Chemistry

Teaching Calculations in Chemistry

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HIGHER STILL

Chemistry

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Support Materials

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INTRODUCTION

These support materials for Chemistry were developed as part of the Higher Still Development Programme. Advice on learning and teaching may be found in *Achievement for All* (SOEID 1996), *Effective Learning and Teaching in the Sciences* (SOEID 1993) and in the Chemistry Subject Guide.

The intention of these support materials is to examine learning and teaching issues that relate to chemical calculations; to alert staff to possible sources of difficulty encountered by students in relation to such calculations; and to suggest strategies whereby those same students may attain greater success in this challenging aspect of chemistry.

Students who have completed a Standard Grade course in chemistry at Credit level or an Intermediate 2 course will already have encountered a number of different types of chemical calculation, for example calculations involving the mole, titrations, empirical formulae and balanced equations. However, students who have followed a purely General course at Standard Grade or an Intermediate 1 course will have considerably less experience of carrying out chemical calculations.

In Standard Grade Chemistry certain types of calculation are regarded as Knowledge and Understanding whereas others are regarded as being Problem Solving. Similarly with Higher Still courses in chemistry, the ability to perform calculations contributes both to the attainment of Outcome 1, i.e. demonstration of knowledge and understanding, and to the attainment of Outcome 2, i.e. the ability to solve problems (see **classification of chemical calculations** for further details).

Certain aspects of mathematical understanding required in chemistry fall outwith this review. For example, the structure of organic molecules brings in three dimensional geometry; flow charts involve considerations of logic; diagrams and graphs use logico-spatial relationships.

Main points

- Direct teaching should be used when students are being introduced to a new type of calculation.
- Difficulties with calculations may be caused by deficiencies in mathematics or language, not in the understanding of the chemistry involved.
- Students should be encouraged to use a verification strategy after every calculation to check for errors.
- Students should be taught to set out calculations on the page in a logical flow of statements as this makes error checking easier.
- While there is no single ‘best method’ of setting out calculations, chemistry staff may wish to consult with mathematics colleagues to ensure a consistent approach to the students in their centre.
- The significance of units in calculations should be emphasised.

IMPORTANCE OF CALCULATIONS

The ability to do chemical calculations correctly is not just a skill that has to be demonstrated in order to pass chemistry exams: it could literally be a matter of life or death. Whether in a laboratory or in an industrial plant, accurate calculation of reacting masses must be carried out before beginning any preparative chemistry and this cannot be done safely unless there is complete mastery of chemical calculations. Patient care in hospitals depends on the ability of medical staff to administer doses of medicine of the appropriate concentration. Research and development in a wide range of industries, from oil to electronics, depends on expertise in performing a wide variety of chemical calculations correctly.

Calculations form an essential part of the study of chemistry. The inability to perform calculations correctly may prevent a student from following a career in chemistry or a wide range of chemistry related occupations.

CLASSIFICATION OF CHEMICAL CALCULATIONS

In Higher Still chemistry courses the ability to carry out calculations is assessed both in Outcome 1 (knowledge and understanding) and in Outcome 2 (problem solving) within the performance criterion ‘Information is processed using calculations where appropriate’.

When the student is only required to use one procedure which can be taught and learned, the assessment will be part of Outcome 1.

For example at Higher:

1. Calculate the OH^-(aq) ion concentration in a solution with a concentration of H^+(aq) ions of 10^{-1} mol l^{-1}.
2. Calculate the volume of 0.2 mol of carbon dioxide if the molar volume is 23.2 litres mol^{-1}.
3. A radioisotope has a mass of 20 g.
   Calculate the mass remaining after 8 days if the half-life is 2 days.

For example at Intermediate 2:

1. Calculate the concentration of a solution which contains 2 mol of sodium hydroxide dissolved in 500 cm^3 of solution.
2. Calculate the volume of HCl(aq) of concentration 0.1 mol l^{-1} required to neutralise 50 cm^3 of NaOH(aq) of concentration 0.2 mol l^{-1}.

