Reversible Reactions

Reversible Reactions Go **Both Ways**

In a reversible reaction, the **products** can react with each other and **change back** into the reactants.

Reactants		Products
A + B	$\rightleftharpoons$	C + D

So there are actually two reactions happening at once: A + B → C + D and C + D → A + B. This can affect the **yield** of a reaction, as some of the products will be converted **back** into reactants.

EXAMPLE: The industrial production of ethanol from ethene.

exothermic →

$$H_2C{=}CH_{2(g)} + H_2O_{(g)} \rightleftharpoons CH_3CH_2OH_{(g)}$$

← endothermic

Catalyst: H_3PO_4
Temperature: 300 °C
Pressure: 60 atm

Because the reaction is reversible you **don't** get a **high yield** — some of the ethanol **converts back** to ethene and water. But you can keep **removing** and **recycling** any ethene that you have left, so you can still end up with a good overall yield.

Reversible Reactions Reach an **Equilibrium**

If a reversible reaction is taking place in a **closed system** it will eventually reach a state of **equilibrium**.

A **closed system** is one where nothing can **get in** or **out**.

1) When a reaction **begins** there will be a **high concentration** of **reactants**, and a **low concentration** of **products** in the system. So the **forward** reaction will be **fast**, and the **reverse** reaction quite **slow**.
2) The concentration of **reactants** will gradually **decrease**, while the products build up. So the **forward** reaction will start to **slow down** while the **reverse** reaction **speeds up**.
3) After a while the forward reaction and the reverse reaction end up going at the **same rate**. From this point on the **concentration** of the **reactants** and **products won't change**.
4) This is called **dynamic equilibrium**. The forward and reverse reactions are **both still happening** — some reactant is being made into product, and some product is being made into reactant.
5) But since these processes are going at **exactly the same rate**, it seems as if nothing's happening.

Dynamic equilibrium — like walking up a down escalator...

1) Compare the rates of the forward and backward reactions of a reversible reaction at the following points:
 a) At the start of the reaction.
 b) At equilibrium.
2) What is dynamic equilibrium?

Le Chatelier's Principle

***Position** of Equilibrium*

The **position** of equilibrium tells you the amount of **reactants compared** to the amount of **products** that are present when the reaction reaches an **equilibrium.**

Reactants Products

$$A + B \rightleftharpoons C + D$$

If the position of equilibrium lies on the **left-hand side**, there are **more reactants** than products in the reaction mixture.

If the position of equilibrium lies on the **right-hand side**, there are more **products** than reactants in the reaction mixture.

*Changing **Conditions** Changes the **Equilibrium Position***

Altering the conditions of a reversible reaction can **move** the position of equilibrium in one direction or the other. Careful control of the conditions can result in a higher yield (more of the products).

Look at the production of ethanol from ethene again as an example:

$$H_2C{=}CH_{2(g)} + H_2O_{(g)} \underset{\text{endothermic}}{\overset{\text{exothermic}}{\rightleftharpoons}} CH_3CH_2OH_{(g)}$$

1) If you increase the **pressure**, conditions will favour the forward reaction and **more ethanol** (CH_3CH_2OH) will be formed.
   This is because there are **more molecules** of gas on the **left-hand side** than on the right-hand side — two molecules of $H_2C{=}CH_2$/H_2O react to form **only one** molecule of CH_3CH_2OH. This **reduces** the pressure.
2) Raising the **temperature** favours the **reverse** reaction. This is because it's **endothermic** (see page 41) and **absorbs** the extra heat energy, **lowering** the temperature.
3) **Removing ethanol** from the container as it forms will push the equilibrium to the **right** to try and make up for the change in concentration between the reactants and products.

These observations can be summarised by an important rule known as **Le Chatelier's Principle**:

A **reversible reaction** will move its **equilibrium position** to **resist** any **change** in the conditions.

Equilibrium reactions are so stubborn — always resisting change...

1) You are making ethanol from ethene and steam using the reaction shown above. What will happen to the yield of ethanol if you increase the amount of steam in the reaction mixture?
2) Ammonia is produced industrially using the following reversible reaction:
   $$N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)}$$
   The forward reaction is exothermic and the backwards reaction is endothermic.
   How will the position of the equilibrium change if you:
   a) Increase the temperature of the reaction?
   b) Remove some ammonia from the reaction?

Equilibrium and Yield

Deciding on the Best Conditions to Use

Thanks to Le Chatelier's principle (see page 35) you might think it would be **easy** to work out the **optimum conditions** for a reversible reaction. But in real life it's not quite that simple.

For most reversible reactions that are used on an industrial scale there are other factors, such as **cost** and **time**, that need to be taken into account.

