

# Lecture # 8.1

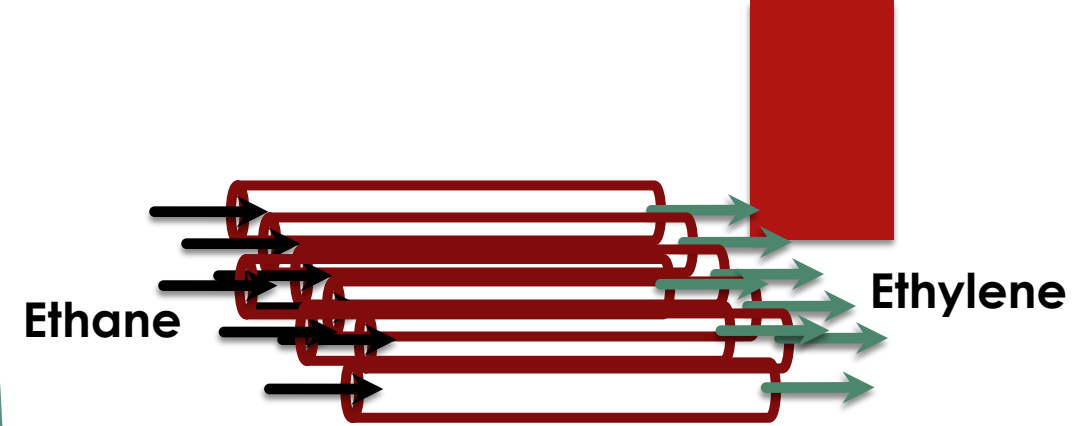
## CHE331A

- ▶ Design of Reactors - Basics
- ▶ Mole balance → Rate Law → Stoichiometry
- ▶ Design and analysis of CSTRs
- ▶ Design/Analysis of PFR with variable volumetric flowrate
- ▶ Pressure drop in a PBR and the production of ethylene oxide

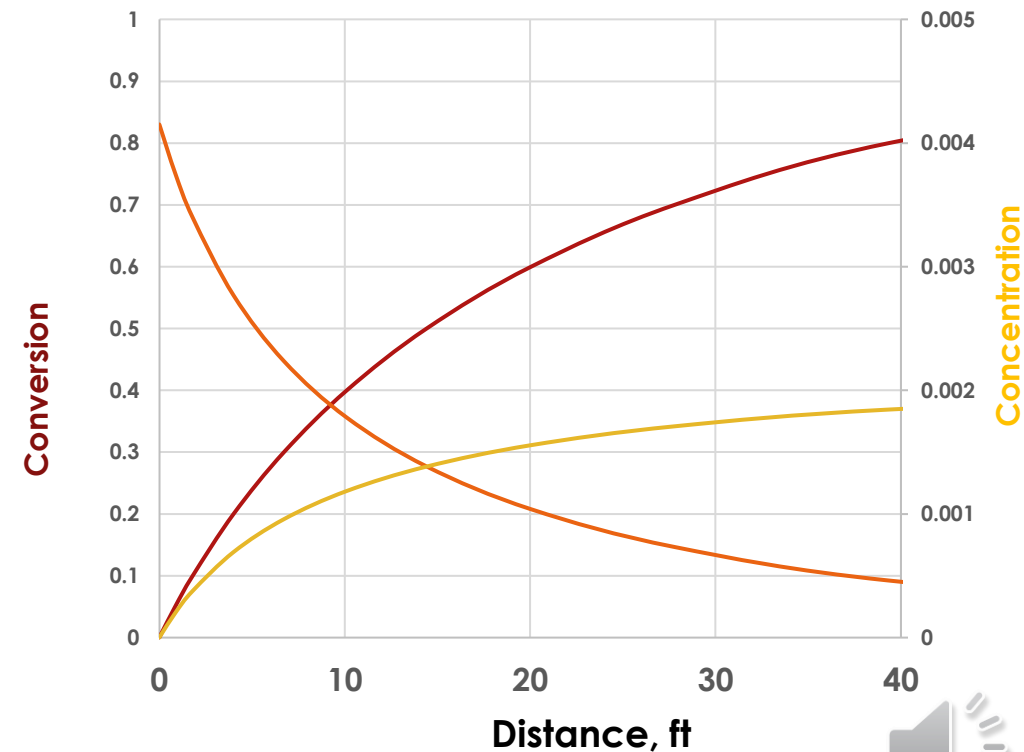
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Conversion/Concentration versus distance for each tube



