

1) Getting the most from reactants

a) The chemical industry

- Industrial processes are designed to maximise profit and minimise the impact on the environment.
- Factors influencing process design include: availability, sustainability and cost of feedstock(s); opportunities for recycling; energy requirements; product yield; marketability of by-products.
- Environmental considerations include: minimising waste; avoiding the use or production of toxic substances; designing products which will biodegrade if appropriate.

b) Chemical calculations

- Balanced equations show the mole ratio(s) of reactants and products. Using the balanced equation and the gram formula masses (GFM), mass to mass calculations can be performed.
- The quantity of a reactant or product can also be expressed in terms of moles. The concentration of a solution can be expressed in mol l<sup>-1</sup>.
- Balanced equations can be used in conjunction with concentrations and volumes of solutions and/or masses of solutes to determine quantities of reactants and/or products.

c) Molar volume

- The molar volume (in units of litres mol<sup>-1</sup>) is the same for all gases at the same temperature and pressure. The volume of a gas can be calculated from the number of moles and vice versa.
- The volumes of reactant and product gases can be calculated from the number of moles of each reactant and product.

d) Percentage yield

- The efficiency with which reactants are converted into the desired product is measured in terms of the percentage yield and atom economy.
- Percentage yields can be calculated from mass of reactant(s) and product(s) using a balanced equation.
- Given costs for the reactants, a percentage yield can be used to calculate the feedstock's cost for producing a given mass of product.

e) Atom economy

- The atom economy measures the proportion of the total mass of all starting materials successfully converted into the desired product.
- It can be calculated using the formula shown below in which the masses of products and reactants are those appearing in the balanced equation for the reaction.
- Atom Economy = (mass of desired product(s) / total mass of reactants) x 100.
- Reactions which have a high percentage yield may have a low atom economy value if large quantities of unwanted by-products are formed.

### f) Excess

- In order to ensure that costly reactant(s) are converted into product, an excess of less expensive reactant(s) can be used.
- By considering a balanced equation, the limiting reactant and the reactant(s) in excess can be identified.
- Whilst the use of excess reactants may help to increase percentage yields, this will be at the expense of the atom economy so an economic / environmental balance must be struck.

## 2) Chemical Equilibria

- Many reactions are reversible, so products may be in equilibrium with reactants.
- At equilibrium, the concentrations of reactants and products remain constant, but are rarely equal.
- This may result in costly reactants failing to be completely converted into products.
- In a closed system, reversible reactions attain a state of dynamic equilibrium when the rates of forward and reverse reactions are equal.
- Le Chatelier's principle states that if the conditions of a chemical system at equilibrium are changed, the system responds by minimising the effect of the changes.
- Changes in concentration, pressure and temperature can alter the position of equilibrium.
- To maximise profits, chemists employ strategies to move the position of equilibrium in favour of products.
- A catalyst increases the rate of attainment of equilibrium but does not affect the position of equilibrium. The effects of altering pressure, altering temperature, the addition or removal of reactants or products can be predicted for a given reaction.

## 3) Chemical energy

### a) Chemical energy

- For industrial processes, it is essential that chemists can predict the quantity of heat energy taken in or given out.
- If reactions are endothermic, costs will be incurred in supplying heat energy in order to maintain the reaction rate.
- If reactions are exothermic, the heat produced may need to be removed to prevent the temperature rising.

### b) Enthalpy

- Chemical energy is also known as enthalpy.
- The change in chemical energy associated with chemical reactions can be measured. The specific heat capacity, mass and temperature can be used to calculate the enthalpy change for a reaction.
- The enthalpy of combustion of a substance is the enthalpy change when one mole of the substance burns completely in oxygen.
- These values can often be directly measured using a calorimeter and values for common compounds are available from data books and online databases for use in Hess's law calculations.

#### c) Hess's law

- Hess's law states that the enthalpy change for a chemical reaction is independent of the route taken.
- Enthalpy changes can be calculated by applying Hess's law.

#### d) Bond enthalpies

- For a diatomic molecule, XY, the molar bond enthalpy is the energy required to break one mole of XY bonds.
- Mean molar bond enthalpies are average values which are quoted for bonds which occur in different molecular environments.
- Bond enthalpies can be used to estimate the enthalpy change occurring for a gas phase reaction by calculating the energy required to break bonds in the reactants and the energy released when new bonds are formed in the products.

### 4) Oxidising or reducing agents

#### a) Elements as oxidising or reducing agents

- A redox reaction is a reaction in which reduction and oxidation occur together, reduction being the gain of electrons by a reactant and oxidation being the loss of electrons by a reactant in a reaction.
- An oxidising agent is a substance which accepts electrons.
- A reducing agent is a substance which donates electrons.
- Oxidising and reducing agents can be identified in redox reactions.
- Elements with low electronegativities (metals) tend to form ions by losing electrons (oxidation) and so can act as reducing agents.
- The strongest reducing agents are found in Group 1.
- Elements with high electronegativities (non-metals) tend to form ions by gaining electrons (reduction) and so can act as oxidising agents.
- The strongest oxidising agents come from Group 7.
- The electrochemical series indicates the effectiveness of oxidising and reducing agents.

#### b) Compounds as oxidising or reducing agents

- Compounds can also act as oxidising or reducing agents.
- Electrochemical series contain a number of ions and molecules.
- The dichromate and permanganate ions are strong oxidising agents in acidic solutions whilst hydrogen peroxide is an example of a molecule which is a strong oxidising agent.
- Carbon monoxide is an example of a gas that can be used as a reducing agent.
- Oxidising and reducing agents can be selected using an electrochemical series from a data booklet or can be identified in the equation showing a redox reaction.

#### c) Use of oxidising agents

- Oxidising agents are widely employed because of the effectiveness with which they can kill fungi and bacteria, and can inactivate viruses.
- The oxidation process is also an effective means of breaking down coloured compounds making oxidising agents ideal for use as 'bleach' for clothes and hair.

#### d) Ion-electron equations

- Oxidation and reduction reactions can be represented by ion-electron equations.
- When molecules or group ions are involved, if the reactant and product species are known, a balanced ion-electron equation can be written by adding appropriate numbers of water molecules, hydrogen ions and electrons.
- Ion-electron equations can be combined to produce redox equations.

#### e) Practical applications

- Displacement reactions are example of redox reactions and oxidising and reducing agents can be identified in these and other redox reactions.
- The technique of titration can be applied to redox reactions, allowing the concentration of a reactant to be calculated from results of volumetric titrations. A potential energy diagram can be used to show the energy pathway for a reaction.

### 5) Chemical Analysis

#### a) Chromatography

- in chromatography, differences in the polarity / size of molecules are exploited to separate the components present within a mixture;
- depending on the type of chromatography in use, the identity of a component can be indicated either by the distance it has travelled or by the time it has taken to travel through the apparatus (retention time);
- the results of a chromatography experiment can sometimes be presented graphically showing an indication of the quantity of substance present on the y-axis and retention time on the x-axis.

Note: Learners are not required to know the details of any specific chromatographic method or experiment

#### b) Volumetric analysis

- volumetric analysis involves using a solution of accurately known concentration in
- a quantitative reaction to determine the concentration of another substance;
- a solution of accurately known concentration is known as a standard solution;
- the volume of reactant solution required to complete the reaction is determined by titration;
- calculations from balanced equations can then be carried out to calculate the concentration of the unknown solution;
- redox titrations are based on redox reactions;
- substances such as potassium permanganate(VII), which can act as their own indicators, are very useful reactants in redox titrations;
- the concentration of a substance can be calculated from experimental results by use of a balanced equation