Prof. Shankar
Lec. 25 20/11/2012

Advanced Reaction Engineering

Gas Solid Reactions

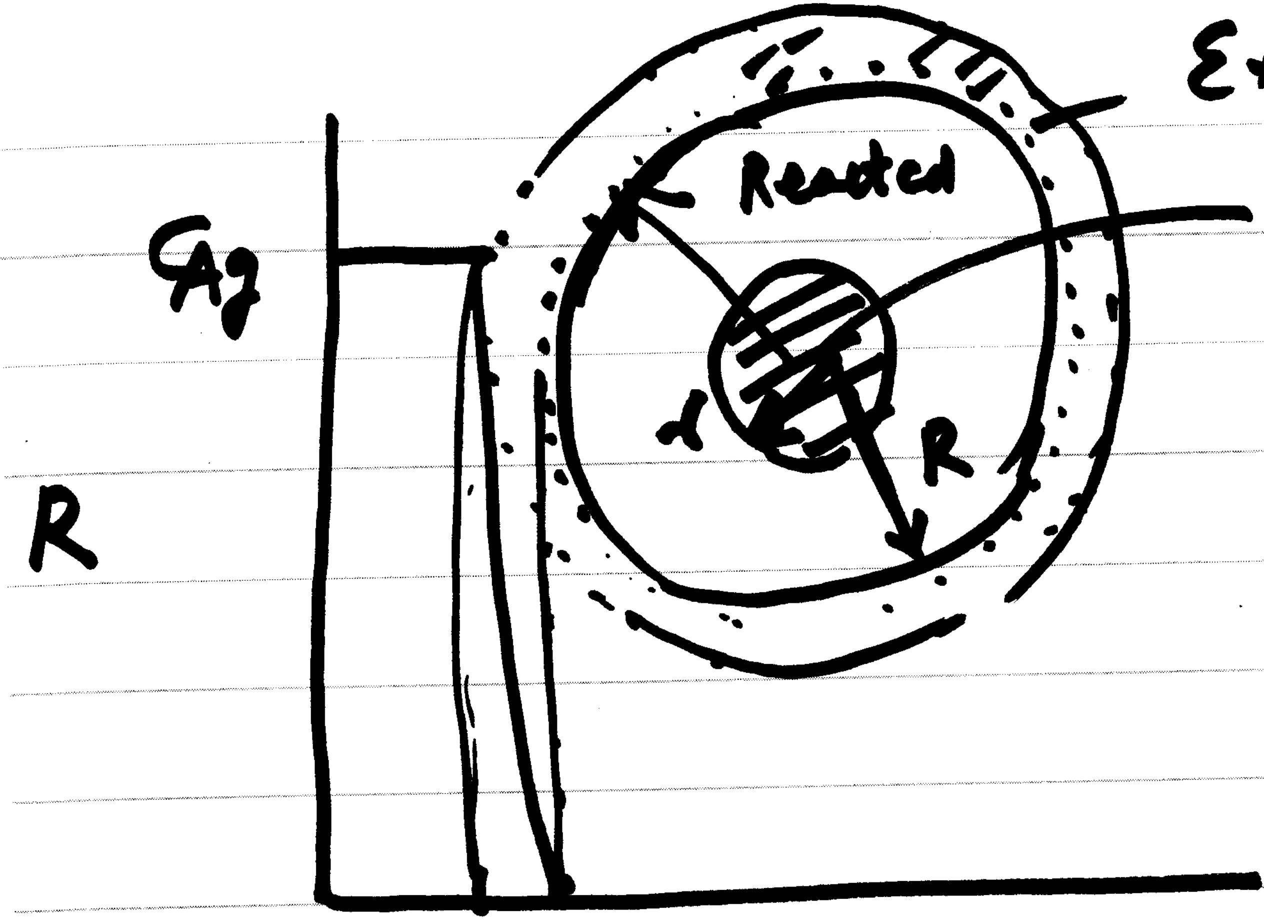
Tuesday
20/NOV/12
14:00-15:00

$$A(g) + b\,B(s) \rightarrow \text{Products}$$

$$CaCO_3 \rightarrow CaO + CO_2$$

$$Fe_2O_3 + CO = \underline{Fe} + CO_2$$

$$ZnS + O_2 = ZnO + SO_2$$



$A(g) + b\underline{B}(s) \rightarrow$

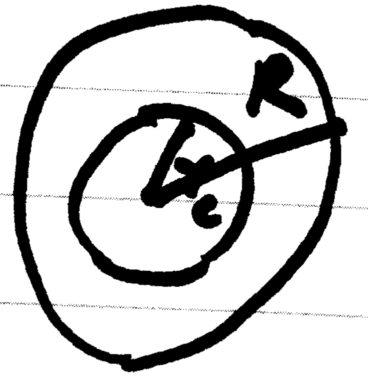
Products

$$\frac{+r_A S}{-1} = \frac{+r_B S}{-b} = \; ; \quad \cancel{-r_A} = \cancel{k_g C_{Ag}}$$

