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Chemical Reaction Engineering I

Chapter 3
Stoichiometry Table

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Chapter Description

Aims

- To differentiate batch and flow system in terms of equation
- To convert design equation in concentration to conversion based design equation

Expected Outcomes

- Set up stoichiometric table for batch and flow system, for constant or variable density of material (liquid or gas)

References & other information

- Elements of Chemical Reaction Engineering',
  by H. Scott Fogler

Subtopics

3.1 Batch System

3.2 Flow System: Liquid Phase Reaction

3.3 Flow System: Gas Phase Reaction

Useful Definitions

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

1. Parameter Θ

$$\Theta_i = \frac{N_{i0}}{N_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

2. Net mole change for the reaction

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

3. Relationship between 'δ' and initial mole fraction of A

$$\varepsilon = \frac{\text{Change in total number of moles when complete conversion of A is attained}}{\text{Total number of moles of all species fed to the reactor}}$$

$$\varepsilon = \frac{N_{AO}}{N_{TO}}\delta = y_{A0} \cdot \delta$$

⇒

$$\frac{N_T}{N_{TO}} = \frac{N_{T0} + \delta \cdot X \cdot N_{A0}}{N_{T0}} = 1 + \varepsilon \cdot X$$

Batch System

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

Stoichiometric Table for a Batch System

Species	Symbol	Initial	Change	Remaining	Concen-trations
A	A	N_{AO}	$-N_{AO}X$	$N_A=N_{AO}(1-X)$	
B	B	$N_{BO}=N_{AO}\Theta_B$	$-b/a\ N_{AO}X$	$N_B=N_{AO}\Theta_B-b/a\ N_{AO}X$	?
C	C	$N_{CO}=N_{AO}\Theta_C$	$c/a\ N_{AO}X$	$N_C=N_{AO}\Theta_C+c/a\ N_{AO}X$	
D	D	$N_{DO}=N_{AO}\Theta_D$	$d/a\ N_{AO}X$	$N_D=N_{AO}\Theta_D+d/a\ N_{AO}X$	
Inert	I	$N_{IO}=N_{AO}\Theta_I$	-	$N_I=N_{AO}\Theta_I$	
		N_{TO}		$N_T=N_{TO}+\delta N_{AO}X$	

Constant Volume Batch System

- With a condition that reaction occurred in liquid form or gas phase that occurred in rigid (e.g. steel) batch reactor, $V=V_o$

$$C_A = \frac{N_A}{V} = \frac{N_{AO}(1-X)}{V_O} = C_{AO}(1-X)$$

$$C_B = \frac{N_B}{V} = \frac{N_{AO}(\Theta_B - \frac{b}{a}X)}{V_O} = C_{AO}(\Theta_B - \frac{b}{a}X)$$

Stoichiometric Table for a Constant Volume Batch System

……	Remaining	Concentrations
…….	$N_A=N_{AO}(1-X)$	$C_A=C_{AO}(1-X)$
…….	$N_B=N_{AO}\Theta_B$-b/a $N_{AO}X$	$C_B=C_{AO}((\Theta_B$-b/a*X)
……	$N_C=N_{AO}\Theta_C$+c/a $N_{AO}X$	$C_C=C_{AO}(\Theta_C$+c/a*X)
…….	$N_D=N_{AO}\Theta_D$ +d/a $N_{AO}X$	$C_D=C_{AO}(\Theta_D$ +d/a*X)
…….	$N_I=N_{AO}\Theta_I$	$C_I=C_{AO}\Theta_I$
	$N_T=N_{TO} + \delta N_{AO}X$	

Variable Volume Batch System

- Usually involve gas phase reaction, $V \neq V_0$.
- The reactor volume may be related to initial reactor volume (V_0) and other operating parameters (P_0, T_0, P, and T)

$$V = V_o \frac{N_T}{N_{TO}} \left(\frac{P_o}{P}\right) \frac{T}{T_o} \left(\frac{Z}{Z_o}\right)$$

