### 3.4 Calculating Amounts of Reactants and Products

## Stoichiometric Equivalences

- Balanced chemical equations contain definite stoichiometric relations between reactants and products $\rightarrow$ stoichiometric mole ratios
Example: $\mathbf{2 H}_{\mathbf{2}}+\mathbf{O}_{\mathbf{2}} \boldsymbol{\rightarrow} \mathbf{2} \mathbf{H}_{\mathbf{2}} \mathbf{O}$
$2 \mathrm{~mol} \mathrm{H}{ }_{2} \Leftrightarrow 1 \mathrm{~mol} \mathrm{O}_{2}$
$2 \mathrm{~mol} \mathrm{H}_{2} \Leftrightarrow \mathbf{2} \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}$
$1 \mathrm{~mol} \mathrm{O}_{2} \Leftrightarrow 2 \mathrm{~mol} \mathrm{H} \mathbf{2}$
$1 \mathrm{~mol} \mathrm{O}_{2} / 2 \mathrm{~mol} \mathrm{H}_{2}$
$2 \mathrm{~mol} \mathrm{H} \mathrm{O} / 2 \mathrm{~mol} \mathrm{H}_{2}$
$2 \mathrm{~mol} \mathrm{H} \mathrm{H}_{2} \mathrm{O} / 1 \mathrm{~mol} \mathrm{O}_{2}$
stoichiometric
equivalences
stoichiometric
mole ratios


## Mole-to-Mole Conversions

- Conversion method
- The mole ratios are used as conversion factors
$(\mathbf{m o l}$ given $) \times($ mole ratio $)=(\mathbf{m o l}$ required $)$
Example: Determine the number of moles of water produced from $3.4 \mathrm{~mol} \mathrm{O}_{2}$.
$\rightarrow$ balanced equation: $\mathbf{2 H}_{\mathbf{2}}+\mathbf{O}_{\mathbf{2}} \rightarrow \mathbf{2} \mathbf{H}_{\mathbf{2}} \mathrm{O}$
$\rightarrow$ mole ratio (conversion factor): [2 mol $\mathbf{H}_{\mathbf{2}} \mathrm{O} / \mathbf{1} \mathbf{~ m o l ~ O} \mathbf{O}_{2}$ ]
$3.4 \mathrm{~mol} \mathrm{O}_{2} \times\left(\frac{2 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}{1 \mathrm{~mol} \mathrm{O}_{2}}\right)=6.8 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}$


## Mass-to-Mass Calculations

- Conversion method


Example: Calculate the mass of oxygen needed to completely burn $\mathbf{5 . 4} \mathbf{~ k g}$ of butane $\left(\mathrm{C}_{4} \mathbf{H}_{\mathbf{1 0}}\right)$.
$\rightarrow$ balanced equation:

$$
2 \mathrm{C}_{4} \mathrm{H}_{10}+13 \mathrm{O}_{2} \rightarrow 8 \mathrm{CO}_{2}+10 \mathrm{H}_{2} \mathrm{O}
$$

$\rightarrow$ mole ratio: $\left[\mathbf{1 3} \mathbf{~ m o l ~ O} \mathbf{2} / \mathbf{2} \mathbf{~ m o l ~ C} \mathbf{4}_{\mathbf{4}} \mathrm{H}_{\mathbf{1 0}}\right]$
$\rightarrow$ molar masses:

$$
\mathrm{C}_{4} \mathrm{H}_{10} \rightarrow 58.1 \mathrm{~g} / \mathrm{mol} \quad \mathrm{O}_{2} \rightarrow 32.0 \mathrm{~g} / \mathrm{mol}
$$

$5.4 \mathrm{~kg} \mathrm{C}_{4} \mathrm{H}_{10} \times\left(\frac{\mathbf{1 0}^{3} \mathrm{~g} \mathrm{C}_{4} \mathrm{H}_{10}}{1 \mathrm{~kg} \mathrm{C}_{4} \mathrm{H}_{10}}\right) \times\left(\frac{1 \mathrm{molC}_{4} \mathrm{H}_{10}}{58.1 \mathrm{~g} \mathrm{C}_{4} \mathrm{H}_{10}}\right) \times$
$\left(\frac{13 \mathrm{molO}_{2}}{2 \mathrm{molC}_{4} \mathrm{H}_{10}}\right) \times\left(\frac{32.0 \mathrm{~g} \mathrm{O}_{2}}{1 \mathrm{molO}_{2}}\right)=1.9 \times 10^{4} \mathrm{~g} \mathrm{O}_{2}=19 \mathrm{~kg} \mathrm{O}_{2}$

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



## 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 $\leq$ Theoretical Yield

- 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 $\left(\mathrm{C}_{3} \mathrm{H}_{8}\right)$ in excess oxygen.
$\rightarrow$ balanced equation:

$$
\mathrm{C}_{3} \mathrm{H}_{8}+5 \mathrm{O}_{2} \rightarrow 3 \mathrm{CO}_{2}+4 \mathrm{H}_{2} \mathrm{O}
$$

$\rightarrow$ mass-to-mass conversion:

