6. Flow Systems XIV

- **Express concentration as a function of conversion**

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

Liquid Phase

Flow $C_B = \frac{F_B}{v}$

Batch $C_B = \frac{N_B}{V}$

No phase change

$$v = v_0 \qquad V = V_0$$

$$C_B = C_{A0}\left(\Theta_B - \frac{b}{a}X\right)$$

$$\varepsilon = y_{A0}\delta$$

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

$$C_{T0} = \frac{P_0}{RT_0}, \quad C_{A0} = \frac{y_{A0}P_0}{RT_0}$$

Gas Phase

Batch $C_B = \frac{N_B}{V}$

$$V = V_0 \frac{N_T}{N_{T0}} \frac{P_0}{P} \frac{T}{T_0}$$

$$C_B = \frac{N_B}{N_T} \frac{N_{T0}}{V_0} \frac{P}{P_0} \frac{T_0}{T}$$

$$C_B = C_{T0} \frac{N_B}{N_T} \frac{P}{P_0} \frac{T_0}{T}$$

Flow $C_B = \frac{F_B}{v}$

$$v = v_0 \frac{F_T}{F_{T0}} \frac{P_0}{P} \frac{T}{T_0}$$

$$C_B = \frac{F_B}{F_T} \frac{F_{T0}}{v_0} \frac{P}{P_0} \frac{T_0}{T}$$

$$C_B = C_{T0} \frac{F_B}{F_T} \frac{P}{P_0} \frac{T_0}{T}$$

No phase change (or semipermeable membrane

$$v = v_0(1+\varepsilon X)\frac{P_0}{P}\frac{T}{T_0}, \quad C_B = \frac{C_{A0}\left(\Theta_B - \frac{b}{a}X\right)}{1+\varepsilon X}\frac{P}{P_0}\frac{T_0}{T}$$

4. Isothermal Reactor Design

- **Objectives**
  - Describe the CRE algorithm that allows the reader to solve chemical reaction engineering problems through logic rather than memorization.
  - Size batch reactors, semibatch reactors, CSTRs, PFRs, PBRs, membrane reactors, and microreactors for isothermal operation given the rate law and feed conditions.
  - Account for the effects of pressure drop on conversion in packed bed tubular reactors and in packed bed spherical reactors

1. Algorithm for Isothermal Reactor Design I

- **Isothermal reactor design algorithm for conversion**

  1) $$F_{j0} - F_j + \int^V r_j dV = \frac{dN_j}{dt}$$

  2) Apply mole balance to reactor type

  3) Is $-r_A = f(X)$ given? ⇒ Then evaluate the equation

  4) If not, determine the rate law in terms of conc.

