1: Relative formula mass

- Relative formula mass (M_r) is just the sum of all the atomic masses (A_r) added together. E.g. $MgCl_2$ = 95.
- The percentage mass of an element in a compound is a way of saying what proportion of the mass of the compound is due to atoms of that element.

$$\text{Percentage mass of an element in a compound} = \frac{A_r \times \text{number of atoms of that element}}{M_r \text{ of the compound}} \times 100$$

Example

Find the percentage mass of magnesium in magnesium oxide, MgO.
Relative atomic masses (A_r): Mg = 24, O = 16

MATHS SKILLS

M_r of MgO = 24 + 16 = 40

$$\% \text{ mass of Mg} = \frac{A_r \text{ of Mg} \times \text{No. of Mg atoms}}{M_r \text{ of MgO}} \times 100 = \frac{24 \times 1}{40} \times 100 = 60\%$$

So magnesium makes up 60% of the mass of magnesium oxide.

5: Limiting Reactants

When a reaction happens, it will stop when one of the reactants ahs been used up. This is called the limiting reactant and all the others are excess. The amount of product formed is directly proportional to the amount of limiting reactant. This is because, if you add more of the limiting reactant, there will be more reactant particles to take part in the reaction, which means more product particles can form. We can use this to calculate the mass of a product formed.

Example 1 **Higher**

What mass of calcium chloride ($CaCl_2$) is produced when 3.7 g of calcium hydroxide ($Ca(OH)_2$) reacts with an excess of hydrochloric acid (HCl)?

MATHS SKILLS

1. The balanced symbol equation for this reaction is:

   $$Ca(OH)_2 + 2HCl \rightarrow CaCl_2 + 2H_2O$$

2. The limiting reactant is $Ca(OH)_2$. The product you want is $CaCl_2$.

   M_r of $Ca(OH)_2$ = 40 + (2 × (16 + 1)) = 74
   M_r of $CaCl_2$ = 40 + (2 × 35.5) = 111

3. Calculate the number of moles of calcium hydroxide in 3.7 g.

   Number of moles = mass ÷ M_r = 3.7 ÷ 74 = 0.050 mol

4. Look at the ratio of moles in the equation to work out how many moles of calcium chloride will be formed.

   1 mole of $Ca(OH)_2$ reacts to produce 1 mole of $CaCl_2$ — the same number of moles are produced. So 0.05 moles of $Ca(OH)_2$ will react to produce 0.05 moles of $CaCl_2$.

5. Calculate the mass of $CaCl_2$ produced.

   mass = moles × M_r = 0.050 × 111 = 5.6 g

2: The Mole

A mole is just a number of particles and is 6.02×10^{23}. It is also called Avogadro's number. The mass of 1 mole of a substance is the same as the number of grams of the M_r. You can find moles using the equation:

$$\text{Number of moles} = \frac{\text{Mass in g (of element or compound)}}{M_r \text{ (of element or compound) or } A_r \text{ (of element)}}$$

Example 2 **Higher**

How many moles are there in 66 g of carbon dioxide (CO_2)?

MATHS SKILLS

M_r of CO_2 = 12 + (16 × 2) = 44

$$\text{No. of moles} = \frac{\text{mass}}{M_r} = \frac{66}{44} = 1.5 \text{ mol}$$

Chemistry

3. Quantitative Chemistry

Amounts of substances

Example 1 **Higher**

8.1 g of zinc oxide (ZnO) reacts completely with 0.60 g of carbon to form 2.2 g of carbon dioxide and 6.5 g of zinc. Write a balanced symbol equation for this reaction.
Relative atomic masses, A_r: C = 12, O = 16, Zn = 65.

MATHS SKILLS

1. First work out M_r (or A_r) for each of the substances in the reaction:

   ZnO: 65 + 16 = 81 C: 12 CO_2: 12 + (2 × 16) = 44 Zn: 65

   Then divide the mass of each substance by its M_r to calculate how many moles of each substance reacted or were produced:

   ZnO: $\frac{8.1}{81}$ = 0.10 mol C: $\frac{0.60}{12}$ = 0.050 mol

   CO_2: $\frac{2.2}{44}$ = 0.050 mol Zn: $\frac{6.5}{65}$ = 0.10 mol

2. Divide by the smallest number of moles, which is 0.050:

   ZnO: $\frac{0.10}{0.050}$ = 2.0 C: $\frac{0.050}{0.050}$ = 1.0

   CO_2: $\frac{0.050}{0.050}$ = 1.0 Zn: $\frac{0.10}{0.050}$ = 2.0

3. The numbers are all whole numbers, so you can write out the balanced symbol equation straight away.

4. So the balanced equation is: $2ZnO + C \rightarrow CO_2 + 2Zn$

3: Conservation of Mass

During chemical reactions, things don't just disappear or appear, the same number of atoms are always present. We show this with the conservation of mass:

During a chemical reaction, no atoms are made or destroyed, so the mass of the products is the same as the mass of the reactants.

