# **3.4 Calculating Amounts of Reactants and Products**

## **Stoichiometric Equivalences**

 Balanced chemical equations contain definite stoichiometric relations between reactants and products → stoichiometric mole ratios

# Example: $2H_2 + O_2 \rightarrow 2H_2O$

 $\begin{array}{c} 2 \ mol \ H_2 \Leftrightarrow 1 \ mol \ O_2 \\ 2 \ mol \ H_2 \Leftrightarrow 2 \ mol \ H_2 O \\ 1 \ mol \ O_2 \Leftrightarrow 2 \ mol \ H_2 O \\ \end{array} \right\} \begin{array}{c} \text{stoichiometric} \\ \text{equivalences} \\ \text{equivalences} \\ \end{array} \\ \begin{array}{c} 1 \ mol \ O_2 / 2 \ mol \ H_2 O \\ 2 \ mol \ H_2 O / 2 \ mol \ H_2 \\ 2 \ mol \ H_2 O / 1 \ mol \ O_2 \end{array} \right\} \begin{array}{c} \text{stoichiometric} \\ \text{stoichiometric} \\ \text{mole ratios} \end{array}$ 

Mole-to-Mole Conversions• Conversion method- The mole ratios are used as conversion factors<br/>(mol given)×(mole ratio) = (mol required)Example: Determine the number of moles of<br/>water produced from 3.4 mol O2. $\rightarrow$  balanced equation:  $2H_2 + O_2 \rightarrow 2H_2O$  $\rightarrow$  mole ratio (conversion factor):  $[2 \mod H_2O/1 \mod O_2]$  $3.4 \mod O_2 \times \left(\frac{2 \mod H_2O}{1 \mod O_2}\right) = 6.8 \mod H_2O$ 

Stoichiometric conversion factors are reaction specific
Example: Calculate the amount of O<sub>2</sub> needed to produce 3.5 mol H<sub>2</sub>O by combustion of methane (CH<sub>4</sub>).
→ balanced equation: CH<sub>4</sub> + 2O<sub>2</sub> → CO<sub>2</sub> + 2H<sub>2</sub>O
→ mole ratio (conversion factor): 2 mol O<sub>2</sub> ⇔ 2 mol H<sub>2</sub>O
[2 mol O<sub>2</sub>/2 mol H<sub>2</sub>O]

$$3.5 \operatorname{mol} \mathrm{H}_{2}\mathrm{O} \times \left(\frac{2 \operatorname{mol} \mathrm{O}_{2}}{2 \operatorname{mol} \mathrm{H}_{2}\mathrm{O}}\right) = 3.5 \operatorname{mol} \mathrm{O}_{2}$$



Example: Calculate the mass of oxygen needed to completely burn 5.4 kg of butane (C<sub>4</sub>H<sub>10</sub>).  $\rightarrow$  balanced equation: 2C<sub>4</sub>H<sub>10</sub> + 13O<sub>2</sub>  $\rightarrow$  8CO<sub>2</sub> + 10H<sub>2</sub>O  $\rightarrow$  mole ratio: [13 mol O<sub>2</sub>/2 mol C<sub>4</sub>H<sub>10</sub>]  $\rightarrow$  molar masses: C<sub>4</sub>H<sub>10</sub>  $\rightarrow$  58.1 g/mol O<sub>2</sub>  $\rightarrow$  32.0 g/mol 5.4 kg C<sub>4</sub>H<sub>10</sub>  $\times \left(\frac{10^3 \text{ gC}_4 \text{ H}_{10}}{1 \text{ kg C}_4 \text{ H}_{10}}\right) \times \left(\frac{1 \text{ mol C}_4 \text{ H}_{10}}{58.1 \text{ gC}_4 \text{ H}_{10}}\right) \times \left(\frac{13 \text{ mol O}_2}{2 \text{ mol C}_4 \text{ H}_{10}}\right) \times \left(\frac{32.0 \text{ gO}_2}{1 \text{ mol O}_2}\right) = 1.9 \times 10^4 \text{ gO}_2 = 19 \text{ kg O}_2$ 

## **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

• Percentage yield:

% 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 ( $C_3H_8$ ) in excess oxygen.