$$r_A = -k_g C_{Ag}$$

$$\left(\frac{d}{dt}N_B\right) = \left(\rho_B S\right) = -bk_g C_{Ag} S$$

$$= -bk_g C_{Ag}\left(4\pi R^2\right)$$



$$N_B = \left(\frac{4}{3}\pi r_c^3\right)\rho_B$$

$$\frac{d}{dt}\left[\frac{4}{3}\pi r_c^3 \rho_B\right] = -\left(k_g C_{Ag}\right)\left(4\pi R^2\right)$$

$$\cancel{3}\,\frac{4}{\cancel{3}}\pi r_c^2 \frac{dr}{dt}\rho_B = -bk_g C_{Ag}\, 4\pi R^2$$

$$\rho_B r_c^2 \frac{dr_c}{dt} = -b k_g C_{Ag} R^2$$

$$\rho_B \left[\frac{r_c^3}{3}\right]_R^{r_c} = - b k_g C_{Ag} R^2 t$$

$$\frac{\rho_B}{3R^2}\left[R^3 - r_c^3\right] = b k_g C_{Ag} \cancel{R^2} t.$$

$$t = \cancel{b k_g C_{Ag}} \frac{\rho_B R}{3 b k_g C_{Ag}} \left[1 - \frac{r_c^3}{R^3}\right]$$

$$t = \frac{\rho_B R_0}{3 b k_g C_{Ag}} \left(1 - \frac{r_c^3}{R^3} \right)$$

$$r_c = 0 \; ; \qquad \tau_F = \frac{\rho_B R_0}{3 b k_g C_{Ag}}$$

$$t = \tau_F \left(1 - \frac{r_c^3}{R^3} \right)$$

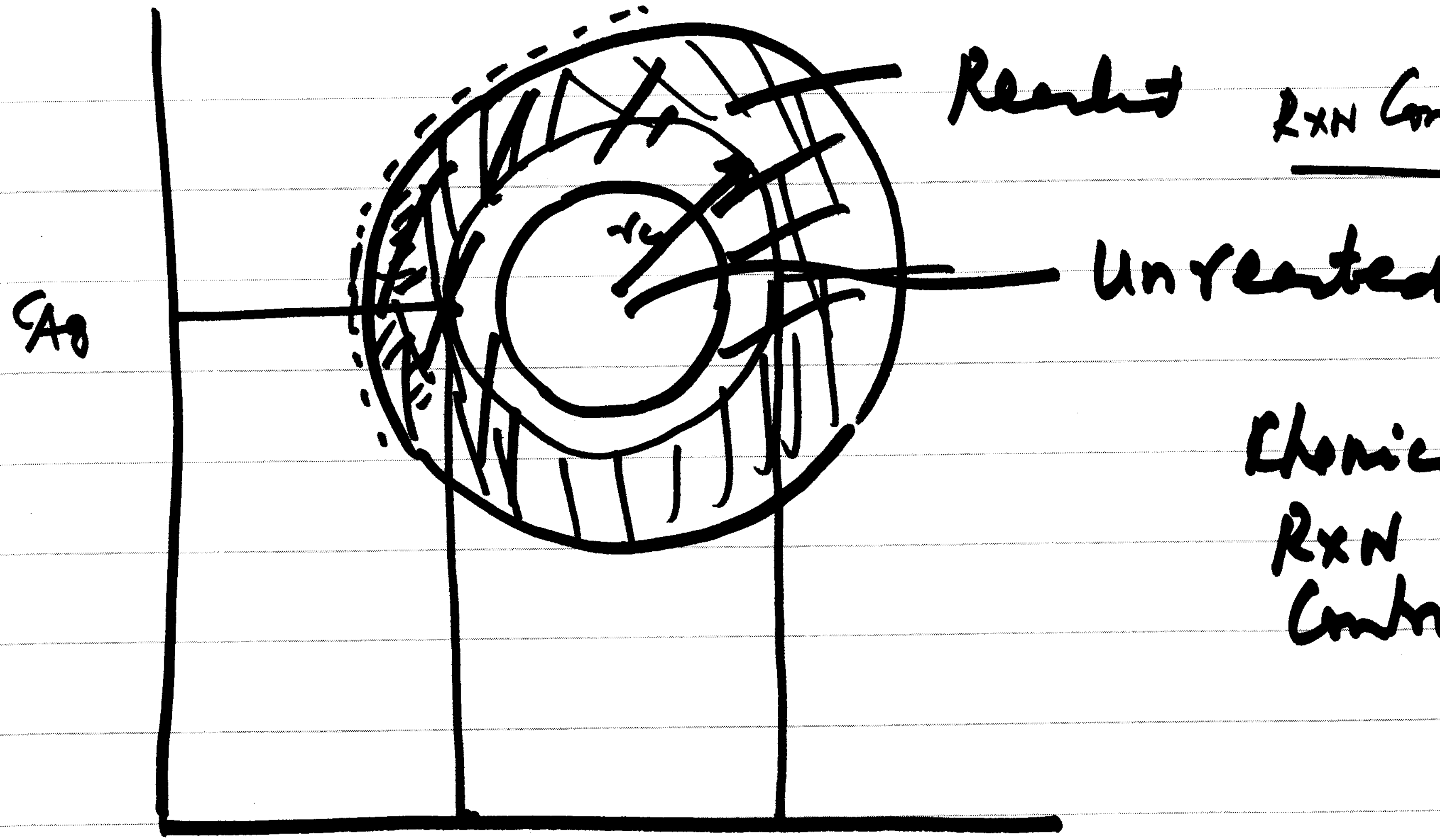
$$\boxed{\frac{t}{\tau_F} = 1 - r_c^3 / R^3}$$ ext Diffusion

