WEEK 3

Materials Balances (Continued)

Degree of Freedom

- Page 98. <u>Degree of Freedom Analysis</u>

$N_{DF} = n_{unknowns} - n_{ind.\ equations}$

When - $N_{DF} = 0$ problem can be solved

- $N_{DF} > 0$ problem is underspecified
- $N_{DF} < 0$ problem is overspecified

Keep in mind that the equations can come from conservation laws and empirical relations.

4.4 Balances on Multiple-Unit Processes

- Notes: Learn how to solve:a1*x+b1*y = c1, a2*x+b2*y = c2
- **Example 4.4-1 Two-Unit Process (in class)**
- **Example 4.4-2 Extraction-Distillation Process (in class): - solute, diluent in a mixture; solvent has more affinity for the solute; raffinate: phase rich in the diluent; extract: phase rich in the solvent; stage in a separation process.**

4.5 Recycle and Bypass

- A chemical reaction (A->B) may not process to completion. The product is composed of B and some A.
- Separate A from B and recycle the unconsumed reactant A.
- **Example 4.5-1 Recycle and bypass (to do in class)**

4.6 Balances on reactive Systems - Chemical Reaction Stoichiometry

4.6a Stoichiometry

- Constraints posed by the stoichiometry (A->B)
- Stoichiometry: proportions at which chemicals combine with one another
- Stoichiometric equation: $2SO_2+O_2 \rightarrow 2SO_3$ The equation must be balanced. Note: SO_2: sulfur dioxide; SO_3: sulfur trioxide

2 mol of SO_3 generated / 1 mol of O_2 consumed

2 lb-mole of SO_2 consumed / 2 lb-mole of SO_3 generated. Note: *Not necessary to relate moles of SO_2 consumed to mol of O_2 consumed!*

Balances on reactive Systems

4.6b Limiting and excess reactants, fractional conversion, extent of reaction

- Are the 2 reactants (A,B) present in stoichiometric proportions?(i.e., (moles A present)/(moles B present) = the stoichiometric ratio?
- “Limiting reactant” would run out if reaction proceed to completion
- The other reactants are “excess reactants”
- $(n_A)_{feed}$ is the number of moles of an excess reactant
- $(n_A)_{stioch}$ is the stoichiometric requirement of A or the amount of A needed to react completely with the limiting reactant.
- $(n_A)_{feed}$- $(n_A)_{stioch}$ amount by which A in feed exceeds amount needed to react completely if reaction goes to completion.
- “Fractional excess” of A = $[(n_A)_{feed} - (n_A)_{stioch}] / (n_A)_{stioch}$
- “Percentage excess” of A = 100X(Fractional excess of A)

Ex: $C_2H_2 + 2H_2 \rightarrow C_2H_6$ (acetylene + hydrogen → ethane)

20 .0 kmol/h of C_2H_2 (limiting) and 50 .0 kmol/h of H_2 (excess)

Feeding ratio: 2.5:1 (50:20)

“Percentage excess” of H_2 is (50.0- 40.0)/40.0 = 0.25

25% excess of hydrogen in the feed

Fractional conversion

- It is possible that some limiting reactants remain because the reactor was not designed for complete conversion.
- “Fractional conversion” f = moles reacted/moles fed
- Fraction unreacted = 1-f

Ex: $C_2H_2 + 2H_2 \rightarrow C_2H_6$ (acetylene + hydrogen → ethane) in a batch reactor: 20 kmol C_2H_2, 50kmol H_2, 50kmol C_2H_6.

After some time, only 30.0 kmol of hydrogen has reacted. How much of each species we have at that time?

Ans. 50 – 30 = 20 kmol of H_2 left; C_2H_2: 30/2 = 15 -> 20 – 15 = 5 kmol of C_2H_2 left; C_2H_6: 50 + 15 = 65 kmol of C_2H_6 left

Stoichiometry and extent of reaction

$C_2H_2 + 2H_2 \rightarrow C_2H_6$

$\nu_{C2H2} = -1$; $\nu_{H2} = -2$; $\nu_{C2H6} = 1$ ---→ ν is a stoichiometric coefficient

In general: $n_i = n_{io} + \nu_i \zeta$ (for a continuous [flow rate] or batch system [number mole])

ζ is called "extent of reaction" [flow rate or number of moles].

Ex: $N_2 + 3H_2 \rightarrow 2NH_3$

Feed to reactor: 100 mol/s N_2; 300 mol/s H_2; 1 mol/s Argon (inert gas); No mole of NH_3.

$n_{N2} = 100$ mol/s – ζ

$n_{H2} = 300$ mol/s - 3ζ

$n_{NH3} = + 2\zeta$

$n_{Argon} = 1$ mol/s

Example 4.6-1 to do in class (page 120)

HMK Page 165: 4.28, 4.29, 4.39, 4.40