This can also be shown with a balanced symbol equation – the M_r on both sides should be equal. We can use this idea to work out the mass of individual reactants and products in reaction. E.g.

Example 1

6 g of magnesium completely reacts with 4 g of oxygen. What mass of magnesium oxide is formed?

MATHS SKILLS

The total mass of the reactants is 4 + 6 = 10 g, so the mass of the product (magnesium oxide) must be 10 g.

However, in some reactions, mass will change.
If a mass seems to increase, it is probably because at least one of the reactants is a gas that is found in air and all the products are either solids, liquids or in an aqueous solution. (The particles in a gas move around, so before the reaction, you can't account for its mass. When it reacts to form a product, the particles become contained, so the mass is counted)
If a mass seems to decrease, it is probably because one of the products is a gas and all of the reactants are solids, liquids, or aqueous. (Before the reaction, all the masses are contained. When a gas is produced, it can escape as it flows free, so its mass can't be counted).

4: The Mole and Equations

In chemical equations, the 'big numbers' in front of the chemical formulas tell you the relative numbers of moles of each reactant and product in the reaction. The 'little numbers' tell you how many atoms of each element there are in the smallest unit of the substance. The ratio of moles of reactants and products always stays the same.

Example 1 **Higher**

How many moles of water are formed if 2 moles of methane combust completely in oxygen? The balanced equation for this reaction is: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

MATHS SKILLS

From the balanced equation, you can see that 1 mole of methane reacts to form 2 moles of water, so the molar ratio is 1:2. So 2 moles of methane will react to form (2 × 2) = 4 moles of water.

We can also use moles to help us balance equations.

1: Concentrations

Lots of reactions in chemistry take place between substances that are dissolved in a solvent to form a solution. The amount of a substance in a certain volume of a solution is called its concentration. The greater the mass of solute in a given volume, the higher the concentration. So, if you take a solution and dissolve more of the solute in it, the concentration will increase. If you do anything to increase the volume, without increasing the amount of solute then the concentration will decrease.

$$\text{concentration (g/dm}^3) = \frac{\text{mass of solute (g)}}{\text{volume of solution (dm}^3)}$$

Example 2

What's the concentration in g/dm³ of iron chloride solution where 10 g of iron chloride is dissolved in 25 cm³ of water?

First, change the units of volume from cm³ to dm³.

volume = 25 ÷ 1000 = 0.025 dm³

Then use the equation to find the concentration of the solution.

$$\text{concentration} = \frac{10}{0.025} = 400 \text{ g/dm}^3$$

All measurements have some uncertainty to them, so will often be repeated to find the average result. The range can also be found – the higher the range, the more uncertain the results are.

2: More on Concentrations

Concentration can also be found with the equation:

$$\text{concentration (mol/dm}^3) = \frac{\text{amount of solute (mol)}}{\text{volume of solution (dm}^3)}$$

However, sometimes, the amount of solute given is in grams. We can work out the concentration in mol/dm³ by using this equation:

$$\text{concentration (mol/dm}^3) = \frac{\text{concentration (g/dm}^3)}{M_r}$$

If you didn't want to do this at the end, then you could of also converted the grams to moles at the start by using the equation:

Moles = Mass/Mr

3: Concentration Calculations

You can find the volume needed for 2 solutions to react together completely using an experiment called a titration. If you know the concentration of one of the solutions, you can use the volumes from the titration experiment, along with the reaction equation, to find the concentration of the other solution. You could be asked to work out the concentration in mol/dm³ or g/dm³

Example **Higher**

You can find the concentration of the acid in the previous example in g/dm³.

Step 1: Work out the relative formula mass of sulfuric acid:
M_r of H_2SO_4 = (1 × 2) + 32 + (16 × 4) = 98

Step 2: Convert the concentration from mol/dm³ to g/dm³.
Concentration (g/dm³) = concentration (mol/dm³) × M_r
= 0.0417 mol/dm³ × 98 = 4.09 g/dm³

Chemistry

3. Quantitative Chemistry

Amounts of substances – Concentration

Example **Higher**

What's the concentration, in mol/dm³, of a solution containing 3.7 g of calcium hydroxide ($Ca(OH)_2$) in 0.25 dm³?