 $\rightarrow$  balanced equation:

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

→mass-to-mass conversion:

$$25.0 \text{ g } \text{C}_{3}\text{H}_{8} \times \left(\frac{1 \text{ mol } \text{C}_{3}\text{H}_{8}}{44.09 \text{ g } \text{C}_{3}\text{H}_{8}}\right) \times \left(\frac{3 \text{ mol } \text{CO}_{2}}{1 \text{ mol } \text{C}_{3}\text{H}_{8}}\right) \times \left(\frac{44.01 \text{ g } \text{CO}_{2}}{1 \text{ mol } \text{CO}_{2}}\right) = 74.9 \text{ g } \text{CO}_{2} \rightarrow \text{Theor. Yield}$$

**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 (from prev. problem): 74.9 g CO<sub>2</sub> → side reaction (consumes some of the propane):  $2C_3H_8 + 7O_2 \rightarrow 6CO + 8H_2O$
- $\rightarrow$  actual yield: 48.5 g CO<sub>2</sub>
- $\rightarrow$  percentage yield:

% Yield =  $\frac{48.5 \text{ g CO}_2}{74.9 \text{ g CO}_2} \times 100\% = 64.8\%$ 

### **Limiting Reactants**

- Reactants present in equivalent amounts
  - All reactants are consumed at the same time
- Nonequivalent amounts of reactants
  - One reactant, called **limiting reactant**, is consumed before the others
  - The other reactants are in excess
- Limiting reactant
  - The reaction stops when the limiting reactant is consumed
  - Limits the maximum amount of product achievable (limits the theoretical yield)
  - Stoichiometric calculations based on the limiting reactant give the **lowest amount of product** compared to calculations based on the other reactants

**Example:** Identify the limiting reactant in the reaction of **5.0 mol H**<sub>2</sub> with **3.0 mol N**<sub>2</sub>, and determine the theoretical yield of  $NH_3$  in this reaction.

 $\rightarrow$  balanced equation:  $3H_2 + N_2 \rightarrow 2NH_3$ 

→calculate the theoretical yield based on each of the reactants and chose the **smaller result**:

3.0 mol N<sub>2</sub> × 
$$\left(\frac{2 \text{ mol NH}_3}{1 \text{ mol N}_2}\right) = 6.0 \text{ mol NH}_3$$
  
5.0 mol H<sub>2</sub> ×  $\left(\frac{2 \text{ mol NH}_3}{3 \text{ mol H}_2}\right) = 3.3 \text{ mol NH}_3 \rightarrow Theor. Yield$   
smaller amount  
 $\Rightarrow$  H<sub>2</sub> is the limiting reactant

**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:

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

→Calculate the theoretical yield based on each of the reactants and chose the smaller result:

$$18 \text{ g} \text{ H}_{2}\text{O} \times \left(\frac{1 \text{ mol H}_{2}\text{O}}{18.0 \text{ g} \text{ H}_{2}\text{O}}\right) \times \left(\frac{2 \text{ mol HNO}_{3}}{1 \text{ mol H}_{2}\text{O}}\right) \times \\ \times \left(\frac{63.0 \text{ g} \text{ HNO}_{3}}{1 \text{ mol HNO}_{3}}\right) = 130 \text{ g} \text{ HNO}_{3}$$

28 g NO<sub>2</sub> × 
$$\left(\frac{1 \text{ mol NO}_2}{46.0 \text{ g NO}_2}\right)$$
 ×  $\left(\frac{2 \text{ mol HNO}_3}{3 \text{ mol NO}_2}\right)$  ×  
× $\left(\frac{63.0 \text{ g HNO}_3}{1 \text{ mol HNO}_3}\right)$  = 26 g HNO<sub>3</sub>  $\rightarrow$  Theor. Yield  
smaller amount