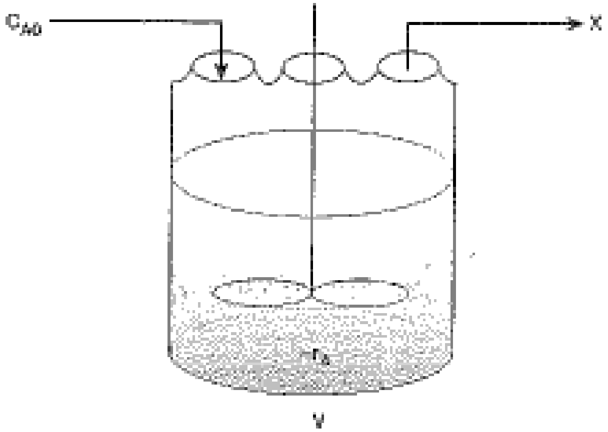
3. Design of CSTRs I



○ **Single CSTR 1**

- **Design equation**

$$V = \frac{F_{A0}X}{(-r_A)_{exit}}$$

- **Substitute $F_{A0} = v_0 C_{A0}$**

$$V = \frac{v_0 C_{A0} X}{-r_A}$$

- **Space time τ**

$$\tau = \frac{V}{v_0} = \frac{C_{A0}X}{-r_A}$$

- **1st order rxn assume**

$$\tau = \frac{C_{A0}X}{-r_A} = \frac{1}{k}\left(\frac{X}{1-X}\right)$$

- **Rearranging**

$$X = \frac{\tau k}{1+\tau k}$$

3. Design of CSTRs II

○ **Single CSTR 2**

- $C_A = C_{A0}(1 - X)$

$$C_\mathrm{A} = \frac{C_\mathrm{A0}}{1 + \boxed{\tau k}}$$

- **Damköhler number ⇒ dimensionless number**
  - **quick estimate of the degree on conversion**

$$\mathrm{Da} = \frac{-r_\mathrm{A0} V}{F_\mathrm{A0}} = \frac{\text{Rate of rxn at entrance}}{\text{Entering flow rate of A}}$$

$$= \frac{\text{A rxn rate}}{\text{A convection rate}}$$

$$= \frac{\text{Characteristic fluid time}}{\text{Charateristic chemical reaction time}}$$

3. Design of CSTRs III

○ **Single CSTR 3**

- Damköhler number for a 1st order irrev. rxn

$$\mathrm{Da} = \frac{-r_{\mathrm{A0}}V}{F_{\mathrm{A0}}} = \frac{kC_{\mathrm{A0}}V}{v_0 C_{\mathrm{A0}}} = \tau k$$

- Damköhler number for a 2nd order irrev. rxn

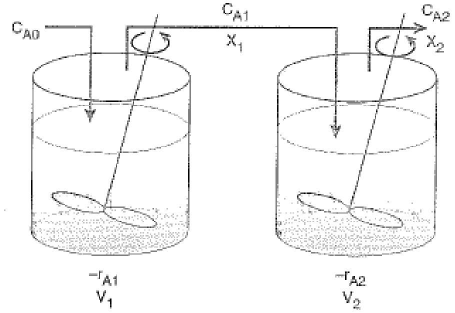
$$\mathrm{Da} = \frac{-r_{\mathrm{A0}}V}{F_{\mathrm{A0}}} = \frac{kC_{\mathrm{A0}}^2V}{v_0 C_{\mathrm{A0}}} = \tau k C_{\mathrm{A0}}$$

- Rule of thumb

- **if Da < 0.1, then X < 0.1**
- **if Da > 10, then X > 0.9**

☞ **1st order rxn, X = Da/(1 + Da)**

3. Design of CSTRs IV



- **CSTR in series 1**
  - **1st order irrev. rxn with no change in volumetric flow rate, effluent of the first reactor**

$$C_{A1} = \frac{C_{A0}}{1+\tau_1 k_1}$$

  - **For 2nd reactor**

$$V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}} = \frac{v_0 (C_{A1} - C_{A2})}{k_2 C_{A2}}$$

  - **Solving for C_{A2}**

$$C_{A2} = \frac{C_{A1}}{1 + \tau_2 k_2} = \frac{C_{A0}}{(1+\tau_2 k_2)(1+\tau_1 k_1)}$$

