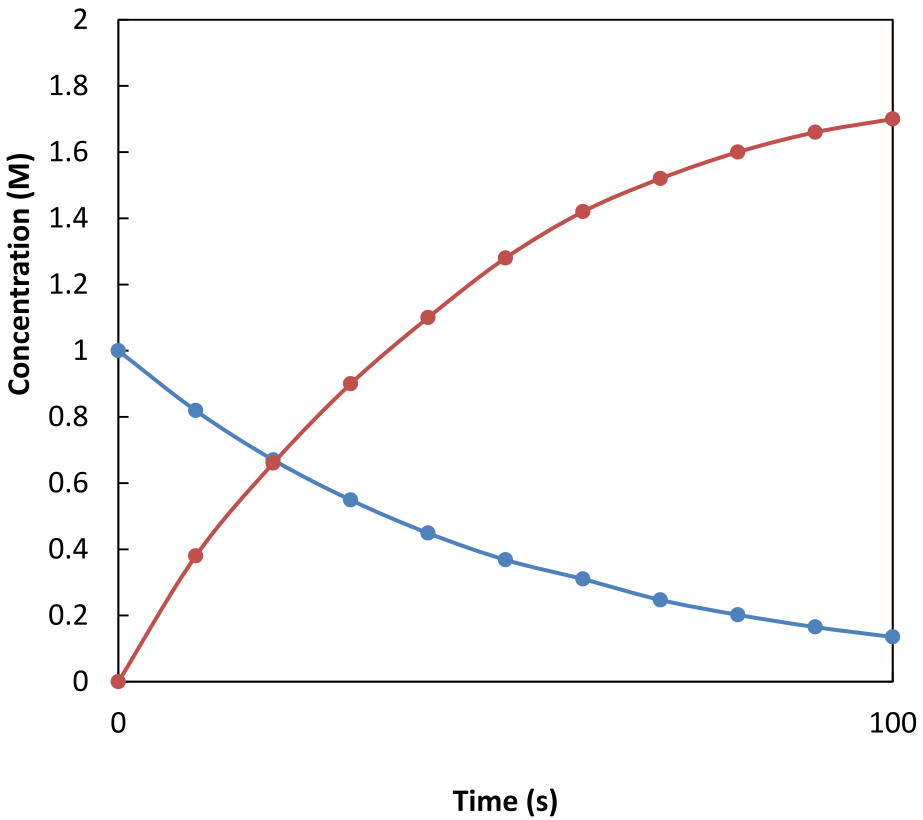
Reaction rate:

$$Rate = \frac{-\Delta[H_2]}{\Delta t}$$

$$Rate = \frac{-\Delta[I_2]}{\Delta t}$$

$$Rate = \frac{1}{2}\frac{\Delta[HI]}{\Delta t}$$

Reactant and Product Concentration as a Function of Time



$$H_2(g) + I_2(g) \rightarrow 2HI(g)$$

The concentration of HI increases at twice the rate the concentration of H_2 or I_2 decreases.

Exercise 1

Calculate the change of H2 concentration for each interval $\Delta[H_2]$ and rate for each interval $\Delta[H_2]/\Delta t$.

Time (s)	$[H_2]$ (M)	$\Delta[H_2]$ (M)	Δt(s)	Rate = $-\Delta[H_2]/\Delta t$ (M/s)
0.00	1.00			
10.00	0.819			
20.00	0.670			
30.00	0.549			
40.00	0.449			
50.00	0.368			
60.00	0.310			
70.00	0.247			
80.00	0.202			
90.00	0.165			
100.00	0.135			

Exercise 1

Calculate the change of H2 concentration for each interval $\Delta[H_2]$ and rate for each interval $\Delta[H_2]/\Delta t$.

