TEACHING ABOUT SCIENCE

D ASSESSING DATA QUALITY: CHEMICAL DATA

This is a lesson aimed at helping students to develop their understanding of how to assess the quality of scientific data.

Teachers' notes

Resources for students and teachers (separate download)

Download from www.nuffieldfoundation.org/aboutscience

OHT D0.1 Aims of the lesson
Activity D1 Cards 1–6 (6 sheets)
Teachers' presentation notes D2.1A and B Dealing with uncertainty (2 pages)
OHT D2.2 Dealing with uncertainty
OHT D2.3A and B Variation of emission rate of a radioactive substance with concentration
OHT D2.4 Variation of emission rate of a radioactive source with concentration
Sheet D2.5A/B What value to choose?
Group task sheets D3.1A–E
Sheet D3.2 'Molar heat capacity and entropy of calcium metal' Reprinted from the *Journal of Chemical Thermodynamics* (5 sheets)
Sheet D4.1 Dealing with errors in A-level Chemistry practical work
Sheet D4.2 Student's report on an experiment to find out how the energy in fuels depends on the structure of the molecules (2 sheets)

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Acknowledgements

These resources were developed as part of a research project at the University of Leeds, funded by the Nuffield Foundation.

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TEACHERS' NOTES

FOCUS

Many of the investigations conducted by professional chemists involve making measurements. However, there is a degree of *uncertainty* about the data sets that result from these measurements.

Quantities that are measured directly, such as the volume of a liquid, include errors arising from the limited resolution of the measuring instrument. The calibration of the measuring instrument itself may also lead to errors.

In many investigations in chemistry (and other fields) theoretical models are used to decide which measurements are made and how the resulting data are analysed. For example, mathematical models of processes in the atmosphere are used to decide how data about climate change are collected and analysed. In considering the implications of such investigations, chemists need to recognise the potential uncertainty that results from the use of models and analogies.

The focus of this teaching is to enable students to recognise a range of different sources of uncertainty in investigations, and to appreciate how this uncertainty can be handled.

RATIONALE

This teaching sequence aims to help students develop their ideas about how data are collected and analysed in science. Chemistry is a quantitative science, and many professional chemists spend time determining values for quantities by making measurements and dealing with uncertainty. However, students tend not to appreciate the need to deal with uncertainty, believing that the process of scientific measurement is unproblematic. In their view, measured data points reveal a 'true' value.

It is quite common for the data collected in school or college science practical work not to produce a result that corresponds to the value published in data books! Not unreasonably, students tend to attribute such discrepancies to human error (that is, their own mistakes) and the limitations of the apparatus available. Professional scientists also make mistakes, and have to deal with the limitations of the apparatus available. As well as mistakes on the part of those making measurements, whether student or professional scientist, measurements are susceptible to other sources of error:

• Systematic errors can result from errors in the calibration of instrumentation. For example, measurements of the radiation emitted from a source will be higher than the 'true' value unless the measuring instrument is calibrated according to the level of background radiation. These errors are called systematic because the error is in one direction only, and can therefore be corrected for after data have been collected.

• Random errors can result from the uncertainty in attributing a value using a measuring instrument. For example, if a ruler graduated in millimetres is used to measure the length of a pencil, the value can only be specified as lying within a range of ± 0.5 mm. As the measured value may fall above or below the 'true' value, this kind of error is called random. Unlike systematic errors, random errors can not be corrected for at the end of the investigation by applying a correction factor.

Various techniques can be used to deal with random errors. Uncertainty in an individual measurement can be estimated by considering the resolution of the instrumentation used to make the measurement. An alternative way of estimating random error is to repeat the measurement many times to obtain a set of data, from which the level of uncertainty can be calculated statistically.

Points plotted on graphs often have error bars to show the range in which the value is likely to lie. Depending on the nature of the particular experiment, results may be presented in one of two possible ways:
• as a measured value ± an error estimate (based on a single measurement);
• as a mean value ± a measure of spread (based on a set of repeated measurements).