When two or more procedures need to be combined or when the procedure or situation is unfamiliar then the assessment will be part of Outcome 2.

For example at Higher:

1. Calculate the OH^-(aq) ion concentration in a solution with a pH of 11.
2. Calculate the volume of 4 g of methane if the molar volume is 23.2 litres mol^{-1}.
3. Calculate the number of atoms in 6 g of carbon.

For example at Intermediate 2:

1. Calculate the mass of sodium hydroxide required to produce 500 cm^3 of 2 mol l^{-1} solution.
2. Phosphoric acid has the formula H_3PO_4.
   Calculate the volume of potassium hydroxide solution, concentration 0.1 mol l^{-1}, required to neutralise 25 cm^3 of phosphoric acid, concentration 0.01 mol l^{-1}.

In the first example at Higher, the student has to combine two procedures:

- stage one is to calculate the concentration of H^+(aq) ions
- stage two involves applying the formula $[H^+(aq)]\ [OH^-(aq)] = 10^{-14}\ mol^2\ l^{-2}$.

In a similar way, in the first example at Intermediate 2 the student has to combine two procedures:

- stage one is to calculate the number of moles from volume and concentration
- stage two is to calculate the mass from the number of moles.

It should be noted that the numbers used in problem solving questions involving the Avogadro Constant (example 3 above at Higher) should be able to be handled by mental arithmetic.

A calculation built around unfamiliar chemistry would also be classed as problem solving. As an example, a calculation involving an EDTA titration to estimate calcium ion concentration in hard water would be problem solving. Although the stoichiometry (a simple 1:1) would be supplied in the text, the unfamiliarity of the chemistry requires students to relate the situation to a more familiar context and to see that it is a generalisable titration calculation. But it is this requirement to make that mental jump that classifies the calculation as problem solving.

THE LANGUAGE OF CHEMICAL CALCULATIONS

Students sometimes have language related difficulties in understanding calculations. These difficulties are often subtle in origin and usually arise from:

- lack of understanding of familiar words used to convey particular meaning in chemistry, e.g. volatile
- lack of understanding of technical terms introduced in the study of chemistry, e.g. intramolecular
- ascribing a familiar meaning to a common word which is being used in a technical sense, e.g. a weak acid.

In a sense, every teacher must be a teacher of language since each subject draws inferences from words in ways that are distinctive to the subject. For example, in everyday use the word ‘strong’ applied to solutions means ‘concentrated’ (as in ‘a strong cup of coffee’) whereas in chemistry the word ‘strong’ has a special meaning with respect to acids and alkalis.

In everyday use of language, communication rarely requires words to be used in a precise sense. In describing things we often have a range of expressions which would do equally well; but in chemistry this is not the case and we require students to employ a precision of meaning that would not normally be needed. Students must therefore be made to see the need for this and then must practise it. A simple but nevertheless highly effective method of doing this is to ask students to form sentences, either in speech or in writing, using particular words or phrases. In this way it can be established whether an individual student understands a particular term.

Although published some years ago by the Scottish Curriculum Development Service (now Scottish CCC), Memorandum No 43 *Language in Chemistry* is still a valuable starting point for considering language issues in chemistry.

THE MATHEMATICS OF CHEMICAL CALCULATIONS

In order to perform chemical calculations correctly students must not only demonstrate mastery of the requisite chemical knowledge but must also exhibit the necessary computational skills. Students who fully understand the chemistry involved may have difficulties due to deficiencies in mathematical skills. Chemistry teachers should liaise with mathematics departments to obtain information about mathematical attainment of students, to seek advice about supporting students with weak computational skills, and to learn something of how key mathematical procedures are taught. In some cases chemistry teachers may have to reinforce the mathematical procedures necessary for a particular type of calculation.

