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The journals, *University Chemistry Education*, published by The Royal Society of Chemistry, (http://www.rsc.org/uchemed/uchemed.htm) and *Chemistry Education Research and Practice*, published from the University of Ioannina, (http://www.uoi.gr/cerp/) have merged with effect from January 1st 2005. The new, fully electronic journal is published by The Royal Society of Chemistry under the title: *Chemistry Education Research and Practice*, and it will continue to be available free of charge on the Internet. There are four issues per year.

The new journal is edited by Georgios Tsaparlis (gtseper@cc.uoi.gr) and Stephen Breuer (s.breuer@lancaster.ac.uk) and intends to maintain the high standards set by its predecessors. Its editorial policy will be the following.

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- research, and reviews of research in chemical education;
- effective practice in the teaching of chemistry;
- in depth analyses of issues of direct relevance to chemical education

Contributions can take the form of full papers, preliminary communications, perspectives on methodological and other issues of research and/or practice, reviews, letters relating to articles published and other issues, and brief reports on new and original approaches to the teaching of a specific topic or concept.

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Equations should be written into the text using the word processing program, either as normal text or using the program's equation facility.

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References should be given by the name of the author (or the first author, if more than one), followed by the year of publication. If an author has more than one reference from the same year, then it should be given as Smith 2001a, Smith 2001b, etc.

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The introduction should set the context for the work to be described; include references to previous related work, and outline the educational objectives.

A concluding section (which need not be headed conclusion) will include an evaluation of the extent to which educational objectives have been met. A subjective evaluation may be acceptable.

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For example:

Osborne R. and Freyberg P., (1985), Learning in science: the implication of children's science, Heinemann, London.

Jackman L.E. and Moellenberg W., (1987), Evaluation of three instructional methods for teaching general chemistry, *Journal of Chemical Education*, **64**, 794-96.

7. All contributions submitted will be referred anonymously by two independent referres. In case of a disagreement a third referre will be consulted. The decision of the Editors on

the acceptance of articles is final.

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Atom and molecule: upper secondary school French students' representations in long-term memory

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Abstract: The purpose of this study is to highlight collectively assimilated knowledge by upper secondary school French students (grades 10 to12) and to identify and describe the students' representations and misconceptions related to the concepts of 'atom' and 'molecule'. In order to understand assimilated knowledge better, the school science curricula and textbooks have been examined so as to identify the intended development of the conceptualisation of these concepts within the school curricula. This study is based on the written answers given by school students to four questions concerning these concepts, submitted a long time after the teaching has taken place. The analysis of the students' answers shows the various representations and misconceptions that concern the concepts of atom and molecule at each student level and allows us to see their evolution over these three years. [Chem. Educ. Res. Pract., 2005, 6 (3), 119-135]

Keywords: didactical transposition, representation, misconception, model, atom, molecule.

Introduction

Students are presented with different models of atom and molecule during their schooling at secondary school level. These models originate from knowledge that has been gradually acquired by the scientific community during the development of science, and which we will name **reference knowledge**. The first task is to turn that knowledge into teaching objects: the **knowledge to be taught** as in Official Instructions and textbooks. Then teachers must bring this knowledge into use by devising class activities that are likely to support the students' learning. It will thus become **school knowledge**. Finally, the last stage of the student's work is to interpret the knowledge 'the way he can' during various steps which will lead him/her to transform it into **acquired or assimilated knowledge** in a particular context.

This personal learner's structured organisation of a system of knowledge has been called 'alternative framework' (Driver et al., 1978; Watts, 1983), 'children's science' (Gilbert et al., 1982) or 'alternative conception' (Gilbert et al., 1985). In reference to the models used by scientists to interpret the data obtained through the experiments and to predict events, such knowledge is also labelled 'mental model' by some. According to Vosniadou (1994) mental models refer to a specific mental representation or analogical representation, made up by an individual during his cognitive functioning. In francophone countries the term 'conception' has been used. Giordan and De Vecchi (1987) define a conception as a "unity of coordinated ideas and coherent clarifying images used by learners to reason when confronted with problem-situations". Later, Watts and Taber (1996) suggested the following distinction: "an alternative conception relates to particular phenomena, and the alternative framework concerns a web of ideas within a particular scientific topic".

The purpose of this study is to highlight the assimilated knowledge collectively by students: which 'teaching models' of the atom and the molecule do they favour in a non-academic context? How does this representation of models develop from the grade 9 to the beginning of grade 12?

Evolution of the presentation of the knowledge to be taught

French Official Instructions don't prescribe any representation or reference model to be taught, just refer to the curricular model. Yet, in textbooks, the description of models is generally paired with a representation in the form of images or molecular models. Authors are therefore free to offer their representations in so far as they are compatible with the knowledge to be taught.

Grade 9 (age 14-15)

In grade 8, an atom is represented by a sphere; a molecule is made of assembled atoms and represented by space-filling molecular model. At this teaching level, an atom consists of a positively charged nucleus and of negatively charged electrons that move (revolve) around the nucleus: the electron suite. The nucleus of the atom contains as many positively charged units as there are electrons around it; the atom is neutral.

- The set of electrons in an atom is labelled the electron suite.
- All electrons are identical, they bear the same mass $(9.11x10^{-31} \text{ kg})$ and the same charge $(e = 1.6x10^{-19} \text{ Coulomb})$.
- The mass of atom is essentially concentrated inside the nucleus.
- The diameter of an atomic nucleus is roughly 100 000 times as small as that of an atom: matter is mostly made of empty space.

Thus, what must be taught is the neutral electric atom, and more precisely, the Rutherford atomic model. As far as molecules are concerned, at the end of grade 9, a student must be able to describe the molecular model of simple molecules: O₂, H₂O, CO₂, and CH₄ (that were met in grade 8).

In grade 9 textbooks, the representation of atoms is more diverse, but the model of the neutral atom (the number of negative charges of electrons equals to the number of positive charges of the nucleus) is that generally presented (Figure 1). In some textbooks, we can find a probabilistic representation of the electron cloud or the solar system model of atom.



Figure 1: Example of representation of a neutral atom model in textbooks

As far as the representation of molecules is concerned, textbooks present space-filling molecular models of the following molecules: H_2O , O_2 , CO_2 and CH_4 .

Grade 10 (age 15-16)

Atom

The atom of mass A is made of a nucleus containing Z protons and (A-Z) neutrons and of an electron suite (or revolving electrons) that contains Z electrons.

- The nucleus of an atom is symbolised ^A_ZX; A is the number of nucleons (protons and neutrons); Z is the atomic number: it characterizes the element and represents the number of protons that the nucleus contains.
- Protons and neutrons have the same mass.
- The mass of the atoms virtually equals the sum of the mass of the nucleons that constitute it
- Isotopes are atoms of one chemical element (identical Z) but with different numbers of neutrons.
- Electrons are distributed in shells, K, L, M that are further and further from the nucleus).
- The highest number of electrons in shells is 2 for K, 8 for L and 18 for M.
- The electronic structure of an atom or a monoatomic ion can be symbolized by $K^XL^YM^Z$ (for example, K^2L^4 for a carbon atom and K^2L^8 for Na^+).
- With the exception of helium, all atoms of noble gases bear 8 electrons on the outer shell.
- During chemical transformations, atoms change so as to acquire the electronic structure of the nearest noble gas in the periodic classification.

Therefore, what must be presented is a mixed model composed of the Rutherford model completed by Chadwick, and of the chemists' model of shells (Lewis, Langmuir and Bohr).

Molecule

In a molecule, atoms are linked by covalent bonding. Each bond is formed by an electron pair that results from the sharing of two electrons, generally one from each of the linked atoms.

- Between two atoms one, two or three bonding electron pairs can be found.
- The electron pairs are represented by dashes.
- An electron pair of the outer shell that is not shared by two atoms is an unshared electron pair.
- The association of atoms within a molecule can be represented by Lewis representation: a planar formula of the molecule showing all the shared and unshared electrons.
- Shared and unshared electron pairs repel one another, and position themselves so as to be as far away from one another as possible.
 - In commentaries, the curriculum authors make it clear that:
- The Lewis representation of atoms with electrons associated in electron pairs must not be used.
- To establish the representation of a molecule, the use of systematic exploration is recommended: the electrons of outer shells in the atoms that make up the molecule are first numbered and then grouped in electron pairs; the electron pairs are then shared between atoms (bonding electron pair) or around atoms (unshared electron pair) so as to satisfy the rules of 'duet' and octet.

In textbooks for grade 10, there exist only a few representations of the atomic model and when they are present, they are similar to the ones that are used in the textbooks of grade 9: neutral atoms and probabilistic representation. In this last representation the electron suite is generally identified, wrongly, with the electron cloud. No representation of the solar system model in shells is provided.

As far as molecules are concerned, the model of a covalent bond has been already introduced, and ball and stick models appear. Each stick between atoms can then be associated with a shared electron pair.

The interpretation of the geometry of some simple molecules is based on taking into account the repulsion of shared and unshared electron pairs around the central atom.

Grades 11 and 12

In grade 11, the representation of molecules with the use of molecular models is generalized in organic chemistry. What is new is the introduction of the polar character of some bonds, and of polar molecules.

Lastly, it is only towards the end of the Physics curriculum in grade 12 that the Bohr model is introduced. It will thus not appear in our study.

Analysis of students' evolving representations of atoms and molecules

Review of the literature

While very few studies have been carried out in this field in France, a lot of research has been conducted in Anglophone countries (UK, Australia, NZ, and Canada). Here, we present the main findings relevant to our work.

Conceptions of the atom

An atom is often described as round, solid, hard (Griffiths and Preston, 1992; Harrison and Treagust, 1996) and defined as a 'ball' or 'sphere' (Harrison and Treagust, 1996). Therefore, the water molecule consists of two or more solid spheres (Griffiths and Preston, 1992).

Charlet-Brehelin (1998) shows that only slightly over a third of students who have followed a traditional course of studies and have left Lower Secondary School (beginning in grade 10) have internalised the minimum formulation level required at the end of grade 9: an atom is made of a nucleus and electrons (electron suite). An identical observation is brought out by Harrison and Treagust, (1996). Students generally produce four categories of models: the atom as a sphere, solar system atom, neutral atom (positive charges of the nucleus equal to negative charges of the electrons), and the atom as a nucleus surrounded by an electron cloud. By the end of a traditional course of studies, the first two models are used by many students, 41% and 48% respectively (Charlet-Brehelin, 1998). According to Harrison and Treagust, (1996), many students represent an atom as a 'simple circle' within a large circle. Even after teaching, there remains among students a certain degree of confusion between the terms used: not only particle, atom, molecule, but also nucleus, proton, neutron and electron and their interrelationships (Osborne and Freyberg, 1985; Johnston, 1988). For some students, the number of electrons, protons and neutrons is the same for a given atom (Tsai, 1998). Keig and Rubba (1993) reveal that for many students (45%), electrons are preassembled in electron pairs within the atom. According to Taber (1998) and Robinson (1998), students use the rule of octet as a basic heuristic principle, to explain chemical bonding, chemical reaction and ion formation. An atom is said to be stable if its valence shell is filled. and is said to be unstable otherwise. The quantum model of the atom gives birth to the representation of the electron cloud. But the fact that the students are willing to use this representation at the end of grade 9 (Charlet-Brehelin, 1998) is no guarantee that they understand its meaning. Harrison and Treagust (1996 and 2000) show that, for students, the electron cloud is considered as a matrix in which electrons are embedded (as water drops in a cloud) and Tsaparlis and Papaphotis (2002) report that upper secondary Greek students' (grade 12) have greater difficulties in understanding the concept of 'atomic orbital'.

Conceptions of molecule

Atoms are generally grouped (Harrison and Treagust, 1996) and molecules are considered as groups of atoms rather than basic chemical entities (Taber, 1998) Such combination of atoms to form molecules is drawn by joining the circles or spheres that represent the atoms (Griffiths and Preston, 1992). As far as molecular models are concerned, three quarters of the students favour space-filling models to represent the molecule whereas the remaining quarter prefers the ball and stick model (Harrison and Treagust, 1996). For the drawn diagrams of molecules (more precisely H₂O), representations evolve, during the process of learning, from space filling model to structural formula (Pereira and Pestana, 1991). Three sorts of mistakes are identified: a) mistakes in representing bonds between atoms; b) mistakes in representing bond angles; c) bond orders (Pereira and Pestana, 1991; Keig and Rubba, 1993). The relative size of atoms is generally disregarded, and the length of the O-H bond increases when one goes from solid to gas state (Pereira and Pestana, 1991). Wrong understanding of the meaning of the formula that represents a molecule leads some students to have an additive misconception of the molecule (de Vos and Verdonk, 1987). The representation: H₂O is then interpreted as the association of one molecule of hydrogen (H₂) and one atom of oxygen (O), or of 'one oxygen atom and two hydrogen atoms (H₂) in the liquid state: $O(g) + H_2(g) \rightarrow H_2O(l)$, which leads to a wrongly drawn diagram of the molecule (Ben Zvi et al. 1988; Keig and Rubba, 1993).

Assimilated knowledge on the modelling of an atom

Methodology and results

The investigation was carried out with 930 students of various upper secondary schools: 239 grade 10 students (age 15-16), 422 grade 11 students (age 16-17), and 269 grade 12 students (age 17-18) of upper secondary schools. In order to collect the data, we asked them to complete a diagnostic questionnaire comprising four open questions. The tasks concerning the concept of atom were:

- Draw a diagram of the hydrogen atom (grade 10), the oxygen atom (grades 11 and 12).
- Describe the hydrogen atom (grade 10), the oxygen atom (grades 11 and 12). The total number and percentage of answers given for each question, from each group is as follows:
- Drawing diagram: grade 10, 185 (77%); grade 11, 400 (95%); grade 12, 246 (91%).
- Description: grade 10, 172 (72%); grade 11, 364 (86); grade 12, 167 (62%).
- Different kinds of drawing diagrams have been identified in the students' answers:
- **D** 0: No answer or answer impossible to classify, biological cell, particle association, atom and molecule confused for one another.
- **D.1**: Atom symbol and symbol and electron pairs for grade 11 and 12 students.
- D.2: Sphere.
- **D.3**: Composition atom model: varied representations where a nucleus and electrons are visible or representation of the neutral atom as in lower secondary school grade 9.
- **D.4**: Solar system (2D or 3D).
- **D.5**: Electron cloud.
 - Examples of such diagrams are given in Figure 2.

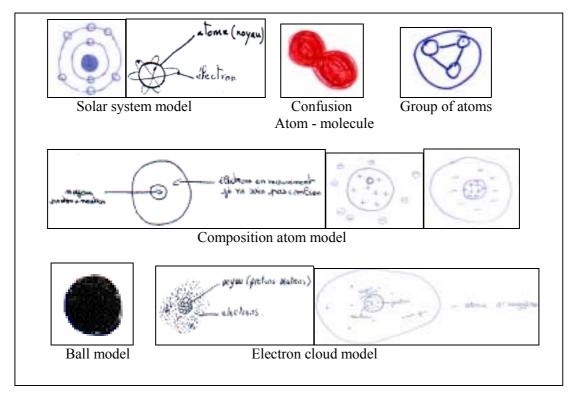


Figure 2. Examples of the student-drawn diagrams of an atom

In order to identify the characteristics of the model that were assimilated, as well as the misconceptions, a certain number of keywords have been picked from the written descriptions. They are shown in Table 1 (see Appendix) and they lead to the definitions of six levels of description:

- **L.0**: Erroneous and no answer.
- **L.1**: An atom composed of a nucleus and an electron suite (or nucleus and electrons).
- **L.2**: A neutral atom composed of a positive nucleus and an electron suite.
- **L.3**: An atom composed of a nucleus that contains protons (Z) and neutrons, and an electron suite (or negative electrons).
- **L.4**: An atom is composed of a nucleus that contains (*Z*) positive protons and an electron suite that contains (*Z*) negative electrons. The number of positive charges equals the number of negative charges. [For oxygen: 8 protons and 8 electrons].
 - **L.5**: An atom is composed of Z protons, A-Z neutrons and Z electrons.
- **L.6**: An atom is composed of a nucleus that contains Z protons and A-Z neutrons, and of an electron suite (or circling electrons) that contain Z electrons (or Z negative electrons).