The precision of an estimate refers to whether the estimated value is thought to lie within a narrow range, or a wider range.

Evidence suggests that AS/A-level students do not appreciate the significance of estimates of values and error bars. For example, when presented with data from repeat measurements, if the same value appears more than once many students will claim that value to be the 'true' value, rather than considering the mean and spread of the data. Similarly, when proposing a line/curve of best fit when data points are plotted with error bars, students will consider it more important that the line/curve hits the data points, rather than considering how the line/curve might be drawn to lie inside all the error bars.

However, errors of the kind discussed above are not the only sources of uncertainty. Many of the investigations carried out by professional scientists are conducted using models, assumptions and theories. For example, predictions about the effects of enhanced global warming are generated from mathematical models of processes in the atmosphere. Those models are used to determine the data which are collected by atmospheric chemists, and the ways in which those data are analysed. The extent to which values and predictions from the investigations of atmospheric chemistry correspond with how atmospheric processes are 'really' happening is therefore dependent upon the appropriateness of the initial model of the atmosphere. The accuracy of a value refers to the extent to which the estimated value corresponds to the 'real' value. It is, of course, possible to have a precise estimate of a value that is not very accurate, because of flaws in the underlying model. However, evidence suggests that AS/A-level students tend to be unaware of uncertainty that arises as a result of the use of analogies and models in investigations.

The teaching sequence aims to show students the various sources of uncertainty in investigations, and how that uncertainty can be dealt with. In particular, teaching focuses upon the various possible sources of spread in measurements, and the difference between a precise estimate and an accurate value. Students are encouraged to think about the quantitative basis of data typically encountered in AS/A level courses in terms of relationships between measured data and explanations of that data.

A NOTE ABOUT LANGUAGE

In everyday English the words 'mistake' and 'error' can be used interchangeably in many situations. For many students the term 'error' implies a mistake. In this activity, the aim is to teach students that experimental errors are the unavoidable consequence of making scientific measurements. It is therefore worth pointing out the difference between the terms 'human error', which implies a mistake, and 'experimental error' as used in science. The term 'uncertainty' is used here to describe errors of all kinds without implying that a mistake has been made.

In activity D2 of the teaching sequence students are shown techniques to deal with experimental error. Single measured values with estimated error bars, and mean values with confidence limits are dealt with together. To avoid the need to distinguish between these we refer to plotted values (either the single measurement or mean value) and to plotted range (either estimated error bars or confidence limits).

Uncertainties arising from assumptions and models are also looked at in activity D2. It may be helpful at this stage to introduce the terms 'precision' and 'accuracy'. These terms are used in the activity to highlight the uncertainty that underlies any measurement, however precise, which is based on assumption or models.

AS/A2 LINKS

Teaching about evaluating the quality of evidence features in the QCA Subject Criteria for Chemistry.

'Students should interpret information gathered from experimental activities including:
i. manipulation of data;
ii. recognition of patterns and trends in a set of data or information;
iii. identification of sources of error and recognition of the limitations of experimental measurements.'

The contexts drawn upon in this task are key parts of the QCA specifications for AS and A2 level chemistry courses. The AS course includes:
The concept of enthalpy change. Standard enthalpy changes of reaction, formation and combustion. Average bond enthalpies (QCA reference 3.8.1)
The use of Hess's Law to calculate enthalpy changes (QCA reference 3.8.2).

KEY SKILLS

The activity gives students the opportunity to gain competence in the following key skill areas:

Communication Level 3
C3.1a Contribute to a group discussion about a complex subject.

Portfolio evidence of this could be in the form of a note from an assessor (the teacher) who has observed the discussion and noted how the requirements of the unit have been met, or an audio/video tape of the discussion.

C3.2 Read and synthesise information from two extended documents about a complex subject.
Portfolio evidence of this could be in the form of a record of what was read including notes, highlighted text or answers to questions about the material.

