Balances with Reactions

Class 13

Quiz:

$2CH_3OH + O_2 \Rightarrow CH_2O + 2H_2O$

$CH_3OH \Rightarrow CH_2O + H_2$

(a) If only the first reaction is considered, and 50 moles of CH_3OH and 20 moles of O_2 are fed to the reactor. Which is the limiting reactant? Find the %excess of the other reactant.

- Limiting reactant = O_2
- Stoichiometric amount of CH_3OH = 40 mol CH_3OH (mol O_2 × 2 mol CH_3OH) = 40 mols CH_3OH
- % Excess CH_3OH = (50-40)/(40) = 1/4, or 25% excess CH_3OH

(b) The reactants from part (a) form 18 moles of CH_2O and 5 moles of H_2. Find the following:

(i) the extents of reaction (ξ_1 and ξ_2),

(ii) the final number of moles (n_i) of each of the other three species at this condition using the extent of reaction method, and

(iii) the fractional conversion of each reactant (f_i).

- CH_2O balance: $18 = 0 + \xi_1 + \xi_2$
- H_2 balance: $5 = 0 + \xi_2$
- So $\xi_2 = 5$ mols, $\xi_1 = 13$ mols
- $n_{CH3OH} = 50 \text{ mol} - 2\xi_1 - \xi_2 = 50 - 2*13 - 5 = 19$ mols
- $n_{O2} = 20 \text{ mol} - \xi_1 = 20 - 13 = 7$ mols
- $n_{H2O} = 2\xi_1 = 26$ mols
- $f_{CH3OH} = (50 - 19)/50 = 1 - 19/50 = 0.62$ (i.e., 62% conversion of CH_3OH)
- $f_{O2} = (20 - 7)/20 = 1 - 7/20 = 0.65$ (i.e., 65% conversion of O_2)

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
  - In = 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

  $n_i = n_{i,o} + \nu_i \xi$, or using flow rates
- One ξ_j for each reaction
  - Use problem info to get ξ_i's, then calculate unknown variables
- Add extent of reaction variables to DOF analysis

  \+ # of unknowns

  \+ # of independent ξ_i's

  \- # of independent reacting molecular species balances

  \- # of independent non-reacting species

  \- # of other equations

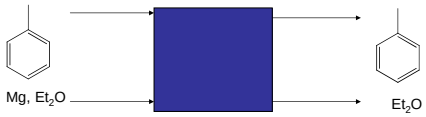
  = DOF

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

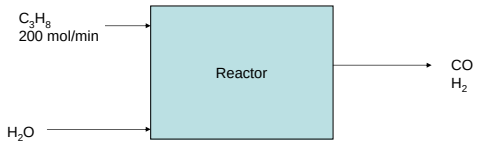


C/H ratio is same in two streams (twice)

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!