Remarks (*in italics above*) concern grade 11 and 12 curricula. We can consider level 1 as the minimum level judged acceptable for students at the end of grade 9 (Lower Secondary), level 2 is the curricular level of description in that class, level 3 is the minimum level judged acceptable in grade 10 (Upper Secondary) and level 6 corresponds to the curricular level of description in that class.

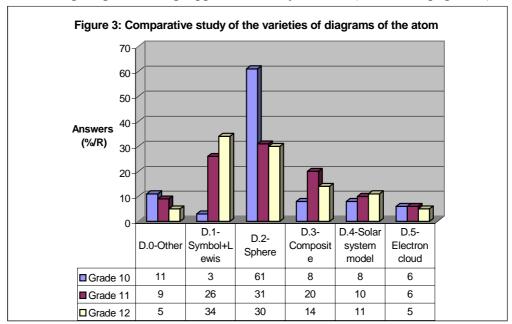
Analysis of results

We recognise that a model can be represented in different ways, with the representations varying according to the aspects of the concept to be illustrated. From our questionnaire it is not possible to know the repertoire of representations that individuals may have. We can only

identify the representations chosen by the students in response to the questions as they understood them. So, as the data from different grades does not refer to individuals, it is only possible to display an average evolution of understanding.

Drawing a diagram of an atom

The percentage of students who produced a representation of an atom was higher at the beginning of grade 11 and 12 than at the beginning of grade 10. Does this mean that the concept of the atom is more familiar to those older students? This is not necessarily so, indeed they are less and less likely to give a description with a diagram. The differences between the use of diagrams and words are: grade 10, -5%; grade 11, -9% and grade 12, -29%. These differences may be explained by the possibility that grade 12 students have forgotten the words used to describe the characteristics of the atom, or more probably, as we shall see later, by the greater emphasis placed on electron pairs that has diverted attention from these characteristics. Figure 3 allows for the comparison of the evolution of choice in the different drawing diagrams along Upper Secondary School. (See list on page 123)



R: percentage worked out from the number of drawing diagrams.

For the majority of students entering grade 10, the atom is represented as a simple sphere (61% of diagrams; 63% if we add the key words sphere or ball as used in the descriptions of other models. If a remarkable decrease in the percentage can be noticed in the following two grades, one is surprised to find still around one-third of the students that remain on the same description in grade 11 (31% of diagrams; 35% diagrams + descriptions) and grade 12 alike (30% of diagrams; 35% diagrams + descriptions). This was already identified by Harrison and Treagust (1996). Moreover, for other representations of the models of atoms exist, a tendency that was already confirmed (Griffiths and Preston, 1992; Harrison and Treagust, 1996; Taber, 1998) to include them into a spherical envelope (around 9%).

One should also consider the second favourite diagram of grade 11 and 12 students, the Lewis representation of the atom (symbol and electron pairs). Indeed, this mode of representation is forbidden by the new Official Instructions. Does this mean that some (older) teachers do not follow the instructions or that the representation is attractive due to its perception as a simplification when modelling the bonding in the molecule? Both are real possibilities, but the second is in agreement with the mental model of 'octet rule' proposed by Taber (1998). Students favour the representation of the eight electrons of oxygen in the form

of four electron pairs around the symbol of the element (and this accounts for 13% and 10%), followed by the showing of the six outside electrons (10% and 7%).

The use of the atomic composition model, and more particularly that of 'neutral atom', reaches a maximum when students enter grade 11, whereas it accounts for a majority of representations in the textbooks of grade 9. It seems therefore, that its adoption, however low, is favoured in the teaching of the electronic structure and nucleus composition. A low percentage in the choice of electron cloud model can be seen among different grades, although it is the description that textbooks authors as well as curricula developers favour. Thus, as Harrison and Treagust (1996, 2000) showed in their work, such a model is not easily grasped by students.

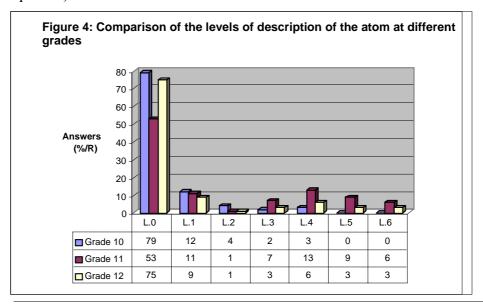
Another interesting observation is that the use of the solar system model of atom increases from grade 10 to grade 12. Yet this model is not often used in textbooks, as it appears only in documents with historical contents. Moreover, although Official Instructions forbid the representation of the solar system model in shells in 2D, some students (8% in grade 10, 10% in grade 11 and 11% in grade 12) choose this diagram. Is that a consequence of school knowledge or is it the students' own conception to represent electronic shells?

Finally, as far as other representations are concerned, they can mainly be explained by the confusion between atom and molecule. One can regret that 5% of grade 12 students still remain at this level!

Description of the atom

A vast majority of students cannot produce a minimum level of description of the concept of atom required at the end of each grade. The differences observed between the three grades prove that if the teaching in grade 10 brings along a clearly positive evolution, the concept is not well absorbed. Indeed, whenever it is not the subject of teaching (i.e. in grade 11), its minimum characteristics appear to have been forgotten by the following year.

The minimum level judged acceptable at the end of grade 9, (L1) is only reached by 21% of grade 10 students, 47% of grade 11 students and down to 25% of students at the beginning of grade 12. As far as the minimal level acceptable at grade10 is concerned (L3), only 35% of grade 11 students and 15% of grade 12 students reach it. (The levels of description are described on p. 124.)



From the diagrams and keywords, we have tried to discover what competences expected at the end of grade 10 appear in the students' answers at grades 11 and 12:

- Knowing the composition of atom knowing that atom is electrically neutral. If 46% of grade 11 students and 47% of grade 12 make it clear that the number of protons equals that of electrons, only 9% and 4% of them state explicitly that the atom is electrically neutral. The composition of the nucleus of the oxygen atom (8 protons and 8 neutrons) is only explicitly referred to by 13% of grade 11 and 10% of grade 12 students;
- Discriminating between the electrons on the inside shells and electrons on the outer shells. 19% and 14% mention a clear organization of electrons in shells, but only 12% and 9% have a clear understanding of the right distribution of electrons in shells K and L (K² L⁶ for oxygen);
- *Numbering the electrons of the outer shell.* The presence of six electrons on the outer shell is clear in some representations (Lewis representation of the oxygen atom, K² L⁶, mentioning the six electrons in the description) among 22% of grade 11 students and 17% among grade 12 students.

Considerations about the mass of atom being concentrated in the nucleus or about the atom as mainly constituted of empty space are only present in very few students' descriptions. Since the question did not explicitly ask that they write down everything they know about the structure of the atom, it is only possible to infer to their preferred representation, not to their total acquired knowledge on this concept.

Students' misconceptions

The representation of atom by Lewis model is very often chosen by grade 11 and 12 students. It is present not only in diagrams but also in the descriptions of atom, either in written or symbolic forms, even when other representations are also used, with a percentage that reaches 46% in both classes. This result is in accordance with Keig and Rubba's work (1996). One may therefore assert with Taber (1995, 1998) and Robinson (1998) that the octet rule corresponds to a 'mental model' that the students have absorbed. Such a model leads them to a static conception of electrons within the atom; they are already grouped in electron pairs: "the atom is made of, consists of, possesses, contains,... electron pairs". And for some of the students, these electron pairs are already organized as bonding electron pairs or as bonds (3%, grade 11 and 10%, grade 12).

Other erroneous conceptions to be seen in diagrams and key words:

- Atom and molecule confused with each other (13%, grade10; 6%, grade 11; 5%, grade 12).
- A confusion between the different concepts used to describe atoms: proton neutron, neutron electron, ion charged particle (respectively 4%, 3% and 2%), as already identified by Osborne and Freyberg (1985).
- Equating the total number of nucleons (16) with the number of electrons (3%, grade 11; 1%, grade 12).

Assimilated knowledge of the modelling of water molecule

The same students, in the same questionnaire were asked to:

Draw a diagram of the water molecule:

Describe the water molecule.

The total number and percentage of answers given for each question, from each group is as follows:

Drawing a diagram: grade 10: 207 (87%); grade 11: 419 (99%); grade 12: 267(99%).

Description: grade 10: 178 (74%); grade 11: 419 (99%); grade 12: 222 (83%).

The analysis of the students' answers leads to various kinds of diagrams and levels of description, as happened for the atom. Key words appearing in the descriptions are presented in Table 2 (Appendix).

Different kinds of diagram:

D.0: Erroneous answer or no answer.

D.1: Space-filling model.

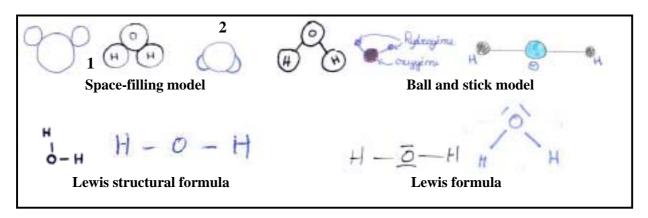
D.2: Ball and stick model.

D.3: Lewis structural formula model.

D.4: Lewis formula model.

Examples of such diagrams are given in figure 5.

Figure 5: examples of diagrams of the water molecule



Levels of description:

- **L.0:** Erroneous description or no answer.
- **L.1:** Water molecule is made of two atoms of hydrogen and one atom of oxygen.
- **L.2:** Water molecule is made of two atoms of hydrogen linked to one atom of oxygen.
- **L.3:** Water molecule is made of two atoms of hydrogen linked to one atom of oxygen by a covalent bond (or simple bond).
- **L.4:** Water molecule is made of two atoms of hydrogen linked to one atom of oxygen by a covalent bond composed of two electrons (or linked electron pair).
- **L.5:** Water molecule is made of two atoms of hydrogen linked to one atom of oxygen by a covalent bond. Each atom contributes one electron to make the bond.

Level 1 is required at the end of grade 9, level 3 is the minimum judged acceptable at the end of grade 10 and level 5 corresponds to the level of formulation in that class.

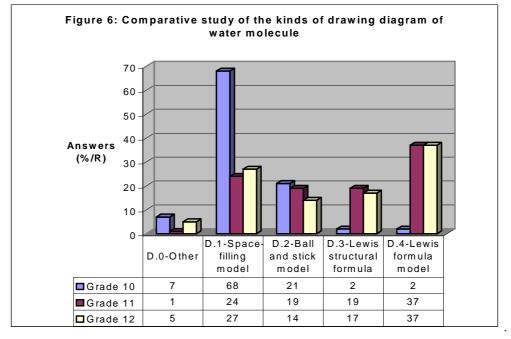
Analysis of results

Diagram of the water molecule

The percentage of total answers to this second question is higher than that to the questions on the atom. Students seem more familiar with the water molecule than with the atom. Yet it is puzzling to note that the difference between these two percentages is higher for grade 12 students (-16%) than for grade 10 (-13%) although the description of water molecule is taught in grade 10 and 11 curricula.

As Pereira and Pestana (1991) and Harrison and Treagust (1996) showed, Figure 6 shows an evolution in the drawing of diagrams along Upper Secondary School. When entering grade 10, the majority of students (68%) choose the model that was introduced at Lower Secondary level: the space-filling model. In grades 11 and 12, they mainly rely on Lewis formula model, which was studied in grade 10 (37%). In grade10, ball and stick models of molecule are also

used to represent molecules. Therefore, it may be remarked that a space-filling model is favoured by a quarter of grade 11 and 12 students and the use of this model decreases from grade 10 to grade 12.



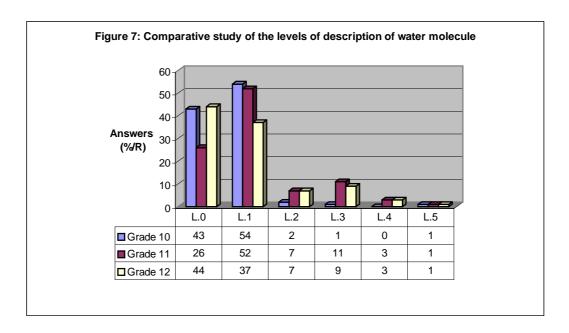
As stressed by Griffiths and Preston (1992), 70% of grade 10 students choose a space-filling model where they put hydrogen atom and oxygen atoms together (diagram 1 in Figure 5), whereas the students in the later grades produce a more acceptable representation: hydrogen atoms are 'integrated' into the oxygen atom (diagram 2 in Figure 5). Lastly, the representation in the guise of angled geometry of these different models increases noticeably from grade 10 (71%) to the higher grades (84%).

Let us note that in grade 11, 3% of the students feel it necessary to represent the molecule by the representation of each constitutive atom with the use of the solar system model in 2D.

Description of water molecule

Figure 7 shows clearly that students seem more familiar with the concept of the molecule than with that of the atom since the percentage of unacceptable descriptions is lower in all grades. Nevertheless, it is surprising to see that grade 12 students are no better than grade 10 students as far as the description of the molecule is concerned. If we consider the minimum level expected at the end of grade 9, it is reached or exceeded by 58% of grade 10 students, 74% of grade 11 students and only 57% of grade 12 students. As far as the minimum level judged acceptable at the end of grade 10 is concerned, only 15% of grade 11 students and 13% of grade 12 students reach it.

As we can see in Table 2 (Appendix), the idea of chemical bonding appears, implicitly (with the use of a verb: attached, jointed, joined, connected, etc.) or explicitly, in few grade 10 students' descriptions (12%); this is not surprising, as it is not in the curriculum at that level. Yet, the idea of bonding, explicitly or implicitly formulated is present in around one-third of the students' answers in the later grades; understandably, since covalent bonding is studied in grade 10. The percentage of students who mention covalent bonding between hydrogen and oxygen atoms is very low: 7% in grade 11 and 5% in grade 12.



In some descriptions of the water molecule, the following can be observed:

- The notion of the polarity of the molecule (11% of grade 11 students), The idea is introduced at the beginning of grade 11, at the same time as the students answer the questions. In grade 12, only 2% of the students refer to it.
- An explicit mention of the angle between the O-H bonds (5%, grade 11 students; 10%, grade 12). The accurate value is not often given.

Students' misconceptions

As noted by Pereira and Pestana (1991), when dealing with the diagrams of molecules with the help of space-filling models and ball and stick models, students do not always show the respective size of atoms: 33%, grade 10; 7%, grade 11; 15%, grade 12. The radiuses of the circles that represent oxygen and hydrogen atoms are generally equal.

Some students confuse atom and molecule in the description: "the water molecule consists of two molecules of hydrogen and one of oxygen" (12%, grade 10; 3%, grade 11 and 8%, grade 12). In grade 10, they also sometimes refer to dihydrogen or dioxygen to name atoms (7%), thus showing confusion in their conceptions.

Attributing colour to atoms in the description of water molecule (for example: "one red circle and two white circles") remains from grade 10 to grade 12 (6%, 3%, 5%) and 8% of grade 12 students still think that the molecule possesses macroscopic properties. These students thus seem to have difficulty in distinguishing model from reality. Indeed, the colour code for atoms was developed when the representation of molecules relied on the use of molecular models.

The poor understanding of what the chemical formula, H₂O, represents (Ben-Zvi et al. 1988; Keig and Rubba, 1993) leads some students to produce an erroneous description or drawing diagram of the water molecule: H and 2O (or H₂ and O): 5%, 4%, 7%.

Lastly, 5% of grade 11 and 4% of grade 12 students believe that the bond between atoms is of the ionic type (molecule consisting of ions or bonding resulting from an exchange of electrons between atoms).

Conclusions

The results of the present study show:

- That the model the students favour through their years of study is that of the spherical atom. Nevertheless, the choice of such drawn diagrams decreases from grade 10 to grade 12 in favour of the Lewis representation (symbol and electron pairs). But, for many students who rely on that representation, electrons are 'pre-assembled' in electron pairs within the atom.
- That for the representation of the water molecule, they move from a strong use of the space-filling model (where all atoms are put side by side) to the diagram according to the Lewis formula as taught in grade 10. But it should be noted that students seldom mention covalent bonding between atoms when describing the water molecule.
- That the levels of assimilation of the concepts of atom and molecule are much lower than those required at the end of the different grades.
- That from grade 10 to grade 12, for some students, confusion remains between atom and molecule and between model and reality.