A wide range of different types of calculation occur in chemistry. Many of them relate in some way or another to the mole concept so it is important that time is spent on reinforcement of this central idea in chemistry. Only the arithmetical operations of addition, subtraction, multiplication and division are employed at Intermediate 1, Intermediate 2 and Higher. The main logical process is that of proportional reasoning. At Higher, the logarithmic nature of the pH scale is implied but an understanding of logarithms is not needed. All other mathematical procedures required should have been encountered in Standard Grade Mathematics but it should be noted that some students may have difficulty in applying what they have learned in mathematics to the context of chemistry.

Performing calculations in chemistry can present daunting challenges to some students due to the large number of different skills, both mathematical and chemical, that have to be assembled in order to arrive at the correct outcome (see **working memory** below). Equations of both the mathematical and the chemical variety have to be manipulated and the relationships between the two types have to be clearly understood.

Proportional reasoning

Proportional reasoning pervades chemistry and there is evidence that it represents a major source of difficulty for some students. It is particularly important in chemistry because so many of the facts of chemistry are described in terms of proportions; formulae and equations are statements of proportional relationships; stoichiometric calculations involving the mole are all based on proportions; rate equations and equilibrium constants involve proportion; defined concepts such as density, pressure, concentration and reaction rate all describe proportional relationships. If students are to make any significant progress in chemistry then possession of proportional reasoning ability is essential.

Proportional reasoning is one of Piaget's formal operations and there is evidence to show that these cannot be learned as one learns factual information. Through teacher mediation in the learning process students must construct proportional reasoning for themselves, by listening to explanations, by trying calculations, **by creating their own mental models**, and by discussion when difficulties arise. Staff can help students to construct proportional reasoning by getting students to explain their reasoning steps in calculations and ensuring that their models for solution are generalisable.

Students tend to compartmentalise learning and may be unaware that skills learned in mathematics can be transferred to chemical calculations. A further task for the teacher then is to show that there is a proportional reasoning ‘bridge’ from mathematics to chemistry by comparing calculations set in a chemical context with familiar everyday examples.

Proportional reasoning involves relationships of the type

$$\frac{\mathbf{A}}{\mathbf{B}} = \frac{\mathbf{C}}{\mathbf{D}}$$

that is the ratio of A to B is the same as that of C to D. However, the application of this idea to chemical settings will be an impossibility for those who have no grasp of proportional relationships. In a chemical context, such a relationship might typically be stated as ‘A moles of *x* give C litres of *y* so B moles of *x* will give D litres of *y* ’. Such a statement assumes a 1:1 correspondence between *x* and *y* but requires no understanding of the mole; A and B could be kilograms of apples and C and D could be litres of apple juice. Processing the calculation depends on being able to see that it involves proportional reasoning, independent of the context.

Having established that the calculation involves proportional relationships and having set these out correctly, the problem remaining for students is to rearrange terms to solve for the unknown term and it is here that great difficulty can often arise. If students are experiencing difficulty it may be of use to give simpler calculations set in familiar contexts which gradually become more difficult, identify the point where understanding breaks down, and then work from there. For example:

- If oranges are 15p each, what is the cost of 5 oranges?
- If 4 oranges cost 60p, what is the cost of 7 oranges?
- A bag of 15 oranges costs £2.25. Another bag, containing 18 oranges, costs £2.52. Which is the better buy?

and so on, eventually reaching chemical calculations.

If students can demonstrate secure understanding of proportional reasoning they could then be introduced to the algorithm known as ‘cross multiplying’ which is a simple but effective method that can be used to solve a wide range of chemical calculations.

Note: Algorithms are carefully developed procedures for getting correct answers to routine calculations with the minimum of effort.

TEACHING CHEMICAL CALCULATIONS

Chemical calculations exist in many forms, ranging along one continuum from simple to complex, and along another from routine to non-routine, with the non-routine ones obviously being the more challenging. However, what is a simple and routine calculation in the hands of an expert may appear to the novice to be distinctly complex and non-routine. The greater the experience gained in doing different types of calculations, the fewer non-routine calculations there are. It is therefore important that chemical arithmetic is seen as an integral part of any chemistry course and that a sufficient amount of time is devoted to it.