  - **For n CSTRs in series**

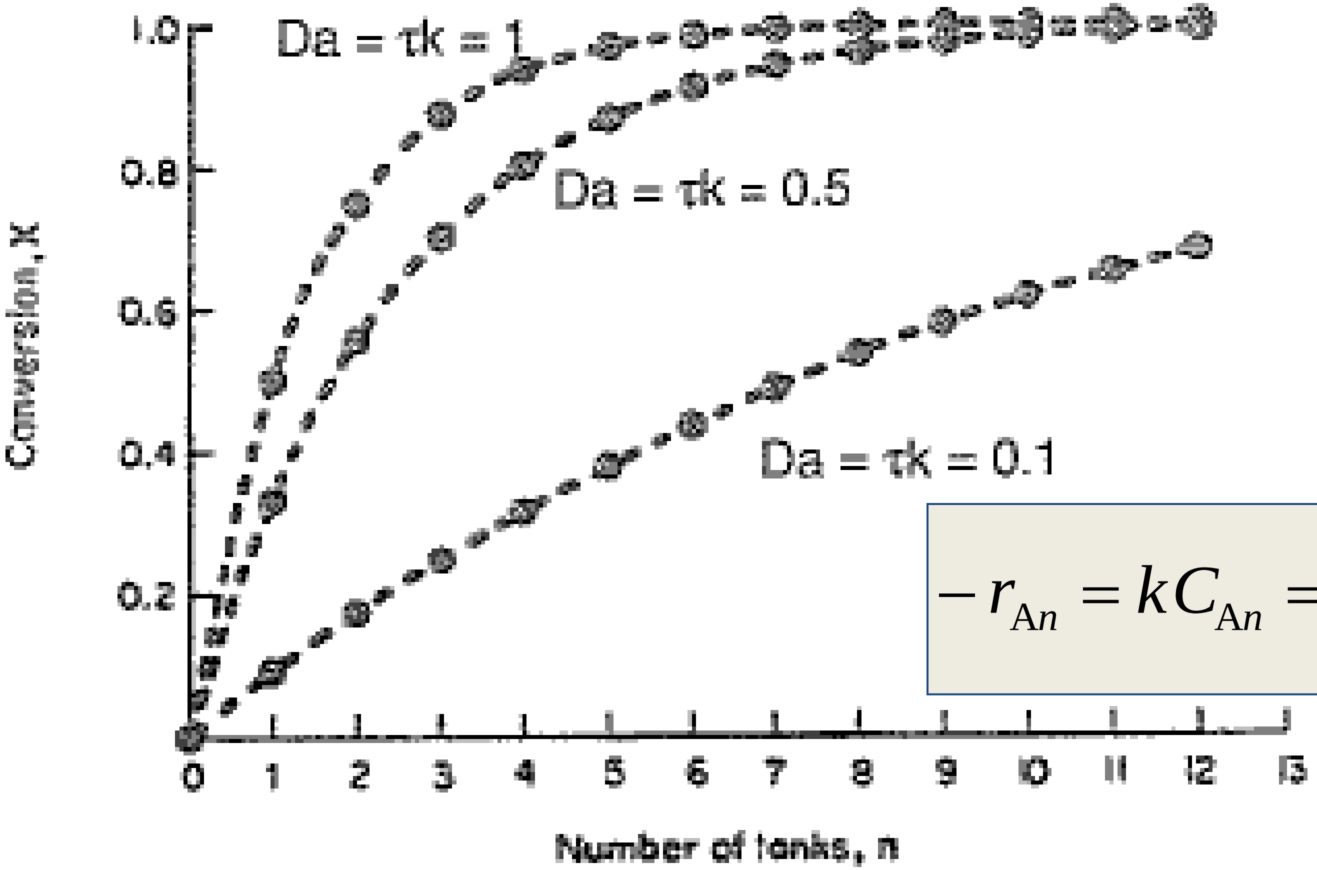
$$C_{An} = \frac{C_{A0}}{(1 + \tau k)^n} = \frac{C_{A0}}{(1 + \mathrm{Da})^n}$$

  - **n tank in series**

$$\boxed{X = 1 - \frac{1}{(1+\tau k)^n} = 1 - \frac{1}{(1+\mathrm{Da})^n}}$$

3. Design of CSTRs V

- **CSTR in series 2**



$$-r_{An} = kC_{An} = k\frac{C_{A0}}{(1+\tau k)^n}$$

3. Design of CSTRs VI

- **CSTR in parallel 1**

  - One large reactor of volume V

- **2^{nd} order reactor in a CSTR**

$$V = \frac{F_{A0}X}{-r_A} = \frac{F_{A0}X}{kC_A^2} = \frac{v_0 C_{A0} X}{kC_{A0}^2(1-X)^2}$$

