Chapter 10
Chemical Calculations and Chemical Equations

An Introduction to Chemistry
by Mark Bishop
Making Phosphoric Acid

- Furnace Process for making $\text{H}_3\text{PO}_4$ to be used to make fertilizers, detergents, and pharmaceuticals.
  - React phosphate rock with sand and coke at 2000 $^\circ$C.
    
    \[ 2\text{Ca}_3(\text{PO}_4)_2 + 6\text{SiO}_2 + 10\text{C} \rightarrow 4\text{P} + 10\text{CO} + 6\text{CaSiO}_3 \]
  - React phosphorus with oxygen to get tetraphosphorus decoxide.
    
    \[ 4\text{P} + 5\text{O}_2 \rightarrow \text{P}_4\text{O}_{10} \]
  - React tetraphosphorus decoxide with water to make phosphoric acid.
    
    \[ \text{P}_4\text{O}_{10} + 6\text{H}_2\text{O} \rightarrow 4\text{H}_3\text{PO}_4 \]
• What is the minimum mass of water that must be added to \(2.50 \times 10^4\) kg \(P_4O_{10}\) to form phosphoric acid in the following reaction?

\[
P_4O_{10} + 6H_2O \to 4H_3PO_4
\]

• The coefficients in the balanced equation provide us with a conversion factor that converts from units of \(P_4O_{10}\) to units of \(H_2O\).

\[
\left( \frac{1\ \text{mol} \ P_4O_{10}}{6\ \text{mol} \ H_2O} \right) \quad \left( \frac{1\ \text{mol} \ P_4O_{10}}{4\ \text{mol} \ H_3PO_4} \right) \quad \left( \frac{6\ \text{mol} \ H_2O}{4\ \text{mol} \ H_3PO_4} \right)
\]
Goal: To develop conversion factors that will convert between a measurable property (mass) and number of particles.

Measurable Property 1  
↓  
Number of Particles 1  
↓  
Number of Particles 2  
↓  
Measurable Property 2  
↓  
Mass 1
↓  
Moles 1
↓  
Moles 2
↓  
Mass 2
• **Tip-off** - The calculation calls for you to convert from amount of one substance to amount of another, both of which are involved in a chemical reaction.

• **General Steps**

1. If you are not given it, write and balance the chemical equation for the reaction.
2. Start your unit analysis in the usual way.

3. If you are not given grams of substance 1, convert from the unit that you are given to grams. This may take one or more conversion factors.

4. Convert from grams of substance 1 to moles of substance 1.
5. Convert from moles of substance 1 to moles of substance 2 using the coefficients from the balanced equation to create the molar ratio used as a conversion factor.

6. Convert from moles of substance 2 to grams of substance 2, using its molar mass.

7. If necessary, convert from grams of 2 to the desired unit for 2. This may take one or more conversion factors.
Equation
Stoichiometry
Steps

Given unit of substance 1
  Unit analysis conversion factors
  Grams of substance 1
    Using molar mass of substance 1: \[
    \frac{1 \text{ mol } 1}{(\text{formula mass } 1) \text{ g } 1}
    \]
    Moles of substance 1
      Using the mole ratio derived from the coefficients in the balanced equation:
      \[
      \frac{(\text{coefficient } 2) \text{ mol } 2}{(\text{coefficient } 1) \text{ mol } 1}
      \]
      Moles of substance 2
        Using molar mass of substance 2: \[
        \frac{(\text{formula mass } 2) \text{ g } 2}{1 \text{ mol } 2}
        \]
        Grams of substance 2
          Unit analysis conversion factors
          Desired unit of substance 2
Given unit of substance 1

If necessary

Mass unit of substance 1

Using \( \frac{\text{coefficient 2 (formula mass 2) (any mass unit) substance 2}}{\text{coefficient 1 (formula mass 1) (same mass unit) substance 1}} \)

Same mass unit of substance 2

If necessary

Desired unit of substance 2
Questions to Ask When Designing a Process for Making a Substance

• How much of each reactant should be added to the reaction vessel?
• What level of purity is desired for the final product? If the product is mixed with other substances (such as excess reactants), how will this purity be achieved?
Limiting Component

The wheels run out first, limiting the number of bicycles to six.