TEACHING SEQUENCE

This teaching sequence includes four activities. Teachers may decide not to use all four activities with all groups. Suggestions about routes through the activities are included in the text below.

Introduction (brief)

Resources OHT D0.1 'Aims of the lesson'.

Points to raise This lesson will be rather different from many science lessons (not much writing and lots of discussion). Students should think and talk!

The focus of this lesson is upon how we interpret data in chemistry. Although students will have already interpreted chemistry data, in this lesson we will look much more closely at what is involved and how learning about data-handling links to other areas of the chemistry course.

Students will be expected to get involved in paired discussion and feed back their ideas to the whole class (link to key skills).

Activity D1 (30 minutes)

This activity aims to alert students to a range of causes of uncertainty. In each case, attention is drawn to uncertainty in the investigation.

This activity could be done before the following activities as an independent part of the sequence.

Resources: Activity cards D1–6

Aims At the end of this activity students should:
1.1 recognise the different sources of uncertainty in measurements:
- human error
- random error
- systematic error
- uncertainty arising from assumptions and models used.

Student activity D1 (10 minutes)

Instructions to the teacher	**Commentary**
Present students, in pairs, with a selection of 3 or 4 of the six cards describing a scientific investigation. For each card, students are asked to discuss • the source of uncertainty • the action scientists should take.	Sources of uncertainty: • human error; • random error; • systematic error; • uncertainty arising from assumptions and models used. The cards give examples of uncertainty due to: • human error – card 3 • random error – cards 1 and 5 • systematic error – card 2 • issues of modelling / assumptions – cards 4 and 6

Teacher-led activity D1 (5 minutes)

Instruction to the teacher	**Commentary**
Take feedback from each group on their decisions about the sources of uncertainty raised by the examples. Develop their answers to give the list of sources of uncertainty: • human error; • random error; • systematic error; • uncertainty arising from assumptions and models used.	Feedback from the group should be used explicitly to refer back to the teaching aim of this activity.

Student activity D1 (10 minutes)

Instruction to the students	**Commentary**
Group all the cards according to the four types of uncertainty given. Decide for each group what action if any the scientists should take.	

Teacher-led discussion of D1 (5 minutes)

Instruction	Commentary
Take feedback on examples of each type of uncertainty and the action the scientists should take.	

Link with the next activity

Instruction	Commentary
Pose the question: 'If uncertainty is present in scientific measurements even when human error is eliminated, how do scientists deal with this uncertainty?'	If there is to be a break here between lessons, the learning outcomes of aim 1.1 should be clearly summarised.

Activity D2 (30 minutes)

The aim of this activity is to build upon the idea of sources of uncertainty raised in activity D1, by getting students to recognise various techniques that can be used to deal with uncertainty. This activity should follow activity D1, although not necessarily in the same session. Activity D2 consists of a teacher presentation followed by a small group discussion amongst students.

Aims At the end of this part of the lesson students should:

2.1 recognise that professional scientists have to deal with human error and experimental error in their work;

2.2 begin to recognise how and why measured data are treated as a set, rather than individual values, and appreciate why repeat measurements with the same value have no special significance;

2.3 begin to appreciate that when a value is quoted with error bars, it means that the quoted value is an estimate thought to lie within a particular range.

Teacher presentation of D2 (10 minutes)

Resources

Teacher presentation notes D2.1A and D2.1B Dealing with uncertainty
OHT D2.2 Dealing with uncertainty
OHTs D2.3A and B Variation of emission rate of a radioactive substance with concentration
OHT D2.4 Variation of emission rate of a radioactive source with concentration

Instructions to the teacher for D2	Commentary
Give a brief presentation on the ways in which scientists deal with uncertainty about measurements. The presentation addresses the following key points.	
1 Random error is dealt with by presenting experimental data in one of two possible ways: • as a measured value ± an error estimate; • as a mean value ± a measure of spread.	OHT D2.2 provides some visual prompts which may help teachers structure their presentation.
2 Error bars give us an estimate of the range of likely values for the measurement. The narrower the range the more precise the estimate. **3** When plotting a line or curve of best-fit, it is important to consider the range of likely values within the error bars not just the central plotted value. **4** Systematic error can usually be dealt with by applying a correction factor. **5** An experimental value may not be accurate, even though it is precise, if the assumptions or theoretical models used to interpret the experimental data are not completely valid.	OHTs D2.3 and D2.4: Teachers' notes D2.1 contain suggestions on how to present this material.

