6. Flow Systems (p. 107)

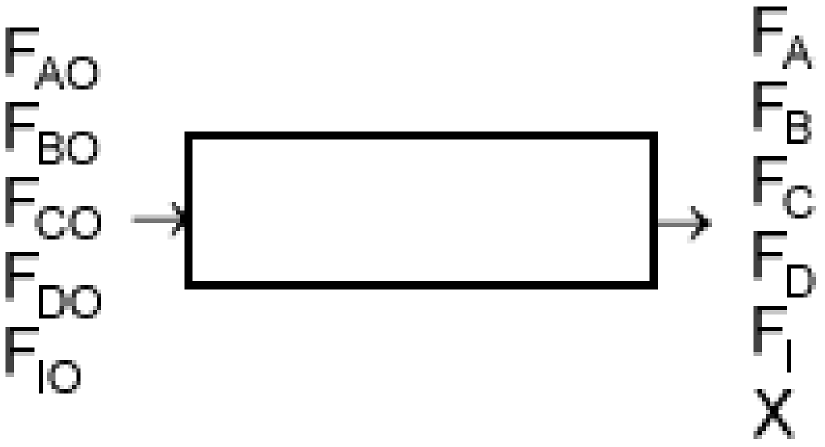
○ **Limiting reactant A**

- Concentration -- Flow System:

$$C_A = \frac{F_A}{v} = \frac{\text{moles/time}}{\text{liters/time}} = \frac{\text{moles}}{\text{liters}}$$

- Liquid phase

$\boldsymbol{v = v_0}$



6. Flow Systems II

Species	Initial (mol)	Change (mol)	Remaining (mol)
A	F_{A0}	$-(F_{A0}X)$	$F_A = F_{A0} - F_{A0}X$
B	$F_{B0} = \Theta_B F_{A0}$	$-\frac{b}{a}(F_{A0}X)$	$F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$
C	$F_{C0} = \Theta_C F_{A0}$	$\frac{c}{a}(F_{A0}X)$	$F_C = F_{A0}\left(\Theta_C + \frac{c}{a}X\right)$
D	$F_{D0} = \Theta_D F_{A0}$	$\frac{d}{a}(F_{A0}X)$	$F_D = F_{A0}\left(\Theta_D + \frac{d}{a}X\right)$
Inert	$F_{I0} = \Theta_I F_{A0}$	$---$	$F_{I0} = \Theta_I F_{A0}$
Totals	F_{T0}		$F_T = F_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)F_{A0}X$

6. Flow Systems III

- **Eqns for conc'n in flow systems**
  - $$C_A = \frac{F_A}{v} = \frac{\text{moles/time}}{\text{liters/time}} = \frac{\text{moles}}{\text{liters}}$$

  - **In general**

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v}$$

$$C_B = \frac{F_B}{v} = \frac{F_{B0} - (b/a)F_{A0}X}{v}$$

$$C_C = \frac{F_C}{v} = \frac{F_{C0} + (c/a)F_{A0}X}{v}$$

$$C_D = \frac{F_D}{v} = \frac{F_{D0} + (d/a)F_{A0}X}{v}$$

$$\Theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}v_0}{C_{A0}v_0} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

6. Flow Systems IV

- **Liquid phase concentrations**
  - **For liquid, volume change of rxn is negligible when no phase change take place,**

  Then $v = v_0$

$$C_A = \frac{F_{A0}(1-X)}{v_0} = C_{A0}(1-X)$$

$$v_j$$

$$C_B = \frac{F_{A0}[\Theta_B - (b/a)X]}{v_0} = C_{A0}\left(\Theta_B - \frac{b}{a}X\right)$$

$$C_C = \frac{F_{A0}[\Theta_C + (c/a)X]}{v_0} = C_{A0}\left(\Theta_C + \frac{c}{a}X\right)$$

$$C_D = \frac{F_{A0}[\Theta_D + (d/a)X]}{v_0} = C_{A0}\left(\Theta_D + \frac{d}{a}X\right)$$

6. Flow Systems V

- **Rxn in gas phase with volume change 1**

  - Either *V* or *v* do vary in some system

  $N_2 + 3H_2 \Leftrightarrow 2NH_3$

  - Batch reactor with variable volume 1

  $PV = ZN_TRT$

  where V = volume

  N_T = total number of moles

  T = Temperature, K

  P = total pressure, atm

  Z = compressibility factor

  R = gas constant = 0.08206 $dm^3 \cdot atm/mol \cdot K$

6. Flow Systems VI

○ **Rxn in gas phase with volume change 2**

- Batch reactor with variable volume 2

- **at time t = 0**

$$P_0 V_0 = Z_0 N_{T0} R T_0$$

- **In general**

$$V = V_0 \left(\frac{P_0}{P} \right) \frac{T}{T_0} \left(\frac{Z}{Z_0} \right) \frac{N_T}{N_{T0}}$$

- **Total number of moles**

$$N_T = N_{T0} + \delta N_{A0} X$$

where

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

$$\delta = \frac{\text{Change in total number of moles}}{\text{Mole of A reacted}}$$

6. Flow Systems VII

○ **Rxn in gas phase with volume change 3**

- Batch reactor with variable volume 3

$$\frac{N_{\mathrm{T}}}{N_{\mathrm{T0}}} = 1 + \frac{N_{\mathrm{A0}}}{N_{\mathrm{T0}}}\delta X = 1 + \delta y_{\mathrm{A0}} X = 1 + \varepsilon X$$

where $$\varepsilon = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)\frac{N_{\mathrm{A0}}}{N_{\mathrm{T0}}} = y_{\mathrm{A0}}\delta$$

