The Limits of Reaction

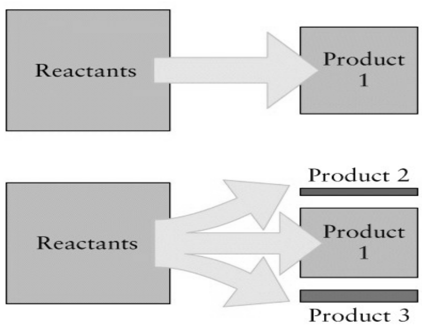
4.3 Reaction Yield

- Theoretical yield - the maximum amount of product that can be expected from a given amount of reactant
- Actual yield - the actual amount of product isolated in a reaction

Actual Yield ≤ Theoretical Yield

- Reasons for the difference between actual and theoretical yield
  - incomplete reaction
  - loss of product
  - side reactions
- Percentage yield:

$$\%\ \text{Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\%$$



- **Example:** Calculate the theoretical yield of carbon dioxide produced by the combustion of **25.0 g** propane in excess oxygen.

⇒ **balanced equation:**

$$\mathbf{C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O}$$

⇒**mass-to-mass conversion:**

$$25.0\ \text{g}\ C_3H_8 \times \left(\frac{1\ \text{mol}\ C_3H_8}{44.09\ \text{g}\ C_3H_8}\right) \times \left(\frac{3\ \text{mol}\ CO_2}{1\ \text{mol}\ C_3H_8}\right) \times$$

$$\times \left(\frac{44.01\ \text{g}\ CO_2}{1\ \text{mol}\ CO_2}\right) = 74.9\ \text{g}\ CO_2 \rightarrow \mathit{Theor.\ Yield}$$

- **Example:** Calculate the percentage yield of carbon dioxide, if the combustion of **25.0 g** propane in excess oxygen yields **48.5 g** carbon dioxide.

⇒ **theoretical yield → 74.9 g CO_2**

⇒ **side reaction (consumes some of the propane):**

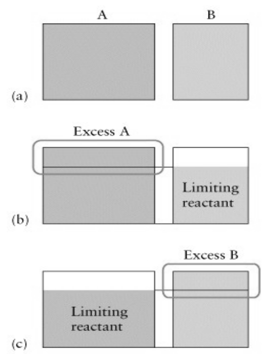
$$\mathbf{2C_3H_8 + 7O_2 \rightarrow 6CO + 8H_2O}$$

⇒**percentage yield:**

$$\%\ \text{Yield} = \frac{48.5\ \text{g}\ CO_2}{74.9\ \text{g}\ CO_2} \times 100\% = 64.8\%$$

4.4 Limiting Reactants

- Reactants present in equivalent amounts
  - all reactants are consumed at the same time
- Nonequivalent amounts of reactants
  - one reactants is consumed before the others
  - the other reactants are in excess
- Limiting reactant
  - consumed before the other reactants
  - limits the maximum amount of product achievable (theoretical yield)
  - stoichiometric calculations based on it give the smallest amount of product



Example: Identify the limiting reactant in the reaction of **5.0 mol H_2** with **3.0 mol N_2**, and determine the theoretical yield of NH_3 in this reaction.

⇒**balanced equation:** $\mathbf{3H_2 + N_2 \rightarrow 2NH_3}$

- ***Method 1:*** **Calculate the amount of one of the reactants needed to react completely with the other reactant:**

5.0 mol H_2×[1 mol N_2/3 mol H_2] = 1.7 mol N_2

⇒**5.0 mol H_2 will consume only 1.7 mol N_2**

⇒**1.3 mol N_2 are in excess (3.0 - 1.7)**

⇒**H_2 is the limiting reactant**

⇒**Calculation of the theoretical yield is based on the limiting reactant:**

$$5.0 \text{ mol H}_2 \times \left(\frac{2 \text{ mol NH}_3}{3 \text{ mol H}_2}\right) = 3.3 \text{ mol NH}_3 \rightarrow \textit{Theor. Yield}$$