Student activity D2 (10 minutes)

Resources: Student sheets D2.5A/B What value to choose?

Instructions	Commentary
Hand out students' sheets D2.5A and B. Instruct students to read the information given and discuss, in groups of 2/3, the points raised on both the student sheets.	

Dealing with the discussion (10 minutes)

Instruction	Commentary
Take feedback from each group on their answers to the questions, ask for explanations / reasons for their answers. Develop students' answers to highlight the teaching aims 2.1, 2.2 and 2.3.	You may wish to split the discussion to follow each of the parts of the student task separately. What does the figure ± 0.8 tell you? This indicates the precision of the estimated value. Why four significant figures? There is no need to provide more than four significant figures given the error range of ± 0.8. Why will CODATA not accept responsibility for consequences of the data? This indicates the problem that even the most precise values are not necessarily accurate. The assumptions and corrections made may not be valid. As a result this could misinform research or development which relies on CODATA values. Discounted result? The aim here should be to encourage discussion of the importance of being critical of results in a data set prior to any analysis. Is the repeat value significant? This question is asked to give the opportunity to correct any misconceptions about the significance of repeated values. What value should be published? Mean value (25.12 J K^{-1} mol^{-1}) ± a measure of spread. This is the mean value of the data points excluding the value 25.80 J K^{-1} mol^{-1}. Using the standard deviation of the values to provide an estimate of spread is beyond the scope of this activity.

Activity D3 (20 minutes, plus homework time)

The aim of this activity is to introduce students to a real research paper where issues of uncertainty are raised explicitly, and to see how these uncertainties can be dealt with. Students work in groups to look at short sections of a real research paper. They are given notes telling them what to look for in the paper, and asking them questions about it. The activity concludes with a plenary session in which the teacher uses the contributions of each group to develop a picture of how the researchers worked to get an estimate of a value.

Activity D3 is optional, in that it covers issues already introduced in activities D1 and D2. Some teachers may feel that the research paper would intimidate their students. However, during pilot work, able students engaged well with the activity. Teachers may feel it appropriate to ask students to read the paper (and prompt questions) as a homework activity before the lesson. However, the difficulty of the reading material should not be underestimated.

Aim at the end of this activity students should
3.1 consolidate their understanding of how professional scientists deal with uncertainty.

Student activity D3 (10 minutes)

Resources
Group task sheets D3.1 A–E
Sheet D3.2 'Molar heat capacity and entropy of calcium metal' Reprinted from the *Journal of Chemical Thermodynamics* (5 sheets)

Instruction	Commentary
Hand out sheet D3.2 (5 sheets) and group task sheets 3.1A–E (one sheet per group) Instruct students to read through their sheet D3.1 and the relevant text from the research paper (D3.2). They are asked to discuss some issues in the text and prepare to feedback their ideas to the rest of the group in a plenary discussion.	

