

WEEK 3

Materials Balances (Continued)

Degree of Freedom

- Page 98. Degree of Freedom Analysis

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

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: $a_1x + b_1y = c_1$,
 $a_2x + b_2y = c_2$
- **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 ($A \rightarrow B$) 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: $2\text{SO}_2 + \text{O}_2 \rightarrow 2\text{SO}_3$ 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”
- $(n_A)_{\text{feed}}$ is the number of moles of an excess reactant
- $(n_A)_{\text{stioch}}$ is the stoichiometric requirement of A or the amount of A needed to react completely with the limiting reactant.
- $(n_A)_{\text{feed}} - (n_A)_{\text{stioch}}$ amount by which A in feed exceeds amount needed to react completely if reaction goes to completion.
- “Fractional excess” of A = $[(n_A)_{\text{feed}} - (n_A)_{\text{stioch}}] / (n_A)_{\text{stioch}}$
- “Percentage excess” of A = 100X(Fractional excess of A)

Ex: $\text{C}_2\text{H}_2 + 2\text{H}_2 \rightarrow \text{C}_2\text{H}_6$ (acetylene + hydrogen \rightarrow 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

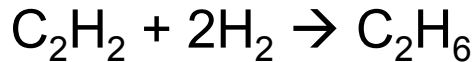
- It is possible that some limiting reactants remain because the reactor was not designed for complete conversion.
- “Fractional conversion” $f = \text{moles reacted} / \text{moles fed}$
- Fraction unreacted = $1 - f$

Ex: $\text{C}_2\text{H}_2 + 2\text{H}_2 \rightarrow \text{C}_2\text{H}_6$ (acetylene + hydrogen \rightarrow ethane)
in a batch reactor: 20 kmol C_2H_2 , 50 kmol H_2 , 50 kmol 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 : $30/2 = 15 \rightarrow 20 - 15 = 5$ kmol of C_2H_2 left; C_2H_6 : $50 + 15 = 65$ kmol of C_2H_6 left

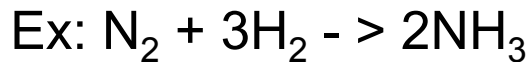
Stoichiometry and extent of reaction



$v_{\text{C}_2\text{H}_2} = -1$; $v_{\text{H}_2} = -2$; $v_{\text{C}_2\text{H}_6} = 1$ --- $\rightarrow v$ is a stoichiometric coefficient

In general: $n_i = n_{i0} + v_i \zeta$ (for a continuous [flow rate] or batch system
[number mole])

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



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

$$n_{\text{N}_2} = 100 \text{ mol/s} - \zeta$$

$$n_{\text{H}_2} = 300 \text{ mol/s} - 3\zeta$$

$$n_{\text{NH}_3} = + 2\zeta$$

$$n_{\text{Argon}} = 1 \text{ mol/s}$$

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

HMK Page 165: 4.28, 4.29, 4.39, 4.40