# Pressure drop in Reactors

- ▶ For liquid phase reactions the effect of pressure drop can be neglected unless mentioned otherwise
- ▶ For gas-phase reactions the concentration of the reacting species is proportional to the total pressure
- ▶ For ideal gas, the concentration of species  $i$  is given by:

$$C_i = C_{A0} \left( \frac{\theta_i + \mu_i X}{1 + \varepsilon X} \right) \frac{P}{P_0} \frac{T_0}{T} \frac{Z_0}{Z}$$

- ▶ For a PFR/PBR the  $\frac{P}{P_0}$  ratio as a function of volume or catalyst weight needs to be determined

# Effect of pressure change $P \neq P_0$ for PBR

- ▶ Mole balance:  $F_{A0} \frac{dX}{dW} = -r'_A$
- ▶ Rate Law for a gas-phase reaction given by:  $-r'_A = k \cdot C_A^2$
- ▶ Stoichiometry:  $C_A = C_{A0} \left( \frac{1-X}{1+\varepsilon X} \right) \frac{P}{P_0} \frac{T_0}{T}$  T and P changes
- ▶ Rate law in terms of conversion:  $-r'_A = k \cdot \left[ C_{A0} \left( \frac{1-X}{1+\varepsilon X} \right) \frac{P}{P_0} \frac{T_0}{T} \right]^2$
- ▶ Thus,  $F_{A0} \frac{dX}{dW} = k \cdot \left[ C_{A0} \left( \frac{1-X}{1+\varepsilon X} \right) \frac{P}{P_0} \right]^2$  for  $T = T_0$  (isothermal)

$$\frac{dX}{dW} = k \cdot \frac{C_{A0}}{\dot{v}_0} \left[ \left( \frac{1-X}{1+\varepsilon X} \right) \frac{P}{P_0} \right]^2 = f(X, P)$$



# Pressure drop in packed porous bed can be calculated using the Ergun equation

► Ergun equation: 
$$\frac{dP}{dZ} = -\frac{G}{\rho g_c D_p} \left( \frac{1-\varphi}{\varphi^3} \right) \left[ \frac{150(1-\varphi)\mu}{D_p} + 1.75G \right]$$

Dominant for laminar flow Dominant for turbulent flow

$\varphi$  = porosity or void fraction =  $\frac{\text{volume of void}}{\text{total volume of bed}}$  and  $1 - \varphi = \frac{\text{volume of solid}}{\text{total volume of bed}}$

$g_c = 1$ ;  $D_p$  = dia. of particle (m);  $P$  in kPa;  $\mu$  = viscosity of gas  $\left( \frac{\text{kg}}{\text{m.s}} \right)$

$Z$  = length of the packed bed (m);  $G = \rho \cdot u$  = superficial mass velocity  $\left( \frac{\text{kg}}{\text{m}^2.\text{s}} \right)$

$u$  = superficial velocity =  $\frac{\dot{v}}{A_c}$ ;  $\rho$  = gas density  $\left( \frac{\text{kg}}{\text{m}^3} \right)$  ← only term changing with  $P$



