Working Method : how to balance chemical equations

The examples below involve reactions of metals. Metals are below and to the left of the metalloids in the periodic table.

Remember that to balance an equation you change the coefficient of a formula (add a number in front of the formula). You do not change the formula itself.

Step 1 : First balance the metallic element on each side of the equation – add a number in front of the symbol on one side if necessary, so that there is the same number of atoms of this element on each side.

Step 2 : Balance any elements that occur in only one formula on the reactant and products side. Sometimes polyatomic ions remain unchanged in reactions and they can be balanced easily at this stage.

Step 3 : Balance the remaining elements if necessary.

Example 1

The alkaline earth metal calcium reacts with water to produce an alkaline solution. Balance the following equation.

Step 1. Balance the metal Ca first. It is balanced

$$Ca(s) + H_2O(l) \rightarrow Ca(OH)_2(aq) + H_2(g)$$

Step 2. Balance O next, as it occurs in only one formula on each side. (H occurs in both products) Multiply H_2O by 2 to balance O.

$$Ca(s) + 2H_2O(l) \rightarrow Ca(OH)_2(aq) + H_2(g)$$

Step 3. You can now see that hydrogen has been balanced by step 2, which often happens. Always check to make sure.

The equation is now balanced over.

Example 2

Potassium hydroxide is a soluble base that can neutralize the diprotic acid sulfuric acid. Diprotic acids produce two hydrogen ions when they dissociate. Balance the following equation.

Step 1. Balance K by doubling KOH on the reaction side.

$$H_2SO_4(aq) + KOH(aq) \rightarrow K_2SO_4(aq) + H_2O(l)$$

Step 2. Both O and H occur in two compounds on both sides of the equation. The sulfate ion is unchanged in the reaction and is balanced, so the coefficient for H_2SO_4 will stay the same. There are 4 H atoms on the reactant side, so multiply H_2O by 2.

$$H_2SO_4(aq) + 2KOH(aq) \rightarrow K_2SO_4(aq) + H_2O(l)$$

$$H_2SO_4(aq) + 2KOH(aq) \rightarrow K_2SO_4(aq) + 2H_2O(l)$$

The equation is now balanced.

Some types of reaction

Combination or **synthesis** reactions involve the combination of two or more substances to produce a single product :

$$C(s) + O_2(g) \rightarrow CO_2(g)$$

Decomposition reactions involve a single reactant being broken down into two or more products :

$$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$$

Single replacement reactions occur when one element replaces another in a compound. An example of this type of reaction is a redox reaction :

$$Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$$

Double replacement reactions occur between ions in solution to form insoluble substances and weak or non-electrolytes, also termed **metathesis** reactions:

$$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$$

The atom economy

The global demand for goods and services along with an increasing world population, rapidly developing economies, increasing levels of pollution, and dwindling finite resources have led to a heightened awareness of the need to conserve resources. Synthetic reactions and industrial processes must be increasingly efficient to preserve raw materials and produce fewer and less toxic emissions. Sustainable development is the way of the future.

To this end the **atom economy** was developed by Professor Barry Trost of Stanford University Stanford, CA, USA. This looks at the level of efficiency of chemical reactions by comparing the molecular mass of atoms in the reactants with the molecular mass of useful compounds.

$$\text{percentage economy} = \frac{\text{mass of atoms of useful products}}{\text{Molecular mass of atoms in reactants}} \times 100\%$$

The atom economy is important in the discussion of Green Chemistry, which we will discuss later in this book. In an ideal chemical process the amount of reactants = amounts of products produced. So, an atom economy of 100% would suggest that no atoms are wasted.

Illustration : The concept of the atom economy gives the measure of the unwanted product produced in a particular reaction.

For example : Conversion of Butan-1-ol to 1-bromobutane

$$\mathbf{CH_3CH_2CH_2CH_2OH + NaBr + H_2SO_4 \rightarrow CH_3CH_2CH_2CH_2Br + NaHSO_4 + H_2O}$$

$$\%\ \text{atom economy} = \frac{\text{mass of (4C + 9H + 1Br) atoms}}{\text{mass of (4C + 12H + 50 + 1Br + 1Na + 1S) atoms}} \times 100$$

$$= \frac{137u}{275u} \times 100 = 49.81\%$$

What is the SI Unit?