The students' conceptualisation of microscopic models of atom and molecule is therefore really problematic. Attempts at interpreting the origins of such difficulty were suggested by Barlet and Plouin (1997), Tsaparlis (1997) and Taber (2004):

- The concepts involved are abstract and cannot be related to everyday experience. Their understanding requires a high level of abstraction from the students, which seems to be the case for only some 50% of them when entering university;
- Real training cannot take place unless students manage to give a meaning to the new knowledge they are presented with. To do so, they rely on the knowledge available in their long-term memory. Whenever such knowledge is not available or wrongly structured, the result leads to superficial, mechanical learning.

Therefore, it is no surprise that in the first confrontation with complex knowledge, students cannot easily absorb it. This is demonstrated by the fact that, after thorough teaching of the models, a positive evolution can be observed in the students' answers. When the topic is not studied any longer, many students go back to their initial levels of drawn diagram and integration. On this subject, Taber (2004) writes: "It is conjectured that recently acquired knowledge – though accessible in response to direct questioning – may not be available in a form suitable to act as the foundation for new learning, not having yet been fully integrated into conceptual schemes".

How can we make the students progress in the appropriation of these abstract concepts? It is not a question of the curriculum, since our observations are in agreement with those carried out in various Anglo-Saxon countries. Our hypothesis is that the possibility of progress is based on activities that allow students to rationalize the organisation of conceptual knowledge. Our first proposal is to work on historical models. Classroom discussion based on arguments/counterarguments on the possibilities and limits of each model can facilitate the students' conceptual understanding (Justi and Gilbert, 2000; Laugier and Dumon, 2000; Niaz et al., 2002). A second proposal is to help students to discern that each representation of one model is a 'purpose-built model' linked to the question asked (Harrison and Treagust, 2000). Finally, inquiry based teaching sequences engaging students to make inferences about the atomic realm can be a good strategy to help them in linking the domains of macroscopic observation, sub-microscopic particles, and symbolic representation (Toomey et al., 2001).

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Official Instructions:

- $B.O.E.N.-N^{\circ}$ 5 du 9 mars 1995, Programmes du cycle central des collèges
- B.O.E.N. –H.S. N° 4 du 22 juillet 1999, Programmes des 3^{ème} des collèges
- B.O.E.N. –H.S. N° 6 du 12 août 1999, Programme de la classe de seconde
- B.O.E.N. –H.S. N° 7 du 31 août 2000, Programme de la classe de 1^{ère}, série scientifique
- B.O.E.N. -H.S. N° 4 du 30 août 2001, Programme de la classe de terminale, série scientifique

Appendix. Summaries of the students' descriptions of the atom and the water molecule

The tables below show, the keywords picked from the written descriptions and classified into different categories. A description of one student may contain more than one keyword. So the total number of the key-words is greater than the total number of students' answers (in parentheses), and the total of percentage is greater than 100%.

Table 1. Summary of the students' descriptions of the atom.

DESCRIPTIONS		Beginning of grade 10		Beginning of grade 11		Beginning of grade 12		
		Nb.	% (172)	Nb.	% (364)	Nb.	% (167)	
ut	Colour		12	7	18	5	16	10
Attribut	Form		20	12	26	7	16	10
Ati	Tota	l	32	19	44	12	32	19
	Symbol		12	7	15	12	4	2
tic	Mass		6	4	7	2	7	4
Characteristics	Charge		12	7	27	7	6	4
	Size		13	8	5	1	1	1
ars	Place in the periodic table		4	2	-		1	1
Ch	Empty space in the atom		1	1	3	1	1	1
	Tota		48	28	57	16	20	12
GR (electro	ons revolve around nucleus)	22	13	88	24	32	19
		$N e^{-} total = Z$	9	5	167	46	79	47
	Su	$N e^{-} total \neq Z$	32	19	13	4	2	1
	Electrons	N valence e correct			8	2	2	1
ition		N e on shells K and L correct			36	10	21	13
Composition		e- on shells K,L,M et N e ⁻ > Z			17	5	2	1
Con	S	Z protons	3	2	79	22	22	13
	len	Z protons and Z neutrons	6	4	48	13	24	14
	Nucleus	Incorrect composition			8	2	3	2
	Total		50	29	376	103	155	93
io	Atom / molecule		14	8	14	4	9	5
lfus	Other		11	6	6	2	3	2
Confusio ns	Total		25	15	20	6	12	7
ling	It can give two bond/two bonded electron pairs				21	6	24	14
Electron pairs/ bonding	Octet rule/ 4 bonds or bonded electron pairs / 4 electron pairs				18	5	14	8
	2 or 3 electron pairs				6	2	1	1
ectro	6 electron pairs / bonds				2	1		
E	Total				47	13		

Table 2: Summary of the students' descriptions of the water molecule.

DESCRIPTIONS		Beginning of grade 10		Beginning of grade 11		Beginning of grade 12	
		Nb.	% (178)	Nb.	% (402)	Nb.	% (198)
	2 H atoms and 1 O atom	110	62	311	77	125	56
Constitution	2 O atoms and 1 H atom (or H ₂ and O)	9	5	18	4	14	7
	2 hydrogen molecules and one of oxygen	22	12	13	3	16	8
	Confusion atom - molecule	36	20	-	-	-	-
	Others (in term of atoms)	14	8	6	1	3	1
Bond	Implicit idea of bond	15	8	57	14	35	16
	Bond	3	2	18	4	11	6
	Covalent bond – bonded electron pair	-	-	28	7	21	5
	Bond by transfer of e ⁻ - molecule composed of ions	-	-	20	5	7	4
	Other	3	2	14	3	2	1
Attributions	Bond angles	-	-	17	4	19	10
	Polarity	-	-	45	11	5	2
	Colours on atoms	10	6	12	3	9	5
1	Macroscopic properties	-	-	6	3	15	8

Molecular visualization in chemistry education: the role of multidisciplinary collaboration

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Abstract: Visualization tools and high performance computing have changed the nature of chemistry research and have the promise to transform chemistry instruction. However, the images central to chemistry research can pose difficulties for beginning chemistry students. In order for molecular visualization tools to be useful in education, students must be able to interpret the images they produce. Cognitive scientists can provide valuable insight into how novices perceive and ascribe meaning to molecular visualizations. Further insights from educators, computer scientists and developers, and graphic artists are important for chemistry educators who want to help students learn with molecular visualizations. A diverse group of scientists, educators, developers, and cognitive psychologists have begun a series of international collaborations to address this issue. The effort was initiated at the National Science Foundation supported Molecular Visualization in Science Education Workshop held in 2001 and has continued through a series of mini-grants. These groups are investigating characteristics of molecular representations and visualizations that enhance learning, interactions with molecular visualizations that best help students learn about molecular structure and dynamics, roles of molecular modeling in chemistry instruction, and fruitful directions for research on molecular visualization in the learning of chemistry. This article summarizes the value of collaboration identified by participants in the workshop and subsequent collaborations. [Chem. Educ. Res. Pract., 2005, 6 (3), 136-149]

Keywords: molecular visualization; modeling; particulate nature of matter; computer-assisted education; collaboration; multidisciplinary.

Do not underestimate the power of kinetic art... Pictures seldom can capture all the subtle nuances of a model, but good pictures and movie clips are not only what are best remembered, they also often enable us to take the next steps in both teaching and research. (Zare, 2002)

The importance of collaboration

Chemistry research today is increasingly focused on phenomena that are understood and communicated by means of visual representations. For example, research on carbon nanotubes, conducting polymers, drug design, and self-assembling materials is carried out and

Chemistry Education Research and Practice, 2005, 6 (3), 136-149

communicated with the help of computer-generated images. Some chemical phenomena are not obvious without the use of visualizations; visualization tools such as molecular modeling programs are required to describe and study them. Using these tools requires the ability to identify and make use of complex visualizations of molecular structures. However, technologies developed for molecular research generally involve interfaces that were optimized for research purposes and may be difficult for beginners to use (Edelson and Gordin, 1997). Fluency with molecular visualization tools is becoming a literacy requirement for chemists, but new interfaces may be required in order for molecular visualization tools to be successful in education.

Visualization tools are now beginning to be used in a central way in the introductory chemistry classroom (Jones, 2001; Tasker, 2004). Beginning chemistry students can now be exposed to a wide array of molecular visualizations: structural formulas, line drawings, physical models, a variety of dynamic three-dimensional computer-generated molecular models, and images generated by instruments such as scanning tunneling microscopes. Learning from these molecular visualizations is challenging for students because they can be complex and require a variety of skills to interpret (Kozma and Russell, 1999). However, the understanding and use of a variety of molecular representations is important in understanding the particulate nature of matter (Griffiths and Preston, 1992; Johnstone, 1993; Bodner and Domin, 2000). The merging of scientific fields with disciplines such as art, psychology, and technology can result in visualizations that are not only effective in communicating concepts, but are also easily interpreted by beginning students (Gordin and Pea, 1995). These interdisciplinary collaborations are important for visualizations of the particulate level of matter to be effective learning tools.

The knowledge and skills required to produce pedagogically effective visualizations and to apply them appropriately for learning go beyond the knowledge of chemistry to encompass the findings of cognitive science and the principles of pedagogy. The need to apply knowledge from multiple disciplines toward the improvement of chemistry education has been recognized by others (Bailey and Garratt, 2002; Bucat, 2004; Gilbert et al., 2004). This paper describes a rationale and model for real-time collaborations between chemists, educators, and cognitive psychologists to develop visualizations, to design effective pedagogical uses of visualizations, and to conduct research studies of learning from visualizations.

In 2001 the United States National Science Foundation supported a project to build collaborations among diverse research communities in order to investigate molecular visualization in the teaching of chemistry. The initial activity of the project was the Molecular Visualization and Science Education Workshop held in Arlington, Virginia, USA, which was organized by the authors of this paper. Thirty-six scientists, developers, cognitive psychologists, and science educators met to examine characteristics of molecular representations, interactions with visualizations of molecular structure and dynamics, the role of molecular modeling in chemistry curricula, and fruitful directions for research on molecular visualization in the learning of chemistry.

The workshop explored the frontier between the physical and cognitive sciences. In particular, the participants examined how research findings from the cognitive sciences can be applied to improve chemical education as well as the design of visualization tools. All types of molecular models were considered, including physical models. However, computer-based multimedia and molecular modeling tools became the primary focus of the workshop, because of their potential to make a profound difference in how molecular-level concepts are learned (Williamson and Abraham, 1995; Hehre and Nelson, 1997; Shusterman and Shusterman, 1997; Smith, 1998; Jones, 1999; Dori and Barak, 2001).

Workshop participants readily saw that each discipline had a separate, but essential role to play in the development and use of molecular visualizations in the learning of chemistry. It

soon became apparent that multidisciplinary collaborations would enable projects more ambitious than participants might otherwise have considered. An independent evaluation of the workshop conducted by José and Williamson (2005) found that immediately following the workshop 72% of the participants agreed with the statement, "The interdisciplinary interactions at this workshop have encouraged me to work with others outside my own perspective on projects." That this effect was fundamental and lasting is suggested by the fact that after one year had passed, 76% agreed with the statement. The workshop report, which summarizes the discussions, is available on-line (Jones et al., 2001).

The next phase of the project was the funding of six small projects called mini-grants to promote collaboration across the disciplines of science, cognition, and education in support of visualization in science education (Jones, 2004; also see the Appendix at the end of this paper). These collaborations, which involve investigators from seven disciplines and seven nations, have begun to address the issues raised at the workshop by initiating pilot research studies and by developing a variety of instructional materials.

This article reports on the potential benefits of interdisciplinary collaboration for molecular visualization that were identified in the workshop and how they have been developed through subsequent collaborations. It also outlines guidelines for such collaborations that have proved beneficial.

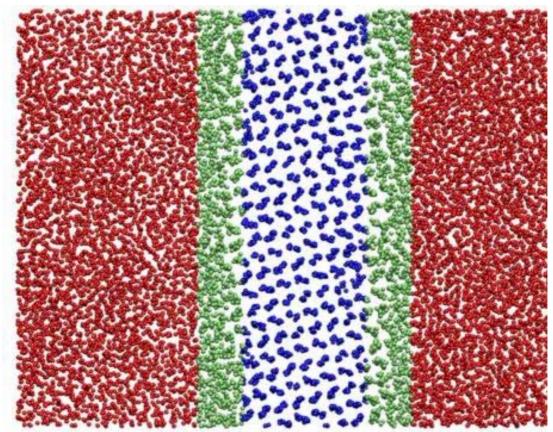
A cognitive science perspective on learning from molecular visualizations

In the past the term *visualization* was used to refer simply to the process of imagining, but the term is now being applied to images that enhance our imagination and visual experience. Visualizations can extend the visual memory and thinking processes of chemists by providing dynamic images of virtual worlds (Shepard and Cooper, 1982). These images are used to convey complex, subtle molecular interactions and dynamics that are difficult to describe in words. For example, they can show chemists the flexibility of proteins, the mechanism by which ions pass through membrane channels, and how heating a molecule affects its reactivity.

A chemist can 'see' the theory underlying a visualization. However, cognitive scientists have shown that the visual system has limited neural resources (Trick and Pylyshyn, 1994). Therefore, visualizations of abstract molecular concepts may be too complex for learners to process. For students to learn from an image, they must attend to its relevant characteristics and understand how they demonstrate new concepts. They must also know the scientific conventions (Habraken, 1996) and learn to tune out irrelevant or distracting information (Kozma and Russell, 1997). For example, Figure 1 was produced for use in research on the structure of water by a molecular dynamics NAMD simulation (Humphrey et al., 1996; Kalé et al., 1999). A chemist involved in this research will see in the image how the structure of water changes when ice melts, but without guidance a beginning student—even a chemist not familiar with the representational conventions—may see only a confusing array of molecules.

Cognitive scientists participating in the workshop and collaborations described in this paper reported that the difficulties students face in understanding and using molecular visualizations can tentatively be divided into four areas: visual subtlety, complexity, abstractness, and conceptual depth (Jones et al., 2001). These difficulties may not be apparent to chemists who are fluent users of visualizations. However, they pose important research and design challenges for chemistry instructors and for developers of molecular visualizations.





What do you see in this picture? The image is a 'snapshot' from a 500 ps molecular dynamics NAMD simulation that shows how the structure of water changes when ice melts. The red spheres represent liquid water molecules, blue spheres represent ice, and green spheres represent water in the interfacial region. The image shows researchers that water molecules form clusters when they melt (the clusters can be seen in the interfacial region). Image provided by Jeffry Madura with the assistance of Pranav Dalal (Center for Computational Sciences), Duquesne University.

Visual subtlety: Spatial relationships in molecular visualizations can be difficult to interpret. Some examples are the two-dimensional display of three-dimensional structures, the fact that a variety of angles other than 90° occur in molecular structures, and the need simultaneously to track the motion or arrangements of multiple objects.

Complexity: Interpreting a molecular structure may be a complex process when the amount and depth of information encoded in the representation is large and when different representations must be used and compared. Although students benefit when different types of representations are used to convey different conceptual content, learning to understand each variety of representation and the interrelations among them is a complex process.

Abstractness and conceptual depth: Molecular visualizations use a set of conventions to represent phenomena not normally visible. The conventions are readily understood by chemists, but beginning students must learn to interpret these conventions. In ball-and-stick molecular models, for example, the balls and sticks are symbols that stand for things that have few of the properties of the symbols themselves. Students must learn to make connections between molecular representations (the balls and sticks) and the concepts they represent (atoms and chemical bonds).

Expert chemists can link theory and appearance to 'see' the theory in a molecular structure. For novice learners the relationship between a visualization and the underlying concepts is much more difficult to understand. In order to learn more about a concept from a visualization they must already have some knowledge about the concept and how it is represented by the visualization (Treagust et al., 2003). The visual subtlety, complexity, and conceptual depth of molecular visualizations present important research and design challenges to chemistry instructors, curriculum developers, and educational researchers.

