Chem Factsheet
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Graphical Techniques

The AS/A2 Specifications state:

Students should be able to:
- plot two variables from experimental or other data;
- understand that $y = mx + c$ represents a linear relationship;
- determine the slope and intercept of a linear graph;
- draw and use the slope of a tangent to a curve as a measure of rate of change (A2 only).

This Factsheet will review the methods and knowledge needed for students to achieve these objectives.

1. Plot two variables from experimental or other data

This clearly refers to plotting a graph: the key elements in doing this correctly are:
- correct allocation of variables to axes
- appropriate choice of scale
- accurate plotting
- correct drawing of line or curve

Allocating variables to axes

The **independent** variable goes on the **x** (horizontal) axis, the **dependent** variable on the **y** (vertical) axis. This means that what you put on the y-axis must depend on what you put on the x-axis.

For example, you could say that rate of reaction depends on concentration of a particular reactant - so that tells you that you put rate on the y-axis and concentration on the x-axis. Similarly, if you are recording the pH change during a titration, since pH depends on volume of alkali (or acid) added, pH is on the y-axis and volume on the x-axis

Similarly, you could say that concentration depends on time - but not that time depends on concentration. So concentration would go on the y-axis and time on the x-axis

> ***Exam Hint:*** *In any graph involving time, time goes on the x-axis*

You may also encounter graphs where one of the variables is not something you actually measure; these include
- graphs of ionisation energy, electron affinity, melting point etc for different elements or corresponding compounds across a period or down a group
- graphs of successive ionisation energies for an element

In cases like this, the non-measured variable (eg the names of the elements or compounds, or the ionisation energy number (1^{st}, 2^{nd} 3^{rd} etc) always go on the horizontal axis; this also coincides with the earlier rule, since the melting point depends on the element, not vice versa.

Note - we always refer to a graph of y against x - eg rate against concentration means that rate is on the y-axis, and concentration on the x-axis.

Choosing a scale

You should always ensure you use **at least half** of the graph paper in both directions - if you don't, your graph is too small and will be hard to read (and may lose you marks!)

The scale you use must be **easy to use** - for example, 5 units to one large square of graph paper is easy, but 3 units to one large square is not, because you'd be using $3^1/_3$ small squares to one unit!

The scale should be **linear** - i.e. the scale goes up in equal units (like 20, 40, 60 etc). (The only exception to this is in **logarithmic graphs**, which you may encounter for ionisation energy etc, but will not be required to plot.)

You do **not** have to:
- use the same scale on each axis (most of the time you won't be able to!)
- start the scale at 0, unless you want to show **proportionality** (i.e. that your line or curve passes through (0, 0)) or need to find the **y-intercept** (in which case, you only have to start the scale on the x-axis at 0)

It is often advantageous not to start a scale at 0 - for example, if you were plotting the values 1050, 2040, 2890 and 3250, you would have no points between 0 and 1000, with the rest of your points comparatively cramped up. If you started the scale at 1000 instead, you could use a larger scale, hence spreading the points out more.

Accurate plotting

Most of the points to be considered here are obvious, but many students lose marks from sloppy work!
- use a pencil not a pen so you can erase mistakes
- use a sharp hard pencil
- make sure you put your dot (or the centre of your cross) exactly on the appropriate point
- take the time to read your scale carefully - work out how many units each small square is worth.
- you probably cannot plot much more accurately than half a small square - but nor should you plot less accurately than this!