- Dividing by v_0

$$\tau = \frac{V}{v_0} = \frac{X}{kC_{A0}(1-X)^2}$$

- For conversion X

$$\boxed{X = \frac{(1+2\mathrm{Da}) - \sqrt{1+4\mathrm{Da}}}{2\mathrm{Da}}}$$

Ex 4-2, p 163

4. Tubular Reactors I

- ○ **Design equation**
  - **- Differential form**
    - **• Q or ΔP**

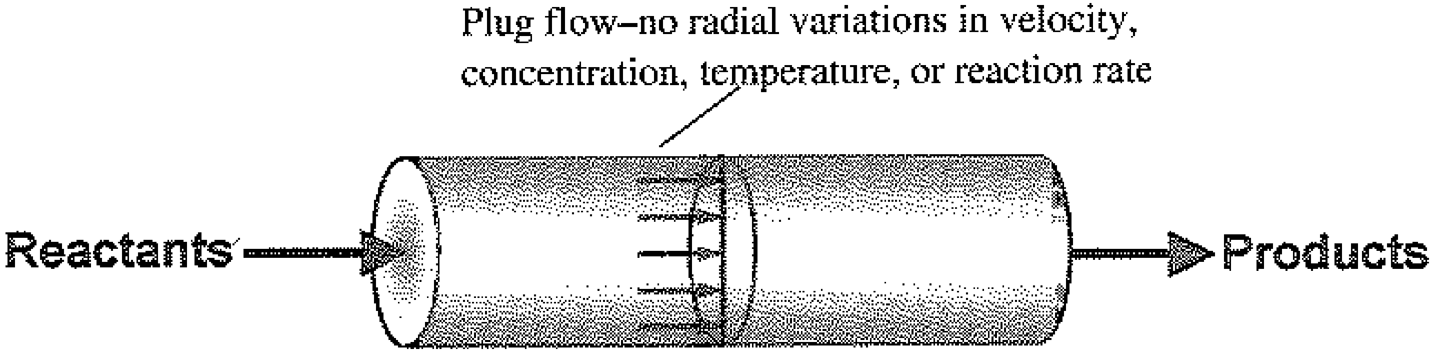
$$F_{A0}\frac{dX}{dV} = -r_A$$

  - **- Integral form**
    - **• no Q or ΔP**

$$V = F_{A0}\int_0^X \frac{dX}{-r_A}$$

- ○ **2nd order reactor in a PFR 1**

$$V = F_{A0}\int_0^X \frac{dX}{kC_A^2}$$



Plug flow–no radial variations in velocity, concentration, temperature, or reaction rate

4. Tubular Reactors II

○ 2nd order reactor in a PFR 2

- Liquid phase reaction ($v = v_0$)

- combining MB & rate law

$$\frac{dX}{dV} = \frac{kC_A^2}{F_{A0}}$$

- conc. of A, $C_A = C_{A0}(1 - X)$
- combining & integrating

$$V = \frac{F_{A0}}{kC_{A0}^2} \int_0^V \frac{dx}{(1-X)^2} = \frac{v_0}{kC_{A0}} \left(\frac{X}{1-X} \right)$$

- solving for X

$$X = \frac{\tau k C_{A0}}{1 + \tau k C_{A0}} = \frac{\mathrm{Da}_2}{1 + \mathrm{Da}_2}$$

4. Tubular Reactors III

- **2nd order reactor in a PFR 3**
  - **- Gas phase reaction ($T = T_0, P = P_0$)**
    - **conc. of A,** $C_A = C_{A0}\left(\frac{1 - X}{1 + \varepsilon X}\right)$
    - **combining**

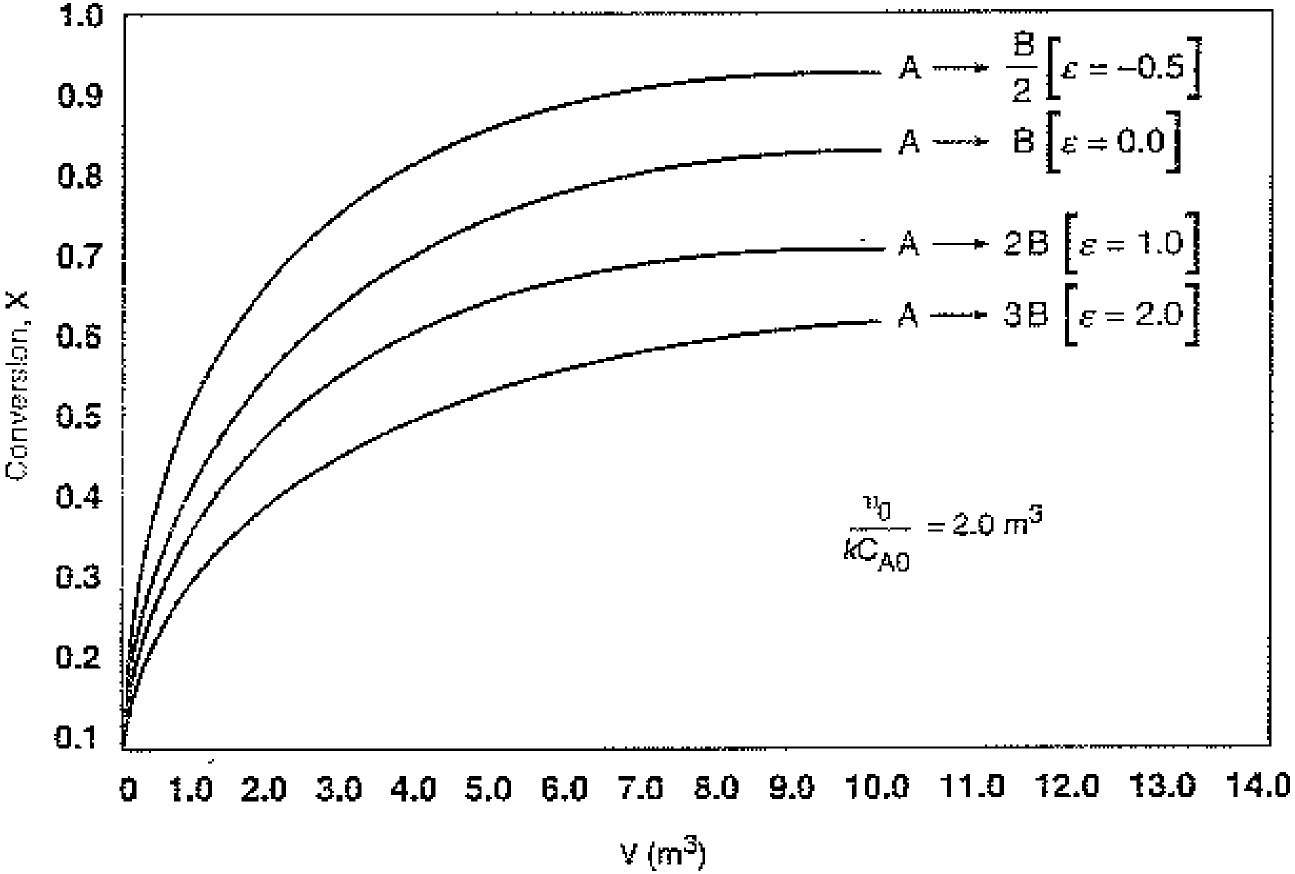
$$V = F_{A0}\int_0^X \frac{(1 + \varepsilon X)}{kC_{A0}(1 - X)^2}dX$$