- ***Method 2:*** **Calculate the theoretical yield based on each of the reactants and chose the smaller result:**

$$3.0 \text{ mol N}_2 \times \left(\frac{2 \text{ mol NH}_3}{1 \text{ mol N}_2}\right) = 6.0 \text{ mol NH}_3$$

$$5.0 \text{ mol H}_2 \times \left(\frac{2 \text{ mol NH}_3}{3 \text{ mol H}_2}\right) = 3.3 \text{ mol NH}_3 \rightarrow \textit{Theor. Yield}$$

Example: Calculate the theoretical yield of HNO_3 in the reaction of **28 g NO_2** and **18 g H_2O** by the chemical equation:

$3NO_2(g) + H_2O(l) \rightarrow 2HNO_3(l) + NO(g)$.

- ***Method 2:*** **Calculate the theoretical yield based on each of the reactants and chose the smaller result:**

$$18 \text{ g H}_2\text{O} \times \left(\frac{1 \text{ mol H}_2\text{O}}{18.0 \text{ g H}_2\text{O}}\right) \times \left(\frac{2 \text{ mol HNO}_3}{1 \text{ mol H}_2\text{O}}\right) \times$$
$$\times \left(\frac{63.0 \text{ g HNO}_3}{1 \text{ mol HNO}_3}\right) = 1.3 \times 10^2 \text{ g HNO}_3$$

$$28 \text{ g NO}_2 \times \left(\frac{1 \text{ mol NO}_2}{46.0 \text{ g NO}_2}\right) \times \left(\frac{2 \text{ mol HNO}_3}{3 \text{ mol NO}_2}\right) \times$$
$$\times \left(\frac{63.0 \text{ g HNO}_3}{1 \text{ mol HNO}_3}\right) = 26 \text{ g HNO}_3 \rightarrow \textit{Theor. Yield}$$

⇒**the smaller amount of product results from the calculation based on NO_2**

⇒**NO_2 is the limiting reactant and 26 g HNO_3 is the theoretical yield**

4.5 Combustion Analysis

- Determination of the elemental composition of organic compounds through combustion in excess O_2
  - – the **C** in the sample is converted to **CO_2** which is absorbed by an excess of **NaOH** and weighed

    $NaOH(s) + CO_2(g) \rightarrow NaHCO_3(s)$
  - – the **H** in the sample is converted to **H_2O** which is absorbed by an excess of **P_4O_{10}** and weighed

    $P_4O_{10}(s) + 6H_2O(l) \rightarrow 4H_3PO_4(l)$

1 mol C from the sample → 1 mol CO_2

2 mol H from the sample → 1 mol H_2O

Example: When 0.236 g aspirin is burned in excess $\mathbf{O_2}$, 0.519 g $\mathbf{CO_2}$ and 0.0945 g $\mathbf{H_2O}$ are formed. Determine the mass % of C, H and O in aspirin.

⇒**Calculate the masses of C and H in the sample based on the masses of CO_2 and H_2O:**

⇒**Calculate the mass of O by subtracting the masses of C and H from the total mass of the sample**

$$0.519 \text{ g CO}_2 \times \left(\frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2}\right) \times \left(\frac{1 \text{ mol C}}{1 \text{ mol CO}_2}\right) \times$$

$$\times \left(\frac{12.01 \text{ g C}}{1 \text{ mol C}}\right) = 0.142 \text{ g C}$$

$$0.0945 \text{ g H}_2\text{O} \times \left(\frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}}\right) \times \left(\frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}}\right) \times$$

$$\times \left(\frac{1.008 \text{ g H}}{1 \text{ mol H}}\right) = 0.0106 \text{ g H}$$

$$0.236 - 0.142 - 0.0106 = 0.084 \text{ g O}$$

$$\%\text{C} = \left(\frac{0.142 \text{ g C}}{0.236 \text{ g sample}}\right) \times 100\% = 60.0\%$$

$$\%\text{H} = \left(\frac{0.0106 \text{ g H}}{0.236 \text{ g sample}}\right) \times 100\% = 4.48\%$$

$$\%\text{O} = \left(\frac{0.084 \text{ g O}}{0.236 \text{ g sample}}\right) \times 100\% = 35.5\%$$

The empirical formula can be determined from the percentage composition in a subsequent step.