Correct drawing of line or curve

There are three cases to consider

<u>Graphs where it is inappropriate to join the points up in any way.</u>

These include any where points half way between the ones plotted are meaningless - for example, there is no element half way between lithium and beryllium, and no ionisation energy half way between the 1^{st} and the 2^{nd}. *(Warning - you will often see these graphs with lines joining the points in textbooks and on the internet! But that doesn't mean it is correct!)*

<u>Graphs where you should draw a best straight line</u>

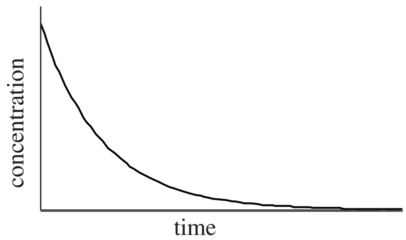
Obviously these need to look at least approximately like a straight line! You must also consider the underlying chemistry - you might expect a graph of rate of reaction against concentration to possibly be a straight line for a first order reaction, but you should be surprised to have a titration curve looking linear. Note that the "best" straight line is not necessarily the one going through the most points; you should aim to have roughly the same number of points above the line and below the line. If you have one obviously strange result, ignore it when drawing the line.

<u>Graphs where you should draw a curve of best fit</u>
As for straight lines, you must make sure that the graph looks like a curve! Ensure you are familiar with the types of curve you are likely to get (see Fig 1 below). Make sure your curve is **smooth** - it's easier to do this if you draw from the inside (concave) side of the curve. It does not have to go through every single point. Do **not** "join the dots" using a ruler.

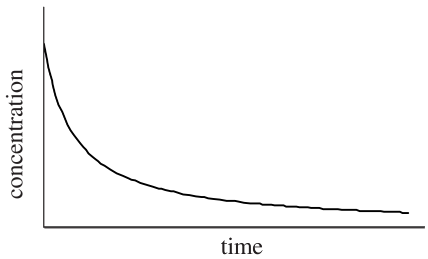
In some cases - for example when determining enthalpy changes experimentally - you will have two sets of points - "before" and "after". The two sets need to be treated individually for drawing lines or curves.

Fig 1. Some common curves

First order reaction; concentration of reactant against time

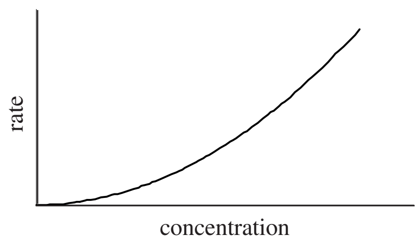


Second order reaction; concentration of reactant against time
(superficially similar to 1st order graph, but does not fall away so quickly, and does not have constant half-life property)

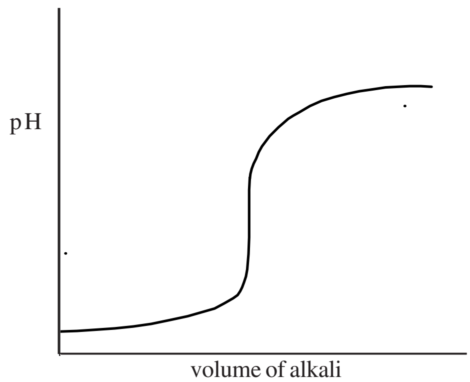


NB The curves for concentration of **product** against time are these shapes turned upside down.

Second order reaction; rate against concentration of reactant



Acid-alkali titration curve



Extrapolating
Extrapolating refers to extending your graph to make predictions, or cross the axes and other lines. Before doing this, you must ask yourself - **is it valid?** Extrapolating assumes that the trend shown by the graph continues before the first measurement and/or after the last measurement. In many cases this is fine - but be aware:

- Many curves look like straight lines if you just consider a limited range of data - so your "linear" data may in fact be part of a curve. Use your theoretical knowledge to judge whether there's any possibility of this.
- There are cases where the trend can definitely not be continued - one example is the effect of enzymes at different temperatures, where too high temperatures cause the enzymes to stop working altogether
- Make sure you have enough data to see what the trend really is - for example, if you used just the first part of a concentration against time curve in a rates experiment, you would not see that the rate slowed down, and any extrapolation would probably be wrong.