SI unit is an international system of measurements that are used universally in technical and scientific research to avoid the confusion with the units. Having a standard unit system is important because it helps the entire world to understand the measurements in one set of unit systems. Following is the table with base SI units:

Property	Unit	Symbol
mass	kilogram	kg
temperature	kelvin	K
time	second	s
amount	mole	mol
electric current	ampère	A
luminosity	candela	cd
length	metre	m

Stoichiometry

A balanced chemical equation provides information about what the reactants and products are, their chemical symbols, their state of matter, and also the relative amounts of reactants and products. Chemical equations may also include specific quantitative data on the enthalpy of the reaction. Stoichiometry is the quantitative method of examining the relative amounts of reactants and products. An understanding of this is vital in industrial processes where the efficiency of chemical reactions, particularly the percentage yield, is directly linked to the success and profitability of the organization.

From a balanced chemical equation the coefficients can be interpreted as the ratio of the amount, in mol, of reactants and products. This is the equation for the reaction used for the manufacture of ammonia in the Haber process :

$$\mathbf{N_2(g) + 3H_2(g) = 2NH_3(g) \qquad \Delta \mathit{H} = -92.22\ kJ}$$

It shows that one molecule of nitrogen gas and three molecules of hydrogen gas combine in an exothermic reaction to produce two molecules of ammonia. However, when setting up a reaction the reactants may not always be mixed in this ratio - their amounts may vary from the exact stoichiometric amounts shown in the balanced chemical equation.

Stoichiometry helps us determine how much substances is needed or is present. Things that can be measured are,

1. *Reactants and products mass*
2. *Molecular weight*
3. *Chemical equation*
4. *Formulas*

In simple words, Stoichiometry as the calculation of products and reactants in a chemical reaction. It is basically concerned with numbers.

Stoichiometry is an important concept in Chemistry that helps us use balanced chemical equations to calculate amounts of reactants and products. Here, we make use of ratios from the balanced equation. In general, all the reactions that take place are dependent on one main factor, that is, how much substance is present.

Stoichiometric Coefficient

The stoichiometric coefficient or stoichiometric number is the number of molecules that participate in the reaction. If you look at any balanced reaction, you can notice that there are an equal number of elements on both sides of the equation. The stoichiometric coefficient is basically the number present in front of atoms, molecules or ions.

Stoichiometric coefficients can be fractions as well as whole numbers. In essence, the coefficients help us to establish the mole ratio between reactants and products.

Balanced Reactions and Mole Ratios

Atoms and molecules are extremely small in size, and their numbers in a very small amount of a substance are very large. Therefore, to represent atoms and molecules in bulk, a mole concept was introduced. One mole of any substance contains 6.022×10^{23} numbers of that substance. This number is also known as Avogadro's number.

The mass of one mole of a substance in grams is called molar mass.

The molar mass of one mole of a substance is numerically equal to the atomic / molecular formula mass.

Let us take one example of a balanced chemical equation,

$$\mathbf{3Fe(s) + 4H_2O(l) \rightarrow Fe_3O_4(s) + 4H_2(g)}$$

The quantitative information drawn from this balanced chemical equation is

1. 3 mole of Fe reacts with 4 moles of H_2O to yield one mole of Fe_3O_4 and 4 moles of H_2.
2. 168g (56×3) of Fe reacts with 72g(18x4) of H_2O to yield 231g of Fe_3O_4 and 8g of H_2 gas.

If the reactants and products are in gaseous form, then the molar volume is taken into consideration. One mole of any gas occupies 22.4 litres.

The limiting reagent

Experimental designers of industrial processes use the concept of a **limiting reagent** as a means of controlling the amount of products obtained. The limiting reagent, often the more expensive reactant, will be completely consumed during the reaction. The remaining reactants are present in amounts that exceed those required to react with the limiting reagent. They are said to be **in excess**.

It is the limiting reagent that determines the amount of products formed. Using measured, calculated amounts of the limiting reagent enables specific amounts of the products to be obtained. The assumption made here is that the experimental or actual yield of products achieved is identical to the theoretical or predicted yield of products. This is rarely the case. Much effort is focused on improving the yield of industrial processes, as this equates to increased profits and efficient use of raw materials.