What is the best way to teach chemical calculations? The recommendation is that the traditional method of direct teaching, working through examples with the whole class, is the most efficient and effective way of introducing a new type of calculation. The distinct advantage that the classroom presentation has over worksheet based individualised methods is that the calculation can be treated as if it were a novel task for the member of staff as well as for the students. The teacher/lecturer could and should think aloud as the calculation is modelled by asking questions such as: What is this calculation about? and How should I tackle this calculation? and What would happen if I ...?. The teacher/lecturer can deliberately select false representations for a calculation and then reject them. This shows students why a particular route is wrong and also lets them see that it may be necessary to explore a number of approaches before arriving at a solution.

Teaching calculations has two purposes: one is to show that many calculations are routine in nature and can be solved by employing suitable general algorithms. This ability is important but it does not prepare students to deal with novel tasks so the use of algorithms should not be overemphasised. The second is to build up expertise and confidence in tackling calculations which are non-routine and which may require non-routine strategies to find solutions. Although one must be wary of generalising, as a rule routine calculations will fall into the category of knowledge and understanding whereas non-routine calculations will belong to problem solving.

Evidence suggests that success at solving calculations becomes more likely if the opportunity has been given (and taken) to practise as wide a variety as possible. Once a new category of calculation has been introduced it is common practice to allow students to work on further examples individually. Building confidence is important at this stage so the chances of early success should be maximised by introducing calculations on a structured, hierarchical basis determined by the complexity of the calculation and the familiarity of the context (see **working memory** below).

To begin with, students should be allowed to attempt simple examples set in familiar contexts. Early questions dealing with mole calculations should be based on familiar chemicals (with the formulae of compounds given) such as calcium, magnesium, CH_4, H_2O, NaOH. It will aid competence if the first examples use only simple whole numbers and students try to do them without the aid of a calculator (see **using calculators** below). Staff should monitor progress and mediate in cases of difficulty. A hierarchy of difficulty can then be introduced by moving on to more complex calculations set in progressively less familiar contexts up to the level of difficulty appropriate to the level of the unit. The difficulty level is established by a combination of the arithmetic and the chemistry involved and in this way materials may be differentiated. For example, it is easier to calculate the number of moles of H^+(aq) ions in 2 litres of 2 mol l^{-1} HCl(aq) than in 27 cm^3 of 0.78 mol l^{-1} H_3PO_4(aq).

Although it is quite acceptable to present students with calculations containing some new twist or other, the temptation to set problems which are far in excess of the difficulty level of the unit should be resisted. There is an erroneous assumption that setting such calculations gives students confidence because they are coping with work of difficulty beyond the required level. In fact the outcome is often the opposite to that desired: many students become demoralised and demotivated because they are unable to solve the calculations.

DOING CHEMICAL CALCULATIONS

It will often be the case that a calculation is set in a wholly familiar context and the application of a well practised algorithm will result in a solution being obtained. However, it is sometimes the case that the context will be unfamiliar and a successful outcome will be more likely if students are conversant with a variety of procedures for handling calculations.

Visualising the calculation

Success at a calculation is more likely if students can visualise the chemical processes and procedures involved. For example, doing calculations involving titrations would be more difficult if students had never had the opportunity to perform them. Similarly, it is worthwhile giving an idea of what 24 litres looks like when discussing the molar volume of gases. It is therefore important to ensure that chemistry courses contain appropriate practical work beyond Prescribed Practical Activities.

Incubating

It is common to get stuck when doing calculations. In such an eventuality students should be advised to leave the calculation and return to it later. In many cases, on returning, the route to the answer becomes apparent. This resting from a calculation or other problem is known as incubation and is particularly effective in all sorts of situations. The mechanism is not known but it is believed that the subconscious mind plays a role.

