

Class 12

Strategy to Finish Ch. 4

Mon (2/4) – 4.6

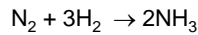
Wed (2/6) – 4.7, but not DOF

Thur (2/7) – Dean's lecture

Fri (2/8) – 4.7 DOF

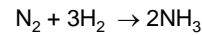
Mon (2/11) – 4.8 Combustion

Stoichiometric



- **Stoichiometric coefficients** (ν_i)
 - Negative for reactants, positive for products
 - $\nu_{\text{N}_2} = -1$, $\nu_{\text{H}_2} = -3$, $\nu_{\text{NH}_3} = 2$
- **Stoichiometric ratio**
 - Molar ratio in stoichiometric equation
 - The stoichiometric ratio here is $\text{N}_2/\text{H}_2 = 1:3$
 - If we actually have a system that has a 1:3 proportion, then we say it is in **stoichiometric proportion**

Non-Stoichiometric



- 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

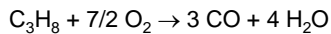
More Terms

- **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 mole of H_2 left after complete reaction
 - % excess = $(n_{i,0} - n_{i,\text{stoich}})/n_{i,\text{stoich}}$
 - = $(7-6)/6$ 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 ($= n_{\text{reacted}}/n_{\text{fed}}$)
 - f_i (or X_i) = $(n_{i,0} - n_i)/n_{i,0} = 1 - n_i/n_{i,0}$
 - Start with 3 moles H_2 , end with 0.3 moles H_2 , then $f_{\text{H}_2} = (3 - 0.3)/3 = 0.9$, or 90% conversion
- **Extent of Reaction** (ξ , pronounced ksee)
 - Amount of reacted, normalized to stoichiometric equation
 - $n_i = n_{i,0} + \xi \nu_i$ or $\xi = (n_i - n_{i,0})/\nu_i$
 - 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 $n_{\text{NH}_3} = 0 + (0.9) \cdot (2) = 1.8$ moles
 - Also, $n_{\text{N}_2} = 1.5 + (0.9) \cdot (-1) = 0.6$ moles
 - note that there is ξ is not species dependent, but there is one ξ for each reaction

Practice (fill-in)

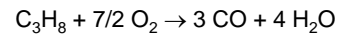


- Start with 2 moles propane, 10 moles O_2
- Limiting reactant:
- %Excess of excess reactant:

If 1.5 moles of propane react,

- Fractional conversion (f) =
- Extent of reaction (ξ) =
- n_{O_2} =
- n_{CO} =
- $n_{\text{H}_2\text{O}}$ =

Practice



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

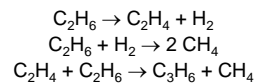
If 1.5 moles of propane react,

- Fractional conversion (f) = $(2 - 0.5)/2 = 75\%$
- Extent of reaction (ξ) = $(0.5 - 2)/(-1) = 1.5$ moles
- $n_{\text{O}_2} = 10 + (1.5) \cdot (-7/2) = 4.75$ moles
- $n_{\text{CO}} = 0 + 1.5 \cdot 3 = 4.5$ moles
- $n_{\text{H}_2\text{O}} = 0 + 1.5 \cdot 4 = 6.0$ 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



Start with 100 moles of C_2H_6

After reaction, we have:

65 moles C_2H_4
15 moles C_2H_6
60 moles H_2
25 moles CH_4
5 moles 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)

- $\text{Yield}_{\text{C}_2\text{H}_4} = 65/100 = 65\%$
- $\text{Selectivity} = 65/(25 + 5) = 2.2$
- Set up each mole balance
 $n_{\text{C}_2\text{H}_6} = 15$ moles = $n_{\text{C}_2\text{H}_6,0} - \xi_1 - \xi_2 - \xi_3$
 $n_{\text{C}_2\text{H}_4} = 65$ moles =
 $n_{\text{H}_2} = 60$ moles =
 $n_{\text{C}_3\text{H}_6} = 5$ moles =

So....

$\xi_3 =$
 $\xi_1 =$
 $\xi_2 =$

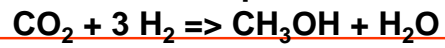
Answers

- $\text{Yield}_{\text{C}_2\text{H}_4} = 65/100 = 65\%$
- $\text{Selectivity} = 65/(25 + 5) = 2.2$
- Set up each mole balance
 $n_{\text{C}_2\text{H}_6} = 15$ moles = $n_{\text{C}_2\text{H}_6,0} - \xi_1 - \xi_2 - \xi_3$
 $n_{\text{C}_2\text{H}_4} = 65$ moles = $0 + \xi_1 - \xi_3$
 $n_{\text{H}_2} = 60$ moles = $0 + \xi_1 - \xi_2$
 $n_{\text{C}_3\text{H}_6} = 5$ moles = $0 + \xi_3$

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:



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 $\text{CO}_2 = (100 - 250/3)/(250/3) = 20\%$

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%)