Day-11

Chemical Kinetics

→ Global reaction:

Eg: $H_2 + \frac{1}{2}O_2 \longrightarrow H_2O$

This doesn't happen in a single step!

→ Elementary reaction:

$$H_2 + M \longrightarrow H + H + M$$

↓

3rd molecule: energy carrier.

→ $H_2 - O_2$ system:

1.) $H_2 + M \rightleftharpoons H + H + M$ (Chain initiation)

2.) $O_2 + H \rightleftharpoons OH + O$ } Chain branching

3.) $O + H_2 \rightleftharpoons OH + H$ }

4.) $H + O_2 + M \rightleftharpoons HO_2 + M$

5.) $HO_2 + H_2 \rightleftharpoons H_2O + OH$

6.) $OH + H_2 \rightleftharpoons H_2O + H$ (Chain propagation)

Other eg: $O + O + M \longrightarrow O_2 + M$

$M + H + H \longrightarrow H_2 + M$

$$H + OH + M \longrightarrow H_2O + M$$

All these are **Chain Termination / Recombination** reactions.

→ $1\ cm^3$ → Initially 1 chain molecule. (= 1 free radical per cm^3).
$N = 10^{19}$ molecules/cm^3, avg. collision rate is 10^9 collision/s. It is chain prop. Reac^n (1 free rad. → 1 free rad.)

a.) $\text{Time} = \frac{10^{19}}{10^9}\ s = 10^{10}\ s \approx 317\ yrs$

b.) Time (chain branching)

$$= \frac{\log_2(10^{19})}{10^9} = \frac{63.1166}{10^9}\ s$$

$$= 63.1166\ ns$$

c.) 1% chain branching, then? (rest 99% nothing).

$$\Rightarrow 1 + 1.01 + 1.01^2 + \ldots + 1.01^N = 10^{19}$$

$$\Rightarrow \frac{(1.01)^{N+1} - 1}{0.01} = 10^{19}$$

$$\Rightarrow (1.01)^{N+1} \approx 10^{17}$$

$$\Rightarrow N \approx 17 \log_{1.01} 10 \approx 3933.9342$$

$$t = \frac{3933.9342}{10^9} \approx 3.93\ \mu s$$

→ Law of mass Action:

$aA + bB \longrightarrow cC + dD$

a, b, c, d are stoichiometric coeffs., elementary reaction.

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

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

$$\frac{1}{c}\frac{d[C]}{dt} = k[A]^a[B]^b$$

$$\frac{1}{d}\frac{d[D]}{dt} = k[A]^a[B]^b$$

k → Rate constant / Arrhenius constant