$$V = \frac{v_0}{kC_{A0}^2}\int_0^X \frac{(1 + \varepsilon X)^2}{(1 - X)^2}dX$$

$$V = \frac{v_0}{kC_{A0}}\left[2\varepsilon(1 + \varepsilon)\ln(1 - X) + \varepsilon^2 X + \frac{(1 + \varepsilon)^2 X}{1 - X}\right]$$

4. Tubular Reactors IV

- 2nd order reactor in a PFR 4
  - Conversion as a function of distance down the reactor



4. Tubular Reactors V

○ **2nd order reactor in a PFR 5**

- Three types of reactions

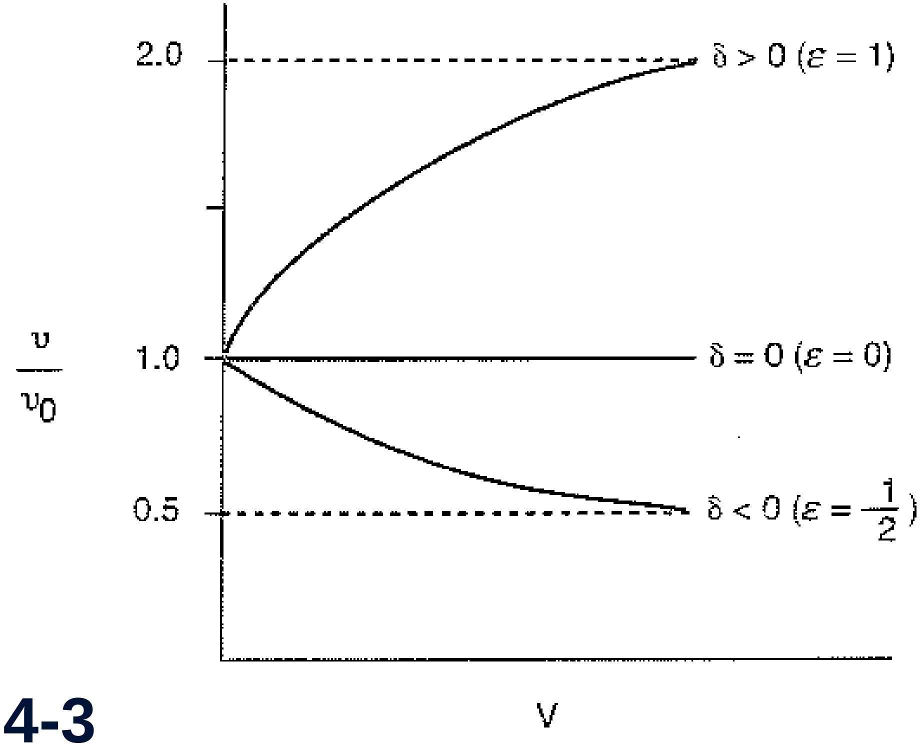
- $\varepsilon = 0$ $(\delta = 0)$ $\Rightarrow v = v_0$
- $\varepsilon < 0$ $(\delta < 0)$