Dealing with the discussion D3 (10 minutes)

Instruction	Commentary
Take feedback from each group on their answers to the two questions. Develop their answers to highlight the teaching aim 3.1. Refer to the commentary for each group.	**Group 1:** From this section of the article, students should be able to identify the implication that the control of the variables in the experiment is not completely precise. Even with the most sophisticated equipment the temperature measurement is approximate and varies during the experiment. **Group 2:** Even the most carefully prepared sample will not be 100% pure, so each measurement will contain errors resulting from the presence of impurities. These can be minimised but not eliminated. The only way to make the result more accurate is to correct for impurities on the basis of assumed content. **Group 3:** The authors needed to estimate the % of each contaminant to be able to correct for them. Each sample used will have contained slightly varying proportions. The % figures used were based on analysis of a small sample of the calcium used. **Group 4:** The title of the table indicates that the results are not corrected for impurities. This will therefore affect all the results. However precise the measurements are, they will differ from the true value for 100% pure calcium. The readings are not repeated at each particular temperature. Since the final value taken is extrapolated from a best-fit curve, the key thing here is that the measurements fit a pattern. **Group 5:** Because of a lack of published data on the heat capacity of calcium hydride, the authors have established a value from combined data with other metal hydrides. They justify this by quoting a 6% error in the match between calcium and other metal hydrides.

Activity D4 (15 minutes, or homework)

The aim of this activity is to help students to appreciate the significance of what they have learnt so far for their own practical work in A-level Chemistry. Students work in groups to look at an account of a practical activity conducted by an A-level student. They are directed to questions about how uncertainty might be dealt with, and in particular how lines of best fit ought to be drawn on graphs where data points are plotted with error bars.

Aim at the end of this activity students should

4.1 appreciate how they might recognise and deal with systematic and random errors in their own practical work in chemistry;

4.2 appreciate how they might recognise the assumptions that underpin data collection and analysis in their own practical work in chemistry;

4.3 understand the basis of routines and algorithms for data handling in chemistry practical work (such as taking the mean value from a set of measurements and commenting on spread, drawing lines/curves of best fit that lie within error bars).

Student activity D4

Resources student sheet D4.1 Dealing with errors in A-level Chemistry practical work

D4.2 Student's report on an experiment to find out how the energy in fuels depends on the structure of the molecules (2 sheets)

Instruction	Commentary
Hand out student sheets D4.1 and D4.2. Instruct students to work in pairs to answer the questions on student sheet D4.1. Alternatively, this activity could be set for homework.	

Dealing with the discussion

Instruction	Commentary
Take feedback from each group on their decisions about the sources of uncertainty raised by the examples. Develop their answers to highlight the teaching aims 4.1, 4.2 and 4.3.	**Question 1** The error bars indicate the degree of spread of the data from the mean value. This gives an indication of how precise the value is. **Question 2** Following the teacher presentation, students should be able to plot a best fit line based on the sets of data for each fuel (that is, using the error bars rather than just the mean values). **Question 3** –2450 to –2510 kJ mol^{-1} **Question 4** This question asks students to consider the accuracy of the experiment, that is, the systematic errors and assumptions. The main systematic error arises from the assumption that all heat energy output goes into heating the water. This ignores inevitable heat losses to the calorimeter and external environment. Students should also consider errors in the mass, volume and temperature measurements.

Closing the teaching sequence (5 minutes)

Resources OHT D0.1 'Aims of the lesson'

Teachers should emphasise the learning outcomes of each part of the sequence. Teachers should comment upon how the ideas introduced during this sequence will be picked up during their AS/A level course.

Points to raise	Commentary
1 Go through the OHT of the learning aims for each of the three activities. Emphasise the key points. **2** Teachers may wish to comment upon how the ideas introduced during this sequence will be picked up during the AS/A level course. Some suggestions follow. • As part of their individual coursework, students will be asked to evaluate their evidence and experimental procedures. They will need to be able to identify different sources of error in their measurements (activity D1) and evaluate the relative importance of each type of error in their particular experiment. • For some coursework activities students may need to be able to evaluate the quality of their measurements using ideas about the error range or spread in their data. They may also need to identify trends in data by plotting lines or curves of best fit which take into account both plotted values and estimated plotted ranges (activity D2).	Trials of this teaching sequence have shown the following. • It is critical that sufficient time is left for a meaningful summary. • It is helpful to summarise clearly for students what has been learnt in the lesson. • It is important to emphasise the links between what they have learnt and the rest of their chemistry/science course(s).