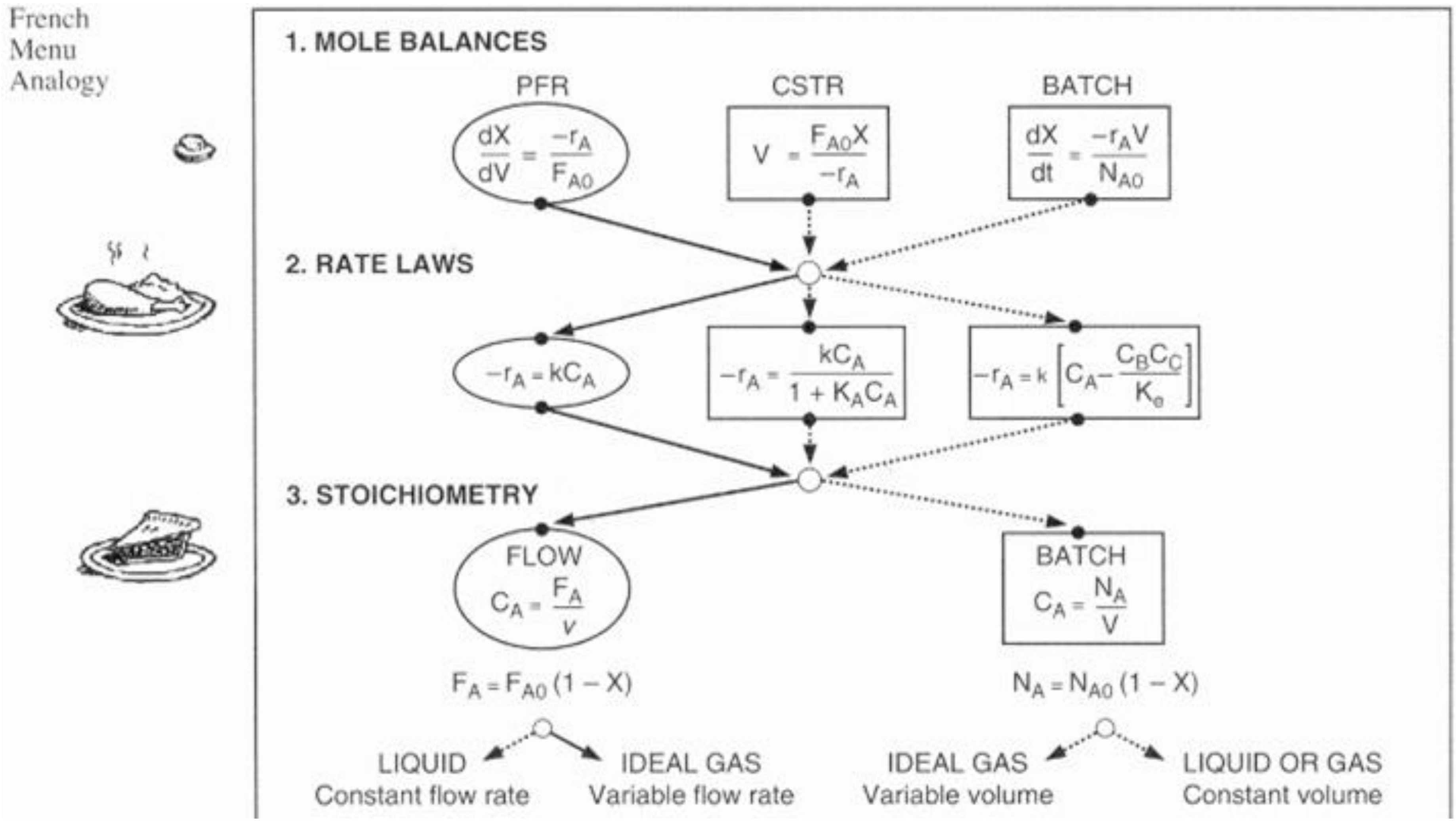
  5) Use stoichiometry to express conc. as a function of conversion

  6) Combine step 4) & 5) to obtain $-r_A = f(X)$

  7) Consider volume change

  8) Combine 4) ~ 7) and solve ODE (Polymath)

1. Algorithm for Isothermal Reactor Design II



1. Algorithm for Isothermal Reactor Design III

$v = v_0$ $\quad v = v_0(1+\varepsilon X)\dfrac{P_0}{P}\dfrac{T}{T_0}$ $\quad V = V_0(1+\varepsilon X)\dfrac{P_0}{P}\dfrac{T}{T_0}$ $\quad V = V_0$

$$C_A = C_{A0}(1-X) \qquad C_A = \frac{C_{A0}(1-X)}{(1+\varepsilon X)}\frac{P}{P_0}\frac{T_0}{T} \qquad C_A = \frac{C_{AO}(1-X)}{(1+\varepsilon X)}\frac{P}{P_0}\frac{T_0}{T} \qquad C_A = C_{A0}(1-X)$$

4. COMBINE (First Order Gas-Phase Reaction in a PFR)

From mole balance — From rate law — From stoichiometry

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}} = \frac{kC_A}{F_{A0}} = \frac{k}{F_{A0}}\left(C_{A0}\frac{(1-X)}{(1+\varepsilon X)}\right)\frac{P}{P_0}\frac{T_0}{T}$$

$$\frac{dX}{dV} = \frac{k}{v_0}\frac{(1-X)}{(1+\varepsilon X)}y\frac{T_0}{T}, \text{ where } y = \frac{P}{P_0} \qquad \text{(A)}$$

Integrating for the case of constant temperature and pressure gives

$$V = \frac{v_0}{k}\left[(1+\varepsilon)\ln\frac{1}{1-X} - \varepsilon X\right] \qquad \text{(B)}$$

2. Applications/Examples of the CRE Algorithm I

Gas Phase Elementary Reaction	Additional Information	
$2A \rightarrow B$	Only A fed	P_0 = 8.2 atm
	T_0 = 500 K	C_{A0} = 0.2 mol/dm^3
	k = 0.5 dm^3/mol·s	v_o = 2.5 dm^3/s

Solve for X = 0.9 for A is limiting

2. Applications/Examples of the CRE Algorithm II

Reactor	Mole Balance	Rate Law	Stoichiometry
Batch	$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$	$-r_A = kC_A^2$	**Gas:** **V = V_0**
CSTR	$V = \frac{F_{A0}X}{-r_A}$	$-r_A = kC_A^2$	**Gas:** **T = T_0, P = P_0**
PFR	$V = F_{A0}\int_0^X \frac{dX}{-r_A}$	$-r_A = kC_A^2$	**Gas:** **T = T_0, P = P_0**