  ⇒ **gas molecule spends longer time**

  ☞ **higher conv.**
- $\varepsilon > 0$ $(\delta > 0)$

  ⇒ **gas molecule spends shorter time**

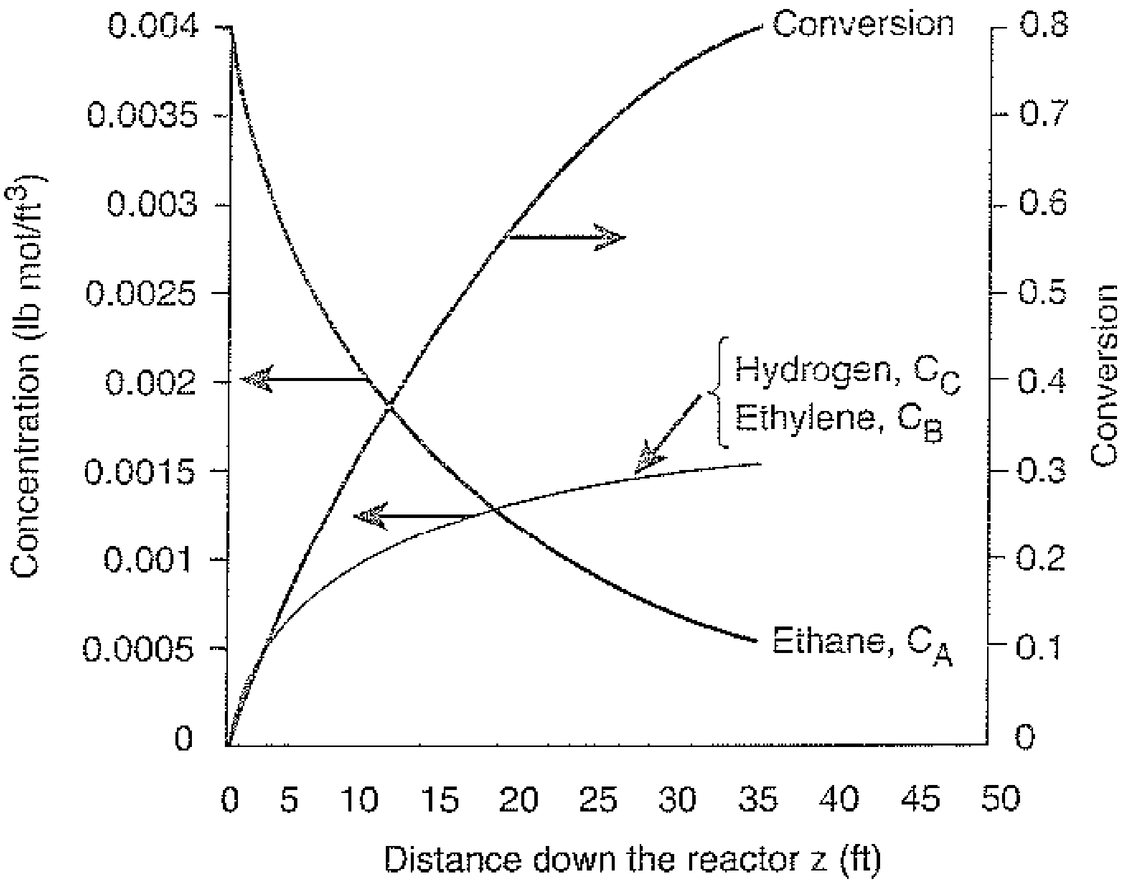
  ☞ **lower conv., p 171 Ex 4-3**



4. Tubular Reactors VI

○ **2^{nd} order reactor in a PFR 6**

- Production of ethylene using PFR



5. Pressure Drop in Reactors I

○ Pressure Drop and the Rate Law

- In PBR in terms of catalyst weight

$$F_{A0}\frac{dX}{dW} = -r_A' \qquad \left(\frac{\text{gram moles}}{\text{gram catalyst}\cdot\text{min}}\right)$$

- **rate equation,** $-r_A' = kC_A^2$
- **stoichiometry** $$C_A = \frac{C_{A0}(1 - X)}{1 + \varepsilon X}\frac{P}{P_0}\frac{T_0}{T}$$
- **isothermal** $$F_{A0}\frac{dX}{dW} = k\left[\frac{C_{A0}(1 - X)}{1 + \varepsilon X}\right]^2\left(\frac{P}{P_0}\right)^2$$

$$\frac{dX}{dW} = \frac{kC_{A0}}{v_0}\left[\frac{(1 - X)}{1 + \varepsilon X}\right]^2\left(\frac{P}{P_0}\right)^2 \qquad \frac{dX}{dW} = F_1(X, P)$$

5. Pressure Drop in Reactors II

- Flow through a Packed Bed 1
  - Ergun equation

$$\frac{dP}{dz} = \frac{G}{\rho g_c D_p}\left(\frac{1-\phi}{\phi^3}\right)\left[\boxed{\frac{150(1-\phi)\mu}{D_p}} + \boxed{1.75G}\right]$$