Have a look at the conditions used for the production of ethanol from ethene again:

$$H_2C{=}CH_{2(g)} + H_2O_{(g)} \underset{\text{endothermic}}{\overset{\text{exothermic}}{\rightleftharpoons}} CH_3CH_2OH_{(g)}$$

Catalyst: H_3PO_4
Temperature: 300 °C
Pressure: 60 atm

Temperature:

1) **Lowering the temperature** would favour the forward reaction and so it should increase the **yield** of ethanol.
2) But lowering the temperature also means that fewer of the particles in the reaction mixture will have **enough energy** to react (see page 32). The particles will also be moving **more slowly**, so there will be **fewer collisions**. So lowering the temperature will **slow down** the **rate** of both the forward and reverse reactions.
3) A low temperature would make the forward reaction **too slow** to be useful. So a compromise temperature of **300 °C** is used.

Pressure:

1) **Increasing the pressure** would favour the forward reaction and increase the **rate** of reaction (as the particles will be **closer together** so will collide **more frequently**). This would increase the **yield** of ethanol.
2) But producing high pressures uses a lot of **energy** and **costs** a lot of money. You'd need some pretty strong equipment to stand up to the high pressures too — and that would be expensive to buy and maintain.
3) To make the reaction economic, a moderately high pressure of **60 atm** is used.

Concentration:

1) Ethanol is **removed** from the reaction vessel as it is produced.
2) This reduces the concentration of products so the equilibrium shifts to favour the **forwards reaction**. This **improves** the **yield** of ethanol.

Catalyst:

1) Using a solid **phosphoric acid(V)** catalyst **increases** the rate of **both** the forward and the backward reactions.
2) The catalyst has **no effect** on the **position** of the equilibrium — it just means the equilibrium is reached **faster** and the **temperature** and **pressure** at which the reaction can happen, at a reasonable rate, are **reduced.**

I should put a dodgy pun here, but I won't yield to the pressure...

1) Explain why the reaction above is not run industrially at a temperature of 40 °C.
2) Explain why the reaction above is not run industrially at a pressure of 500 atm.

The Mole

A Mole is a Number of Particles

If you had a sample of a substance, and you wanted to **count** the number of atoms that were in it, you'd have to use some very **big numbers**, and spend a very long time counting. So you need a **unit** to describe the **amount** of a substance that you have — that unit is the **mole.**

One mole of a substance contains $\mathbf{6.02 \times 10^{23}}$ particles.
6.02×10^{23} mol^{-1} is known as **Avogadro's constant**.

The particles can be **anything** — e.g. atoms or molecules (or even giraffes).
So 6.02×10^{23} atoms of **carbon** is 1 mole of carbon,
and 6.02×10^{23} molecules of CO_2 is 1 mole of CO_2.

Molar Mass is the Mass of One Mole

One mole of atoms or molecules has a **mass in grams** equal to the **relative formula mass** (A_r or M_r) of that substance.

For **carbon**, A_r = **12.0** so 1 mole of carbon weighs **12 g** and the **molar mass** is **12 g mol^{-1}**.
For $\mathbf{CO_2}$, M_r = **44.0** so 1 mole of CO_2 weighs **44 g** and the **molar mass** of CO_2 is **44 g mol^{-1}**.
So, **12.0 g** of **carbon** and **44.0 g** of $\mathbf{CO_2}$ must contain the **same number of particles.**

You can use molar mass in calculations to work out how many moles of a substance you have.
Just use this formula:

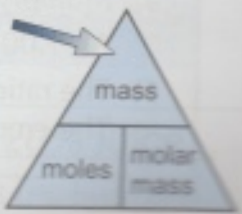
$$\text{Number of moles} = \frac{\text{Mass of substance (g)}}{\text{Molar mass (g mol}^{-1}\text{)}}$$

g mol^{-1} is the same as g/mol.

EXAMPLE: How many moles of sodium oxide are present in 24.8 g of Na_2O?

Molar mass of Na_2O $= (2 \times 23.0) + (1 \times 16.0) = 62.0$ g mol^{-1}
Number of moles of Na_2O $= 24.8$ g $\div 62.0$ g mol^{-1} = **0.400 moles**

You can **rearrange** the formula above and use it to work out the mass of a substance or its relative formula mass (see page 3). It can help to remember this triangle:



EXAMPLE: What is the mass of 1.30 moles of magnesium oxide (MgO)?

Molar mass of MgO $= (1 \times 24.3) + (1 \times 16.0) = 40.3$ g mol^{-1}
Rearranging the formula, mass = moles × molar mass
So mass of MgO $= 1.30 \times 40.3 =$ **52.4 g** (3 s.f.)

Avocado's constant: how much I need to satisfy my guacamole craving

1) Find the molar mass of sulfuric acid, given that 0.700 moles weighs 68.6 g.
2) How many moles of sodium chloride are present in 117 g of NaCl?
3) I have 54.0 g of water (H_2O) and 84.0 g of iron (Fe). Do I have more moles of water or of iron?