Time (s)	$[H_2]$ (M)	$\Delta[H_2]$ (M)	Δt(s)	Rate = - $\Delta[H_2]/\Delta t$ (M/s)
0.00	1.00			
10.00	0.819	-0.181	10.00	0.0181
20.00	0.670	-0.149	10.00	0.0149
30.00	0.549	-0.121	10.00	0.0121
40.00	0.449	-0.100	10.00	0.0100
50.00	0.368	-0.081	10.00	0.0081
60.00	0.310	-0.067	10.00	0.0067
70.00	0.247	-0.054	10.00	0.0054
80.00	0.202	-0.045	10.00	0.0045
90.00	0.165	-0.037	10.00	0.0037
100.00	0.135	[illegible]	10.00	0.0030

Rate of Reaction

The rate of a chemical reaction is a measure of how fast the reaction occurs.

Fast rate of chemical reaction:
a large fraction of molecules react to form products in a given period of time.

Slow rate of chemical reaction:
only a relatively small fraction of molecules react to form products in a given period of time.

The Rate Law: The Effect of Concentration on Reaction Rate

The rate of a reaction often depends on the concentration of reactants.

$$A \rightarrow products$$

If the reverse reaction is negligibly slow, the relationship between the rate of the reaction and the concentration of the reactant (called the rate law):

$$Rate = k[A]^n$$

Where

k = constant of proportionality called the rate constant

N = reaction order.

The value of *n* determines how the rate depends on the concentration of the reactant

n = 0	n = 1	n = 2
$Rate = k[A]^0 = k$	$\text{Rate} = \text{k}[\text{A}]^1$	$\text{Rate} = \text{k}[\text{A}]^2$
• If **n = 0,** rate is independent of the concentration of reactant. • The concentration of the reactant decreases linearly with time. • The slope of the line is constant, indicating a constant rate.	• If **n = 1**, rate is directly proportional to the concentration of reactant. • The rate slows down as the reaction proceeds because the concentration of the reactant decreased.	• If **n = 2**, rate is proportional to the square of the concentration of reactant. • The rate is more sensitive to the reactant concentration.

Exercise 2

Consider the reaction between nitrogen dioxide and carbon monoxide:

$$NO_2(g) + CO(g) \rightarrow NO(g) + CO_2(g)$$

The initial rate of the reaction is measured at several different concentrations of the reactants, and tabulated in Table 1.

From the data, determine:

a) The rate law for the reaction

b) The rate constant (k) for the reaction

$[NO_2]$(M)	[CO](M)	Initial Rate (M/s)
0.10	0.10	0.0021
0.20	0.10	0.0082
0.20	0.20	0.0083
0.40	0.10	0.033

- The rate laws show the relationship between the rate of a reaction and the concentration of a reactant.
- How to check the relationship between the concentration of a reactant and time?

The Integrated Rate Law

The **integrated rate law** for a chemical reaction is a relationship between the **concentrations of the reactants** and **time**.

First-Order Integrated Rate Law

$$A \rightarrow product$$

- Rate = k[A]=-Δ[A]/Δt
- Rearrange:

