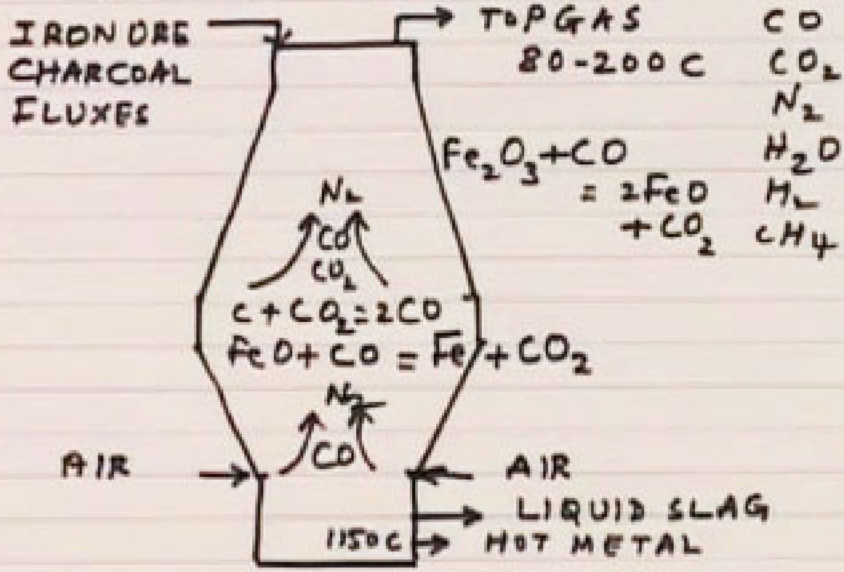
GAS SOLID NONCATALYTIC REACTIONS

EFFECT OF EQUILIBRIA.

SOME EXAMPLES



why Not: $Fe_2O_3 + 3H_2 = 2Fe + 3H_2O$

$\cancel{}_2$ =

$$CaCO_3 = CO_2 + CaO$$

A (s) B (g) C (S)

Kp (mmHg)	T (K).
0.0722	773
1.84	873
22.0	973
167	1073
1793	1173
2942	1273

$$r_A = k_2' C_C C_B - k_1' C_A$$

$$r_A = k_2 C_c - k_1$$

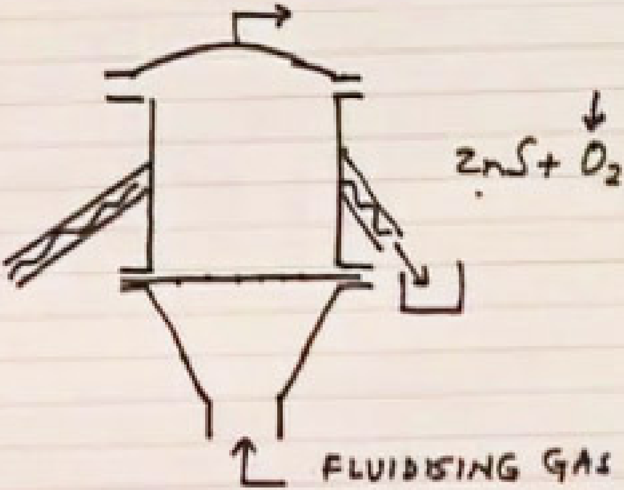
$$= k_2 \left(C_c - \frac{k_1}{k_2} \right)$$

$$= k_2 (C_c - K_c)$$

$$r_A = \frac{k_2}{RT} (P_c - K_p)$$

$CaCO_3 : CO_2 + CaO$

FLUID BED REACTOR.



$ZnS + O_2 = ZnO + SO_2$

Effect of changing Gas Composition

$$A(g) + B(s) = C(g) + D(s)$$

cocurrent flow.

$$F_A = F_{A0}(1 - X_A)$$

$$F_B = F_{B0} - F_{A0} X_A$$

$$F_C = F_{C0} + F_{A0} X_A$$

$$F_D = F_{D0} + F_{A0} X_A$$

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1 - X_A)\, T_0}{v_0 T}$$

$$C_C = \frac{(F_{C0} + F_{A0} X_A)\, T_0}{v_0 T}$$

$$C_C = (C_{C0} + C_{A0} X_A)\frac{T_0}{T}$$

$$K_p = \left(\frac{P_C}{P_A}\right)^* = \left[\frac{C_{C0} + C_{A0} X_A}{C_{A0}(1 - X_A)}\right]^*$$

$$K_p = \left[\frac{C_{C0} + C_{A0} X_A}{C_{A0}(1 - X_A)}\right]^*$$

$$X_A^* = \left(\frac{K_p - \theta_C}{1 + K_p}\right) \qquad \theta_C = \frac{F_{C0}}{F_{A0}}.$$