$$N_B = \frac{4}{3}\pi r_c^3 \rho_B$$

$$N_{B0} = \frac{4}{3}\pi R^3 \rho_B$$

$$1 - X_B \quad \frac{N_B}{N_{B0}} = \frac{r_c^3}{R^3}$$

$$X_B = 1 - \frac{r_c^3}{R^3} ; \quad \boxed{t/\tau_F = X_B}$$



RXN Control.

Chemical RXN Control.

$$\frac{dN_B}{dt} = r_B(S) \; ; \quad \frac{r_A S}{-1} = \frac{r_B S}{-b}$$

$$r_A = -k_s C_{Ag}$$

$$r_B = -b k_s C_{Ag}$$

$$\frac{r_A}{-1} = \frac{r_B}{-b}$$

$$\boxed{\frac{dN_B}{dt} = -b k_s C_{Ag} \left(4 \pi r_c^2\right)}$$

Surface area

$$\frac{d}{dt}\left(\frac{4}{3}\pi r_c^3 \cdot \rho_B\right) = - b k_s C_{Ag} \cdot 4\pi r_c^2$$

$$\frac{\cancel{4\pi} \cancel{3} \cancel{r_c^2}}{\cancel{3}} \rho_B \frac{dr_c}{dt} = - b k_s C_{Ag} \cancel{(4\pi r_c^2)}$$

$$\frac{dr_c}{dt} = - \frac{b}{\rho_B} k_s C_{Ag}$$

$$(r_c - R) = - \frac{b}{\rho_B} k_s C_{Ag} t$$

$$(R - r_c)\,\rho_B = -\; b\,k_s\,C_{Ag}\,t$$

$$R\left(1 - \frac{r_c}{R}\right)\rho_B = b\,k_s\,C_{Ag}\,t$$

$$\boxed{\frac{\rho_B R}{b\,k_s\,C_{Ag}}\left(1 - r_c/R\right) = t}$$ RxN Contrl.

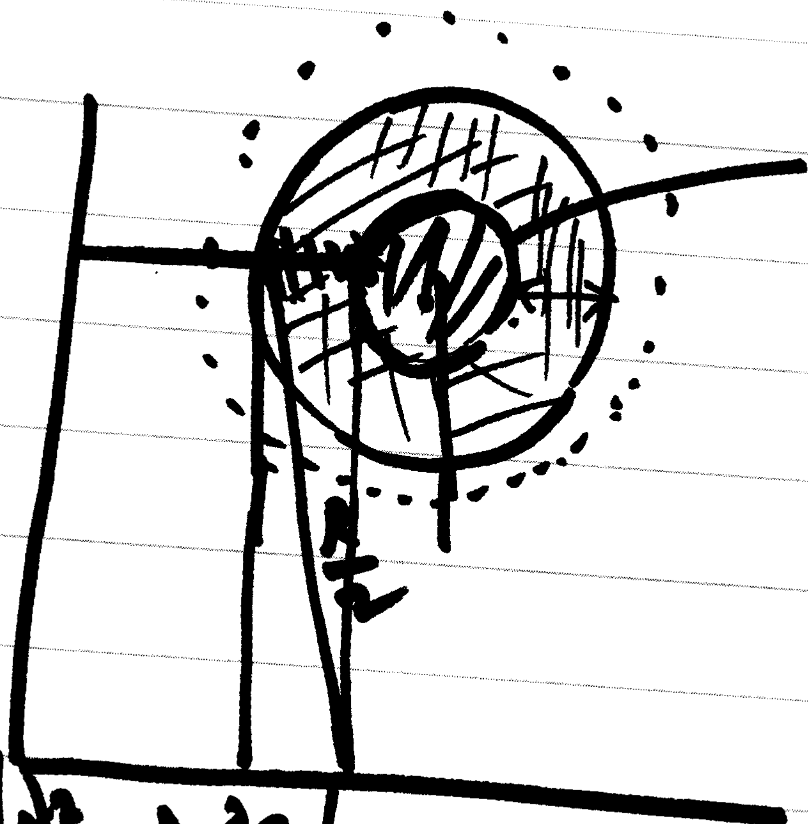
$$r_c = 0\;; \qquad t = \tau_s = \frac{\rho_B R}{b\,k_s\,C_{Ag}}$$