In a chemical reaction, it is possible that one of the reactants is present in excess amount. Some of these excess reactants will, therefore, be left over when the reaction is complete; the reaction stops immediately as soon as one of the reactants is totally consumed.

The substance that is totally consumed in a reaction is called the limiting reagent.

Let us take one example of a chemical reaction to understand the limiting reagent concept.

$$\mathbf{N_2 + 3H \rightarrow 2NH_3}$$

Suppose we have one mole of N_2 reacting with one mole of H_2. But from the balanced chemical equation, one mole of N_2 requires three moles of H_2. So, the limiting reagent in this reaction is H_2.

How to find Limiting Reagent?

The determination of the limiting reactant is typically just a piece of a larger puzzle. In most limiting reactant stoichiometry problems, the real goal is to determine how much product could be formed from a particular reactant mixture. The limiting reactant or reagent can be determined by two methods.

1. *Using the mole ratio*
2. *Using the product approach*

In order to calculate the mass of the product first, write the balanced equation and find out which reagent is in excess. Using the limiting reagent calculate the mass of the product.

The following points should be considered while attempting to identify the limiting reagent :

- When there are only two reactants, write the balanced chemical equation and check the amount of reactant B required to react with reactant A. When the amount of reactant B is greater, reactant A is the limiting reagent.

- The reactant which is in a lesser amount than is required by stoichiometry is the limiting reactant.

- In an alternate method of finding the limiting reagent, the amount of product formed by each reactant is calculated.

- The limiting reactant is the reactant from which the minimum amount of product is formed.

- Also, if we calculate the amount of one reactant needed to react with another reactant, then the reactant which is in shortage would be the required limiting reactant.

Thus, the required limiting reagent for the reaction can be identified using the points provided above. These reagents are very important while calculating the percentage yield of a given reaction.

Limiting Reagent Examples

Consider 1 mol of oxygen and 1 mol of hydrogen are present to undergo the following reaction.

$$2H_2 + O_2 \rightarrow 2H_2O$$

Since the reaction uses up hydrogen twice as fast as oxygen, the limiting reactant would be hydrogen.

Example : 100g of hydrochloric acid is added to 100g of zinc. Find the volume of hydrogen gas evolved under standard laboratory conditions.

Solution :

The chemical equation for these reactions is given below.

$$2HCl(aq) + Zn(s) \rightarrow ZnCl_2(aq) + H_2(g)$$

Zinc chloride is formed in excess so the limiting reagent here is hydrochloric acid.

73g of HCl = 22.41 of H_2
100g of HCl = YL of H_2

Y/ 22.4 = 100/73
Y = (100 x 22.4) / 73
Y = 30.6L

Therefore, 33.6L of H_2 is produced under standard laboratory conditions.

Theoretical and experimental yields

The balanced chemical equation represents what is theoretically possible when a reaction is carried out under ideal conditions. It allows the expected amount of products to be calculated - the **theoretical yield**.

Scientists in industry work to maximize the yield of reactions and maximize profits. However, under experimental conditions and especially in large-scale processes, many factors result in a reduced yield of products. These factors could include :

- loss of products from reaction vessels
- impurity of reactants
- changes in reaction conditions, such as temperature and pressure
- reverse reactions consuming products in equilibrium systems
- the existence of side-reactions due to the presence of impurities.

To calculate the **percentage yield** a comparison is made between the theoretical yield and the actual amount produced in the process - the **experimental yield :**

$$\%\text{ yield} = \frac{\text{experimental yield}}{\text{theoretical yield} \times 100\%} \text{ x } 100\%$$

Worked example : determining theoretical yield

Respirators are being used increasingly with concern for workplace safety and rising levels of environmental pollution. Iodine (V) oxide, I_2O_5 reacts with carbon monoxide, CO and can be used to remove this poisonous gas from air :

$$\mathbf{I_2O_5\ (s) + 5CO(g) \rightarrow I_2(g) + 5CO_2\ (g)}$$

100.0 g of I_2O_5 reacts with 33.6 g of CO. Calculate the theoretical yield of carbon dioxide and given an experimental yield, in mol, of 0.900 mol CO calculate the percentage yield.