$$A(g) + B(s) = C(g) + D(s).$$

$$\frac{dF_A}{dV} = \left(r_A' \, a_s \right)$$

$$r_A' = -k_g \left(C_A - C_A^* \right)$$

$$r_A' = -k_g \left(C_{A0}(1-x_A) - C_{A0}(1-x_A^*) \right)$$

$$\frac{dF_A}{dV} = -k_g C_{A0} \left[x_A^* - x_A \right] a_s$$

$$-F_{A0} \frac{dx_A}{dV} = -k_g C_{A0} \left(x_A^* - x_A \right) a_s .$$

$$\frac{dx_A}{d\tau_g} = k_g \cancel{C_{A0}} \left(x_A^* - x_A \right) a_s .$$

$$\tau_g = V / v_0$$

$$\frac{dx_A}{d\tau_g} = k_g\left(x_A^* - x_A\right) a_s .$$

$$a_s = \left(4\pi R^2\right) N/V$$

$$\epsilon_R = \left(\frac{4}{3}\pi R^3\right) N/V .$$

$$a_s = 3\epsilon_R/R .$$

$$\frac{dx_A}{d\tau_g} = k_g\left(x_A^* - x_A\right) 3\epsilon_R/R . \quad (1)$$

$$\tau_g = \left(V/v_g\right) \qquad V = v_0 \tau_g$$

Reaction Control.

$$A(g) + B(s) = C(g) + D(s).$$

$$\frac{dF_A}{dV} = r_A' \, a_s.$$

$$r_A' = k_c (C_A - C_A^*)$$

$$\epsilon_R = \frac{4}{3} \pi R^3 N/V \quad \text{(expt quantity)}$$

$$a_s = \frac{4 \pi r_c^2 N}{V}$$

$$a_s = \frac{3 \epsilon_R}{R} \left[r_c^2 / R^2 \right] = \frac{3 \epsilon_R}{R} (1 - X_B)^{2/3}$$

$$a_s = \frac{3 C_R}{R}\left(1 - X_B\right)^{2/3}$$

$$= \frac{3 C_R}{R}\cdot\left(1 - \frac{X_A}{\theta_B}\right)^{2/3}$$

$$\frac{dF_A}{dV} = -k_s\left(C_A - C_A^*\right)\frac{3 C_R}{R}\cdot\left(1 - \frac{X_A}{\theta_B}\right)^{2/3}$$

$$-F_{A0}\frac{dX_A}{dV} = -k_s\left(C_A - C_A^*\right)\frac{3 C_R}{R}\left(1 - \frac{X_A}{\theta_B}\right)^{2/3}$$

$$\frac{dX_A}{d\tau_s} = k_s\left(X_A^* - X_A\right)\frac{3 C_R}{R}\left(1 - \frac{X_A}{\theta_B}\right)^{2/3}$$

Ash Diffusion Control.

$$\frac{dF_A}{dV} = (r_A' s)\frac{3\epsilon_R}{4\pi R^3}$$

$$\frac{-4\pi D(C_A - C_A^*)}{\left(\frac{1}{r_c} - \frac{1}{R}\right)} \frac{3\epsilon_R}{4\pi R^3}$$

$$-F_{A0}\frac{dX_A}{dV} = \frac{-\left[4\pi D\, C_{A0}\,(X_A^* - X_A)\right]3\epsilon_R}{\left(\frac{1}{r_c} - \frac{1}{R}\right)4\pi R^3}$$

$$\frac{dX_A}{d\tau_s} = \frac{4\pi D(X_A^* - X_A)\,3\epsilon_R}{4\pi R^2(R/r_c - 1)}$$

Ash Diffusion Contd.

$$\frac{dX_A}{d\tau_g} = \frac{\dfrac{3\epsilon_R D}{R^2} \cdot \left[\dfrac{K_g - \theta_c}{1+C_p} - X_A \right]}{\left[\left(1 - \dfrac{X_A}{\theta_B}\right)^{-1/3} - 1 \right]}.$$

$\tau_g = 0 \qquad X_A = 0$

$$\frac{dF_A}{dV} = -k_g C_{A0} (X_A^* - X_A) \frac{3\epsilon_R}{R} \quad \text{Film}$$

$$\frac{dF_A}{dV} = -C_{A0} (X_A^* - X_A) \frac{3 k_r \epsilon_R}{R} \left(1 - \frac{X_A}{\theta_B}\right)^{2/3}$$

Reaction

$$\frac{dF_A}{dV} = \frac{-3 \epsilon_R D C_{A0} (X_A^* - X_A).}{R^2 \left\{(1-X_B)^{-1/3} - 1\right\}} \quad \text{Ash. Control.}$$

$\Omega_i =$ Potential / Flux.

$$\Omega_1 = -\frac{1}{3k_g \epsilon_R / R}$$ FILM.

$$\Omega_2 = -\frac{1}{3k_s \frac{\epsilon_R}{R}\left(1-\frac{X_A}{\theta_B}\right)^{2/3}}$$ RXN.

$$\Omega_3 = \frac{-\left\{\left(1-X_B\right)^{-1/3}-1\right\}}{\left(3\epsilon_R D/R^2\right)}$$ Ash Contr.

