WEEK 4

Material Balances (Continued)

Balances on reactive systems

4.6 Chemical Equilibrium: A+B <-> C + D

$K(T) = (y_C.y_D)/(y_A.y_B)$ "equilibrium constant"

Example 4.6-2 on page 122 in class.

4.6d Multiple reactions, yield and selectivity. In a reaction, undesired by-products are formed as well as desired products. The goal is to maximize the production of the desired products while keeping the undesired by-products at a minimum.

Yield: (moles of desired product formed)/(moles that would have been formed if there were no side reactions and the limiting reactant had reacted completely)

Selectivity: (moles of desired product formed)/(moles of undesired product formed)

The concept of extent of reaction is also applicable in the case of multiple reactions: $n_i = n_{io} + Sum_j(\nu_{ij}\zeta_j)$

Example at the end of page 123 (in class)

4.7 Balances on reactive systems

- We distinguish between balance on molecular versus balance on atomic species
- Example 4.7a to do in class: molecular balance (i.e., H_2), atomic balance (i.e., H), extent of reaction.

4.8 Combustion reactions: rapid reaction of a fuel with oxygen → CO_2, H_2O, CO, SO_2

Ex: fuel: propane - C_3H_8

$C_3H_8 + (7/2)O_2 \rightarrow 3CO + 4H_2O$ (partial combustion or incomplete combustion since CO is formed)

Balances on reactive systems

- “Composition on a wet basis” : water is accounted for
- “composition on a dry basis”: water is not accounted for
- Convert from “wet basis” to “dry basis”

Example 4.8-1 page 143

4.8b Theoretical and Excess Air

Feed more air than what is needed

* Feed less expensive reactant in excess.

Theoretical oxygen: moles or molar flow rate of O_2 needed for complete fuel combustion

Theoretical air: quantity of air that contains the theoretical oxygen

Excess air: Amount by which the air fed to the reactor exceeds the theoretical air

Percent excess air: $[(\text{mole air})_{fed} – (\text{mole air})_{theor}]/(\text{mole air})_{theor} \text{X } 100\%$

Example 4.8-2 in class

Chapter 5. Single-phase system

- We need to estimate the properties before using mass balance equations.
- **5.1** Liquid and solid densities: source: Perry's chemical engineering handbook

Mixture of a liquid:

1) Volume additivity: $$\frac{1}{\bar{\rho}} = \sum_{i=1}^{n} \frac{x_i}{\rho_i}$$

Similar molecular structure ex: n-pentane, n-hexane etc.
x_i is the mass feaction of component i

2) The average: $$\bar{\rho} = \sum_{i=1}^{n} x_i \rho_i$$

Single-phase system

5.2 Ideal gas: Equation of state: mole, volume, pressure and temperature

- Ideal gas: PV = nRT (low pressure)

$$PV = nRT \Leftrightarrow P\dot{V} = \dot{n}RT$$

P = absolute pressure of a gas

V = volume

R = gas constant

T = absolute temperature

$\hat{V} = \frac{V}{n}$ "Specific molar volume"

HMK Page 4.42, 4.64 (a), 5.5