Solution :

Step 1 : Calculate the initial amount in mol of reactants and determine the limiting reagent:

$$n(I_2O_5) = \frac{m}{M}$$

$$\frac{(100.0g)}{(2x(126.9) + 5(16.00)\ g\ mol^{-1})}$$

$$= 0.2996\ mol$$

$$n(CO) = \frac{m}{M}$$

$$= \frac{(33.6g)}{(12.01 + 16.00\ g\ mol^{-1})}$$

$$= 1.2\ mol$$

Step 2 : Using mole ratios, determine the limiting reagent.

$$I_2O_5 : CO$$
$$1 : 5$$

$$0.3000 : \alpha = 0.3000 \times 5$$
$$\alpha = 0.3000 \times 5/1$$
$$\alpha = 1.500 \text{ mol}$$

The reaction of 0.3000 mol of I_2O_5 requires 1.50 mol of CO for completion. However, only 1.20 mol of CO is available; therefore, this is the limiting reagent.
The ratio of limiting reagent CO to product CO_2 is 5:5 or 1:1. The number of mol of CO_2 that is theoretically possible is therefore 1.2 mol.
It was found that 0.90 mol or 39.61 g of CO_2 was produced. This is the **experimental yield**.
To determine the percentage yield of CO_2 we first need to calculate the theoretical yield of CO_2 :

$$m = M \times n$$
$$= [12.01 + 2(16.00)] \text{ gmol}^{-1} \times 1.2 \text{ mol}$$
$$= 52.8 \text{ g}$$

Then :

$$\% \text{ yield} = \frac{\text{experimental yield}}{\text{theoretical yield} \times 100\%}$$

$$= \frac{(39.61\text{g})}{(52.8\text{g})\ 100\%} = 75.0\%$$

Concentration

In a typical laboratory the majority of reactions carried out are in solution rather than in the gaseous phase. Chemists need to make up solutions of known concentrations.

A **solution** is a homogenous mixture of a solute that has been dissolved in a **solvent**. The solute is usually a solid, but could be a liquid or gas. When the solvent is water the solution is described as an **aqueous solution**.

The **molar concentration** of a solution is defined as the amount (in mol) of a substance dissolved in 1 dm^3 of solvent. 1 dm^3 = 1 liter (1 L).

$$\text{concentration } c/\text{mol dm}^{-3} = \frac{\text{amount of substance } n/\text{mol}}{\text{volume of solution } V/\text{dm}^3}$$

Units of concentration

Units of concentration include :

- mass per unit volume, g dm^3
- mol per unit volume, mol dm^3
- parts per million (ppm) : one part in 1×10^6 parts.
  1 ppm = 1 mg dm^{-3}

Worked Examples : Concentration Calculation

Example 1 : Molarity of Solution

Calculate the concentration, using the unit mol dm^{-3}, of a solution formed when 0.475 g of magnesium chloride, $MgCl_2$ is completely dissolved in water to make a solution with a volume of 100 cm^3.

Solution :

$$N(MgCl_2) = \frac{m}{M} = \frac{0.475 \text{ g}}{24.34 + 2(35.45) \text{ g mol}^{-1}}$$

$$= 4.99 \times 10^{-3} \text{ mol}$$

Convert the volume in cm^3 to dm^3 :

$$100 \text{ cm}^3 \times \frac{1 \text{ dm}^3}{1000 \text{ cm}^3} = 0.1 \text{ dm}^3$$

Calculate the concentration of the solution :

$$[MgCl_2] = \frac{n}{V} = \frac{0.475 \text{ g}}{24.34 = 2(35.45) \text{ g mol}^{-1}}$$

$$= 4.99 \times 10^{-2} \text{ mol dm}^{-3}$$

Example 1 : Concentration of ions

Determine the concentration, in mol dm^{-3} of the chloride ions in examples 1 above.