The place of molecular visualization in the curriculum

Mathematics curricula based on multiple representations have been found to provide teachers with a greater variety of instructional and assessment approaches than do traditional curricula (Cuoco and Curcio, 2001). Similar findings have also been reported in chemistry classrooms (Russell et al., 1997). Participants in the collaborations described here devised a set of characteristics that should be considered when introducing molecular visualizations into the tertiary general chemistry curriculum (Jones et al., 2001). These include providing opportunities for practice and feedback on learning, appropriate annotation of visualizations, gradual introduction of conventions and structural complexity, comparative presentation of related visualizations, the use of animations, provisions for appropriate interactions with the visualizations, and instructional materials designed for concept mastery and inquiry.

Interactive computer-generated molecular visualizations provide many opportunities for instructional innovation. They are being used not only to encourage students to think about chemistry in terms of molecules, models, and symbols, but also to provide opportunities for students to become more independent learners (Agapova et al., 2002). In addition, interactive visualizations can help instructors interest and motivate students with a variety of learning styles (Suits, 2003). To achieve these goals, more activities incorporating visualizations that are easy for students to use and interpret will need to be developed.

Many topics in chemistry require learners to understand structures in three dimensions, changes over time, and causality. Molecular animations can be powerful tools for learning these dynamic and three-dimensional chemistry concepts (Tasker, 2004). However, a problem with the use of animations for teaching molecular structure and dynamics is that merely viewing a visualization may lead to learning at a lower level than would drawing or building a molecular structure. Consequently, it may be beneficial for computer-based visualizations to provide opportunities for students actively to explore concepts (Khan, 2001).

At the high end of technological development are novel learning environments that help students to visualize complex or invisible phenomena through immersion in a virtual reality (Johnson et al., 2001). Virtual reality offers the potential for exploring complex molecular structures from many vantage points, even from the inside out. However, the more complex the representations the more guidance and scaffolding is required for students to interpret them (Suits and Diack, 2002; Ardac and Akaygun, 2004; Kuo et al., 2004).

Research on molecular visualizations in chemical education

Because molecular visualization plays a central role in much chemistry and biology research, research into the characteristics and modes of interaction with visualizations used by scientists is as important as research into learning with visualizations. Although some work is currently being conducted in these areas, our knowledge of how visualizations can best be created and used is still tentative. Interdisciplinary collaborations involving chemists, biologists, cognitive scientists, and science educators may enhance these research studies.

Research on characteristics of molecular visualizations can address such questions as, "What are the effects of visualizations on intuitions, research questions, conceptions, and misconceptions?" and "What principles of graphic design are important for the design of effective molecular visualizations?" Research on modes of interaction with visualizations can address questions such as, "How do student mental models of matter change as a function of interaction with molecular visualizations?" and "Which learning method is most appropriate for a given learning situation?" Research on curriculum issues is needed to study issues such as the problem-solving skills required for interpreting different kinds of visualizations, how the curriculum can be restructured to incorporate visualizations, the extent of guidance students need to interpret specific types of visualizations, and how learning from visualizations can best be assessed.

Building fruitful collaborations between disciplines

At the 2001 Gordon Research Conference on Visualization in Science and Education the US National Science Foundation solicited and funded six small projects called mini-grants to promote collaboration across the disciplines of science, cognition, and education in support of visualization in science education (see the Appendix at the end of this paper). Each project received US\$5000 to facilitate interdisciplinary and multidisciplinary collaboration. These collaborations, which involve participants representing thirteen disciplines, have begun to address the issues raised at the workshop by conducting pilot research studies and by developing a variety of instructional materials. A second round of five mini-grants, administered by Mary Jane Shultz, Tufts University, were awarded in 2003. The Appendix at the end of this article contains a brief description and contact information for each of the six completed projects.

Outcomes of the mini-grant program

The outcomes of the mini-grant projects far exceeded expectations. The participants reported that they had carried out projects not otherwise possible without the multidisciplinary collaborations, had initiated additional collaborative research and development efforts, and had identified barriers to collaboration between disciplines for work in this area. The six collaborations involved participants from more than twenty-five institutions and seven nations. Research studies on learning from visualizations were conducted in nine of the institutions. Twenty conference presentations reported the results of these projects, two articles have been published (Dori et al., 2003; Velázquez-Marcano et al., 2004), and several articles are in preparation.

A variety of products were produced in the collaborations, including new evaluation instruments, websites for research or dissemination, digital videos of chemical demonstrations and experiments, a set of animations, instructional software programs, paper instructional materials, and two annotated bibliographies.

Three major obstacles were encountered by the mini-grant teams. One was the need to overcome different views on project goals and activities that often arose from differences in disciplines and types of institutions. The second was the need to frame projects in such a way that they would be acceptable for promotion of participants within science departments. Some promotion and tenure committees did not understand how to evaluate the work being done. The third was the difficulty of maintaining frequent communication among participants at geographically distant institutions. Minor problems reported included the difficulty in finding times when all the collaborators were available to meet, coping with the time required for the work, and changes in personnel.

Many benefits of the collaborations were cited by project participants, including new ties across disciplines, the development of new instructional tools, research instruments, and protocols, and the new perspectives gained from other disciplines. The participants felt that the collaboration between disciplines was a strength of their projects and they reported that they would not have been able to tackle the projects alone. The scientists felt that they had gained the ability to set appropriate learning objectives, had developed a greater awareness of student learning needs, an appreciation of the difficulties of evaluating major instructional change, the ability to design assessment tools, and the confidence to tackle complex projects that require expertise in other disciplines. One investigator, Peter Mahaffy, reported the following (Lewis and Mahaffy, 2003):

"In my experience, the most valuable dimension to the mini-grant was the way it formalised working across learning communities. Natural scientists with experience in visualization, social scientists, teachers, and curriculum planners all engaged in conversation and testing to learn how visualizations are culturally laden. In the process of trying to understand the cultural dimensions to visualization, we have also carefully identified some more fundamental questions about what constitutes an effective visualization."

Recipients of the mini-grants reported that they would not have been able to carry out the interdisciplinary projects without the stimulus of the mini-grant funds. Although the dollar amount was very small, it was enough to bring together individuals with complementary expertise. The majority of the mini-grant participants reported that they plan to continue their work in the area of scientific visualization in education.

The mini-grant recipients reported a number of factors that they felt led to successful collaborations. These factors include common goals, mutual interests in the educational applications of scientific visualizations, additional funds from other sources, pre-existing connections among the participants and with other, related projects, proximity of the participants to one another, and supportive colleagues and institutions. The following case study illustrates how the efforts of one mini-grant team managed to overcome difficulties and achieve a synergy beyond that which team members could have managed individually.

Testbeds for new visualizations in organic chemistry: Case study of a mini-grant

One of the authors of this paper, Neil Stillings, was the Co-Principal Investigator of a mini-grant project. The work was carried out under the leadership of Carl Wamser, a chemist at Portland State University (PSU) in Oregon, on the West Coast of the U.S., while Stillings, a cognitive psychologist, is based on the East Coast, 3000 km and three time zones away. Locations of the additional participants and consultants, Pratibha Varma-Nelson (Northeastern Illinois University), Jack Kampmeier (University of Rochester), Don Wedegaertner (University of the Pacific), and Gwen Shusterman (Portland State University), were equally widespread.

The majority of the work was performed at Portland State University, where the subject students were enrolled, and where the two Principal Investigators met to administer the new tests and surveys. The project was carried out in an organic chemistry course in which an innovative teaching environment, Peer-Led Team Learning workshops, had been introduced (http://www.sci.ccny.cuny.edu/~chemwksp/). The goal of the project was to create new visualization exercises and assessments of stereochemistry that could be used within this workshop learning environment and would also be valuable in traditional classrooms. Wamser would develop the exercises and Stillings the assessments.

Stillings felt that he needed to know more about the chemistry before he could begin. Therefore, one of his first activities was to visit PSU, where he attended organic chemistry classes and workshop sessions as an unobtrusive observer. He studied how the students used

molecular models and 3D computer visualizations to develop an understanding of stereoisomerism. He also obtained a model kit and an organic chemistry textbook in order to learn the stereochemistry concepts taught in the course. This initial background work allowed him to create a specialized organic chemistry analog of a commonly used generic mental rotation test (Peters et al., 1995).

The new test was administered to students along with a questionnaire that asked the students to characterize their mental rotation strategies and to reflect on the ways in which three-dimensionality can be perceived and manipulated. Preliminary results show that students significantly improved their scores after participating in peer-led workshops in which they were required to build three-dimensional models to illustrate stereochemistry concepts.

The team kept in touch through frequent email exchanges and conference calls. They felt that maintaining frequent contact allowed the development of the testing and assessment methods to proceed smoothly despite the distance and the different disciplinary backgrounds. They also felt that the work would not have been possible without the collaboration fostered by the mini-grant (Wamser and Stillings, 2003):

"This work would not have happened without the stimulus of the NSF mini-grant. The specific manner in which it was carried out could not have happened without the blending of the two unique approaches brought by the two PIs. Each of us has become much more aware of the other's field of study and the potential for interrelationships between the fields. In particular, neither of us would have had the expertise or confidence to have tackled an interdisciplinary project like this alone."

Summary

The workshop and projects described in this paper show that the field of molecular visualization can benefit from collaborations that involve chemists, educators, cognitive psychologists, and other professionals. The workshop, which brought together multiple disciplines with a common agenda, was found to be instrumental in promoting these collaborations. José and Williamson reported in an evaluation of the workshop (2005) that the workshop "made progress toward defining the role/nature of molecular visualization in science education," served as a model of successful interdisciplinary collaboration, and acted as a catalyst for research into learning from molecular visualization. The workshop also served to raise awareness within the cognitive science community of molecular visualization as a research area. This multidisciplinary workshop model has now been successfully applied in geoscience education (Manduca et al., 2004).

Participants in the Workshop for Molecular Visualization in Science Education found that communication between disciplines is not only important between educational researchers and classroom teachers (de Jong, 2000), it is necessary between educational researchers and chemists, psychologists, and professionals from other fields. Collaborations involving chemists, cognitive scientists, science educators, and others are needed to carry out research studies on learning with molecular visualizations. The success of the mini-grant program suggests that small multidisciplinary projects that promote collaboration on such research efforts may be successful.

Individuals wanting to become involved in multidisciplinary collaborations in molecular visualization can find willing collaborators at conferences such as the Gordon Research Conference on Visualization in Science and Education, which is currently scheduled in odd-numbered years in Oxford, England. Information on this conference series is available at http://www.grc.org/programs/2005/visualiz.htm. Several other conference series promote multidisciplinary collaboration for scientific visualization in instruction. Two are the IEEE

Visualization Conference, http://vis.computer.org/, and Ed-Media, which is sponsored by the Association for the Advancement of Computing in Education, http://www.aace.org/conf/edmedia/.

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Appendix: Summaries of the Mini-grant Projects

This listing includes only the Principal Investigators and Co-Principal Investigators of each project and a brief summary of the accomplishments. Many additional participants were involved and extensive additional activities were carried out. Principal Investigators can be contacted for further information on the individual projects. All participants are from the United States unless otherwise indicated.

1. Towards the general chemistry course of the year 2050

Principal Investigator: Peter Garik, Boston University

Co-Principal Investigators:

Yehudit Dori, Technion, Israel University of Technology, Haifa, Israel

Morton Hoffman, Boston University Kenneth Jordan, University of Pittsburgh Contact: Peter Garik, garik@bu.edu

Summary: This project was designed to set up pilot tests of new instructional approaches incorporating visualization in a small honors course at Boston University. The investigators were able to modify their goals to include the large introductory chemistry course, due to the interest of an additional faculty member at Boston University. Their final goals included the refinement of a computer-based visualization tool for learning quantum mechanics, creating an instructional unit for the tool, develop an instrument to measure the effect of the tool on students' knowledge and beliefs, and providing access to the software through a website.

2. Cross-cultural issues in building science education capacity through visualizations in chemistry and physics

Principal Investigator: Nathan Lewis, California Institute of Technology and Caltech Chemistry Animation Project

Co-Principal Investigators:

Peter Mahaffy, The King's University College, Edmonton, Alberta, Canada

Natalia Tarasova, Professor and Director, Institute for Problems of Sustainable Development, Moscow, Russia

Zafra Lerman, Columbia College, Chicago

Brian Martin, The King's University College, Edmonton, Alberta, Canada, and Alberta Modular Approach to Physics Project

Clarence Joldersma, Associate Professor of Education, Calvin College, Michigan

Leanne Willson, Psychology, University of Alberta, Canada

Contacts:

Nathan Lewis, <u>nslewis@its.caltech.edu</u> Peter Mahaffy, <u>pmahaffy@KingsU.ab.ca</u>

Summary: This proposal provided seed funding to bring together developers of significant visualization tools in chemistry and physics with experts in cognition, education, pedagogy, assessment, and cross-cultural issues. It piloted the use of these visualization tools in a development context, thus extending discussions about visualization in science to include collaborators from Eritrea in the science of learning and the learning of science. A detailed annotated bibliography on cross-cultural issues in science education was prepared and disseminated among project participants. Project materials were evaluated then implemented in the Chemical Liceum in Khimki, Moscow region of Russia, and at several institutions in Eritrea: the Chemistry, Physics, and Education Departments of the University of Asmara, the Eritrean Ministry of Education (for a panel of curriculum leaders), and a library in Decamare.

3. Assessment strategies for instruction using molecular visualizations

Principal Investigator: Duane W. Sears, University of California-Santa Barbara

Co-Principal Investigators:

Robert C. Bateman, University of Southern Mississippi

Brian T. White, University of Massachusetts

David Uttal, Northwestern University

Contact: Duane Sears, sears@lifesci.ucsb.edu

Summary: This project was designed to address the question, "Do visualizations really help students learn?" The investigators compared and evaluated available molecular visualization software programs that are used widely by instructors in biochemistry, biology, chemistry, and related disciplines. A cognitive psychologist critiqued assessment instruments and provided guidance in the analysis of assessment data. The project investigators participated with others in developing a research plan to investigate the teaching of biochemical concepts and scientific thinking skills by interactive investigation of the properties of hemoglobin.

4. The influences of external representations on introductory chemistry student's learning of particulate structures and processes

Principal Investigator: Mark Walter, Oakton Community College Co-Principal Investigators:
Dorothy Gabel, Indiana University
David H. Uttal, Northwestern University
Zafra Lerman, Columbia College, Chicago
John K. Gilbert, The University of Reading, UK

Summary: This minigrant initiated a collaboration that focused on using students' explanations of self-constructed external models to monitor conceptual change and the influence of the external representations on this process. The work involved studying the effect of allowing students to create atomic and molecular models from pliable, nontoxic Play-Doh. The project conducting experiments to compare the Play-Doh visualization tool with a visualization created using pen and paper and explored the contributions of cognitive psychology to understanding the Play-Doh visualization. The visualization experiments were conducted at Oakton Community College and Indiana University, Bloomington. The results, though preliminary, showed enhanced learning when the Play-Doh visualization method was used.

5. Peer-led chemistry workshops as testbeds for new visualizations in organic chemistry

Principal Investigator: Carl C. Wamser, Portland State University Co-Principal Investigator: Neil Stillings, Hampshire College

Contact: Carl Wamser, wamserc@pdx.edu

Contact: Mark Walter, mwalter@oakton.edu

Summary: This project created new visualization exercises and assessments on stereochemistry for organic chemistry courses. The new materials were tested with students in peer-led team learning (PLTL) workshops in the organic chemistry class at Portland State University. The assessment of student learning emphasized mental rotation skills judged by student scores on standardized tests for mental rotation as well as on course-based stereochemistry problems. The project developed instruments to investigate correlations between student success in understanding and applying stereochemistry in an organic chemistry context with a more general ability to perform mental rotation of three-dimensional objects. New molecule-based mental rotation tests were developed and have been tested in the PLTL workshops.

