Day - 14

→ $O_2 \rightleftharpoons 2O$ at equilibrium (2000 K)

$$K_p = \exp.\left(\frac{-2\times 121709}{8.314\times 2000}\right)$$

$$= 4.389 \times 10^{-7}$$

Now, $K_p = \frac{x_O^2}{x_{O_2}}\left(\frac{1}{1}\right)^{2-1}$

$$= \frac{x_O^2}{x_{O_2}}$$

And $K_p = K_c\,(RT)^{2-1}$

$$= K_c RT$$

$$\Rightarrow K_c = \frac{4.389\times 10^{-7}}{8.314\times 2000}$$

$$= 2.64\times 10^{-11} = \frac{[O]^2}{[O_2]} = \frac{K_f}{K_r}$$

not required, just wrote it ☺

$$x_O = \sqrt{4.389\times 10^{-7}\times 0.21}$$

$$\approx 3.036\times 10^{-4}$$

$$= 303.6 \text{ ppm}$$

assumed 21% of O_2 in air

→ Reaction mechanism:

(i) NO formation

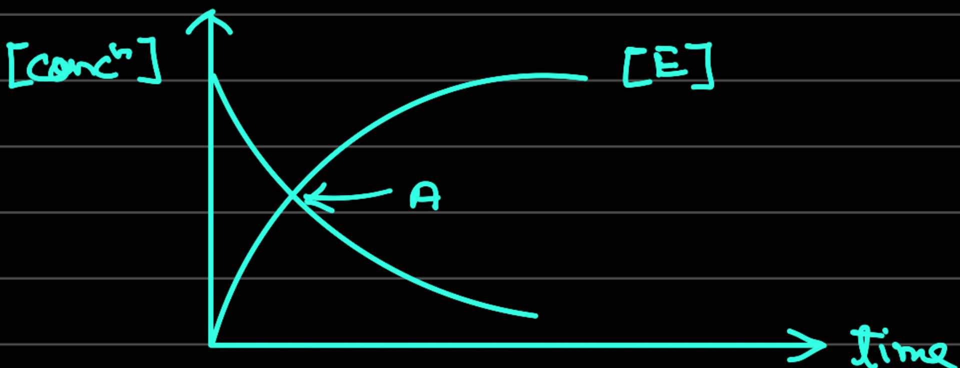
(ii) H_2-O_2 reaction

☆ Reduced mechanism –

- Partial equilibrium
- Steady state approximation

$$A + B \longrightarrow C$$
$$C + D \longrightarrow E$$

[C] is very low and gets consumed very quickly.



→ NO formation –
(Thermal NO)

$$N_2 + O_2 \longrightarrow 2NO \qquad (>1800\ K)$$

$$N_2 + O \longrightarrow NO + N$$

$$k_{f_1} = 1.8 \times 10^{14} \exp\left(\frac{-38370}{T}\right)$$

$$N + O_2 \longrightarrow NO + O$$

$$k_{f_2} = 1.8 \times 10^{10}\, T \exp\left(\frac{-4680}{T}\right)$$

$$\frac{d[N]}{dt} = k_{f_1}[N_2][O] - k_{f_2}[N][O_2]$$

Using steady-state approximation,

$$\frac{d[N]}{dt} = 0 \implies [N] = \frac{k_{f_1}}{k_{f_2}} \frac{[N_2][O]}{[O_2]}$$