Using verification strategies

Once the answer has been obtained it should be a matter of habit for students to verify it. The way this is done will depend on the calculation. With certain types it will be possible to substitute the answer into the information supplied and arrive at the figures given in the question; this is known as working back. As an example of this, consider an enthalpy diagram question in which an unknown enthalpy change has to be calculated. When the value has been calculated correctly, combining it with the other known values will result in equal totals for endothermic and exothermic processes.

With other calculations, the units in which the answer is expressed may be used as a clue to verification. Different types of calculation have different methods of verification and students should be encouraged to develop verification strategies. Many students do not verify their answers despite knowing the value of the procedure. Why is this? One suggestion is that they are not confident about the calculation process to begin with and are then even less sure about which verification strategy to adopt.

Working memory

When doing calculations we rely on information stored in memory. The amount of information that we can store appears to be limitless. However, we are not able to access all of it at once and this inability has implications for doing calculations.

It would appear that we have a ***long-term memory*** of unlimited capacity and a ***short-term or working memory*** of limited capacity. A good analogy would be a computer with a hard disk of unlimited storage and the RAM of limited size which is accessed when any information processing is to be carried out. Without trying to define the nature of a ‘bit’ too precisely it is reckoned that the average person can hold about seven ‘bits’ of information in the working memory at any given time although this varies with maturity and intellect.

Working memory can be used to hold information ‘bits’ and processing ‘bits’: the more of one that is held, the fewer there can be of the other. It is then not surprising that students have difficulty with more complex calculations involving several steps even although they can complete each step correctly. For this reason it is important that students are taught to tackle complex problems by breaking them down into manageable chunks and then integrating the answers to the sub-tasks to give the final answer.

There are a number of strategies for compensating for limitations in working memory:

External memory

The first, which is frequently overlooked, is to use an external memory which can consist simply of rough notes or working made at the side of the page. Setting out the calculation step by step eases the demand on working memory and should be encouraged. Ironically, use of a calculator may sometimes cause overload of the working memory since some students have a tendency to process all the information mentally which uses up too many ‘bits’ of memory space. The result is confusion and an incorrect or incomplete calculation.

Chunking

Other strategies depend on gaining experience at doing calculations. Space can be conserved in the working memory by a well known phenomenon called chunking where smaller ‘bits’ are amalgamated into larger ‘bits’. An unfamiliar mathematical formula of four terms might use four ‘bits’ of space but as it becomes progressively more familiar the formula starts to be perceived as a single entity and becomes one ‘bit’ of information thus leaving more space for more complex calculations.

Automatisation

Automatisation is a further means of maximising working memory and means overlearning to the point that performance of a task requires little or no attention. For example, if enough practice is given then mathematical processes such as multiplying and dividing by 10 can be carried out without resorting to use of a calculator. However, care needs to be exercised in applying chemical knowledge automatically since close attention will always need to be paid to chemical formulae as these can alter the outcome of a calculation. To illustrate this point, a student may have learned that a metal M forms a chloride of formula MCl_2 but may encounter an unfamiliar form MCl_3 in a calculation. Unless care is taken, automatisation may lead to the formula being read as MCl_2 with the result that the calculation will be performed incorrectly. See also **reading errors** below, which deals with a slightly different situation.

ACHIEVING SUCCESS WITH CALCULATIONS

Reading errors

Many difficulties with calculations arise from misreading the information given. Both good and bad calculation solvers misread information but the good ones usually catch their errors. Transcription errors arise from misreading formulae, for example NO_2 for N_2O; from transposing figures, e.g. reading 9. 532 instead of 9.352; or from reading g instead of kg. Such errors are very common and will persist until deliberate attention is paid to the difficulty. Although students are not severely penalised for such errors in tests they could have serious consequences elsewhere. **Paired working** (see below) can reduce the incidence of reading errors.