6. Visualization to promote conceptual change

Principal Investigator: Vickie M. Williamson, Texas A & M University

Co-Principal Investigators:

Guy Ashkenazi, Hebrew University, Jerusalem, Israel Roy Tasker, University of Western Sydney, Australia *Contact*: Vickie Williamson, williamson@tamu.edu

Summary: The participants in this project developed a web-based instrument, collected research data with that instrument, and investigated whether video demonstrations or molecular animations helped students to understand chemistry concepts and if the order of presentation of the macroscopic video or animation affected learning. Students showed improvement after each visualization. A significant improvement in responses was seen between the first and second visualization. These results were interpreted to mean that it is important to combine both types of visualizations, but that the specific order may not be important.

The strategies used by distance education students when learning basic chemistry; implications for electronic delivery

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Abstract: The already developed learning profiles of distance education students could be a determining factor in whether or not electronic forms of instruction will be successful. Several groups of distance education chemistry students were interviewed to discover the strategies they use when studying from their present printed material. A number of strategies were identified and grouped into two major categories and several subcategories, depending on the content of the material being studied and time available for study. It was found that the students used a cognitive linear style of learning, using three distinct types of learning strategies revolving around the core strategy of taking, summarising and rewriting of notes. They then used a separate, but similar, set of strategies to validate their knowledge. A computer based learning program would have some advantages over print, but would need to support the present style of learning adopted by the students. Suggestions are made for an integrated program that may encourage students to adopt alternative strategies. [Chem. Educ. Res. Pract., 2005, 6 (3), 150-165]

Keywords: distance learning; learning profiles; learning strategies; note taking; deep and surface learning; facts and concepts; computer based learning.

Introduction

In Australia, because of its large area and small population, the distance education students usually receive instruction on their own, and often at a remote site where they cannot physically meet with their fellow students. Printed study guides and textbooks are still the primary learning resources, and students have adopted their study methods around these. However, the rapid expansion of information technology combined with economic forces is forcing institutions to investigate more (supposedly) cost-effective methods to deliver their courses (Gladieux, 2000), and there is considerable pressure on educators to use modern technology to provide more flexible ways of delivering high quality educational programs (McNamara and Strain, 1997). This push to use technology has caused difficulties, not the least of which have been a failure to maintain a quality product (Vidovich and Porter, 1999), and the extra stress on the students brought about by a new and different form of communication (Hara, 2000). In his review of distance education, Dhanarajan (2001) pointed out the necessity to adapt the current teaching pedagogy to better exploit the technology.

Such a pedagogical change needs to be based on a learner-centred approach where the educational process is supported by the technology rather that being driven by it (Rumble, 2001; Petrides, 2002). Laurillard (2002) pointed out that it is a mistake to base the design of learning materials on the capabilities of the instructional media, and that good design must take into account the students' present state of understanding and the already established methods they use to acquire that understanding.

Students develop their own profiles of learning depending on their particular orientation, described as "the predisposition of a learner to adopt a particular process" (Biggs, 1993), which, in turn, depends on the students' approach, motivation, mental model and environment. It is suggested that this learning profile is relatively stable, but not unchangeable, and results in a set of strategies that the students use when confronted with a learning task (Vermunt, 1996).

Another barrier to electronic forms of delivery is that distance education students are reluctant to accept new ways of receiving instruction because their time is limited. They need to be convinced that there is some immediate benefit, measured by their learning outcomes, in adopting an alternative study method, and that they do not have to go through a period of relearning how to study (Lyall and McNamara, 2000a).

In the first part of a study into the learning profiles of distance education chemistry students, their orientations to learning were explored (Lyall and McNamara, 2000b). This study found that these students are highly motivated and independent. They are pragmatic about their studies and tend to use a flexible 'strategic' or 'achieving' approach, which is concerned with the efficiency of learning and attainments by the use of planning, time management and the systematic use of study skills (Biggs, 1993; Richardson, 1994).

This paper continues the study of learning profiles by examining the learning strategies used by distance education chemistry students, where learning strategies are defined as the tactics or procedures students adopt for handling a learning task (Christensen et al., 1991). Recognition of these strategies is important in the first instance to assess, and possibly improve, the present method of instruction. A further aim was to use this information to assist the student in the transition to electronic delivery by suggesting a computer aided learning program (CAL) that would utilize the already existing learning strategies of the student and identifying those strategies that might be readily modified, and possibly enhanced, by the use of electronic media. The intention is that the data gained from this study will provide distance education chemistry educators with scientifically based tools to develop their teaching methods.

Methodology

The study was carried out on several groups of first year chemistry students at two Australian universities over a five-year period. The content and level of the units was similar, as was the form of instruction used by all groups. The universities supplied a printed unit book, and the students were expected to purchase a prescribed textbook. The unit books contained a series of study guides, the purpose of which was to guide the students' study within the particular areas of the unit by providing some information on specific concepts, referring students to areas in the prescribed textbook, and providing examples and self-assessment questions. Students in the latter years of the study did have access to electronic material, including interactive computer simulations, but it was left to the individual students to use as they saw fit. About half the students were compelled to attend a "laboratory" session of computer generated questions and answers.

A grounded theory approach was used. In this method, rather than start with a theory and try to prove (or disprove) it, the theory is "discovered, developed and provisionally verified" (Strauss and Corbin, 1990). This can be achieved by using ethnographic interviews, which are largely unstructured, with the interviewers adapting their questions during the course of the interview. The data from these interviews is then analysed according to a systematic set of procedures.

Conducting the interviews and analysis of the results was an ongoing process. The students were interviewed three times over the academic year. Most interviews were conducted in private

with only the interviewer and interviewee present. For the first interview a battery of guiding questions was developed and tested in a pilot study. These questions were mainly open-ended and were modified as the interviews proceeded, depending on the participant's response (or lack of response). The interviews were recorded by audiotape and transcribed in full with the addition of any notes made by the interviewer. The data was then analysed and used as a basis for the second interviews. Similarly, results from the second interview were used for the third.

Analysis of the interviews was carried out using a three stage coding procedure outlined in Strauss and Corbin (1990). First, 'open' coding was used to identify and categorise phenomena relevant to the study. Phenomena are defined as being ideas, events, happenings or incidents. These were then given conceptual labels and classified into categories and subcategories pertaining to a similar phenomenon. Properties (characteristics or attributes) and dimensions (some measure of the properties) of the phenomena were identified.

'Axial' coding procedures were then applied to the data to determine connections and links between the phenomena. The processes of open and axial coding were not performed in isolation of each other, nor in a strict sequence, but were often being conducted at the same time, it being found necessary to return often to the original transcripts and to modify the open coding categories during axial coding.

A final list of categories and sub-categories of phenomena relevant to the learning strategies of the students was prepared and presented to a panel of four experienced education researchers for their comments. They were amended in light of their recommendations. A 'selective' coding process was then carried out to integrate the categories to form the grounded theory and to identify the core category, which is the central category around which the others are integrated.

Students were also asked to submit (copies of) any written notes or other material they generated while studying, so that this could be examined in conjunction with the interviews.

Results

In all, fifty-nine students were interviewed from several different intakes of science students at two Australian universities. This represented about 22% of the students enrolled at the time.

Using the analysis procedure recommended by Strauss and Corbin (1990) the learning strategies used by the students were grouped into two major and intrinsically separate categories. These were called *studying* and *validating*. Studying could be identified as the actual mental and physical activities the student used to try and remember new material. Validating is a set of strategies used by the student to test and correct his or her newfound knowledge and understanding. These categories were then further divided into several sub-categories each with their own set of learning strategies. The results are presented as a general description of each learning strategy with specific findings and/or student comments in italics.

Studying

Studying was identified as being the 'core' category since this was where the students did most of their learning. All other categories and sub-categories related, in some way, to the studying category. Studying was divided into four sub-categories called absorbing, note taking, memorising and understanding. Note taking refers to the writing of notes by the learner and is the 'key' learning strategy. The other three are groups of learning strategies (see Figure 1).

studying absorbing notetaking memorising understanding preliminary primary listing objectives reading notes repetitive linking in-depth making writing alternative reading summaries practicing explanations identifying recall practical key points repetitive exercises alternative observation grouping reading highlighting ageing applying revisiting

Figure 1. Strategies associated with the 'study' category.

Absorbing

Absorbing involves the learner in 'non-discriminating' activities including reading and writing and is generally the first learning activity undertaken by the student. There are *five* learning strategies associated with absorbing: *preliminary reading*, *in-depth reading identifying the key points*, *alternative reading*, and *ageing*.

1) Preliminary reading through the study guide is a recommended study practice at both universities, but the majority did not do this for their chemistry units. Most claimed it was a waste of time since science in general, and chemistry in particular, was a hierarchical subject where new information was built on previous knowledge and therefore the study guides were designed to be read in sequence.

Peter claimed that he had very good recall, provided he "got it right first time", so he didn't need a preliminary read through, and Brian needed to take notes as a memory aid so a preliminary read was not helpful.

2) *In-depth reading* was where the 'serious' study began. All interviewees bar one worked through their study guides in a sequential manner, reading each topic in-depth one after another as they occurred in the study guide, for the same reasons as given above. Some worked through it slowly, doing examples and trying to master each concept thoroughly before going on to the next. Others would continually read the whole topic over and over again until, in the words of one, "it clicked".

Lynne worked through each chapter three times whereas Margaret claimed she re-read the topics up to 15 times. Margaret's continual re-reads were more than simple absorbing since she highlighted key and difficult points in the first reading and in her re-reading did all the examples and problems in the study guide. One interviewee claimed that he did not study sequentially but instead tried to structure the material at the beginning of the topic. His method was to divide a topic into two or three groups and then to divide that further into more groups, forming what he called a "pyramid tree", which is a type of linking technique that will be discussed later.

3) Identifying the key points of the topic was an important strategy for most. This appeared to be an inductive process since they could not describe how it was done. Some key words were already highlighted in the study guide and textbook. Not surprisingly these key

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words were nearly always chemical or scientific terms such as 'formula weight' or 'alkanes' and sometimes headings to describe a chemical process such as 'condensation reaction'. Often these key points were not identified until summaries of their notes had been made.

4) Alternative reading was a strategy used by nearly all the students. This refers to the use of textbooks other than the prescribed text. There were two main reasons for doing this. The first was to obtain different explanations for content that the student found difficult. The other was as an adjunct to the study guide in order to expand the material used for studying. Most students had obtained two or three alternative texts, some considerably more.

Judith had about six other textbooks and said "I usually use textbooks much more than I use the study guides – I read the study guide to find out what it is I'm supposed to know then I use textbooks to get to know it."

5) Ageing is a passive learning tool referring to the process of leaving content that is causing difficulty and coming back to it after a period of time. In some ways it is forced on the learner since the lecturer can seldom be contacted at the time needed, but several used it as a positive learning strategy.

Joanne commented "If I can't work it out I'll stop because I'm not getting anywhere, and then I'll go away and either come back later that day or the next day and start from there again to try and work it out and I tend to find that if I do that I can usually work out most of my own problems".

Note taking

Possibly the most important strategy for most students was note taking. The content and detail varied considerably but their main function was to put descriptions and explanations 'into their own words'. One example, shown in Figure 2, is typical of the less detailed style of note taking.

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Figure 2: An example of 'brief' notes.

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The primary level notes were generally summaries of the content in the study guide and/or textbook(s), taken directly from the study material and written down in the students' own words. Some of the interviewees made summaries of their own notes from time to time during the course of their study. Some made summaries of their summaries, up to three times. Many more made summaries at the end of semester when studying for the examinations.

Brent made summaries and noted better explanations in his notes on one side of a sheet of paper. He then made further notes, on the other side of the paper, when revising and a third set when studying for the examinations. Lynne also made three summaries, an overview on the preliminary read, a one-page summary of each chapter on working through and a summary of those pages for the examination. Maria and Steven made brief notes on cards, which they could carry around with them.

As can be seen from the above example the notes were mainly simple explanations of chemical terms used in the study guides and almost invariably made use of chemical equations in the explanations. The terms were usually highlighted and as such were used as the key points discussed previously.

Any content that the students could not understand or they had difficulty in understanding was included in their notes. Often the key points were modified, or even not identified, until the second or third reading.

Steven said "I think it is very important, the key parts, because the first time around I failed to... not being used to studying for a long period, I failed to see certain key suggestions".

There were generally two reasons for making notes. First, several of the students thought that the mere act of translating and writing it down helped them in remembering the content. The other reason was to ensure that when the student revised the material, especially for examinations, he or she would have it in words that could be understood more easily. Most used the notes for further study and revision, particularly around examination time.

Memorising

Memorising has two dimensions. One is as a part of the preferred studying routine where the information is expected to be retained for a long period. The other is used as a short-term strategy to pass examinations, which is called swotting. Most of the interviewees admitted that they had made use of swotting at some time or another, but regarded it as undesirable and claimed that they used it as a last resort, usually because of a lack of time to 'study properly'. In general the techniques used for memorising and swotting were similar. Without exception all the interviewees used some form of memorising or rote learning techniques, but regarded it as somehow being inferior to understanding.

There were four major learning strategies associated with memorising: *listing*, *repetitive* writing, practicing recall, and repetitive observation.

1) Listing is a learning strategy for memorising and is often inter-related to the 'understanding' strategy of grouping, in which the learner groups together different topics that appear to have some common characteristics. Once grouping is used to gain an understanding of the underlying concepts, it often then becomes a list, which is more easily memorised. For instance, a list of the important organic functional groups can be memorised but it is first necessary to understand the concept of functional groups. A majority of the students made up

their own lists or groups in addition to the lists and tables given to them in study guides and textbooks.

Alice was typical of this group. She made up lists, such as the ending of chemical names and what they meant, and kept them as references with her study books. Greg would make lists, such as the names and formulas of polyatomic ions, and memorise the first entry. He claimed he could then more easily remember the rest.

2) Repetitive writing was regarded as an important strategy for learning, with about half claiming to use it regularly. Most students would try to use different words when rewriting, which introduced a further level of activity in that it required the student to think about alternative wording for the material.

Greg would keep writing material down until he felt he had retained it and may need to do this up to 20 times.

- 3) Practicing recall is a well-known technique for memorising, but surprisingly, less than half the students acknowledged using it as a learning strategy. It was, however, commonly used for 'testing'.
- 4) Repetitive observation by putting up lists, such as the structures and names of organic functional groups and polyatomic ions, in a place where they would be constantly seen, was used by a few students, often for swotting just before the examinations.

Understanding

This was one of the more difficult sub-categories to assess since many of the phenomena associated with understanding are mental processes, and as such an in-depth explanation of them is outside the context of this study. What was important was to identify the strategies the students used to aid their understanding. Seven such strategies were used: *objectives*, *linking*, *finding alternative explanations*, *applying theory to the solving of practice exercises*, *grouping highlighting material*, and *revisiting study material*.

1) Objectives were regarded as a useful learning tool. Most of interviewees did not rely on the objectives given in their study guides but defined their own from assignments and past examination papers. The majority of students regarded these as a more reliable guide to what they were expected to know.

Roger and Rhonda claimed they always defined objectives by looking through the assignments and in this way they could gauge the depth of knowledge the lecturer required. Phillip thought that assignments also helped in his understanding and when reviewing his notes, and Margot used past examination papers to set her objectives early in her studies, and thought that she probably based her notes on what was in the papers.

2) Linking was finding how the newly learned content fitted in and connected with already acquired knowledge. Most assumed that what they had been studying immediately prior would provide that starting point or base. This reinforced the view previously expressed that the students regarded chemistry as being highly hierarchical.

As Rhonda said "chemistry sort of builds up, as you go you've got to remember and have a comprehension of what went on before, you need to know about electrons before you know about bonds". Richard related it to a snowball effect using a similar example of "atoms then electrons

then bonds then compounds then reactions". Roger explained it as "once your knowledge reaches a critical mass you just tack on ideas at the end".

About half of the interviewees made some kind of effort to connect items of content together by making up diagrams and flowcharts to see the connections between topics.

Steven claimed that he didn't deliberately try to build on material but was always looking to see where it actually 'fitted in'. He used the example of using covalent bonds in organic chemistry, which was studied in the ninth week of semester, but to understand this he had to refer back to week three when bonding was first introduced. Several others said they worked backwards and forwards through the study guides trying to make links.