2. Understand that y = mx + c represents a linear relationship/ Determine the slope and intercept of a linear graph

This means that you must be able to:

- recognise the equation of a straight line graph (without seeing the graph)
- understand how the slope (gradient) and intercept of a straight-line graph relate to its equation
- be able to determine the slope and intercept - and hence the equation - of a straight line from its graph

As stated above, the equation of a straight line is of the form

whatever variable goes on the vertical axis
*the **gradient** - how steep the line is*

$$y = mx + c$$

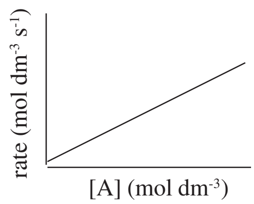
*the **y-intercept** - where it crosses the vertical axis.*
whatever variable goes on the horizontal axis

Any equation that can be rearranged into this form will also be the equation of a straight line - for example, $2y - x = 6$ can be rearranged into the form $y = \frac{1}{2}x + 3$ (so $m = \frac{1}{2}$ and $c = 3$).

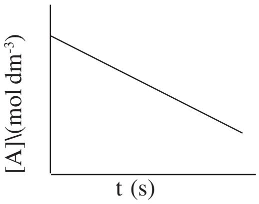
The strategy for rearranging is:
First get the y-axis variable on its own by adding or subtracting as necessary. Then divide both sides of the equation by any numbers in front of the y-axis variable. (A later Factsheet will concentrate on rearranging equations).

> ***Exam Hint:*** *Any equation just involving x, y and numbers, without the x's and y's being multiplied together or raised to any powers, will be the equation of a straight line*

One example you will certainly meet is
rate = k[A] where [A} is the concentration of a reactant.
Here, our two variables are rate (y-axis) and [A] (x-axis). The gradient is k (it's the number in front of the variable on the x-axis) and the y-intercept is zero - there is no number added to or subtracted from the "k[A]" on the right hand side of the equation. An intercept of zero means that the straight line passes through the origin - this means we have **direct proportionality**.



Another example you may encounter is if you plot concentration of reactant against time for a zero-order reaction. This gives a line with a slope of -k (where k is the rate constant) and y-intercept equal to the initial concentration of the reactant.

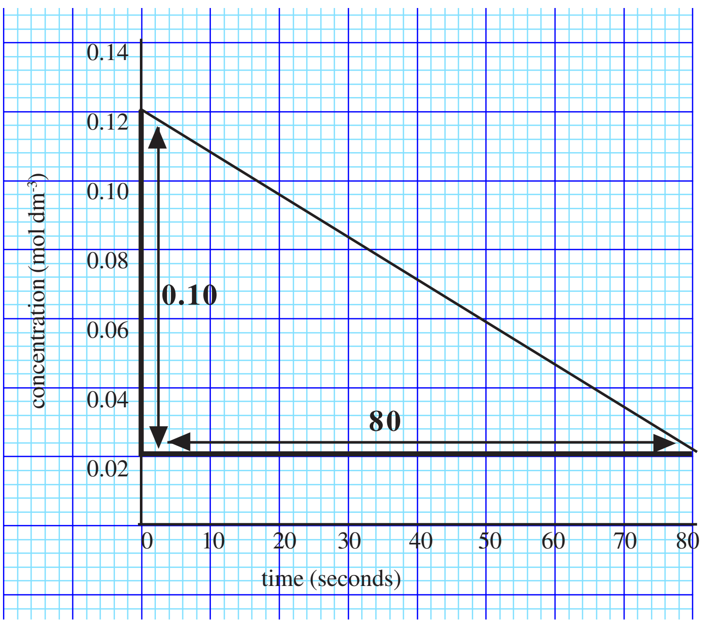


To determine the intercept from the graph:
- make sure your scale on the x-axis starts at 0
- continue your line back to the y-axis
- write down the point at which the line crosses the y-axis - this is the intercept