Dominant for turbulent flow

Dominant for laminar flow

where P = pressure

φ = porosity = void fraction

g_c = conversion factor relating gravity

D_p = diameter of particle in the bed

μ = viscosity of gas passing through the bed

z = length down the packed bed of pipe

u = superficial velocity

ρ = gas density

G = ρu = superficial mass velocity

5. Pressure Drop in Reactors III

- **Flow through a Packed Bed 2**

- Pressure drop in packed bed 1

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

$$\boxed{\frac{dP}{dz} = -\beta_0 \frac{P_0}{P}\left(\frac{T}{T_0}\right)(1+\varepsilon X)}$$

$$\beta_0 = \frac{G(1-\phi)}{\rho_0 \, g_c \, D_P \, \phi^3}\left[\frac{150(1-\phi)}{D_P} + 1.75G\right]$$

where β_0 is a constant depending on the properties of the packed bed and the entrance conditions

5. Pressure Drop in Reactors IV

- **Flow through a Packed Bed 3**

- Pressure drop in packed bed 2

- **interested in more in catalyst weight rather than the distance z**

$$W = (1\text{-}\varphi)A_c z \times \rho_c$$

$$\overbrace{\text{Weight of catalyst}} = \overbrace{\text{Volume of solids}} \times \overbrace{\text{Density of solid catalyst}}$$

- **catalyst weight,** $W = zA_c\rho_b = zA_c(1\text{-}\varphi)\rho_c$

$$\frac{dP}{dW} = -\frac{\beta_0}{A_c(1-\varphi)\rho_c}\frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}}$$

5. Pressure Drop in Reactors V

- **Flow through a Packed Bed 4**
  - **Pressure drop in packed bed 3**

$$\frac{dP}{dW} = -\frac{\beta_0}{A_c(1-\varphi)\rho_c}\frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}}$$

- **let**

$$\alpha = \frac{2\beta_0}{A_c\rho_c(1-\varphi)P_0}$$

- **then** $\dfrac{dP}{dW} = -\dfrac{\alpha}{2}\dfrac{P_0}{\left(P/P_0\right)}\dfrac{T}{T_0}\dfrac{F_T}{F_{T0}}$ $\quad \dfrac{d\left(P/P_0\right)}{dW} = -\dfrac{\alpha}{2}\dfrac{1}{\left(P/P_0\right)}\dfrac{T}{T_0}\dfrac{F_T}{F_{T0}}$

$$\boxed{\frac{dy}{dW} = -\frac{\alpha}{2}\frac{1}{y}\frac{T}{T_0}\frac{F_T}{F_{T0}}}$$