Being unclear about the goal of a calculation

Students are often unclear about what they have to calculate although it is clearly stated in the text of the question. This is due to the fact that they are unable to decode information inherent in written sentences and diagrams. In cases where this is a serious problem the advice of the learning support service should be sought. Staff should check that students understand what they are being asked to do and get students to make a habit of checking they are clear about the goal with every calculation they attempt. It is also not uncommon for students to lose track of the goal of a calculation while they are in the process of solving it. This problem can be overcome by writing down the goal before starting the calculation.

Paired working

A technique which has proved successful is for students to work in pairs when solving problems. One student acts as the calculation solver while the other acts as a checker. Each student in turn reads through a calculation then thinks aloud and talks through his/her method for tackling the calculation while the other student acts as a checker monitoring the process, for example by verifying that the calculation has been correctly read and the correct figures have been used. The checker may stop the solver if a mistake is spotted or the strategy is unclear. Two heads being better than one, correct solutions have a greater chance of occurring. The teacher/lecturer intervenes in the process to check on progress and give help when needed. The teacher/lecturer also has an important role in assuring the quality of the dialogue between students.

Real improvement is observed since students are forced to confront their strategies for thinking about calculations. There is also evidence to suggest that pairs of students of similar ability have more success than pairs of widely varying ability. The technique can serve two purposes: it can assist those who habitually make reading errors and it can help those whose calculation strategies need developing.

USING CALCULATORS

Calculators are very useful tools in studying chemistry but, like all tools, they need to be used effectively and selectively. This means that students should learn **when** to use them as well as **how**.

A common image of the professional scientist is someone spending many hours doing complicated calculations. Although very complex calculations can be carried out on a calculator, chemists often make use of rough calculations done on the back of an envelope or even in their head. Students need to know how to do calculations by hand for three reasons:

- Sometimes a rough answer will do in an exploratory experiment.
- Can the result from the calculator be trusted? A rough calculation with simplified numbers will give an estimate. It is very easy to press a wrong key.
- They may not always have access to a calculator.

The importance of making an estimate cannot be stressed enough. When using calculators students should also be taught to repeat each calculation to check the answer and ensure that no keying errors have been made.

There are three main types of calculator available: arithmetical, scientific, and graphical. The scientific calculator is suitable for Higher, Intermediate 2 and Intermediate 1 chemistry courses. Students should be made aware that in SQA examinations the use of certain types of programmable calculator is prohibited.

Unfortunately, for students and staff alike, different makes of calculator use different algorithmic languages. It is the responsibility of students to familiarise themselves with the operation of their own calculators. Many students do not know the correct method of working with powers of 10 for their particular calculators so some time should be allocated to ensuring that students are proficient at this routine.

Students should be taught to work through a calculation in a logical flow of statements set out in written form on the page as they use the calculator to work out the answer. There is a tendency for students to key in calculation data without setting out the calculation. This is bad practice and leads to a greater frequency of errors. It should therefore be strongly discouraged.

Significant figures

Students should be aware that the answer to a calculation cannot be more accurate than the data and that answers should have no more significant figures than the least accurate measurement. Significant figures are used a lot in science because the uncertainties have some relationship to the size of what has been measured but many students do find the concept difficult to understand. With calculators it takes no effort to produce answers to eight decimal places but students need to be taught that such answers are invalid unless the input data was of a similar accuracy. Practice should be given at working with the idea of significant figures to build up a gradual familiarity with the concept, for example by doing estimation exercises.

SCIENTIFIC NOTATION (STANDARD FORM)

Students should understand that since chemistry has a lot of very big numbers and a lot of very small numbers it would be very time consuming and involve a lot of zeros to write them in the way we write everyday numbers like 23.47, called ordinary form; also we would run out of spaces on a typical 10 digit calculator display. So we use scientific notation with which scientific and graphical calculators can deal.

Students may need practice at converting from ordinary form to scientific notation and vice versa, and should understand the significance of positive and negative indices. Numbers smaller than 1 may give difficulties. Students should also be able to read the numbers in words, e.g. 6.42×10^{-6} as six point four two times ten to the power negative six.