$$\frac{\Delta[A]}{\Delta t} = k[A]$$ - also known as the differential rate law

- The integrated rate law:
- $\ln[A]_t = -kt + \ln[A]_0$

$$ln\frac{[A]_t}{[A]_0} = -kt$$

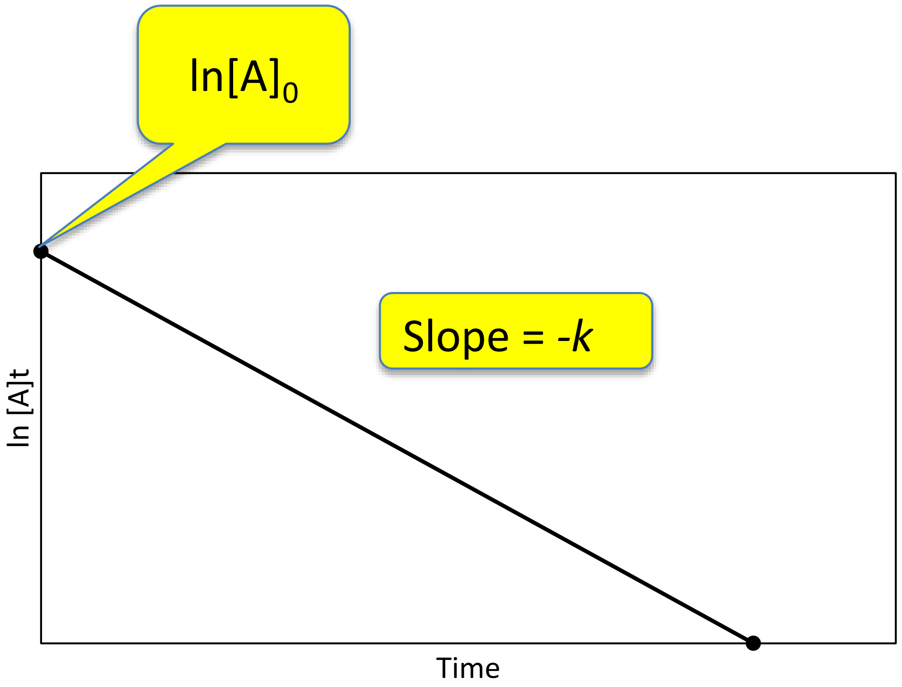
Where

$[A]_t$ = concentration of A at any time t

k = rate constant

$[A]_0$ =initial concentration of A

First-Order Integrated Rate Law



- The integrated rate law has the form of an equation for a straight line.
- $\ln[A]_t = -kt + \ln[A]_0$
- $y = mx + c$

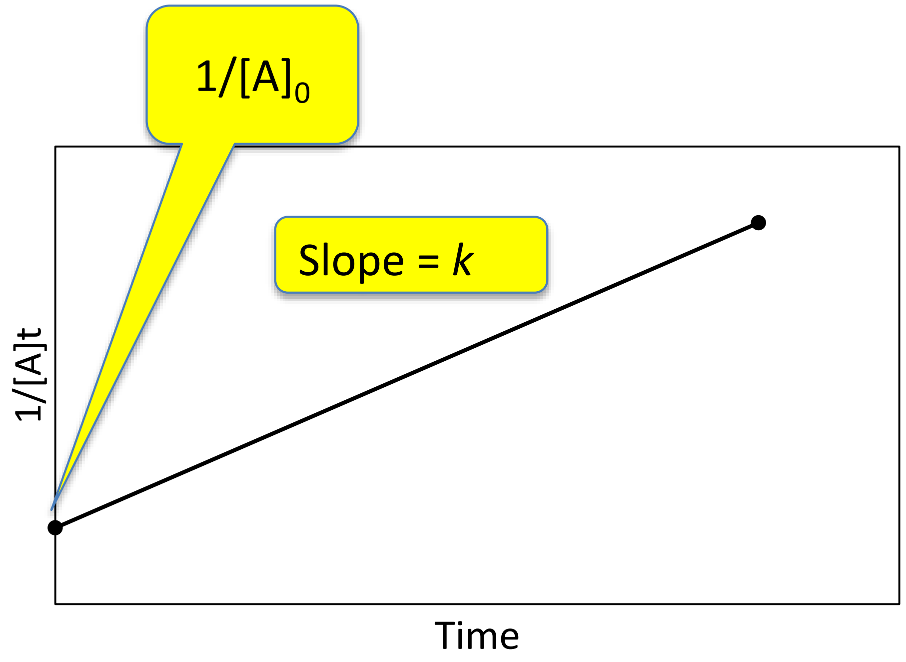
Second-Order Integrated Rate Law

$$A \rightarrow product$$

- Rate = $k[A]^2 = -\Delta[A]/\Delta t$
- Rearrange: differential rate law
- $\frac{\Delta[A]}{\Delta t} = k[A]^2$
- The second-order integrated rate law:
- $\frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$

Form equation for a straight line

Second-Order Integrated Rate Law



- A plot of the inverse of the reactant concentration vs time yields a straight line.

Conclusion of The Chapter

This chapter discussed about rate of reaction, rate law, and integrated rate law.

Chemistry, A molecular Approach, Nivaldo J. Tro, Pearson, 4th Edition, 2017