where $y = P/P_0$

5. Pressure Drop in Reactors VI

○ **Flow through a Packed Bed 5**

- Pressure drop in packed bed 4

- **for single reactions**

$$\frac{dy}{dW} = -\frac{\alpha}{2}\frac{1}{y}\frac{T}{T_0}(1+\varepsilon X)$$

- **isothermal operation**

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

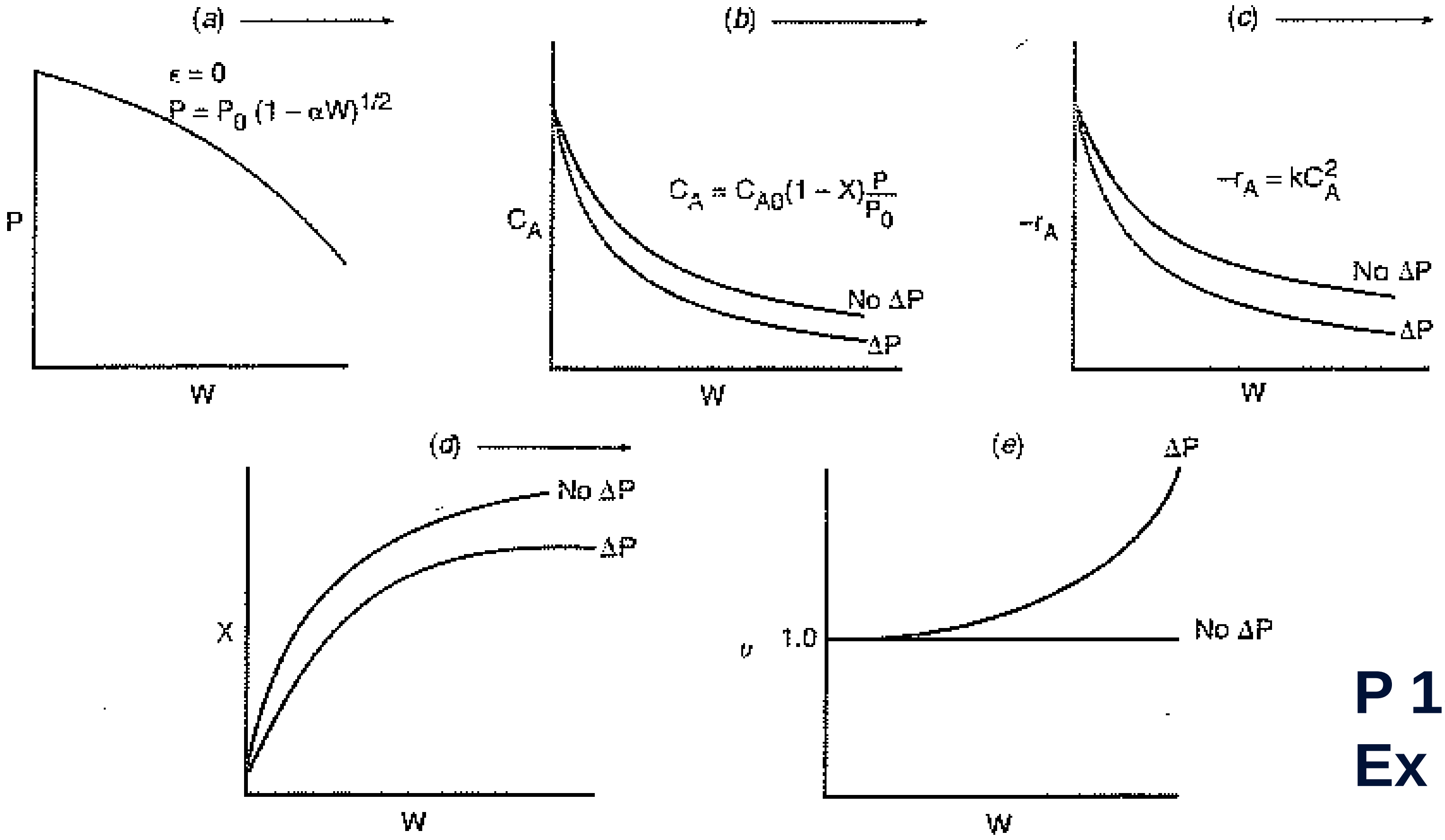
- **notice that**

$$\frac{dX}{dW} = f(X,P) \text{ and } \frac{dP}{dW} = f(X,P) \text{ or } \frac{dy}{dW} = f(X,P)$$