$$\frac{t}{\tau_s} = \left(1 - \frac{r_c}{R}\right)$$

R×N control.

$$r = 0 \qquad t = \tau_s = \frac{\rho_B R}{b k_s C_{Ag}}.$$

Ash Diffusion Control.



unreacted surface.

I/P − O/P + Gen = Acc

$$\left[4\pi r^2 D \frac{\partial c}{\partial r}\bigg|_{r+\Delta r} - 4\pi r^2 D \left(\frac{\partial c}{\partial r}\right)_r \right] + 0 = \frac{\partial}{\partial t}\left[4\pi r^2 dr\, \varepsilon\, c \right]$$

$$\frac{dN_B}{dt} = r_B S$$

$$(-r_A S) = \left(-\frac{r_B S}{mb}\right) = D\left(\frac{\partial c}{\partial r}\right)4\pi r^2$$

$$-r_A S b = -r_B S$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\frac{\partial c}{\partial r}\right)=\epsilon\frac{\partial c}{\partial t}$$

$$\underline{y = r/R};\qquad \theta = {}^{Dt}/_{\tau_D};$$

$$\tau_D = \frac{\frac{4}{3}\pi R^3 \rho_B}{D\left(\frac{\partial c_0}{R/2}\right)4\pi R^2} = \frac{\rho_B R^2}{6 D \Delta c_0}$$

$$\frac{1}{R^2 y^2}\frac{\partial}{R\,\partial y}\left[R^2 y^2\frac{D}{R}\frac{\partial\psi}{\partial y}\right]=\frac{\epsilon}{\tau_D}\left(\frac{\partial\psi}{\partial\omega}\right)$$

$$\frac{1}{r^2}\left[\frac{\partial}{\partial r}\cdot\left(r^2 D\frac{\partial c}{\partial r}\right)\right]$$

$$\boxed{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\frac{\partial c}{\partial r}\right) = \epsilon\frac{\partial c}{\partial t}}$$

Porosity.

$y = r/R$; $\theta = t/\tau_D$

$$\tau_D = \frac{\frac{4}{3}\pi R^3 \rho_B}{(D\, c_0/R/2)\; 4\pi R^2} =$$

$$\tau_D = \rho_B R^2 / 6 b D C_0$$

$$\frac{1}{\cancel{R^2}\, y^2}\frac{\partial}{\partial y}\left(y^2 \cancel{D} \frac{\partial \psi}{\partial y}\right) = \frac{\epsilon}{\tau_D}\frac{\partial \psi_0}{\partial \theta}$$

$$= \frac{\epsilon\, 6 b \cancel{D} C_0}{\rho_B \cancel{R^2}}\frac{\partial \psi_0}{\partial \theta}$$

$$\boxed{\frac{1}{y^2}\frac{\partial}{\partial y}\left(y^2 \frac{\partial \psi}{\partial y}\right) = \left(\frac{6 \epsilon C_0}{\rho_B}\right)\frac{\partial \psi_0}{\partial \theta}}$$

Small

$$\frac{1}{y^2}\frac{\partial}{\partial y}\left(y^2 \frac{\partial \psi}{\partial y}\right) = \cancel{\left(\frac{6\,\epsilon\, C_0}{\rho_B}\right)\frac{\partial \psi}{\partial \theta}}$$

QSSA

C_0 typically 0.05 gmol/L

ρ_B 10 gmol/L

$\epsilon = 0.2 - 0.4.$

$$\frac{6\,\epsilon\, C_0}{\rho_B} \simeq \frac{(6)(0.3)(0.05)}{10} = (9\,10^{-3})$$

$$\frac{1}{y^2}\frac{\partial}{\partial y}\left(y^2\frac{\partial\psi}{\partial y}\right) = \frac{6\epsilon G}{\rho_B}\cancel{\left(\frac{\partial\psi}{\partial\theta}\right)} \quad \text{QSSA.}$$

$$= 0$$