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

☜ **Holds for both batch & flow systems**

$$\varepsilon = \frac{N_{\mathrm{T}f} - N_{\mathrm{T0}}}{N_{\mathrm{T0}}}$$

$$= \frac{\text{Change in total number of moles for comlpete conversion}}{\text{Total moles fed}}$$

6. Flow Systems VIII

○ **Rxn in gas phase with volume change 4**

- Batch reactor with variable volume 4

- **in terms of volume**

$$V = V_0\left(\frac{P_0}{P}\right)\frac{T}{T_0}\left(\frac{Z}{Z_0}\right)(1+\varepsilon X)$$

- **compressibility factor will not change significantly**

$$V = V_0\left(\frac{P_0}{P}\right)(1+\varepsilon X)\frac{T}{T_0}$$

6. Flow Systems IX

○ **Rxn in gas phase with volume change 5**

- Flow reactor with variable volume 1

$$PV = ZN_T RT$$

- **total concentration** $$C_T \left(= \frac{N_T}{V} \right) = \frac{F_T}{v} = \frac{P}{ZRT}$$
- **entrance condition with negligible compressibility change**

$$\boxed{v = v_0 \left(\frac{F_T}{F_{T0}} \right) \frac{P_0}{P} \left(\frac{T}{T_0} \right)}$$

- **in general**

$$\boxed{C_j = C_{T0} \left(\frac{F_j}{F_T} \right) \frac{P}{P_0} \left(\frac{T_0}{T} \right)}$$

6. Flow Systems X

- **Rxn in gas phase with volume change 6**

- Flow reactor with variable volume 2

$$\frac{F_{\mathrm{T}}}{F_{\mathrm{T0}}} = 1 + \frac{F_{\mathrm{A0}}}{F_{\mathrm{T0}}}\delta X = 1 + \delta y_{\mathrm{A0}} X = 1 + \varepsilon X$$

$$v = v_0\left(\frac{F_T}{F_{T0}}\right)\frac{P_0}{P}\left(\frac{T}{T_0}\right)$$

$$\boxed{v = v_0(1+\varepsilon X)\frac{P_0}{P}\left(\frac{T}{T_0}\right)}$$

- **concentration of species j is $C_j = F_j/v$**

$$C_j = \frac{F_{\mathrm{A0}}(\Theta_{\mathrm{j}} - \nu_j X)}{v_0(1+\varepsilon X)\frac{P_0}{P}\left(\frac{T}{T_0}\right)}$$

$$\boxed{C_j = \frac{C_{\mathrm{A0}}(\Theta_{\mathrm{j}} - \nu_j X)}{1+\varepsilon X}\left(\frac{P_0}{P}\right)\frac{T}{T_0}}$$

6. Flow Systems XI

- **Example: Calculate ε**

- For the gas phase reaction,

$2A + B \rightarrow C$

the feed is equal molar in A and B. Calculate ε.

<u>Solution</u>

A is the limiting reactant

$A + \frac{1}{2}B \rightarrow \frac{1}{2} C$

$$\delta = \frac{1}{2} - 1 - \frac{1}{2} = -1$$

$$\varepsilon = y_{A0}\delta = (\tfrac{1}{2})(-1) = -0.5$$

6. Flow Systems XII

○ **Stoichiometric Table - production of ethyl benzene 1**

2Ethylene + Toluene → Ethylenebenzene + Propylene

- Gas feed consists of 25% toluene and 75% ethylene.

a) Set up a stoichiometric table

b) Write the rate of reaction solely as a function of conversion

※ Assume the reaction is elementary with $k_T = 250$ ($dm^6/mol^2 \cdot s$). The entering pressure is 8.2 atm and the entering temperature is 227°C and the reaction takes place isothermally with no pressure drop.

6. Flow Systems XIII

- **Stoichiometric Table - production of ethyl benzene 2**

  2Ethylene + Toluene → Ethylenebenzene + Propylene

  - Basis of calculation

  - Entering concentrations of ethylene and toluene

  - What are ε and δ

  - Row in the stoichiometric table for toluene

  - Row in the stoichiometric table for ethylene

  - The complete stoichiometric table including total molar flow rates

  - Volumetric flow rate in terms of conversion

  - Conc of toluene and ethylene in terms of conversion

  - $-r_A$ solely as a function of conversion

6. Flow Systems Stoichiometry Table

Species	Initial (mol)	Change (mol)	Remaining (mol)
A	F_{A0}	$-(F_{A0}X)$	$F_A = F_{A0} - F_{A0}X$
B	$F_{B0} = \Theta_B F_{A0}$	$-\frac{b}{a}(F_{A0}X)$	$F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$
C	$F_{C0} = \Theta_C F_{A0}$	$\frac{c}{a}(F_{A0}X)$	$F_C = F_{A0}\left(\Theta_C + \frac{c}{a}X\right)$
D	$F_{D0} = \Theta_D F_{A0}$	$\frac{d}{a}(F_{A0}X)$	$F_D = F_{A0}\left(\Theta_D + \frac{d}{a}X\right)$
Inert	$F_{I0} = \Theta_I F_{A0}$	$---$	$F_{I0} = \Theta_I F_{A0}$
Totals	F_{T0}		$F_T = F_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)F_{A0}X$