5. Pressure Drop in Reactors VII

- **Flow through a Packed Bed 6**

- Pressure drop in packed bed 5 – effect of *P* drop

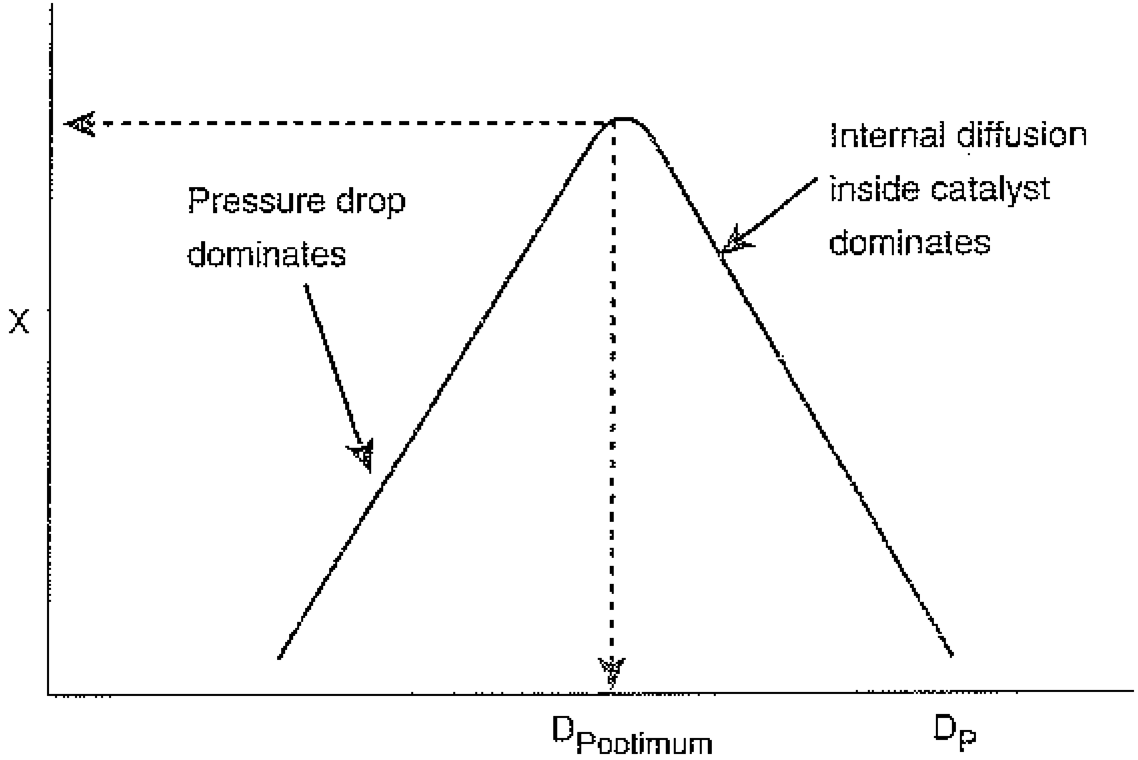


P 187
Ex 4-5

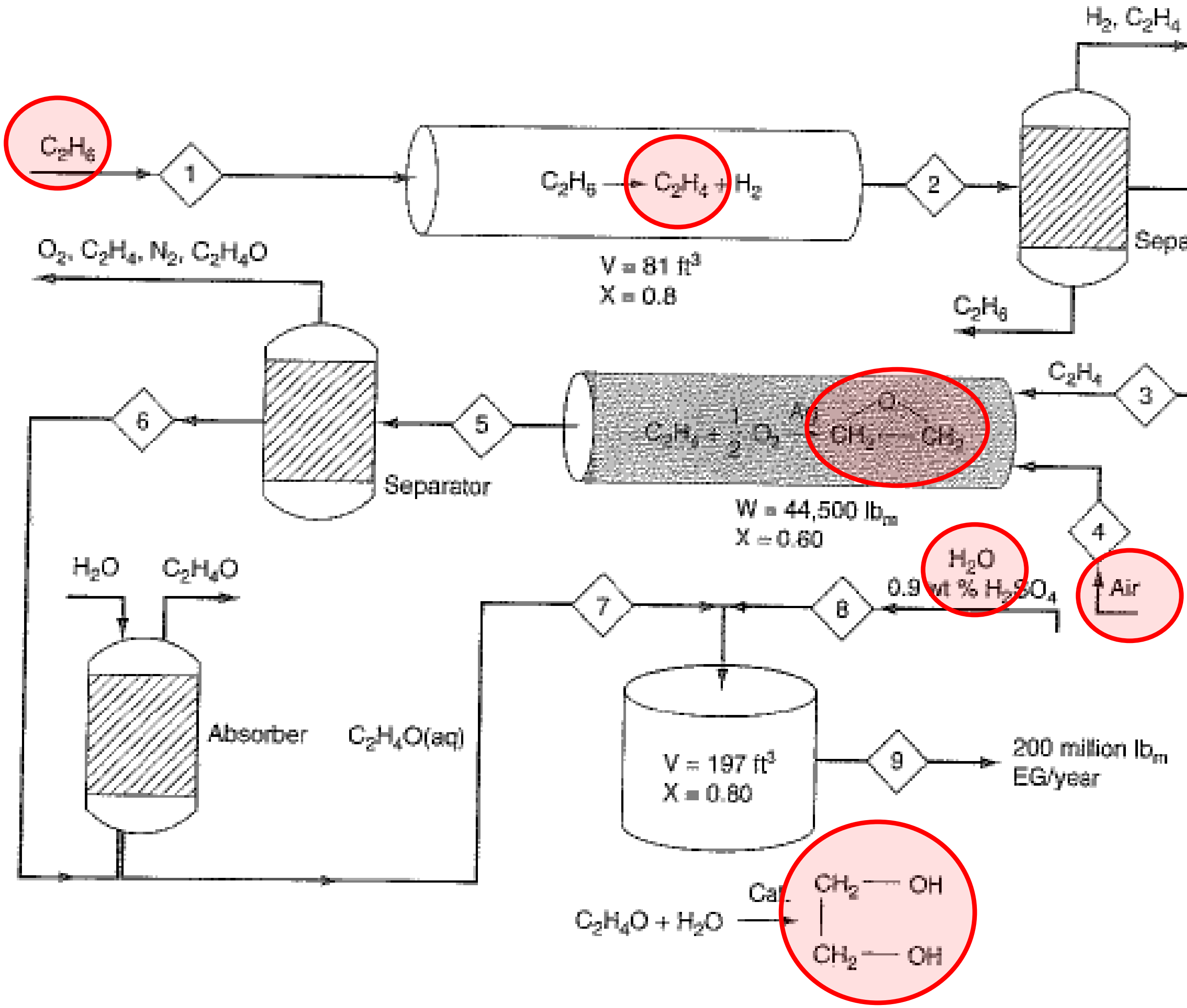
5. Pressure Drop in Reactors VIII

- **Flow through a Packed Bed 7**

  - Finding optimum particle diameter



6. Synthesizing for Design of a Chemical Plant I



6. Synthesizing for Design of a Chemical Plant II

- **Manufacturing of ethylene glycol**

  - Economy

Profit = **EG cost** - **Ethane cost**

$$\frac{\$0.38}{lb_m} \times 2 \times 10^8 \frac{lb_m}{year} \qquad \frac{\$0.04}{lb_m} \times 4 \times 10^8 \frac{lb_m}{year}$$

- **SA cost** - **Operating cost**

$$\frac{\$0.43}{lb_m} \times 2.26 \times 10^6 \frac{lb_m}{year} \qquad \$8,000,000$$

= \$76,000,000 - \$16,000,000 - \$54,000 - \$8,000,000

= \$52 million