Students should be made familiar with the rules for manipulating numbers written in scientific notation i.e.

$$10^m \times 10^n = 10^{m+n}$$

and

$$10^m \div 10^n = 10^{m-n}$$

and also that for addition and subtraction numbers must be converted to the same degree of magnitude.

If students find difficulty in working with powers of 10 using a calculator they could be taught how to manipulate the powers of 10 separately by hand, use the calculator for the remaining terms, and then combine the two in the final answer.

Using powers of 10 alone can sometimes give a very quick estimation method.

UNITS

Students have been familiar with handling numbers in mathematics for many years before they start doing chemistry. Unfortunately they may also become accustomed to treating the number as the quantity in itself and do not always understand the significance of the fact that a physical quantity of the type we deal with in chemistry requires a unit to be stated if the number is not to be meaningless. Even when the significance is appreciated it is not always thought to be that important.

Staff need constantly to emphasise the fact that calculations are dealing with physical quantities and that units are required to give the figures meaning. Appropriate quantities should be expressed in the same units before any mathematical operation is carried out, for example, by converting all volumes to either litres or cm^3.

Units are written using symbols which often have to represent more than one unit and when chemical symbols are included there is clearly the potential for confusion. For example, C is the symbol for carbon but it is also used as ^oC to indicate temperature; in the lower case, c represents the specific heat capacity of water and it also crops up in cm^3. Learning difficulties can be avoided if care is taken to explain a symbol and its correct usage on first encountering it.

Units can be combined, as in expressing concentration. In line with the use of such units in SQA unit and course assessments, the solidus, e.g. g/l, should be used at Intermediate 1, and negative index form, e.g. mol l^{-1}, should be used at Intermediate 2 and Higher. The latter form allows units to be manipulated in the same manner as powers of 10. Higher students could be shown how units can be used in this way.

There should be consistency within a department over the naming of units. For example, cm^3 might be called cubic centimetre by one teacher, centimetre cubed by a second, and millilitre by a third. All of these expressions are in common use and students should know that they mean the same thing but nevertheless confusion will be minimised if a common naming policy is adopted.

More information about units is contained within Memorandum 37, *Units, Symbols and Terminology for Science and Engineering*, originally published by the Scottish Curriculum Development Service (now Scottish CCC).

APPENDIX 1 - WHERE DO CALCULATIONS OCCUR?

The following examples of calculations are drawn from the contents statements in the Arrangements to illustrate the contexts in which students at the various levels will meet calculations.

Access 3

There are no references to calculations in the content statements but the suggested activities indicate various possibilities.

Intermediate 1

There are no references to calculations in the content statements but the suggested activities indicate various possibilities.

Intermediate 2

Building Blocks

Calculate the average rate of a reaction, or stage in a reaction, from initial and final quantities and the time interval.

Calculate the number of protons, neutrons and electrons from the atomic number and mass number, and vice versa.

Calculate the relative atomic mass of an element from the mass numbers of the isotopes and their relative abundances.

Calculate the relative formula mass of a substance from the relative atomic masses.

Calculate the number of moles of a substance from its mass and vice versa.

Calculate the mass of a reactant or product using a balanced equation.

Acids, Bases and Metals

Calculate either the number of moles of solute, or the volume, or the concentration of a solution from the other two variables.

Calculate the concentration of acids and alkalis from the results of volumetric titrations.

Higher

Energy Matters

Calculate the average rate of a reaction, or stage in a reaction, from initial and final quantities and the time interval.

Calculate the amount of reactant that is in excess.

Calculate enthalpy change from potential energy diagrams.

Calculate activation energy from potential energy diagrams.

Calculate enthalpy changes using $cm\Delta T$.

Calculate the volume of a gas from the number of moles and vice versa.

Calculate the volumes of reactant and product gases from the number of moles of each reactant and product.

The World of Carbon

Calculate percentage yields from masses of reactants and products using balanced equations.