3) Finding alternative explanations was an important strategy for understanding. As has been mentioned previously, most of the students obtained several different textbooks. One of the reasons for this was to find alternative explanations for concepts. The majority of the students consistently searched for definitions and explanations until they found one they could understand.

Judith said "If I couldn't understand the study guide I'd go to another textbook ... another, then section." As Brent commented "if I think there was something in the textbook that says it better then I'll note this down in my notes". Greg liked different angles to "illuminate something you haven't seen".

4) Applying the theory to the solving of practice exercises was considered to be a very important learning technique for most interviewees and most used practice exercises of some kind to gain an understanding of concepts. Assignments and, less commonly, examination papers were also used as a source of practice exercises.

Typical views were expressed by Margot who described doing exercises as "pushing in" the content and Mary who commented "I use examples a lot and I find that by working through the examples and working through the problems I learn more than I do by reading the text". Steven used worked examples in the text and made sure his notes contained the information to solve them.

This was particularly true for topics that the students found were conceptually difficult, especially those requiring mathematical solutions such as pH of acids, bases and buffers. Understanding of organic reactions was also achieved by doing multiple examples. In this case students were adamant that they wanted 'real' compounds, with 'real' names rather than generic examples. In particular, many students disliked the use of R to denote an undefined alkyl group. There was a slight preference for having examples throughout the text rather than at the end of topics.

5) Grouping (mentioned previously in memorising) is a learning strategy for concepts where related information is formed into small groups in order to learn it more efficiently. It is a strategy most of the students used, although many did not recognise it as such, as only a few deliberately went looking for patterns between content, most thinking that associations were obvious or would be referred to in the study material.

The act of summarising their notes, which was mentioned previously under note taking, was an example of grouping. This was not a passive activity, as the students needed to make decisions about what to include in their summary, that is, what keywords and concepts were important, and to make links between the topics.

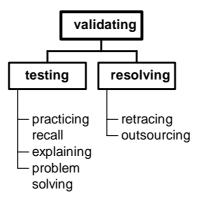
Samantha and Simone thought that they could understand things better if they could put them into groups themselves. Brent liked to group content and look for patterns and both James and Steven made summaries and diagrams grouping items together.

- 6) Highlighting material in their own notes, and less frequently in their study guides or textbooks, was used by most students to identify important passages or words that would act as a trigger for their memory. Generally, they wanted to be able to do this themselves as, when it was suggested that a list of key words at the beginning of each chapter would be useful, most felt that it would not really help them learn. As previously mentioned, chemical names, symbols and reaction equations were often highlighted.
- 7) Revisiting or looking back over study material had two dimensions. Most interviewees mentioned reviewing the material at regular intervals during the semester, and recognised that this was beneficial to their learning and should be done. Nearly all revised their material just before the exam.

Validating

Validating is the set of procedures that the learners use to determine how well they have retained their newfound knowledge. It is strongly related to studying, and many of the strategies involved are similar to, and practiced at the same time as, those in memorising and understanding. However, it is regarded as a different category, since validating occurs after the learning processes. Validating has two sub-categories referred to as *testing* and *resolving* (see Figure 3).

Figure 3: Strategies associated with the 'validating' category.



Testing

Most of the students interviewed agreed that they did test themselves in some way, and that it was an important strategy in their learning. Nearly all thought it was a good idea to test regularly through the semester, but the degree to which this was done varied considerably. There were three strategies identified with testing: *practicing recall, explaining*, and *problem solving*.

- 1) Practicing recall, as well as being used as an understanding tool, was considered as an important testing strategy.
- 2) Explaining was describing a concept to another person, often their partner. Students thought that if they were able to talk about a concept in a simple but clear way, so that non-chemists could understand it, then they had themselves understood it.

3) Problem solving was the most common form of testing, most often by answering the self assessment questions (SAQs) in the study guide and in the textbook, but also by attempting past examination papers. They were generally done as the students were going through the material, and were often attempted again before examinations.

One group had access to assessable online computer tests where they could get an immediate answer to a multiple choice or short answer question. Most considered it to be an excellent way of learning and testing. Although many did not like the pedantic nature of the computer, they also recognised that chemistry is often pedantic and that the difference of a single letter can be important, such as in the naming of organic compounds, pentene being a very different compound from pentane.

Several students commented that, once they got over their initial disappointment when they gave a wrong answer in a test, they realised that they had learned a valuable lesson without being penalised greatly (there were 120 questions through the semester worth a total of 30% of the marks).

This view is not shared by on-campus students, which demonstrates the self-sufficiency of distance education students and their strong view that they are primarily responsible for their own learning. Similarly to recall, problem solving was used for more than one purpose. Apart from testing, it was also used when studying in order to understand the material, as discussed in applying theory, so it was difficult to separate these two outcomes.

Resolving

Resolving was the set of strategies the students used to solve any problems or shortfalls in memory retention following testing. Many of the strategies used in resolving are similar to those used in studying, but are different in that resolving is a short term strategy used, in the words of two students, "to add pockets of information" and "to top up the larger pool of knowledge" and as such is an irregular procedure, and not done in sequence like studying. Apart from those already discussed, resolving has two new strategies: retracing the appropriate sections of the subject, and outsourcing.

- 1) Once a lack of knowledge had been determined, the student needed to *retrace* the appropriate sections of the subject so that the missing parts could be fitted in. Often the students used a dictionary or a textbook glossary to fill in any perceived lack of knowledge. Several students used the exercises to identify and resolve problems
- 2) Outsourcing was necessary when the students could not find or understand material in their study guides. Prescribed and other textbooks were the next source. If these failed then a few would simply bypass the topic and let the information already gained age for a day or two. Using the university library was not popular since it took time, and in many cases a suitable alternative library was not available. Some students would use the Internet, but most were unsure of the accuracy of information obtained this way. Students who worked in scientific organisations indicated that the scientists at their place of work were a useful source. In most cases the final resort was to ring the lecturer concerned, but there was a reluctance to do this.

The learning model

The strategies employed by the students for learning from the study materials were very similar. The students studied sequentially, by going through the study guide page by page,

using three distinct types of learning strategies, absorbing, memorising and understanding, which were based on producing their own notes from the study guides and textbooks.

The sequential nature of the learning process may have been due to the way the study guides had been written, but it was also the way the students expected to learn, that is, building up their knowledge by adding to their existing knowledge base and experiences. This coincides with the view that science is strongly hierarchical where advanced knowledge is based on previously learned material (Bennett et al., 1995).

This, and the fact that they produced their own notes, written in their own words, would indicate that the students were using a constructivist-cognitive model of learning where the learners construct their own meanings and are therefore actively participating in the learning process. However, in this case the preferred dialogue, which is considered so important (Garrison, 1993 and Jonassen et al., 1995) in this type of learning model, was mainly between the learner and the study material rather than with the teacher.

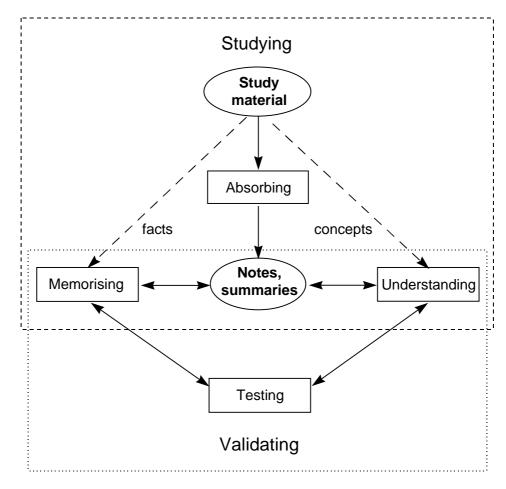


Figure 4: The learning model for distance education chemistry.

It has been suggested that chemical content can be divided into facts, concepts and rules, each of which requires a different set of strategies for learning (Middlecamp and Kean, 1988). Facts are statements about how the world is and how it is to be represented, and they cannot be determined or worked out they just 'are'; concepts are ideas about matter where each concept is related to other concepts, and rules are generalisations about how things behave or how they relate to one another. For example, a fact would be: 'glacial acetic acid is a colourless liquid at room temperature'. A concept would be 'an acid is a compound which donates a proton to another compound called a base'. A rule would be 'an acid cannot exist unless a base is present'.

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The students were able to distinguish two different types of chemistry content: facts and concepts. They recognised that there were different methods for learning these, memorising strategies for facts and understanding strategies for concepts. However, students did not accept rules as separate entities, regarding them more as a subset of concepts, which could be learnt by doing examples (which is a strategy associated with understanding).

The way the students utilised the three types of learning strategies as they proceeded through the study material was reasonably straightforward, although it is important to note that all three processes were usually being carried out at the same time. The core activity, around which the other three revolved, was the making, and remaking, of notes and summaries. In many cases the notes ended up as lists of key points or memory triggers, which could be readily memorised.

Absorbing strategies were generally used first, and students typically read sections of the study guide several times, making notes as they went. After this the content was recognised as facts or concepts to enable the appropriate learning strategies to be utilised. The process of deciding whether a particular content was a fact or a concept was not a conscious deductive activity by the students, but appeared to be an inductive decision where the student claimed they could 'just recognise' what the content was. Overall, the interviewees were accurate when asked to nominate whether sections of content were facts or concepts.

Generally, the memorising and understanding strategies were applied mainly to the student-prepared notes and summaries, although students would sometimes return to the study guide for this. A few interviewees did not use the notes at all, but applied their memorising and understanding strategies directly to the study guides and textbooks.

Once the studying process had been carried out, students then validated their knowledge by testing themselves by various means, and then attempting to resolve any problems by returning to the studying process and reapplying some of the memorising and understanding strategies. There was a very definite hierarchy involved in resolving problems. First the student would consult the study guide, then the textbooks, sometimes other sources of information such as the library and then, as a last resort, the lecturer.

The memorising, understanding, testing process was a limited cyclic one, that is, students would (say) memorise, test, then memorise again, and test, a few times until they considered they had either retained the knowledge or could not afford to spend any more time on that topic.

That this model was a successful one is indicated by the success rate of the students interviewed. Only three failed their subject and about one-third of them were in the top 25%.

Implications for electronic delivery

It would appear from this study that for a computer based learning program to be immediately acceptable to the current distance education chemistry students it would need to follow the pattern of a book in its design. Only such a pattern would be able to match the existing strategies of these students. In particular the key strategy of making notes and summaries is one that could be done better on the computer, due (rather unexcitingly) to its word processing capabilities. However, this would depend on the students being able to learn as well from the computer screen as from the printed page, a key question that was not addressed here.

One of the most significant advantages of such a computer program would be the linking of relevant concepts together to promote the learning process of building up of knowledge. Whilst the students expect this to be a linear process, and it is designed into the study guides as far as possible, the learning of chemistry is not, and cannot be, entirely sequential. It is inevitable that at some time in the learning process students will need to revisit a previously

studied concept. In this case a glossary may be all that is needed, otherwise the student may need to retrace the original material (a validating strategy). For instance, the concept of ionic and covalent bonding is introduced early in the semester following on from a discussion of electronic structure. The study guides then concentrate on ionic bonding, inorganic compounds and reactions, equilibrium, acids and bases etc, which is a logical and linear progression. It is not until late in the semester that organic chemistry is studied and the students need to refer back to the original concept of covalent bonding studied several months before. Both operations can be done with the click of a button on the computer without the student losing his or her place in the learning program.

A further advantage of a computer program is in the presentation of exercises, problems and self-assessment questions, which can be embedded in the program and hidden to varying degrees until required by the student.

Whether or not the student will see these advantages, let alone be prepared to use them, is a vexed question. A previous study (Lyall and McNamara, 2000a) has shown that distance education chemistry students are reluctant to move out of their "zone of comfort" and use a different mode of delivery. The current study serves to reinforce this view. These students will need to be convinced that they can use their existing learning strategies and will not have to relearn how to study.

When the results of this study are integrated with those of the previous one on orientations of learning (Lyall and McNamara, 2000b), which was conducted on a similar cohort of students, some interesting observations can be made. First is that the students are not interested in the interactive nature of the computer insofar as it can make use of non-linear teaching strategies. These might include, for instance, online tutorials, accessing the web or databases for information, or self-selection of concepts to be studied depending on their perceived knowledge (self-paced learning). Nor do they regard the graphical and motion capabilities of programs to be critical to their primary learning, as for example, Rasmol in which molecules can be rotated and manipulated to better show their bonding etc. To use these attributes would require the students to change their learning strategies.

This is not to suggest, however, that computer interactive programs using graphics and motion do not have a place in the learning program. Whitnell et al. (1994) espoused the use of multimedia in chemistry lectures because it allows the lecturer to portray complex chemical concepts and processes, particularly those which occur at the molecular level, by the use of computer animation, three dimensional graphics and video. Kirkwood (2003) pointed out that distance students recognise the benefits of having learning materials presented a in a variety of media. This was also shown in our previous study (Lyall and McNamara, 2000a) when a few students, who moved out of their comfort zone and used an alternative CAL program, which presented a basic course in organic chemistry, enjoyed their experience, all regarding it as an equal or better way of learning.

Any synchronous activity with instructors or other students, even when computer generated and therefore more likely to be accessible to a distance student, was rejected. Even non-synchronous communication, which involved other students (bulletin boards), was not popular as a means of solving academic problems, although they were used in a limited way for social contact. Even the more private email contact with the lecturer was used only as a last resort. This observation is in direct contrast to the widely held view that distance education students require interaction with their teachers (Boyle 1995; Lemmer et al., 1997; Garrison et al., 2001; for instance).

Most of the previous studies were conducted in disciplines in which social interactions are essential, such as business studies and teacher education. In science this may not be so important. However, it is suggested that a more important reason for this is that the students regarded the working out of their own problems as a very powerful learning strategy. In

reality it is a set of strategies categorised under understanding and resolving. This explains a personal observation that computer regulated bulletin boards and discussion group activities are not popular with science students even when actively encouraged by the instructor by posting material such as problems and answers. If this material is used at all it is used by 'sleepers', students who read the discussions but very seldom make comments themselves.

Design of a suitable computer program

To overcome the reluctance of students to move to a new form of learning (CAL) the following approach is suggested. The computer program would present the major study material in a linear format giving written explanations and moving from screen to screen as in the printed study guide. The written text, however, would not necessarily be the same as in the study guides, since full advantage would be taken of the computer's ability to show demonstrations in both graphics and animation as appropriate, to support, but not replace, the textual information. The use of lists to summarise material in the text is recommended (for both electronic and printed study guides).

The computer program would have a facility where the students could write their own notes and summaries without exiting from the screen. The notes pages should also be able to be accessed in a linear way, that is, the students could follow the content from notes page to notes page without reference to the main text, if required. The ability to print out notes and to highlight text on the screen would be an advantage.

Specific objectives, and other resource material such as the Periodic Table, lists of functional groups etc. relating to the text, and worked examples of problems would be accessible from each screen.

A glossary of terms should be included with brief (one or two line) explanations of each term to be accessed from the main text by using a pointing device on the term itself to activate a hypertext link. Links would also be provided between the text and previous related text, or where appropriate, simpler and more basic explanations.

Wherever appropriate, problem exercises would be accessible from the main screen. The answers would be hidden and only accessed after the problem has been completed. If the student's answer is wrong they should be able to make a choice of repeating the exercise, revising relevant material through means of a hypertext link or accessing the worked answer.

A CAL program following this design would take advantage of most of the students' existing learning strategies and they would be less inclined to reject it on the grounds that they needed to learn a new way of studying. Furthermore, the program introduces new media such as graphics and motion, ready access to previous concepts and embedded exercises, which have the potential to enhance the learning of the students without interfering with their already established methods. That this can be done at the click of a mouse without the student leaving the main body of text may prove to be attractive to the student. However, satisfactory progress through the course would not depend on the student accessing this enhanced material.

Conclusion

This study has identified the important learning strategies used by distance education chemistry students, with the expectation that these could be used to improve instructional material. The implications of the study for the design of alternative delivery methods using electronic technologies are mixed. Whereas a computer based learning program would have some advantages over print, it would need to support the cognitive linear style of learning adopted by the students. It is suggested that a package containing printed notes, student

selected textbooks, CAL, email and telephone communication would be a powerful educational tool which would satisfy most of the students present learning strategies and encourage them to adopt new ones which could be advantageous to their learning.