2. Applications/Examples of the CRE Algorithm III

Reactor	Stoichiometry 2	
Batch	**Per mole A ?**	$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V_0}$ $= C_{A0}(1-X)$
CSTR	**Per mole A** **A $\rightarrow$ ½B** **ε = 1.0(1- ½) = -0.5**	$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)}$
PFR	**Per mole A** **A $\rightarrow$ ½B** **ε = 1.0(1- ½) = -0.5**	$= C_{A0}\frac{(1-X)}{(1+\varepsilon X)}$

2. Applications/Examples of the CRE Algorithm IV

Reactor	Stoichiometry 3	
Batch	$C_B = \frac{N_B}{V} = \frac{N_{A0}(+\frac{1}{2}X)}{V_0} = \frac{C_{A0}X}{2}$	
CSTR	$C_B = \frac{F_B}{v} = \frac{F_{A0}(+\frac{1}{2}X)}{v_0(1+\varepsilon X)}$	
PFR	$= \frac{C_{A0}X}{2(1+\varepsilon X)}$	

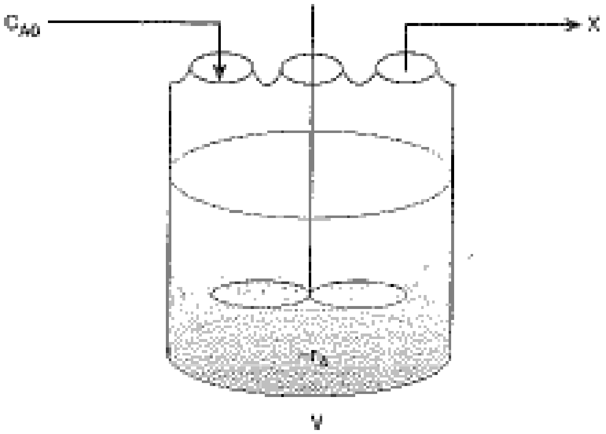
2. Applications/Examples of the CRE Algorithm V

Reactor	Combine	Integration
Batch	$t = \frac{1}{kC_{A0}} \int_0^X \left[\frac{1}{(1-X)^2} \right] dX$	$t = \frac{1}{kC_{A0}} \left[\frac{X}{(1-X)} \right]$
CSTR	$V = \frac{F_{A0} X (1-0.5X)^2}{kC_{A0}^2 (1-X)^2}$	
PFR	$V = \frac{F_{A0}}{kC_{A0}^2} \int_0^X \left[\frac{(1-0.5X)^2}{(1-X)^2} \right] dX$	$V = \frac{F_{A0}}{kC_{A0}^2} \left[2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X} \right]$

2. Applications/Examples of the CRE Algorithm VI

Reactor	Evaluate	For X = 0.9
Batch	$kC_{A0} = (0.5)(0.2)$ $= 0.1\ s^{-1}$	$t = 90\ s$
CSTR	$kC^2_{A0} = (0.5)(0.2)^2$ $= 0.02 mol/dm^3 \cdot s$ $F_{A0} = C_{A0} \cdot v_0$ $= (0.2)(2.5) = 0.5\ mol/s$	$V = 680.6\ dm^3$ $\tau = V/v_0 = 272.3\ s$
PFR		$V = 90.7\ dm^3$ $\tau = V/v_0 = 36.3\ s$

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**

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

$$C_A = \frac{C_{A0}}{1+\tau k}$$

- Damköhler number ⇒ dimensionless number

- **quick estimate of the degree on conversion achieved by continuous reactors**

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

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

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

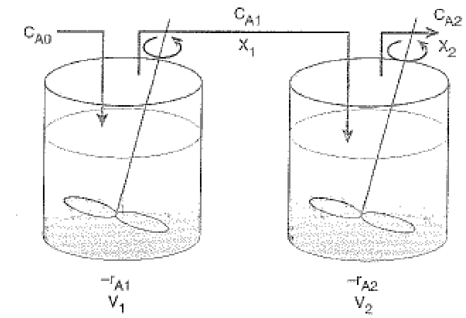
$$\mathrm{Da} = \frac{-r_{\mathrm{A0}}V}{F_{\mathrm{A0}}} = \frac{kC_{\mathrm{A0}}^2V}{v_0 C_{\mathrm{A0}}} = \tau k C_{\mathrm{A0}}$$

