Day-15

→ Thermal NO formation-

$N_2 + O \xrightarrow{k_{f_1}} NO + N$, $k_{f_1} = 1.8\times10^{14} \exp.\left(\frac{-38370}{T}\right)$

$N + O_2 \xrightarrow{k_{f_2}} NO + O$, $k_{f_2} = 1.8\times10^{10} T \exp.\left(\frac{-4680}{T}\right)$

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

Using steady-state approximation,

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

$$\frac{d[NO]}{dt} = k_{f_1}[N_2][O] + k_{f_2}[N][O_2]$$

$$= 2k_{f_1}[N_2][O]$$

Partial equilibrium > 1800 K : $O_2 \rightleftharpoons 2O$

$$[O] = \sqrt{k_p [O_2] \left(\frac{RuT}{P_o}\right)^{-1}}$$

$$\text{So } \frac{d[NO]}{dt} = 2k_{f_1}[N_2]\sqrt{k_p [O_2]\left(\frac{RuT}{P_o}\right)^{-1}}^{1/2}$$

$$\Rightarrow \frac{d[NO]}{dt} \propto k_{f_1}[N_2][O_2]^{1/2}$$

→ H_2-O_2 reaction mechanism –

$H_2 + M \longrightarrow H + H + M$ → very high T

$H_2 + O_2 \longrightarrow HO_2 + M$ → All other T

$H + O_2 \longrightarrow O + OH$

$H_2 + OH \longrightarrow H_2O + H$

$O + H_2O \longrightarrow OH + OH$

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

$O + O + M \longrightarrow O_2 + M$

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

mass diffusion $\propto \frac{1}{P}$

$H + O_2 + M \longrightarrow HO_2 + M$

↳ unreactive

$HO_2 + H \longrightarrow OH + OH$

$HO_2 + H \longrightarrow H_2O + O$

$HO_2 + O \longrightarrow O_2 + OH$

$HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$

$HO_2 + H_2 \longrightarrow H_2O_2 + H$

$H_2O_2 \longrightarrow OH + OH$