Lecture 1
Introduction of kinetics chemistry

Objective of the course

A detailed study of the rate of the reaction and the factors affecting it and and their various applications.

- Introduction to chemical kinetics reaction 1
- rate law 4
- Set the order of the reaction 3
- Kinetics of complex interactions 3
- The effect of temperature on the rate of the reaction 1
- reaction rate theories 2

Kinetics Chemistry :

-A branch of physical chemistry deals with the speeds or rates in which a chemical reaction occurs.

-The study of how fast reactions take place.

-The study of laws that express mathematically the effect of a change in concentration on the rate of a reaction.

The importance of chemical kinetics:

- Studying the rate of reactions
- Study the time required for the completion of the reaction
- Determine the reaction mechanism

- A **reaction mechanism** is the sequence of elementary steps by which a chemical reaction occurs.

  or A detailed and complete description of the chemical changes at the molecular level and the different stages that the reaction takes

Rate of reaction:

The change in the concentration of a reactant or a product with time (M/s).

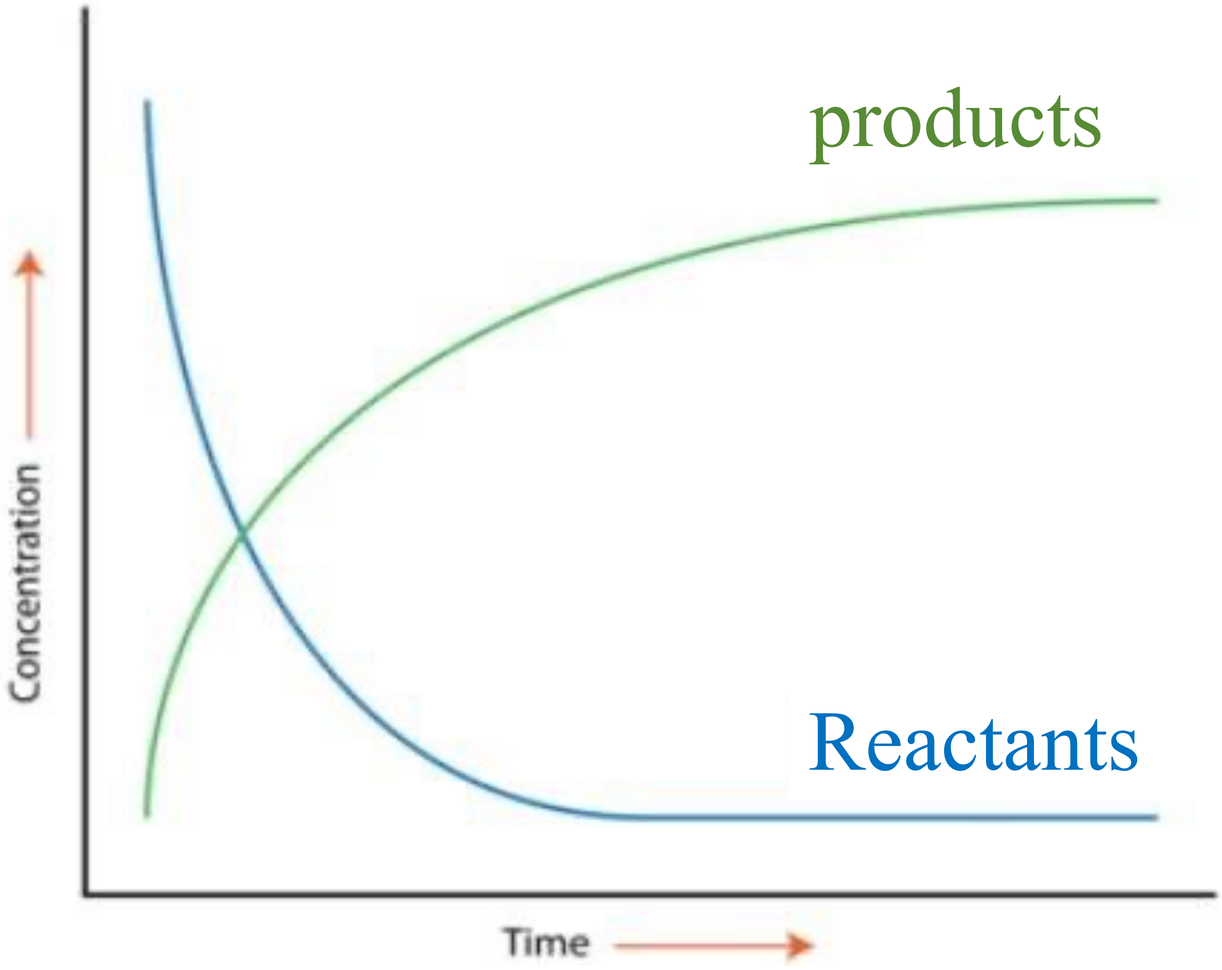
Many familiar reactions , such as the photosynthesis happen almost in a fraction of second, while others , such as the rusting of iron or the conversion of diamond to graphite may take millions of years to complete.