- 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**

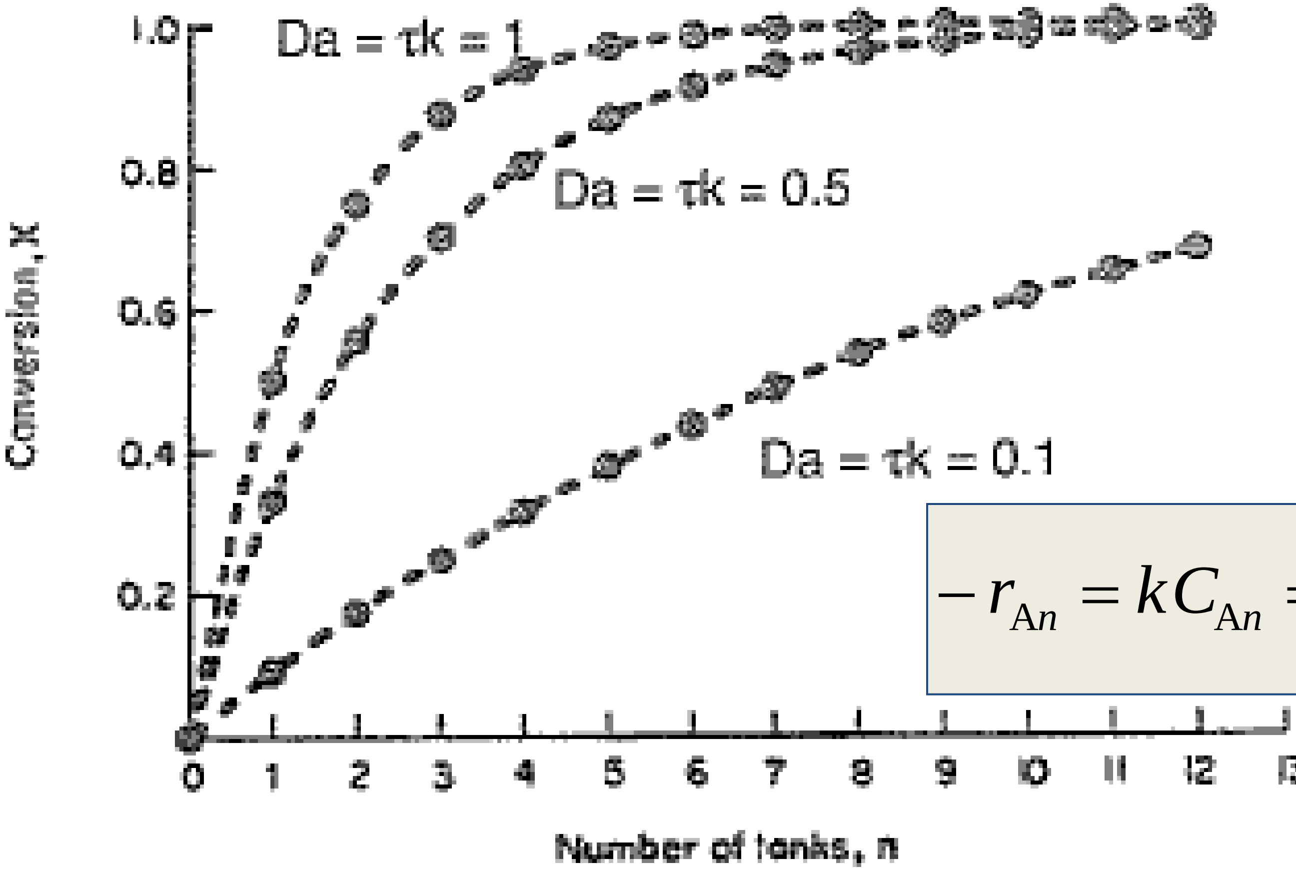
$$C_{An} = \frac{C_{A0}}{(1 + \tau k)^n} = \frac{C_{A0}}{(1 + \mathrm{Da})^n}$$

  - **n tank in series**

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

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

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

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**

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

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**

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

- **solving for X**

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

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**

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

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

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

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**

$$F_{A0}\frac{dX}{dW} = k\left[\frac{C_{A0}(1-X)}{1+\varepsilon X}\right]^2\left(\frac{P}{P_0}\right)^2$$

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

5. Pressure Drop in Reactors II

- **Flow through a Packed Bed**

- Ergun equation

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

- **pressure drop in packed bed**

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

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

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