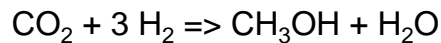


Balances with Reactions

Class 13



Quiz:



Suppose you had 100 mol of CO_2 and 250 mol of H_2 , find limiting reactant and % excess of other reactant

- Limiting reactant = H_2
- Stoichiometric amount of $\text{CO}_2 = 250 \text{ mol H}_2 (\text{mol CO}_2/3 \text{ mol H}_2) = 83.3 \text{ mols CO}_2$
- % Excess $\text{CO}_2 = (100-83.3)/(83.3) = 0.20$, or 20% excess CO_2

Suppose 80 mol of CH_3OH was formed, find ξ and f_{H_2} .

- $n_{\text{CH}_3\text{OH}} = (1) \cdot (\xi) = 80 \text{ mol } (= n_{\text{H}_2\text{O}})$
- $n_{\text{CO}_2} = 100 \text{ mol} - (1) \cdot (\xi) = 20 \text{ mol}$
- $n_{\text{H}_2} = 250 \text{ mol} - (3) \cdot (\xi) = 10 \text{ mol}$
- $f_{\text{H}_2} = (250 - 10)/250 = 1 - 10/250 = 0.96$ (i.e., 96%)

ADVICE

☞ Work through the examples in sections 4.7, 4.8

☞ Don't just browse through!

(Otherwise you will not learn this material)

3 Different Methods of Balances for Reacting Systems

- Molecular Species Balances
- Atomic Element Balances
- Extent of Reaction

Molecular Species Balances (reacting systems)

- Use **generation** and **consumption** terms
- Use ratios of species based on stoichiometry
 - Moles species j generated/moles species i consumed
- Add # of independent chemical rxns to DOF analysis
 - + # of unknowns
 - + # of independent chemical reactions
 - # of independent molecular species balances
 - # of other equations
 - = DOF

Atomic Element Balances (reacting systems)

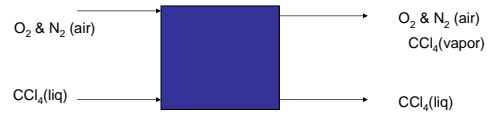
- No generation and consumption terms
 $\text{In} = \text{Out}$
- Count moles of atoms
 - Split up species into atoms
- Add # of independent atomic element balances to DOF analysis
 - + # of unknowns
 - # of independent atomic element balances
 - # of independent non-reacting molecular species balances
 - # of other equations
 - = DOF

Balances Using Extent of Reaction

- Use definition of ξ
 $n_i = n_{i,0} + \nu_i \xi$, or using flow rates
- One ξ_j for each reaction
 - Use problem info to get ξ_j 's, then calculate unknown variables
- Add extent of reaction variables to DOF analysis
 - + # of unknowns
 - + # of independent ξ_j 's
 - # of independent reacting molecular species balances
 - # of independent non-reacting species
 - # of other equations
 - = DOF

Recommendations

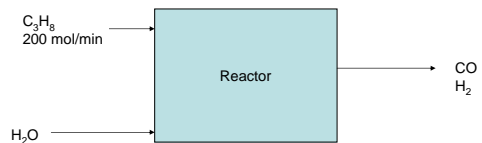
- Book recommends element balances (I agree)
 - If not, try extent of reaction approach
- **Caution:** Element balances are not always independent!!!
 - If ratio of two elements is constant everywhere, the element balances are not independent!
 - Not common, but occurs occasionally



Cautions

- If no reactions occur in the subunit, use the DOF for non-reacting systems
- If reactions occur in the block, you must use the DOF for reacting systems

Example Problem



Assignment: Work this problem in one of three ways:

1. Molecular Balances
2. Element Balances
3. Extent of Reaction

Start with DOF!