Solution :

When Solid $MgCl_2$ is dissolved in water, the constitution ions are liberated :

$$\mathbf{MgCl_2\,(s) \rightarrow Mg^{2+}\,(aq) + 2Cl\,(aq)}$$

$$[Cl^-] = \frac{n}{V} = \frac{2x(4.99 \times 10^{-3}\ mol)}{0.1\ dm^3}$$

$$= 9.98 \times 10^{-2}\ mol\ dm^{-3}$$

Example 1 : Mass of Solute

Calculate the mass, in g, of potassium hydrogen phthalate, $C_8H_5O_4K$ (a primary standard) in 250 cm^3 of a 1.25 mol dm^{-3} solution.

Solution :

$$n(C_8H_5O_4K) = V \times [C_8H_5O_4K]$$

$$= 250\ cm^3 \times \frac{1\ dm^3}{1000 cm^3} \times 1.25\ mol\ dm^{-3}$$

$$= 0.313\ mol$$

$$m = n(C_3H_5O_4K) \times M$$

$$= 0.313\ mol \times [\ 8\ (12.01) + 5\ (1.01) + 4\ (16.00) + 39.10\ ]\ g\ mol^{-1}$$

$$= 63.9\ g$$

Example 1 : Concentration of Standard Solution

A standard solution is prepared by dissolving 5.30 g of sodium carbonate, Na_2CO_3 in 250 cm^3 of distilled water in a volumetric flask. A 10.0 cm^3 sample of this solution is removed by bulb pipette and diluted with water to the final volume of 0.100 dm^3. Calculate the concentration, in mol dm^3, of the diluted solution.

Solution :

First calculate $n(Na_2CO_3)$ in a 10.0 cm^3 sample of the standard solution:

$$n(Na_2CO_3) = \frac{m}{M} \times \frac{10.0\ cm^3}{250\ cm^3}$$

$$= \frac{5.30\ g}{2(22.99) + 12.01 + 3(16.00)\ g\ mol^{-1}} \times \frac{10.0\ cm^3}{250\ cm^3}$$

$$= 0.00200\ mol$$

Finally calculate the concentration of the diluted solution in mol dm^{-3} :

$$[Na_2CO_3] = \frac{n}{V} = \frac{0.00200\ mol}{0.100\ dm^3}$$

$$= 0.0200\ mol\ dm^{-3}$$

Volumetric Analysis

The volumetric analysis involves the quantitative measurement of substance in terms of volume.

Principle: In volumetric analysis, a known volume (V_1) of the substance, whose concentration (N_1) is known, is reacted with the unknown volume (V_2) of the solution of the substance, whose concentration (N_2) is to be calculated. The volume V_1 is noted at the endpoint of the reaction. The concentration N_2 is calculated using the following equation.

$$\boxed{N_1 \times V_1 = N_2 \times V_2}$$

The endpoint of such a reaction is indicated by a change in colour or precipitation etc.

Terms involved in volumetric analysis are as follows :

1. **Titration -** The process of finding out the volume of solution required to react completely with the volume of another solution is called titration.
2. **Titrant -** The solution of known strength is called titrant.
3. **Titrate -** The solution whose concentration is to be estimated is called titrate.
4. **Indicator -** Indicators are reagents which change their colour when the reaction is complete.

Worked example : acid – alkali titration calculation

Example 1 : Calculate the volume, in dm^3, of 0.390 mol dm^{-3} potassium hydroxide, KOH solution that will neutralize 25.0 cm^3 of 0.350 mol dm^{-3} sulfuric acid, H_2SO_4.

$$2KOH(aq) + H_2SO_4(aq) \rightarrow K_2SO_4(aq) + 2H_2O(l)$$

Solution :

Step 1 : Calculate the amount, in mol, of H_2SO_4 :

$$n(H_2SO_4) = c \times V$$

$$= 0.350 \text{ mol dm}^{-3} \times 0.0250 \text{ dm}^3$$

$$= 8.75 \times 10^{-3} \text{ mol}$$

Step 2 : The mole ratio of acid : alkali is 1:2. Therefore 8.75×10^{-3} mol of acid reacts with $2(8.75 \times 10^{-3}$ mol$) = 1.75 \times 10^{-2}$ mol of KOH.