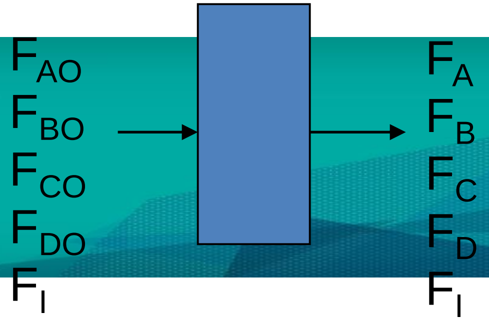
$$= V_o (1 + \varepsilon X) \left(\frac{P_o}{P}\right) \frac{T}{T_o} \left(\frac{Z}{Z_o}\right)$$

For Ideal Gas

$$V = V_o \frac{N_T}{N_{TO}} \left(\frac{P_o}{P}\right) \frac{T}{T_o}$$

$$= V_o (1 + \varepsilon X) \left(\frac{P_o}{P}\right) \frac{T}{T_o}$$

Flow System



Consider reaction where A is a limiting reactant in a flow reactor with the reaction,

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D \qquad \text{where } \Theta_i = \frac{F_{iO}}{F_{AO}} = \frac{y_{iO}}{y_{AO}}$$

Stoichiometric Table for a Flow System

Species	Initial	Change	Remaining	Concen-trations
A	F_{AO}	$-F_{AO}X$	$F_A=F_{AO}(1-X)$	
B	$F_{BO}=F_{AO}\Theta_B$	$-b/a\ F_{AO}X$	$F_B=F_{AO}\Theta_B-b/aF_{AO}X$	?
C	$F_{CO}=F_{AO}\Theta_C$	$c/a\ F_{AO}X$	$F_C=F_{AO}\Theta_C+c/a\ F_{AO}X$	
D	$F_{DO}=F_{AO}\Theta_D$	$d/a\ F_{AO}X$	$F_D=F_{AO}\Theta_D+d/a\ F_{AO}X$	
Inert	F_I	-	F_I	
	F_{TO}		$F_T=F_{TO}+\delta F_{AO}X$	

Flow System: Liquid Phase Reaction

$v = v_O$

- $F_A = F_{AO}(1-X)$
  Since $F_A = C_A v$
  $C_A v = C_{AO} v_O (1-X)$
  $C_A = C_{AO}(1-X)$
- $F_B = F_{AO}\Theta_B - b/aF_{AO}X$
  $C_B = C_{AO}(\Theta_B - b/a*X)$

Stoichiometric Table for a constant volumetric flow rate system

Change	Remaining	Concentrations
……	$F_A=F_{AO}(1-X)$	$C_A=C_{AO}(1-X)$
……	$F_B=F_{AO}\Theta_B-b/aF_{AO}X$	$C_B=C_{AO}(\Theta_B-b/a*X)$
……	$F_C=F_{AO}\Theta_C+c/a\ F_{AO}X$	$C_C=C_{AO}(\Theta_C+c/a*X)$
……	$F_D=F_{AO}\Theta_D\ +d/a\ F_{AO}X$	$C_D=C_{AO}(\Theta_D+d/a*X)$
……	F_I	C_I
	$F_T=F_{TO} + \delta F_{AO}X$	

Similar with batch system

Flow System: Gas Phase Reaction

- In a gas phase flow system,

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

- Thus,

$$C_A = \frac{F_A}{v} = \frac{F_{AO}(1-X)}{v_O(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0} = C_{AO}\frac{(1-X)}{(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0}$$

$$C_B = \frac{F_B}{v} = \frac{F_{AO}(\Theta_B - \frac{b}{a}X)}{v_O(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0} = C_{AO}\frac{(\Theta_B - \frac{b}{a}X)}{(1+\varepsilon X)}\frac{T_0}{T}\frac{P}{P_0}$$

At constant temperature and pressure, if the rate of reaction was

$$-r_A = kC_A^2 C_B^1$$

$$C_{A0} = \frac{P_{A0}}{RT}$$

$$r_A = \frac{kC_{AO}{}^3(1-X)^2(\Theta_B - \frac{b}{a}X)}{(1+\varepsilon X)^3}$$

$$\Theta_B = \frac{y_{B0}}{y_{A0}} = \frac{C_{B0}}{C_{A0}} = \frac{F_{B0}}{F_{A0}}$$

Authors Information

Credit to the authors:

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