Combined Resistances

$$\frac{dF_A}{dV} = \frac{\text{Potential}}{\sum \Omega}$$

$$\frac{dX_A}{d\tau_g} = \left(X_A^{*} - X_A\right)\left\{ \frac{3 k_g C_R}{R} + \frac{3 k_s C_R}{R}\left(1 - \frac{X_A}{\sigma_B}\right)^{2/3} + \frac{3 C_R D}{R^2\left\{\left(1 - \frac{X_A}{\sigma_B}\right)^{-1/3} - 1\right\}} \right\}$$

$X_A = 0 \quad \tau_g = 0$

Conversions from RTD.

Film Diffusion.

$$1 - X_B = 1 - t/\tau_F$$

$$RTD = E(t).$$

$$\overline{(1-X_B)} = \int_0^\infty (1-X_B)\, E(t)\,dt$$

$$\bar{C}_A = \int C_{A,\text{element}}\, E(t)\,dt$$

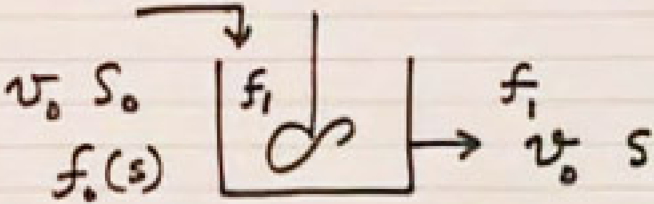
FILM DIFF.

$$\overline{(1-X_B)} = \int_0^{\tau} (1-X_B)\, E(t)\, dt.$$

$$+ \int_{\tau}^{\infty} (1-X_B)\, E(t)\, dt$$

$$\overline{(1-X_B)} = \int_0^{\tau} \left(1 - t/\tau_F\right) E(t)\, dt.$$

Population Balance Modelling



$$v_0 \bar{S}_0 - v\bar{s} + \bar{r}V = \frac{\partial}{\partial t}(V\bar{s})$$

$$\bar{S}_0 = \int s f_0(s)\,ds$$

$$\bar{S} = \int s f_1(s)\,ds$$

$$\bar{r} = \int r f_1(s)\,ds$$

$$v_0 \int s f_0(s)\, ds - v_0 \int s f_1(s)\, ds + \int \underbrace{v r f_1(s)}_{I}\, d\underline{s} = \frac{\partial}{\partial t}\left[v \int s f_1\, ds\right]$$

$$v_0 \int s f_0(s)\, ds - v_0 \int s f_1(s)\, ds$$

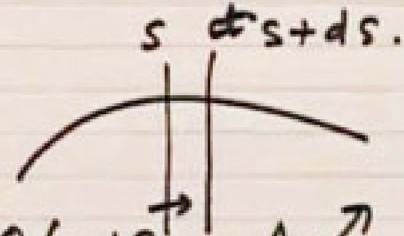
$$1 + \left[r v f_1(s)\, s\right] - \int s \cdot \frac{\partial}{\partial s}(r f_1) \cdot ds \cdot V$$

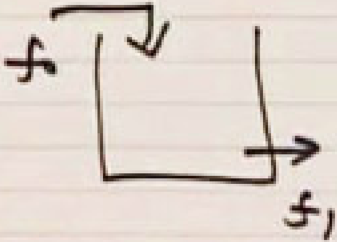
$$= \frac{\partial}{\partial t}\left[V \int s f_1\, ds\right]$$

$$\Rightarrow \quad v_0 f_0 - v_0 f_1 - \frac{\partial}{\partial s}(r_1 V f_1) = \frac{\partial}{\partial t}(f_1 V) \quad -(*)$$

Setting up PBE from Basics.

$\mathcal{R}_1 =$





I/p - O/p + Gen = Acc.

$$v_0 f_0(s) ds - v_0 f_1(s) ds$$

$$\left[f_1(s) r_1 W\big|_s - f_1(s+ds) r_1(s+ds) W \right]$$

$$= 0$$

$$v_0 f_0 - v_0 f_1 - \frac{d}{ds}\left(f_1 r_1 W\right) = 0$$

$$f_0 - f_1 - \frac{d}{ds}\left(f_1 r_1 \bar{F}_1\right) = 0$$