Find the number of moles of calcium hydroxide:

$M_r(Ca(OH)_2)$ = 40 + 2 × (16 + 1) = 74

moles = mass ÷ M_r = 3.7 ÷ 74 = 0.050 mol

Now you've got the number of moles and the volume, just stick them in the formula:

Concentration = 0.050 ÷ 0.25 = 0.20 mol/dm³

Examples **Higher**

- The concentration of a 270 g/dm³ solution of magnesium sulfate ($MgSO_4$, M_r = 120) in mol/dm³ is 270 ÷ 120 = 2.25 mol/dm³.
- The concentration of a 0.15 mol/dm³ solution of potassium hydroxide (KOH, M_r = 56) in g/dm³ is 0.15 × 56 = 8.4 g/dm³.

Example **Higher**

In an experiment, 25.0 cm³ of a 0.100 mol/dm³ solution of sodium hydroxide (NaOH) is neutralised by 30.0 cm³ of sulfuric acid (H_2SO_4) with an unknown concentration.

You can work out the concentration of the acid in moles per dm³.

Step 1: Work out how many moles of sodium hydroxide you have:
Number of moles = concentration (mol/dm³) × volume (dm³)
You need to know the volume in dm³, so first convert 25.0 cm³ into dm³ by dividing by 1000: 25.0 cm³ ÷ 1000 = 0.0250 dm³
Number of moles = concentration × volume
= 0.100 mol/dm³ × 0.0250 dm³
= 0.00250 moles of NaOH

Step 2: Write down the balanced equation for the reaction.
$$2NaOH + H_2SO_4 \rightarrow Na_2SO_4 + 2H_2O$$
Using the equation, you can see that for every two moles of sodium hydroxide there is one mole of sulfuric acid. So if you had 0.00250 moles of sodium hydroxide you must have had 0.00250 ÷ 2 = 0.00125 moles of sulfuric acid.

Step 3: Work out the concentration of the sulfuric acid.
Concentration (mol/dm³) = number of moles ÷ volume (dm³)
You need to know the volume of acid in dm³, so start by converting 30.0 cm³ into dm³ by dividing by 1000:
30.0 cm³ ÷ 1000 = 0.0300 dm³.
Concentration (mol/dm³) = number of moles ÷ volume (dm³)
= 0.00125 mol ÷ 0.0300 dm³ = 0.0417 mol/dm³

6: Volume of gases

At the same temperature and pressure, equal numbers of moles of any gas will occupy the same volume. At room temperature and pressure (r.t.p. = 20°C and 1atm) one mole of any gas occupies 24 dm³.

$$\text{Volume of gas (dm}^3) = \frac{\text{Mass of gas (g)}}{M_r \text{ of gas}} \times 24$$

Examples **Higher**

- At r.t.p., 24 g of oxygen (O_2) will occupy $\frac{24}{32} \times 24 = 18$ dm³.
- At r.t.p., 14.2 g of chlorine (Cl_2) will occupy $\frac{14.2}{71} \times 24 = 4.8$ dm³.

For reactions between gases, you can use the volume of 1 gas to find the volume of another. You just need to look at the molar ratio of the gases in the balanced equation – this will be the same as the ratio of the volumes of the gases in the reaction.

Example 1 **Higher**

How much carbon dioxide is formed when 30 dm³ of oxygen reacts with carbon monoxide? $2CO_{(g)} + O_{2(g)} \rightarrow 2CO_{2(g)}$

From the balanced equation, 1 mole of O_2 reacts to form 2 moles of CO_2. This means that the ratio of the volumes of O_2:CO_2 is 1:2.

So 30 dm³ of O_2 reacts to form (2 × 30 dm³) = 60 dm³ of CO_2

1: Atom Economy

The atom economy of a reaction tells you what percentage of the mass of the reactants ends up as useful products when manufacturing a chemical. From this, you can also work out what percentage is wasted. 100% atom economy means that all the atoms in the reactants have been turned into useful (desired) products. The higher the atom economy the 'greener' the process.

$$\text{atom economy} = \frac{\text{relative formula mass of desired products}}{\text{relative formula mass of all reactants}} \times 100$$

Example

a) Calculate the atom economy of the following reaction to produce magnesium chloride: $MgO_{(s)} + 2HCl_{(aq)} \rightarrow MgCl_{2(aq)} + H_2O_{(l)}$

Here, the desired product is magnesium chloride.