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Using a context-based approach to undergraduate chemistry teaching – a case study for introductory physical chemistry

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Abstract: This paper describes the rationale for using a context-based approach to the teaching of undergraduate physical chemistry, together with an overview of a case study, which has been developed to teach aspects of thermodynamics, kinetics and electrochemistry usually associated with the early stages of undergraduate chemistry courses. The context is that of the next generation of energy for an emerging city (Los Verdes) located in the south-west region of the USA. Working in groups, students use an array of physical chemistry principles to examine the combustion of fossil fuels and hydrogen, the use of hydrogen in fuel cells, solar power, and energy from a geothermal source. Students gain experience in working with both familiar and novel types of problem solving. [Chem. Educ. Res. Pract., 2005, 6 (3), 166-179]

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Introduction

Employers, educators and funding bodies continue to emphasise the importance of the development of a wide range of subject-specific and transferable skills during university courses. This view has been reinforced in the UK by the QAA Subject Benchmarking activity and the Programme Specification Template in which subject specific skills, cognitive and transferable skills are very prominent.^{1, 2} Within the new system of quality assurance, UK chemistry departments will need to demonstrate that students have developed and been assessed in a range of these skills. Such skills include, for example, working with novel problems and planning strategies for their solution, interpretation of chemical information and presentation of scientific arguments, as well as the usual range of transferable skills such as communication, group work, information retrieval and time management. Although some traditional methods of teaching and learning chemistry do not enable students to gain many of these skills or, at least, do not provide academics with evidence that they have done so, various strategies have been developed for addressing these issues. Some of these teaching and learning styles involve discipline-related activities (Bailey, 1997), while others are discipline independent (Wyeth, 1997). Problem-based case studies have a long history in many subject areas and their value within chemistry has long been recognised (Garratt and

² http://www.qaa.ac.uk/academicinfrastructure/programSpec/progspec0600.pdf

¹ http://www.qaa.ac.uk/academicinfrastructure/benchmark/honours/chemistry.asp

Mattinson, 1987; Pontin et al., 1993). More recent examples within the main sub-disciplines of chemistry e.g. organic (Bennett and Cornely, 2001), inorganic (Breslin and Sanuodo-Wilhelmy, 2001) and physical (Holman and Pilling, 2004) chemistry, and subjects allied to chemistry such as biochemistry (Cornely, 1998) and environmental science (Breslin and Sanuodo-Wilhelmy, 2001; Cheng, 1995) have also been described. Problem-based approaches in laboratory work are also gaining in popularity (McGarvey, 2004; Jervis et al., 2005; Tsaparlis and Gorezi, 2005).

An increasing number of students entering into higher education to study chemistry do so having studied in a context-related way in schools and colleges, and a review of such an approach has illustrated its popularity for students studying chemistry in the UK (Holman and Pilling, 2004; Burton et al., 1995). The employment of more 'real-life' examples has also been identified as a recommendation for the teaching of chemistry following a review of the science curriculum in schools in the UK.³ This context-based approach is not necessarily continued into first year courses although there are materials readily available for use in later stages of programmes. Such materials tend to focus on applied areas of chemistry, such as industrial, pharmaceutical, forensic, and environmental chemistry. This is not surprising, given the linear degree structure traditionally adopted by the majority of university chemistry courses, with core chemistry being taught early in the programme and applications appearing later. Our own experience (Belt & Phipps, 1998; Belt et al., 1999, 2002; Summerfield et al., 2003) in producing case studies for analytical chemistry revealed that not only could the problem-based approach deliver curriculum content, but it also succeeded in engaging, enthusing and motivating undergraduates in chemistry. Therefore, we decided to produce a series of problem solving case studies, which focussed on core areas of organic, inorganic and physical chemistry usually encountered during the early stages of undergraduate chemistry courses. One of these case studies, which is concerned primarily with fundamental aspects of physical chemistry, is described here.

Case studies in physical chemistry

A review of the chemical education literature indicates that many teachers of physical chemistry believe that their students find this sub-discipline of chemistry to be 'hard' (Sözbilir, 2004), although we remain unconvinced that this perception is any truer for physical chemistry than for any other chemical sub-discipline. What is clearer is that this perception has prompted some researchers to investigate the reasons *why* students find physical chemistry difficult (Nicoll & Francisco, 2001; Hahn & Polik, 2004). A number of factors appear to contribute to this perception. Perhaps surprisingly, these are not simply limited to students' abilities in mathematics, despite physical chemistry having such a high mathematical component. Factors such as motivation, logical thinking and prior knowledge are also important. In any case, there exist a substantial number of examples in the literature where teachers of physical chemistry have attempted to alleviate this perceived problem using a diverse array of teaching methods, and these are reviewed elsewhere (Hamilton, 2003).

It is clear that teaching chemistry within an applied context is gaining in popularity and Zielinksi and Schwenz have identified the importance of context-rich teaching materials in the teaching of physical chemistry in the 21st century (Zielinski and Schwenz, 2001). Emerging out of the success of the Salters chemistry course used in pre-university chemistry teaching in the UK (Burton et al., 1995), Holman and Pilling have adopted a contextualised approach to the teaching of thermodynamics for university students, concluding that such a method seems to be successful in enhancing students' interest in, and understanding of, thermodynamics,

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³ http://www.planet-science.com/sciteach/review/Findings.pdf

though they expressed some doubts over how successful it is in developing students' abilities in problem-solving (Holman and Pilling, 2004). In the US, high school students taking a context-based course (ChemCom) outperformed those students studying more traditional courses. This success was attributed, at least in part, to higher levels of interest and motivation amongst the students, together with their perception of the relevance of the topics (Sutman and Bruce, 1992; Gutwill-Wise, 2001). However, there can be an apparent mismatch between the teaching styles that school students experience (and their prior knowledge) with expectations of tutors in universities, and this has been identified as a possible cause of students' difficulties in understanding thermodynamics (Carson and Watson, 1999).

Having considered these points, our rationale for producing some context-based teaching material for physical chemistry appears justified. That apart, when we first set about designing a case study for physical chemistry teaching, it was also our aim to produce a resource that would complement other teaching activities, rather than substitute for them, especially as it is also clear that different students respond to contrasting learning environments, often at different times. In addition, we chose to concentrate on selected topics of physical chemistry with an emphasis on revisiting these themes rather than attempting to cover an entire syllabus. By taking this approach, we believed that the case study would enable students to reinforce their knowledge and understanding of topics, make links between different areas of chemistry, and to integrate theory with applications. The case study has been designed to use as an entire package, but individual activities can be used with appropriate introduction and background information. This feature enhances its flexibility. Finally, in selecting a context, we decided that students would be motivated by a 'domestic energy' related theme, since it is topical (and will continue to be so in the foreseeable future), relevant to all students, and encompasses both economic and environmental considerations. From a tutor's perspective, it has the additional appeal that various physical chemistry principles can be investigated within this theme.

Capital City

The chemistry covered in the *Capital City* case study is concerned with, but not exclusively, introductory thermodynamics and kinetics, the latter having been identified as a particularly key topic for 21st century physical chemistry teaching (Zielinski and Schwenz, 2001). The case study uses the context of identifying fuel sources for an emerging city (Los Verdes, located in the south-west USA) by evaluating and interpreting a range of physical chemistry data. These fuels include both traditional energy sources (e.g. fossil fuels) and renewable energy sources (e.g. fuel cells, solar cells). In terms of scientific skills, students need to manipulate 'core' thermodynamic and kinetic equations and evaluate the outcomes of these. As the case study evolves, students need to make estimations and approximations where traditional approaches are inappropriate. In order to complete the case study, students need to develop and use a range of other skills such as effective group work, communication, organisation, problem solving and critical thinking.

Overview

The case study is delivered over 8 1-2 hour sessions and all the paper-based material required for each session is provided by the tutor (see **Case Study Layout - Editorial considerations**). In Plymouth, the case study is compulsory for all the students and is timetabled towards the end of the first year of the degree programmes in order that it complements and builds upon the relevant background lecture courses, particularly in thermodynamics, kinetics and electrochemistry, which are delivered earlier in the year. The

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format of the study consists of a 3-way liaison between the head of a city council department (unseen), a project manager of a power consultancy company (the tutor) and a project advisory team (the entire student cohort). This advisory team is subdivided into smaller groups (3-5 students) and these retain their membership for each session. Each sub-group works on a common theme during each session, although in some cases, the datasets with which they are working are different. Having begun the case study with a general discussion of potential energy sources (Session 1), the groups accumulate a portfolio of data and analyses for various fuels in the subsequent sessions (Sessions 2-7), re-visit the overall project aim in the final session (Session 8), and deliver a short oral presentation and/or report, the content of which is informed by the outcomes of the previous sessions. A summary of the sessions in terms of their principal themes and tasks is shown in Table 1. A tutor guide has also been produced which gives outline time plans for the sessions, model or suggested solutions to the individual tasks, topics for discussion and blank templates where needed.

Individual sessions

Session 1: New energies – new futures: the Capital City project

In the first session, students are introduced to the case study in terms of their roles, the overall aims and the assessment. Having also discussed the philosophy behind the study and overviewed the scientific and transferable skills that will be developed, the groups are given the first e-mail correspondence from the project manager (the tutor), which describes the expectations for the session. Accompanying this e-mail is a letter from the Head of the Department of Energetic Affairs (DEA) at the Los Verdes City Council who is responsible for the overall energy project, inviting the project manager and his/her team to provide some early feedback on potential energy sources. An extract from a previous 'initial needs' study is also included in the correspondence. After discussing these documents, the students produce a short summary outlining their suggestions for future power generation. At this early stage of the case study and, with the absence of more detailed information, the students need to rely principally on their prior knowledge and engage in group discussions. There is no single 'correct' solution to the first session, but each group is briefed to make a single proposal that is 'Economical, Environmental and Eye-catching'. As such, the first session acts as a suitable 'ice-breaker' and can give an early indication to the tutor of students' prior knowledge of energy production and possibly of physical chemistry (Carson and Watson, 1999).

Session 2: Steam power plant using fossils fuels

At the beginning of the second session, the groups are informed that their initial proposals have been considered by the DEA, along with those provided by competitors. The outcome of these deliberations reveals that a total of six named energy sources should be investigated in more detail. These are presented to the group by the project manager together with a brief rationale for why some alternatives have been rejected (e.g. negative public opinion for nuclear power, limited water supply for hydroelectric). By doing this, all the group's suggestions are acknowledged, but the tutor is able to keep the subsequent investigations within his/her control.

 Table 1. Summary of the Capital City case study

Session	Title	Tasks / Activities	Problem-solving
1	New energies – New futures: The Capital City project	Discussion of potential energy sources based on prior knowledge. Propose a solution which is 'Economical, Environmental and Eye-catching'	Evaluation of prior knowledge within a group. Working within a restricted timescale (all sessions)
2	Steam power plant using fossils fuels	Use of the Carnot cycle and determination of the cost efficiencies of fossil fuel combustion. To consider the potential environmental impact of fossil fuel combustion	Carnot cycle and Gibbs free energy calculations. Conversion of thermodynamic terms to costs. (Homework: Quantitative determination of CO ₂ , NO and SO ₂ from combustion)
3	Air pollution from fossil fuel burning in steam power plants	Determination of production of the greenhouse gas NO due to combustion of fossil fuels and direct oxidation of nitrogen at high temperatures. Evaluation of the total contributions of CO ₂ , NO and SO ₂	Influence of temperature on equilibrium constants. Making estimations from graphical data and applying approximations to determine equilibrium constants
4	H_2 production by steam reforming of methane (SRM)	Assessment of the generation of hydrogen by the Steam Reforming of methane (SRM) and subsequent combustion	Determination of rate parameters for a catalytic process. Calculation of optimal conditions for a series of catalysts and temperatures according to specified criteria
5	Fuel cells	Assessment of the use of hydrogen in fuel cells by calculation of energy efficiencies from two contrasting methods	Calculation of thermodynamic data from electrochemical measurements. Identification and quantification of errors. Conversion of thermodynamic terms to cost efficiencies
6	Solar power	Determination of the efficiencies of two types of solar energy conversion and up-scaling to a power plant	Interpretation of graphical data. Using estimations and approximations to solve numerical problems. Interconversion of units and manipulation of unfamiliar parameters
7	Geothermal power	Investigation of the potential to use pressurised steam from a natural source as an energy source	Carnot cycle (re-visited). Interpreaetion of unfamiliar graphical data and numerical manipulations
8	Final recommendations	Synthesis of previous findings and presentation of final recommendations	Interpretation of a large dataset including both quantitative and qualitative data

The first potential power source to be investigated in more detail is fossil fuel combustion. Each group receives a briefing paper on 'Steam Power Plants', which describes the principles of their operation together with some relevant thermodynamic relationships. Individual groups are allocated a different fossil fuel type (further e-mail) ranging from coal of various grades to oil and gas. The objective for each group is to determine the efficiency of each fuel expressed as the cost per unit power output (\$ MWh⁻¹). In order to do this, the groups need to perform thermodynamic calculations (e.g. free energy calculations) and combine these with power plant operational parameters such as fuel consumption rates and fuel costs (see Appendix 1 for briefing paper, e-mail correspondence and fuel data for one group). As such, this session involves the students performing the types of calculations that they are likely to have some familiarity with, even if the exact procedure is new. This type of problem solving was perceived by the authors as being an important feature of the early stages of the case study to promote the students' confidence. At the end of the session, the results of the individual group calculations are collated by the tutor, compared with model answers and feedback is given. The session concludes with a further e-mail to each group that acknowledges their economic considerations and raises the potential environmental significance of fossil fuel burning (viz. the production of CO₂, NO and SO₂ as atmospheric pollutants). In order to investigate these impacts more rigorously in the subsequent session, the groups are asked to calculate quantities of CO₂, NO and SO₂ emissions for their respective fuels, and present these data at the beginning of Session 3 (note: this is the only formal 'homework' for the entire case study).

Session 3: Air pollution from fossil fuel burning in steam power plants

Once the atmospheric gas calculations from Session 2 (homework) have been collated and summarised, the groups receive a further e-mail stating that the project team may not be aware that NO production can also take place due to direct reaction between N2 and O2 in air, particularly at elevated temperatures (e.g. in combustion chambers). The groups are advised that this is in need of further investigation if the true environmental significance of fossil fuel combustion is to be evaluated, and they are given some further thermodynamic data, along with a briefing paper on greenhouse gases. In order to complete this task, students need to combine thermodynamic terms (determination of a free energy of reaction and subsequent determination of an equilibrium constant, K) and evaluate the effect of temperature on K for a reaction. Whilst the former type of calculation may well be familiar, the second has been designed so as to require the students to make estimations from graphical data and, in turn, make assumptions about variations in atmospheric partial pressures of gases. In this particular case, since the equilibrium constant for the formation of NO from N2 and O2 is always small, even at high temperature ($K = 6.3 \times 10^{-3}$ at 2700 K; the highest combustion temperature encountered by any group), a reasonable assumption to be made is that the N_2 (ca. 0.78 atm) and O₂ (ca. 0.21atm) partial pressures are essentially constant. As such, reasonable NO concentrations can be determined from a simple consideration of the dependence of K on T (graphical data supplied). This type of 'one-step' estimation/assumption for a quantitative calculation enables the students to observe the outcome quickly, which is particularly useful for students who have little experience with this type of problem solving.

This session ends with a tutor-led discussion (optional) on the potential significance of NO and SO_2 generation in terms of the production of acid rain (further chemistry is involved before HNO_3 and H_2SO_4 are generated as shown via a handout/overhead transparency).