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

Example: Calculate the percentage yield of carbon dioxide, if the combustion of $\mathbf{2 5 . 0} \mathbf{g}$ propane in excess oxygen yields $\mathbf{4 8 . 5} \mathbf{g}$ carbon dioxide.
$\rightarrow$ theoretical yield (from prev. problem): $\mathbf{7 4 . 9} \mathbf{g ~ C O}_{\mathbf{2}}$ $\rightarrow$ side reaction (consumes some of the propane):

$$
2 \mathrm{C}_{3} \mathrm{H}_{8}+7 \mathrm{O}_{2} \rightarrow 6 \mathrm{CO}+8 \mathrm{H}_{2} \mathrm{O}
$$

$\rightarrow$ actual yield: $\mathbf{4 8 . 5} \mathrm{g} \mathrm{CO}_{2}$
$\rightarrow$ percentage yield:

$$
\% \text { Yield }=\frac{48.5 \mathrm{~g} \mathrm{CO}_{2}}{74.9 \mathrm{~g} \mathrm{CO}_{2}} \times 100 \%=64.8 \%
$$

Example: Identify the limiting reactant in the reaction of $5.0 \mathbf{~ m o l ~ H}_{\mathbf{2}}$ with $\mathbf{3 . 0 ~ \mathbf { ~ m o l ~ }} \mathbf{N}_{\mathbf{2}}$, and determine the theoretical yield of $\mathrm{NH}_{3}$ in this reaction.
$\rightarrow$ balanced equation: $\quad \mathbf{3 H}_{\mathbf{2}}+\mathbf{N}_{\mathbf{2}} \rightarrow \mathbf{\mathbf { N H } _ { \mathbf { 3 } }}$
$\rightarrow$ calculate the theoretical yield based on each of the reactants and chose the smaller result:
$3.0 \mathrm{~mol} \mathrm{~N}_{2} \times\left(\frac{2 \mathrm{~mol} \mathrm{NH}_{3}}{1 \mathrm{~mol} \mathrm{~N}_{2}}\right)=6.0 \mathrm{~mol} \mathrm{NH}_{3}$
$5.0 \mathrm{~mol} \mathrm{H}_{2} \times\left(\frac{2 \mathrm{~mol} \mathrm{NH}_{3}}{3 \mathrm{~mol} \mathrm{H}_{2}}\right)=3.3 \mathrm{~mol} \mathrm{NH}_{3} \rightarrow$ Theor. Yield smaller amount
$\Rightarrow \mathrm{H}_{2}$ is the limiting reactant

## 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: Calculate the theoretical yield of $\mathrm{HNO}_{3}$ in the reaction of $\mathbf{2 8} \mathrm{g} \mathrm{NO}_{\mathbf{2}}$ and $\mathbf{1 8 ~ \mathrm { g } \mathrm { H } _ { \mathbf { 2 } } \mathrm { O } \text { by the }}$ chemical equation:

$$
\mathbf{3 \mathrm { NO } _ { 2 }}(\mathrm{g})+\mathrm{H}_{2} \mathrm{O}(\mathrm{l}) \rightarrow \mathbf{2} \mathrm{HNO}_{3}(\mathrm{l})+\mathrm{NO}(\mathrm{~g}) .
$$

$\rightarrow$ Calculate the theoretical yield based on each of the reactants and chose the smaller result:

$$
\begin{aligned}
& 18 \mathrm{~g} \mathrm{H}_{2} \mathrm{O} \times\left(\frac{1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}{18.0 \mathrm{~g} \mathrm{H}_{2} \mathrm{O}}\right) \times\left(\frac{2 \mathrm{~mol} \mathrm{HNO}_{3}}{1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}\right) \times \\
& \times\left(\frac{63.0 \mathrm{~g} \mathrm{HNO}_{3}}{1 \mathrm{molHNO}_{3}}\right)=130 \mathrm{~g} \mathrm{HNO}_{3}
\end{aligned}
$$

$$
\begin{aligned}
& 28 \mathrm{~g} \mathrm{NO}_{2} \times\left(\frac{1 \mathrm{~mol} \mathrm{NO}_{2}}{46.0 \mathrm{~g} \mathrm{NO}_{2}}\right) \times\left(\frac{2 \mathrm{~mol} \mathrm{HNO}_{3}}{3 \mathrm{~mol} \mathrm{NO}_{2}}\right) \times \\
& \times\left(\frac{63.0 \mathrm{~g} \mathrm{HNO}_{3}}{1 \mathrm{~mol} \mathrm{HNO}_{3}}\right)=26 \mathrm{~g} \mathrm{HNO}_{3} \rightarrow \text { Theor. Yield } \\
& \text { smaller amount } \\
& \Rightarrow \text { The smaller amount of product results } \\
& \text { from the calculation based on } \mathrm{NO}_{2} \\
& \Rightarrow \mathrm{NO}_{2} \text { is the limiting reactant and } 26 \mathrm{~g} \mathrm{HNO}_{3} \\
& \text { is the theoretical yield }
\end{aligned}
$$