Chemical Reactions

Calculate enthalpy changes by application of Hess's Law.

Calculate the concentration of $H^+(aq)$ or $OH^-(aq)$ in a solution from the concentration of the other by using $[H^+(aq)][OH^-(aq)] = 10^{-14}$ mol^2 l^{-2}.

Calculate the concentration of a reactant from the results of volumetric titrations.

Calculate the mass or volume of an element discharged from the quantity of electricity passed and vice versa.

Calculate the quantity of radioisotope or half-life or time elapsed given the value of the other two variables.

Advanced Higher

Electronic Structure and the Periodic Table

Calculate quantities in the contexts of electromagnetic radiation and spectroscopy using: $c = \lambda\nu$; $E = h\nu$; and $E = Lh\nu$.

Calculate oxidation numbers/states of elements in different species.

Principles of Chemical Reactions

Carry out calculations in volumetric and gravimetric analysis based on stoichiometric equations, working with masses, moles, concentrations and percentage by mass.

Carry out calculations involving equilibrium constants given by:
$K = [C]^c[D]^d / [A]^a[B]^b$, including calculation of the units of K.

Carry out calculations involving the ionic product of water given by:
$K_w = [H_3O^+]\,[OH^-]$

Carry out calculations based on $pH = -\log_{10}[H^+]$

Carry out calculations involving the pH of weak acids expressed as:
$pH - 1/2\ pK_a - 1/2\ \log_{10}c$

Estimate the pH range over which an indicator changes colour using pK_{In}.

Carry out calculations relating the pH of an acid buffer solution to its composition and the acid dissociation constant.

Carry out calculations based on enthalpy changes, including bond enthalpies, by application of Hess's Law.

Calculate the standard enthalpy change for a reaction from the standard enthalpies of formation of the reactants and products.

Carry out calculations based on Born-Haber cycles.

Calculate the standard entropy change for a reaction from the standard entropies of the reactants and products.

Calculate the change in entropy of the surroundings from the temperature and the enthalpy change for a reaction system.

Carry out calculations based on the relationship: $\Delta G° = \Delta H° - T\Delta S°$

Calculate the standard free energy change for a reaction from the standard free energies of formation of the reactants and products.

Calculate the temperature at which a reaction becomes feasible using an Ellingham diagram.

Calculate the emf of a cell under standard conditions (E°) from standard reduction potentials.

Carry out calculations based on the relationship: $\Delta G° = - nFE°$

Determine the order of a reaction with respect to each reactant, and the overll order of the reaction, based on the relationship: $rate = k[A]^m[B]^n$

Calculate the rate constant for a reaction using initial rate data for a series of reactions in which the initial concentrations of reactants are varied.

Organic Chemistry

Use data from elemental microanalysis to calculate the masses of C, H, S and N in a sample of an organic compound in order to find its empirical formula.

Calculate wavenumber as the reciprocal of the wavelength in infrared spectroscopy.

APPENDIX 2 - CHARACTERISTICS OF STUDENTS WHO HAVE DIFFICULTY WITH CALCULATIONS[1]

The following list summarises the behaviours exhibited in varying degrees by students who have difficulty with calculations:

- they do not believe that they can solve calculations; they seem to feel that you either know the answer or you do not
- they are impatient; if they do not see the answer quickly, they give up
- they are careless readers; they often misread what is written; they may begin working the problem before they know what the problem asks
- they jump to conclusions and guess; they expect to go in one step from what is given to the answer; if they cannot, they give up
- they organise their work carelessly or not at all; they are unable to trace their thinking at the end of a problem
- they seldom check their work
- they have only one approach to problems; usually they try to recall an algorithm; if they cannot, or it is not appropriate, they do not know what to do and give up.

These support materials offer some understanding of these behaviours and some strategies to assist such students.

[1] This list is adapted from Whimbey and Lockhead, 1983. *Problem Solving and Comprehension*. The Franklin Institute Press, Philadelphia