The frames are in excess.
Limiting Component (2)

\[
\left( \frac{1 \text{ bicycle}}{1 \text{ frame}} \right) \quad \text{and} \quad \left( \frac{1 \text{ bicycle}}{2 \text{ wheels}} \right)
\]

? bicycles = 7 frames \( \left( \frac{1 \text{ bicycle}}{1 \text{ frame}} \right) = 7 \) bicycles

? bicycles = 12 wheels \( \left( \frac{1 \text{ bicycle}}{2 \text{ wheels}} \right) = 6 \) bicycles
The reactant that runs out first in a chemical reaction limits the amount of product that can form. This reactant is called the \textit{limiting reactant}. 
Why substance limiting? (1)

• To ensure that one or more reactants are converted to products most completely.
  – Expense
    \[
    \text{P}_4(s) + 5\text{O}_2(g) \rightarrow \text{P}_4\text{O}_{10}(s) + \text{excess } \text{O}_2(g)
    \]
  – Importance
    \[
    \text{SiO}_2(s) + 2\text{C}(s) \rightarrow \text{Si}(l) + 2\text{CO}(g) + \text{excess } \text{C}(s)
    \]
Why substance limiting? (2)

• Concern for excess reactant that remains
  – danger
  \[ P_4(s) + 5O_2(g) \rightarrow P_4O_{10}(s) + \text{excess } O_2(g) \]
  – ease of separation
  \[ \text{SiO}_2(s) + 2C(s) \rightarrow \text{Si}(l) + 2\text{CO}(g) + \text{excess } C(s) \]
Limiting Reactant Problems

• **Tip-off** - You are given two amounts of reactants in a chemical reaction, and you are asked to calculate the maximum amount of a product that can form from the combination of the reactants.

• **General Steps**

  1. Do two separate calculations of the maximum amount of product that can form from each reactant.

  2. The smaller of the two values calculated in the step above is your answer. It is the maximum amount of product that can be formed from the given amounts of reactants.
Percent Yield

Percent Yield = \( \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\% \)

- **Actual yield** is measured. It is given in the problem.
- **Theoretical yield** is the maximum yield that you calculate.
Why not 100% Yield?

• Reversible reactions
• Side reactions
• Slow reactions
• Loss during separation/purification
Conversions to Moles

- Measurable property
- Mass
- Volume of solution
- Moles
- Moles of pure substance
- Moles of solute
Molarity

\[ \text{Molarity} = \frac{\text{moles of solute}}{\text{liter of solution}} \]

- Converts between moles of solute and volume of solution

volume 1 solution $\rightarrow$ mol 1 $\rightarrow$ mol 2 $\rightarrow$ volume 2 solution
Stoichiometry

Start here when mass of mixture is given.

\[
\frac{\text{(number from \%)} \times \text{(mass unit) \_1}}{100 \times \text{(same mass unit) total}}
\]

any mass unit \_1

\[
\frac{\text{--- g}}{\text{--- (any mass unit)}}
\]

grams \_1

\[
\frac{1 \text{ mol \_1}}{\text{(formula mass) \_1}}
\]

moles \_1

\[
\frac{\text{(number from molarity)} \times \text{mol \_1}}{1 \text{ L (or } 10^3 \text{ mL soln) \_1}}
\]

(L or mL) of solution \_1

\[
\frac{\text{--- (L or mL)}}{\text{--- (any volume unit)}}
\]

any volume unit of solution \_1

Start here when mass of pure substance is given.

\[
\frac{100 \times \text{(same mass unit) total}}{\text{(number from \%)} \times \text{(mass unit) \_2}}
\]

mass mixture with substance \_2

any mass unit \_2

\[
\frac{\text{--- (any mass unit)}}{\text{--- g}}
\]

grams \_2

\[
\frac{\text{(formula mass) \_2}}{1 \text{ mol \_2}}
\]

moles \_2

\[
\frac{1 \text{ L (or } 10^3 \text{ mL soln) \_2}}{\text{(number from molarity) \_mol \_2}}
\]

(L or mL) of solution \_2

\[
\frac{\text{--- (any volume unit)}}{\text{--- (L or mL)}}
\]

any volume unit of solution \_2

Can be converted into mass or into volume of solution.

This is the core of any equation stoichiometry problem.
• **Tip-off** - The calculation calls for you to convert from amount of one substance to amount of another, both of which are involved in a chemical reaction.

• **General Steps**
  1. If you are not given it, write and balance the chemical equation for the reaction.
  2. Start your unit analysis in the usual way.
3. Convert from the units that you are given for substance 1 to moles of substance 1.

- For pure solids and liquids, this means converting mass to moles using the molar mass of the substance.
- Molarity can be used to convert from volume of solution to moles of solute.
4. Convert from moles of substance 1 to moles of substance 2.

5. Convert from moles of substance 2 to the desired units for substance 2.
   – For pure solids and liquids, this means converting moles to mass using the molar mass of substance 2.
   – Molarity can be used to convert from moles of solute to volume of solution.

6. Calculate your answer and report it with the correct significant figures (in scientific notation, if necessary) and unit.