To determine the slope (gradient) from the graph:
- draw a triangle on the line - make it as large as possible but make sure you are clear where its sides are on the scale (try to use "easy" numbers if you can)
- **using your scale**, work out the height and base of your triangle
- work out height ÷ base
- make sure you have the right **sign**:
  - lines with **positive gradient** slope **upwards**
  - lines with **negative gradient** slope **downwards**
- put in the **units** -it's the units from the y-axis divided by the units from the x-axis

***Exam Hint:-** even though you may be quite happy calculating the gradient without drawing a triangle, doing so means you are showing your working - which can be useful if you make a numerical slip.*

Worked Example. The graph below shows how the concentration varied with time in the course of a reaction.
(a) State the order of the reaction
(b) Find the value of k.



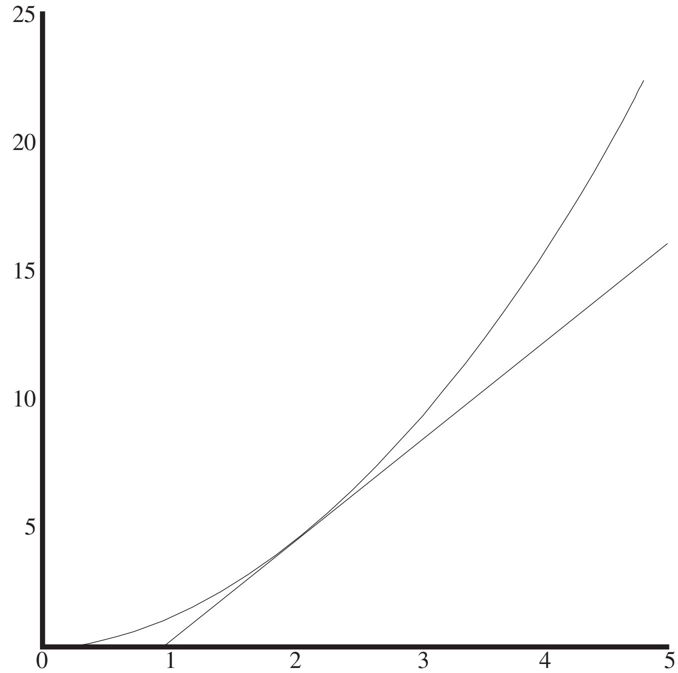
(a) the reaction is zero order (concentration against time a straight line)
(b) gradient = -0.10÷ 80 = -0.00125.   So k = 0.00125 mol dm^{-3} s^{-1}

***Exam Hint:** One of the commonest mistakes when calculating a gradient is "counting squares" rather than using the scale.*

Draw and use the slope of a tangent to a curve as a measure of rate of change

This means that you must be able to:
- understand what a tangent is
- be able to draw a tangent accurately
- be able to find the slope of a tangent and understand what it means

A tangent to a curve is used to find its **gradient** at a particular point. It is a straight line which must just touch the curve at the specified point. The diagram below shows the tangent to the curve at the point (2, 4)



The gradient of the tangent is $\frac{16-0}{5-1}$ = 4 - so that tells us the gradient of thecurve at the point (2, 4) is 4.

Accuracy is very important when drawing tangents – use as fine a pencil as possible for both the original curve and the tangent, and spend some time ensuring the tangent is just touching the curve, rather than missing it altogether or crossing it twice.

As always when finding a gradient, make your "triangle" as large as possible; this minimises the effects of any errors.

In chemistry, you are most likely to need to draw tangents in rates experiments to determine the rate at a given time (or times) from a concentration-time graph. The **units** of the gradient will be, in this case, concentration/time (i.e. mol dm^{-3}s^{-1}).

If you have to draw several tangents in order to plot a rate against concentration graph, then make your life simpler by plotting them at "easy" values of concentration (eg 0.1 rather than 0.076). You should always draw them at regular intervals.

***Exam Hint:** Do not erase your tangents after you have drawn them and calculated the gradient - they are an essential part of your working.*

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