Session 4: H₂ production by steam reforming of methane (SRM)

Having spent two sessions considering the combustion of fossil fuels, students turn their attention to the utilisation of hydrogen as a fuel in Sessions 4 and 5. In Session 4, the groups

are given a briefing paper that describes the Steam Reforming of Methane (SRM, the catalytic production of hydrogen from methane and water) as a source of hydrogen, because hydrogen itself is not readily available directly from natural resources. Since the thermodynamic parameters for hydrogen combustion are known and there would be little benefit to the students in terms of further calculations of this type, we decided to introduce some kinetics into this part of the case study. It also occurred to us that the majority of kinetics-based calculations that most students perform during the early stages of physical chemistry courses relate to the determination of orders of reaction (which are nearly always integer values), rate constants (k) and activation energies (E_a). The types of calculation that appeared to us to be less common, but valuable for students to perform, included the determination of rates of change of reactants or products (this is somewhat surprising, given that this is the basis of chemical kinetics!) and the temperatures at which such processes should be carried out in order for a rate of reaction to be optimised or for some other specific criteria to be met. The production of hydrogen via the SRM process for combustion purposes provided an opportunity to achieve both of these.

In the first part of the session, and as a means of re-familiarising the groups with the terms usually associated with chemical kinetics, the groups need to realise that orders of reaction cannot be predicted from the reaction stoichiometry but have to be determined experimentally. Having then been given some experimental data (concentrations of reactants versus time), the groups identify up to 3 methods for determining the order of reaction (with respect to [H₂O]; the groups are advised that the rate of reaction is linear with respect to [CH₄]), perform one of these calculations, and evaluate the results. Since each group works with the results obtained from a different catalytic system, the orders of reaction with respect to water are different, and they turn out to have non-integral values. In the next step, the groups are informed that in order to be considered further, the catalytic processes must operate as efficiently as possible in terms of (a) costs and (b) a production rate of hydrogen such that subsequent combustion will be competitive with fossil fuels encountered previously (Sessions 1-2). In order to address the production rate criterion, rate constants are determined at different temperatures using the activation energies provided. Since all terms in the rate equation are now known, the rates of reaction, expressed in terms of rates of formation of hydrogen, can be determined as a function of temperature. However, the overall solution to the task is not simply to carry out the SRM reaction at the highest temperature (as might be predicted a priori) since the operational costs increase with temperature. The groups need to determine the optimal trade-off between H₂ production rate and increasing costs.

Collation of the results from each group reveals the identity of the most cost efficient catalyst for further consideration and one of the catalysts that is incapable of satisfying both criteria. However, since the groups are allocated different catalytic systems at random, it is not appropriate to identify individual groups as 'winners' or 'losers'.

Session 5: Fuel cells

In this session, the groups evaluate the potential use of hydrogen in fuel cells as an alternative to combustion. The groups receive data from the DEA in the form of a FAX document, which summarises certain fuel cell data provided by two rival companies working in 'alternative technologies'. However, as the accompanying e-mail describes, the data is both incomplete and questionable in terms of its accuracy. It is, therefore, up to the team to complete the data by performing some electrochemical calculations, determine any discrepancies that are present and identify the cause of these if appropriate. Having done this, and discussed whether either of the providers are sufficiently reputable, the preferred alternative is decided upon and the electrochemical efficiency is converted into a cost efficiency, which permits comparison with the other fuels considered thus far.

Session 6: Solar power

The student groups consider the use of solar power in Session 6. Although most students will have some familiarity with the basic principles of solar power, it is unlikely that many (if any) will have performed any calculations associated with it. Therefore, at the beginning of the session, the students discuss their perceived pros and cons of using solar-derived energy. The groups are then given a briefing paper describing two types of solar energy technology, solar cells and a solar plant. The latter operates on a collector/converter principle used to drive a turbine encountered previously in combustion plants. They are also given some graphical data, which includes efficiencies of collectors/converters, solar irradiance information such as a photon response curve for a semiconductor, a typical irradiation spectrum for the Los Verdes region and temporal irradiance curves (daily/monthly).

The main task for this session is to determine the scale of operation needed for each solar power method in order for them to be at least equivalent in power generation compared with more conventional fuel sources, and then determine the respective costs (see Appendix 2 for the solar energy briefing paper, e-mail correspondence and solar data information). What may appear on first inspection to be an 'impossible' problem, becomes achievable once simplified into a series of more recognisable tasks. Thus, having roughly converted the energies for a Si response curve (expressed in eV) into a wavelength equivalent (nm), the response curve can be mapped directly onto the solar spectrum in order to estimate the fraction of the irradiance that can be utilised (simplifying the solar spectrum by averaging intensities over larger wavelength ranges further simplifies this approach, Appendix 2). This efficiency can then be combined with an estimate of the average daily and monthly irradiance intensity (taken from further graphical data) to yield the overall harnessing of a solar cell for an extended period. There are, of course, alternatives to tackling this problem and the students are encouraged to consider how the task could be tackled more rigorously. However, what is important is that students recognise that meaningful solutions to physical chemistry problems can sometimes be achieved by taking approximations and/or estimations of data, and without the need of equations or prescribed methods. This is one of the desired outcomes from this session. By combining the power output from an individual cell with the associated costs and the power requirements for the city of Los Verdes given in the first session, a direct comparison between this technology and more conventional sources can be made to conclude the session.

Session 7: Geothermal power

The final type of power to be considered by the team is that derived from geothermal energy since the Los Verdes region of the USA is considered to be a suitable location to exploit such technology. Due to the complexities of geothermal energy use, this session focuses on one aspect (viz. heat transfer from pressurised steam), which, despite the oversimplification, provides a further opportunity for students to engage in unfamiliar problem solving. The groups need to familiarise themselves with new terminology (the technology is probably new to them too) and proceed through a series of thermodynamics calculations to determine the optimum combination of well depth and wellhead pressure to maximise on power output. Collectively, the groups consider a series of permutations and use the optimum conditions to determine the economic parameters, thereby enabling a direct comparison with the other energy sources investigated. The task involves critical analysis of the accompanying briefing paper (an extract from a review article written previously by the project leader) together with interpretation of graphical data as per Session 6. Having completed the calculations, the session concludes with a discussion on how geothermal resources may be utilised further, including integration with other energy sources.

Session 8: Final recommendations

In the final session, the groups re-visit the original aims of the case study. They are given some additional information relating to how the DEA currently predict the future developments of various energy sources ('insider information' provided as a private e-mail from a DEA employee/friend of the project manager). Together with this information, the groups need to synthesise their results from the previous sessions and present their recommendations within the time restrictions of a 1-hour workshop. The session concludes with a discussion of the entire case study, including a reflection on students' learning.

Managing the case study including assessment

To date, the Capital City case study has been piloted with groups of ca. 30 students studying for degrees in Analytical Chemistry and Applied Chemistry at the University of Plymouth, so the observations described here are primarily those of the main tutor (STB). Evidence from our previous work using case studies as teaching material has shown that a key to the success of such an approach is to ensure that the students are 'on-board' with the teaching approach and the expectations of the tutor from the outset (Belt & Phipps, 1998; Belt et al., 1999, 2002; Summerfield et al., 2003). While this may seem obvious, we feel it is of particular importance for this style of teaching for a number of reasons. Firstly, the case study is taught over a number of sessions (and in our case, a number of weeks), so for this reason alone, it is important to establish a modus operandi early on. Secondly, the context-based approach will probably be different from that used in other areas of the course which are taught in parallel (this is certainly the case in Plymouth), even though some students will have encountered the teaching of chemistry in context pre-university. Thirdly, most of the sessions have more than one component, with at least one of these having a discussion or calculation that does not necessarily have a 'correct' or unique solution. This too, may be unfamiliar to many students, particularly with disciplines like thermodynamics and kinetics, which have such a significant mathematical base. As a result of this third point, it was decided not to assess the students summatively, but to give rapid formative feedback during the sessions. By doing so, it was predicted that students would engage more positively with the philosophy of the case study approach, without concerning themselves with levels of reward normally associated with 'correct' answers, particularly with the types of tasks that demand making estimations and assumptions.

It is probably also the case that for most undergraduate degree courses in chemistry, evaluation of students' learning focuses on subject related knowledge and understanding during the first year, with formal assessment of other key skills such as critical thinking and communication occurring later on, once students have gained further experience in these (e.g. via project work). In addition, since some of these so-called key or transferable skills rely more heavily on subjective testing, it is probably more effective, from an encouragement point-of-view, to avoid formal summative assessment of these skills too early in undergraduate courses. Of course, there can be the risk that a lack of formal assessment results in poor attendance, so students are required to attend and contribute to all of the sessions in order to complete the module. In addition, the open-ended nature of several of the tasks with incomplete or poorly defined solutions means that the tutor potentially runs the risk of losing some control over managing the sessions, or even of suffering loss of credibility with the students, features that have been identified by others (Hinde and Kovac, 2001; Bailey and Garratt, 2002). With all of these points in mind, the tutor conducting the piloting in Plymouth (STB) dedicated a significant time period in the first session (ca. 30 minutes) to explain the case study philosophy, including his role as tutor and his expectations of the students.

Subsequent sessions concluded with a feedback period during which the results of the groups' conclusions were collated and discussed. This provided an opportunity for students to raise issues and for the tutor to review the session in general terms, to give credit for correct and/or partially correct solutions (Bailey and Garratt, 2002) and to provide model solutions (if necessary) such that groups were 're-aligned' before the beginning of the next session.

Observations

Tutor observations

On the basis of feedback obtained from end-of-session discussions, it is clear that the students welcome the opportunity to work within a real-life context even though the topic itself may appear far removed from their normal day-to-day experiences. The first session is mainly concerned with small group discussions, so each student is able to make a positive contribution and to familiarise themselves with group members. Similarly, the groups seem more comfortable with the calculations associated with the early sessions once they recognise how the tasks can be broken down into more recognisable thermodynamical calculations. As expected, once the tasks require the students to make approximations and estimations, or demand mapping of an unfamiliar scenario onto a familiar algorithm of calculations, more guidance from the tutor is required. However, in most cases, it is the recognition that such methods are needed or acceptable rather than the **performing** of them *per se*, that would appear to be important to the students' progress with the tasks. As such, one benefit of the case study approach is that its session-by-session continuity means that most groups find themselves rediscovering novel approaches to problem solving and using them with increased confidence as the case study progresses, which is a clear demonstration of transferable skills development.

Student feedback

In terms of student evaluation of the case study, feedback questionnaires were used at the end of the final session in addition to end-of-session discussions with the tutor. Students were asked to identify their perceptions of ease/difficulty in carrying out the tasks, to describe their individual contributions, and discuss how they might approach such problems differently in the future. They were also asked to classify the tasks using their own terms (physical chemistry, maths, environmental chemistry, problem solving, industrial, etc.) and to describe whether they had needed to use prior knowledge and/or learn something new in order to complete the tasks. A selection of questions and responses are given in Table 2. Consistent with the tutor's observations, the majority of students welcomed the opportunity to 'put theory into practice' by studying physical chemistry in an applied context and to work as part of a group. When it comes to students' perceptions of difficulty, probably the most significant point is that the majority of the students found the calculations to be difficult until they recognised a familiar method that they could apply. At this point, many of the determinations then became relatively straightforward. This is in-line with Bodner's description of the transition between problem-solving and performing exercises (Bodner, 2003).

Table 2. Selected feedback from chemistry students having completed the Capital City case study

Q: Which part(s) of the session did you find easy / difficult?

Easy Calculations that I already knew how to do. Most of the calculations up until the last cost per MWh were not too difficult and well within my	Difficult New calculations that I had to get my head around. Getting confused with units. Minor errors made last session (MWh) difficult.	
capability. Most parts were within my capability.	Talking at group discussions.	
The first session when we had to think about energy sources was easy. First session – advantages/disadvantages of different fuels	Some demanding calculations, discussion helped solve these. Calculations (x2)	
First task in first session (discussion)	Some of the calculations, not enough time (x2)	
Discussion at start to think about positives and negatives of different fuels Methane / coal powered plant.	Calculations, units made things difficult. When sorted out, it was straightforward. Identifying the information needed was hard.	
The harder tasks were easier when longer time period was given made it easier to work out what to do.	Working out how to arrive at the answers. Maths was simple but difficult to know which values to use.	
	Calculations and working out how to approach the tasks. Manipulating information and equations.	
	Estimating power use for solar power plant.	
	Shorter time period made it more difficult.	
	Knowing where to start was a problem.	
	Session 6 was very difficult (x2)	
	Understanding what is being asked for amidst all the information. Most of the sessions were fairly difficult. However, after discussion / feedback sessions the answers were a lot easier to understand. Deciphering each task to know which bits of information to use was difficult, but once this was done it was OK. Session 6 (Solar Power) was very difficult – would never have got to the end answer. Most was challenging, but rewarding. Most of it. Found energy cell sessions quite complex.	
	Ensuring units are correct was difficult. Perhaps a little more guidance in that area (importance of units)	

would be useful.

Q: Would you approach the task(s) differently in the future? If so, what would the differences be?

Yes NO 9 17

Yes – Units would be monitored much more carefully

Being able to think for myself, equipped me with the knowledge to know what principles are applied.

Be more confident in trying my ideas.

I would be more confident in my original thought processes.

Look at units, more time thinking.

Read up before, learn equations.

Spend more time organising the tasks and working through them.

Background reading.

More delegation.

Q: To what extent did you need to use prior knowledge / learn something new?

Other lectures had equations that needed to be used, but this put in practice what I had learnt.

Prior knowledge of thermodynamics, but we learned how to use knowledge in real life situations.

All was prior knowledge, but learnt how to apply it to real life. (x 7)

Helpful to see how theory is used

Gained more experience on practical application of theory.

Prior knowledge not needed (x 3)

Formulas would have been nice.

Learnt new things in every session (x 5)

Mostly new (x 2)

A lot of prior knowledge of algebra was needed.

Prior knowledge: physical chemistry, maths. Learned lots of new ways of working things out.

Learnt a bit about solar power.

Prior knowledge included Partial pressures, Carnot cycle, renewable energy.

Used prior knowledge and learnt something In all tasks

On a less positive note, several students said that they would have benefited from more time or clearer guidance and help from the tutor. However, they thought that the feedback/discussion sessions helped in their understanding, and a number of students concluded that the case study had given them increased confidence in problem solving and taught them the need for working in a more organised way.

Case study layout – editorial considerations

In addition to the scientific content required for each session, we also decided that students (and tutors) would benefit from consistency and quality in format, and that the context-based philosophy would be supported via the use of 'familiar' and 'external' documentation. Each session has some (hard copy) e-mail correspondence together with additional information, which takes the form of extracts from technical reports, published articles, FAX documents and datasheets (see Appendices 1 and 2). As such, consistency in delivery is maintained across each session and all the necessary information is available for the tasks to be completed in-class. We believed that this consistency in the formatting of the documentation would also help students in their cross-referencing of material towards the later stages of the case study, when it was hoped that the data from each session would be synthesised. In summary, students work with each of the following for each session:

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- A cover page for each session with a relevant graphic and description of the session aims
- An e-mail communication giving feedback from the previous session
- Background paper(s) to provide relevant numerical data, equations, graphs
- A further e-mail setting tasks and guidance for the current session (the individual tasks are further highlighted by the use of 'Post-It' type notes)
- Blank tables and other materials (as decided by the tutor)

The tutor's notes have been written with the intention of being as comprehensive and navigable as possible. These comprise the following for each session:

- A cover page, similar to that received by the students, with further elaboration of the key aims
- An outline of the session including a suggested time plan
- Model or suggested solutions to the tasks showing both questions and answers (answers are presented in shaded boxes for ease of navigation)
- Additional material that might be useful (e.g. completed tables)
- Overhead transparency templates

Conclusions

At the outset of this project, it was our intention to produce a case study that would enable chemistry students to develop their understanding of various aspects of physical chemistry during the early stages of their undergraduate degree course. Students would perceive the relevance of the context-based approach and this would lead to greater motivation. We decided to limit the number of topics in order that they would be revisited and this would reinforce learning. We also believed that the evolving storyline of the case study would provide an opportunity for students to work with different problem types, from the familiar to the novel. Further, it was hoped that students would recognise the differences between these problem types and that they would particularly benefit from working with unfamiliar problem-solving scenarios.

The early piloting of the *Capital City* case study indicates that we have made some progress in achieving our aims. Our evaluation suggests that students welcome studying chemistry within an applied context and that this can lead to the development of their subject knowledge and their perception of its relevance. Some students expressed increased confidence in approaching problem solving in the future.

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The Appendixes associated with this paper can be found as separate PDF files at http://www.rsc.org/Education/CERP/issues/2005_3/index.asp