Class 12

Strategy to Finish Ch. 4

Mon (2/4) – 4.6

Wed (2/6) – 4.7, but not DOF

Thur (2/7) – Dean's lecture

Fri (2/8) – 4.7 DOF

Mon (2/11) – 4.8 Combustion

Stoichiometric

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

- **Stoichiometric coefficients** (ν_i)
  - Negative for reactants, positive for products
  - $\nu_{N2} = -1$, $\nu_{H2} = -3$, $\nu_{NH3} = 2$
- **Stoichiometric ratio**
  - Molar ratio in stoichiometric equation
    - The stoichiometric ratio here is $N_2/H_2 = 1:3$
  - If we actually have a system that has a 1:3 proportion, then we say it is in **stoichiometric proportion**

Non-Stoichiometric

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

- Occurs quite a bit!
- **Limiting reactant** – whichever reactant will be consumed first!
  - If we start with 1 mole N_2, 2 moles H_2, then H_2 is the limiting reactant
    - If the 2 moles of H_2 are consumed, there will still be N_2 left!
- **Excess reactant** – whichever reactant will be left over
  - In the example above, N_2 is the excess reactant

More Terms

- **Stoichiometric Requirement**
  - Given x number of moles, how many moles of the other reactant(s) are needed in stoichiometric proportion?
    - Given 2 moles of N_2, what is the stoichiometric requirement of H_2 to form NH_3? (6 moles)
- **Percent Excess**
  - Suppose we have 2 moles N_2 and 7 moles H_2
    - There will be 1 moles of H_2 left after complete reaction
    - % excess = $(n_{i,0} - n_{i,\,stoich})/n_{i,\,stoich}$
    - = (7-6)/6 in this case = 1/6, or 16.7% excess H_2

Reaction-Related Terms

- **Fractional Conversion** (f_i in our text, X_i in others)
  - Relative amount of reactant converted (= $n_{reacted}/n_{fed}$)
  - f_i (or X_i) = $(n_{i0} - n_i)/n_{i0} = 1 - n_i/n_{i0}$
    - Start with 3 moles H_2, end with 0.3 moles H_2, then $f_{H2} = (3 - 0.3)/3 = 0.9$, or 90% conversion
- **Extent of Reaction** (ξ, pronounced ksee)
  - Amount of reacted, normalized to stoichiometric equation
  - $n_i = n_{i0} + \xi\nu_i$ or $\xi = (n_i - n_{i0})/\nu_i$
  - note that ν_i is negative for a reactant, positive for a product
  - Example
    - Start with 3 moles H_2, 1.5 moles N_2, 0.3 moles of H_2 are left after rxn
    - $\xi = (0.3 - 3)/(-3) = 2.7/3 = 0.9$ moles
    - So $n_{NH3} = 0 + (0.9) \cdot (2) = 1.8$ moles
    - Also, $n_{N2} = 1.5 + (0.9) \cdot (-1) = 0.6$ moles
  - note that there is ξ is not species dependent, but there is one ξ for each reaction

Practice (fill-in)

$C_3H_8 + 7/2\ O_2 \rightarrow 3\ CO + 4\ H_2O$

- Start with 2 moles propane, 10 moles O_2
- Limiting reactant:
- %Excess of excess reactant:

If 1.5 moles of propane react,

- Fractional conversion (f) =
- Extent of reaction (ξ) =
- n_{O2} =
- n_{CO} =
- n_{H2O} =

Practice

$C_3H_8 + 7/2\ O_2 \rightarrow 3\ CO + 4\ H_2O$

- Start with 2 moles propane, 10 moles O_2
- Limiting reactant: propane
- %Excess of excess reactant:
  (10 – 7)/7 = 3/7 = 42.8%

If 1.5 moles of propane react,

- Fractional conversion (f) = (2 – 0.5)/2 = 75%
- Extent of reaction (ξ) = (0.5 – 2)/(-1) = 1.5 moles
- $n_{O2} = 10 + (1.5) \cdot (-7/2) =$ 4.75 moles
- $n_{CO} = 0 + 1.5 \cdot 3 =$ 4.5 moles
- $n_{H2O} = 0 + 1.5 \cdot 4 =$ 6.0 moles

Yield & Selectivity

- These both have to do with multiple products, only one of which is most desired
- **Yield** = (moles of desired product)/
  (max possible moles at complete conversion)
- **Selectivity** = (moles desired product)/
  (sum of undesired products)

Practice

$C_2H_6 \rightarrow C_2H_4 + H_2$

$C_2H_6 + H_2 \rightarrow 2\ CH_4$

$C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$

Start with 100 moles of C_2H_6

After reaction, we have:

65 mols C_2H_4
15 mols C_2H_6
60 mols H_2
25 mols CH_4
5 mols C_3H_6

- Find yield and selectivity if C_2H_4 is the desired product
- Find ξ_1, ξ_2, and ξ_3

Answers (fill-in)

- $Yield_{C2H4} = 65/100 = 65\%$
- Selectivity = 65/(25 + 5) = 2.2
- Set up each mole balance

$n_{C2H6} = 15$ moles $= n_{C2H6,0} - \xi_1 - \xi_2 - \xi_3$
$n_{C2H4} = 65$ moles =
$n_{H2} = 60$ moles =
$n_{C3H6} = 5$ mols =

So….

ξ_3 =
ξ_1 =
ξ_2 =

Answers

- $Yield_{C2H4} = 65/100 = 65\%$
- Selectivity = 65/(25 + 5) = 2.2
- Set up each mole balance

$n_{C2H6} = 15$ moles $= n_{C2H6,0} - \xi_1 - \xi_2 - \xi_3$
$n_{C2H4} = 65$ moles $= 0 + \xi_1 - \xi_3$
$n_{H2} = 60$ moles $= 0 + \xi_1 - \xi_2$
$n_{C3H6} = 5$ mols $= 0 + \xi_3$

So….

$\xi_3 =$ 5 mols
$\xi_1 = 65 + 5 = 70$ mols (from C_2H_4 balance)
$\xi_2 = 70 - 60 = 10$ mols (from H_2 balance)

Example:
$CO_2 + 3 H_2 \Rightarrow CH_3OH + H_2O$

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
- % Excess CO_2 = (100-250/3)/(250/3) = 20%

Suppose 80 mol of CH_3OH was formed, find ξ and f_{H2}.

- $n_{CH3OH} = (1)*(\xi) = 80$ mol ($= n_{H2O}$)
- $n_{CO2} = 100$ mol – $(1)*(\xi) = 20$ mol
- $n_{H2} = 250$ mol – $(3)*(\xi) = 10$ mol
- $f_{H2} = (250 – 10)/250 = 1 – 10/250 = 0.96$ (i.e., 96%)