Step 3 : Calculate the volume of KOH :

$$V = \frac{n}{C}$$

$$V(KOH) = \frac{1.75 \times 10^{-2} \text{ mol}}{0.390 \text{ mol dm}^{-3}}$$

Stoichiometry Problems with Solutions

1. Calculate the mass of sodium hydroxide required to make 500 ml of 0.10 M solution.

Solution :

The molar mass of NaOH = 40g

Volume of NaOH = 500ml = 0.5 L

Molarity = 0.10M

Molarity = moles / volume in litres

= weight of NaOH = molarity x molar mass of NaOH x volume

= 0.10 x 40 x 0.5

= 2 g

2. How much volume of 11M HCl has to be diluted with water to prepare 3M of 400 ml HCl?

Solution :

M_1 = 11M

M_2 = 3M

V_1 = ?

V_2 = 400 ml

Now, $M_1 \times V_1 = M_2 \times V_2$

V_1 = (3 x 400) / 11

= 109 ml

3. How many carbon atoms are present in 0.5 moles of oxalic acid ($C_2H_2O_4$)?

Solution :

1 mole of oxalic acid = 6.022×10^{23} number of oxalic acid

0.5 mole of oxalic acid = $6.022 \times 10^{23} \times 0.5$ number of oxalic acid

Since there are 2 carbon per oxalic acid,

The number of carbon atoms in 0.5 moles of oxalic acid = 6.022×10^{23}

$\times 0.5 \times 2$

$= 6.022 \times 10^{23}$

4. 0.5216g of a solid mixture containing Na_2SO_4 is dissolved in water and treated with an excess of $BaCl_2$, resulting in the precipitation of 0.6168g What percentage of the mixture was $BaSO_4$?

Solution :

$Na_2SO_4 + BaCl_2 \rightarrow BaSO_4 + 2NaCl$

233g of BaSO4 is obtained from 142g of Na_2SO_4

So, 0.6168g of $BaSO_4$ is obtained from = $(142 \times 0.6168) / 233$

$= 0.37g$

Since the mass of the solid mixture is 0.5216 g,

The percentage of $BaSO_4$ is solid mixture = $(0.37/0.5216) \times 100$

$= 70.34\%$

5. **A solution containing 5 g of KOH and $Ca(OH)_2$ is neutralized by an acid. If it consumes 0.1 g equivalents of the acid, calculate the composition of the solution.**

Solution :

Let the mass of KOH present in mixture = x

Mass of $Ca(OH)_2$ = (5-x)g

Equivalent mass of KOH = 56; Equivalent mass of $Ca(OH)_2$ = 37

Gram equivalent of KOH + Gram equivalent of $Ca(OH)_2$ = Gram equivalent of acid

$$\frac{x}{56} + \frac{(5-x)}{37} = 0.1$$

⇨ x = 3.83g

Mass of KOH in the sample = 3.83g

Percentage of KOH = (3.83/5) x 100

= 76.6%

Percentage of $Ca(OH)_2$ = (1.17/5) x100

= 23.4%

6. **How many ml of 0.45 m HCl must be added to 25 ml of 1.00 m KOH to make neutral solution?**

Solution :

1. Write balanced equation :

$HCl + KOH \rightarrow KCl + H_2O$

0.4m 9.00m

? ml 25ml

2. Find moles of known solution :

Here, KOH is the known solution.

$$\text{Molarity, } M = \frac{\text{Moles}}{\text{Volume in litre}}$$

$$\text{Moles} = M \times L = 1.00M \times 0.0025\ L$$

$$= 0.025 \text{ mol KOH}$$

3. Use mole ratio to find moles of unknown solution :

$$0.025 \text{ mol KOH} \times \frac{1 \text{ mol HCl}}{1 \text{ mol KOH}} = 0.025 \text{ mol KOH}$$

[As, 1 mol KOH gets neutralized by 1 mol HCl]

4. Solve the unknown solution :

Here, HCl is the unknown solution.

$$M = \frac{m}{L}\ ;\ L = \frac{m}{M} = \frac{0.025 \text{ mol HCl}}{0.45 \text{ M HCl}} = 0.056\ L = 56\ ml$$

Therefore, 56 ml of 0.45m HCl will be needed to neutralize 25 ml of 1.00m KOH.