# Change in pressure has an effect on the density of the reacting gas-phase

- ▶ For steady-state flow, mass flow rates are equal:  $\dot{m} = \dot{m}_0$
- ▶ Thus,  $\rho \cdot \dot{v} = \rho_0 \dot{v}_0$  also  $\dot{v} = \dot{v}_0 \frac{P_0}{P} \frac{T}{T_0} \frac{F_T}{F_{T0}}$  ( $Z = Z_0$ )
- ▶ As per the Ergun equation the pressure drop depends on  $\frac{1}{\rho}$  ( $= \frac{\dot{v}}{\rho_0 \dot{v}_0}$ )

$$\frac{dP}{dZ} = -\frac{G}{\rho_0 g_c D_p} \left( \frac{1-\phi}{\phi^3} \right) \left[ \frac{150(1-\phi)\mu}{D_p} + 1.75G \right] \frac{P_0}{P} \left( \frac{T}{T_0} \right) \frac{F_T}{F_{T0}}$$

$$\frac{dP}{dZ} = -\beta_0 \frac{P_0}{P} \left( \frac{T}{T_0} \right) \frac{F_T}{F_{T0}}$$

where,  $\beta_0 = \frac{G}{\rho_0 g_c D_p} \left( \frac{1-\phi}{\phi^3} \right) \left[ \frac{150(1-\phi)\mu}{D_p} + 1.75G \right] \rightarrow D_p \text{ decreases, } \beta_0 \text{ increases}$



# Packed bed reactor calculations continued

- Weight of catalyst:  $W = (1 - \varphi)A_c Z \rho_c$

$A_c$  = cross-section of tube     $\rho_c$  = true density of solid catalyst  
 $\rho_b = \rho_c(1 - \varphi)$  is the bulk density of solid catalyst, and  $W = A_c Z \rho_b$

- The mole balance equation is in terms of  $dW \rightarrow dW = A_c \rho_b dZ$

- Thus,  $\frac{dP}{dZ} = -\beta_0 \frac{P_0}{P} \left( \frac{T}{T_0} \right) \frac{F_T}{F_{T0}} \rightarrow \frac{dP}{dW} = -\frac{\beta_0}{A_c \rho_b} \frac{P_0}{P} \frac{F_T}{F_{T0}}$  for  $T = T_0$

- With  $y = P/P_0 \rightarrow P_0 dy = dP$ , Thus, we have for  $\alpha = \frac{2\beta_0}{A_c \rho_b P_0}$

$$\frac{dy}{dW} = -\frac{\alpha}{2y} \cdot \frac{F_T}{F_{T0}}$$

a decrease in  $D_p$  increases  $\beta_0$  and  $\alpha$

Example 4-4 for  
calculation of  $\alpha$



# Pressure drop depends on several factors related to the bed and reacting system

► With  $\frac{F_T}{F_{T0}} = (1 + \varepsilon X)$  then  $\frac{dy}{dW} = -\frac{\alpha}{2y} \cdot \frac{F_T}{F_{T0}} = -\frac{\alpha}{2y} (1 + \varepsilon X) = g(X, P)$

$$\frac{dy}{dW} = -\frac{\alpha}{2y} (1 + \varepsilon X)$$

► For  $\varepsilon = 0$  then  $\frac{dy}{dW} = -\frac{\alpha}{2y}$  and  $y^2 = 1 - \alpha \cdot W$  ( $y = 1$  @  $W = 0$ )

○ For  $\varepsilon < 0$  then  $\frac{dy}{dW} = -\frac{\alpha}{2y} (1 + \varepsilon X)$  and  $\frac{dy}{dW}$  will be less

○ For  $\varepsilon > 0$  then  $\frac{dy}{dW} = -\frac{\alpha}{2y} (1 + \varepsilon X)$  and  $\frac{dy}{dW}$  will be more



# Design equations for PBR with pressure drop requires the solution of 2 ODEs

► Mole balance:  $\frac{dX}{dW} = f(X, P)$

► Pressure drop:  $\frac{dy}{dW} = g(X, P)$  and

$$\frac{dX}{dW} = k \cdot \frac{C_{A0}}{\dot{v}_0} \left[ \left( \frac{1-X}{1+\varepsilon X} \right) \frac{P}{P_0} \right]^2 = f(X, P)$$

$$\frac{dy}{dW} = -\frac{\alpha}{2y} (1 + \varepsilon X) = g(X, P)$$

► These two coupled ODEs need to be solved simultaneously