$M_r(MgO) = 24 + 16 = 40$ $\quad M_r(HCl) = 1 + 35.5 = 36.5$

M_r of all reactants $= 40 + (2 \times 36.5) = 113$

M_r of the desired product is $M_r(MgCl_2) = 24 + (2 \times 35.5) = 95$

$$\text{Atom economy} = \frac{\text{relative formula mass of desired products}}{\text{relative formula mass of all reactants}} \times 100$$

$$= \frac{95}{113} \times 100 = 84\%$$

b) Calculate the percentage mass wasted in this reaction.

Percentage mass wasted = 100 – 84 = 16%

Reactions with only one product always have an atom economy of 100%, as all the reactants end up as the 'useful' product.

Companies in the chemical industry will often choose to use reaction with few products, as they have high atom economies, which have environmental and economic benefits.

- **Economic Advantages**

Reactions with low atom economy aren't usually profitable, as they need lots of raw materials to produce a certain amount of the desired product. Raw materials are very expensive to buy, and the waste products are also very expensive to remove and dispose of – meaning that reactions with a high atom economy are cheaper.

- **Environmental Advantages**

Reactions with high atom economy use fewer raw materials, which will run out eventually so need to be used efficiently. They also produce a lot less waste, which is better for the environment as waste chemicals are often harmful and can be difficult to dispose of in a way that minimizes their harmful effects.

2: Percentage Yield

Percentage yield is a measure of the amount of product you'd expect to get from a reaction compared to the amount of product that's formed. It is always somewhere between 0% and 100%. You can always calculate the percentage yield if you know the theoretical yield and the actual yield of a reaction.

The theoretical yield of a reaction is the amount you would get if all the reactants formed the desired products and none were wasted. This can be calculated from the balanced reaction equation, or from the masses of the reactants.

The amount of product you get in the reaction is known as the yield. The yield depends on the amount of reactant that you start with and the method that you use.

Chemistry
3. Quantitative Chemistry
Atom Economy and Yield

3: Reactions and Industry

Industrial reactions are carried out on a much bigger scale, so they are a lot more expensive and produce a lot more waste. When choosing which reaction to use to make a substance, industries need to consider several factors to make sure the process is economical and sustainable.

1) Atom Economy - Reactions with high atom economy use less raw materials and have less waste.
2) Yield – Reactions with a high percentage yield have less wasted products and are more sustainable.
3) Rate – The rate of reactions is how quickly the reaction happens to form the products. This needs to be at a reasonable rate in industrial processes.
4) Equilibrium position – In a reversible reaction, the point where the rate of reaction between the reactants and products is equal, is known as equilibrium. Being able to control the position of equilibrium to maximize the amount of product, makes industrial processes profitable – if the amount of products is high and amount of reactants left low.
5) Usefulness of by-products – By-products are things produced by chemical reactions that aren't 'desired'. Often, they are waste, but sometimes they are useful for something else. So, one way to reduce waste in a reaction, is to choose one that forms useful by-products as well as the intended product.

$$\text{percentage yield} = \frac{\text{mass of product actually made (g)}}{\text{maximum theoretical mass of product (g)}} \times 100$$

Example

A reaction with a theoretical yield of 36 g only made 28.2 g of product. Calculate the percentage yield of the reaction.

$$\text{Percentage yield} = \frac{\text{mass of product actually made (g)}}{\text{maximum theoretical mass of product (g)}} \times 100$$

$$= \frac{28.2}{36} \times 100$$

$$= 78\%$$

Even though no atoms are made or destroyed in reactions, in real life, you will never get a 100% yield. Some product or reactant will always get lost along the way. How this happens depends on what sort of reaction it is and what apparatus is being used. The 3 common problems are:

1) The reaction is reversible

A reversible reaction is one where the products of the reaction can react themselves to produce the original reactants. They are shown like this: $A + B \rightleftharpoons C + D$

If a reaction is reversible, it means that the reactants will never be completely converted to products because the reaction goes both ways. Some of the products are always reacting together to change back to the original reactants. This will mean a lower yield.

2) Product is lost when it's separated from the reactants.

When you filter a liquid to remove solid particles, you nearly always lose a bit of liquid or solid. If you want to keep the liquid, you'll lose the bit that remains with the filter paper and solid (as they are always a bit wet). If you want to keep the solid, some of it will get left behind when it is scraped off the filter paper. Material can also sometimes be lost when transferring it from one container to the next.

3) Unexpected reactions may be happening

Sometimes there can be other unexpected reactions happening, known as side-reactions. For example, the reactants may react with gases in the air, or impurities in the reaction mixture, rather than reacting to form the product you want. Again, this means a lower yield.

Example **Higher**

One of the reactions used in the production of nylon gives ammonium sulfate as a by-product. Ammonium sulfate can be used as a fertiliser, so even though it's not the desired product of this reaction, it's still a useful by-product, rather than waste.