A chemical reaction can be represented by the reactants in the general equation :

$$\text{Reactants} \longrightarrow \text{Products}$$

$$A \longrightarrow B$$

This equation tells us that during the reaction, the reactants are consumed during the formation of products.


products
Reactants
Concentration
Time

The general equation:

$$aA + bB \rightarrow dD + fF$$

products

Reactants

$$R = +\frac{d[D]}{dt} = +\frac{d[F]}{dt}$$

$$R = \frac{+1}{d}\frac{d[D]}{dt} = \frac{+1}{f}\frac{d[F]}{dt}$$

$$R = -\frac{d[A]}{dt} = -\frac{d[B]}{dt}$$

$$R = \frac{-1}{a}\frac{d[A]}{dt} = \frac{-1}{b}\frac{d[B]}{dt}$$

Reaction rate unites:

$$\boldsymbol{R = (conc)(time)^{-1}}$$

$$\boldsymbol{R = mol/L(s, min, day, year \ldots.)^{-1}}$$

$$\boldsymbol{R = M/(s, min, day, year \ldots.)}$$

Example:

When ammonia reacts with oxygen at high temperatures, nitrogen oxide and water vapor are formed, if you know that the rate of ammonia consumed equals $3.5\times10^{-2} Ms^{-1}$ calculate the rate of oxygen consumed?

1- Writing the equation for the reaction:

$$NH_3 + O_2 \rightarrow NO + H_2O$$

2- Balance the chemical equation:

$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$$

3 - Write the following relationships between reactants and products

$$R = \frac{-1}{4}\frac{d[NH_3]}{dt} = \frac{-1}{5}\frac{d[O_2]}{dt} = \frac{1}{4}\frac{d[NO]}{dt} = \frac{1}{6}\frac{d[H_2O]}{dt}$$

$$R = \frac{-1}{4} V_{NH_3} = \frac{-1}{5} V_{O_2} = \frac{1}{4} V_{NO} = \frac{1}{6} V_{H_2O}$$

The rate of oxygen consumed can be found in terms of the consumed of ammonia, as in the question:

$$\frac{-1}{4} \frac{d[NH_3]}{dt} = \frac{-1}{5} \frac{d[O_2]}{dt}$$

$$\frac{d[O_2]}{dt} = \frac{-5}{-4}(3.5 \times 10^{-2}) = \qquad Ms^{-1}$$

Factors influencing the rate of reaction:

1. Reactant concentration :

Increasing the concentration of one or more reactants will often increase the rate of reaction. This occurs because a higher concentration of a reactant will lead to more collisions of that reactant in a specific time.

Factors influencing the rate of reaction:

2. Physical state of the reactants and surface area:

If we have a heterogeneous mixture, the rate of reaction will be limited by the surface area of the phases that are in contact. For example, if a solid metal reactant and gas reactant are mixed, only the molecules present on the surface of the metal are able to collide with the gas molecules. Therefore, increasing the surface area of the metal by cutting it into many pieces will increase its reaction rate.

Factors influencing the rate of reaction:

3. Temperature:

An increase in temperature typically increases the rate of reaction. An increase in temperature will raise the average kinetic energy of the reactant molecules. Therefore, a greater number of molecules will have the minimum energy necessary for collision.

Factors influencing the rate of reaction:

4.Presence of a catalyst:

A catalyst is a substance that accelerates a reaction by participating in it without being consumed. Catalysts provide an alternate reaction pathway which has lower activation energy to obtain products.

The rate constant (K):

The change in the concentration of a reactant or a product when the degree of concentration of all its reactants is equal the unit.

$$K = \frac{dx}{dt} = mol^{1-n}.L^{n-1}.time^{-1}$$

Reaction Order(n):

-The sum of the exponents of its concentration terms.

-The sum of the number of molecules, atoms or moles of the reactants whose concentration determines the rate of the reaction.

- The order of the reaction is an experimental or process result
- It is not related to a balanced chemical equation
- Take correct and mixed numbers

Reaction Order(n):

$$aA + bB \rightarrow dD + fF$$

-The order of the reaction for A is a and for B is b, and the overall order of the reaction is a+b and can take integer, fractional or zero numbers.

The molecularity of a reaction:

-The molecularity of a reaction is defined as the number of molecules or ions or substances that participate in the initial chemical reaction (which occurs during one step)

-If a chemical reaction proceeds by more than one step or stage, its overall velocity or rate is limited by the slowest step, the rate-determining step.

- The reaction molecule is related to the reaction mechanics
- It is not related to a balanced chemical equation
- Just take the right numbers

Example:

For the following reaction Find the reaction order and molecularity of a reaction?

1) $C_4H_9OH \rightarrow C_4H_8 + H_2O$

Order of a reaction=1

Molecularity of a reaction =1

The law of the reaction rate :

$$Rate = K[A]^a[B]^b$$

The rate of the reaction depends on the concentrations of the reactant A and B, that mean multiplying the concentrations of [A] and [B] each concentration raised to a power of the number of its moles in the balanced chemical equation.

Whereas K = velocity constant.
X, Y = reaction order
It is not possible to know the rate of reaction from knowing the chemical equation, but only through the practical experiments.

Example:

$$NO_2 + CO \rightarrow CO_2 + NO$$

We find from experiment that the relationship between focus and speed:

$$Rate = K\,[NO_2]^2$$

So the rate does not depend on the concentration of CO, but on the square of the concentration of NO_2, and therefore the reaction is of the second order of NO_2 and the zero order of CO.