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The journal is aimed at those who teach chemistry in higher education. As a journal for all practising teachers of chemistry at this level it deals with any topic of practical relevance and use to those involved. It is a place to publish effective methods and ideas for the teaching and learning of chemistry and issues related to the effectiveness of teaching and learning. Contributions are particularly welcome if the subject matter can be applied widely and is concerned with encouraging active and independent learning, with increasing student motivation for learning, with helping them to become effective exploiters of their chemical knowledge and understanding, or with assessment. Contributions should be of clear practical interest to those who teach chemistry.

There are no hard and fast rules for subdividing manuscripts. However, an introduction should provide a clear statement of the relationship of what is described to previous work and opinion (and is likely to include some references to some aspects of educational theory), and also the overall purpose of the article (including, where appropriate, the educational objectives, intended learning outcomes and why these are not satisfactorily achieved by other approaches). Other sections may be equivalent to 'methods', 'results', and 'discussion' as used in conventional scientific papers; these sections would describe how the work was carried out, show or illustrate the outcomes (new teaching materials etc) which have been created, and critically evaluate how far the original objectives have been met. It is accepted that evaluation will rarely involve the use of rigorous control groups; but manuscripts should include a discussion of some appropriate method of evaluation leading to critical assessment of the effectiveness of the work described.

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Full Papers: these describe a specific method of or approach to teaching, or some teaching material which has been used by the author; papers should explain the educational objectives which led to the use of the method and indicate its potential usefulness in other institutions. Where appropriate, information about the availability of supporting material should be given.

Communications: these are brief accounts of work still undergoing evaluation and development, but of sufficient interest to merit publication because it is likely either to be widely adaptable by other institutions or to provoke widespread discussion.

Perspectives: these provide an opportunity for contributors to present a concise but in-depth analysis of a topic of general interest, with clear conclusions likely to be directly useful to other academics involved in teaching. Articles intended as a perspective should deal with a topic of immediate interest and relevance.

Letters: these are a medium for the expression of well argued views or opinions on any matter falling within the remit of Journal, including comments on and experience with previous publications.

All contributions, whether or not they were solicited, are rigorously reviewed. Referees are required to evaluate the quality of the arguments presented, and not to make subjective judgements involving their personal views of what constitutes good or effective teaching. Contributions are judged on:

(i) originality and quality of content;
(ii) the appropriateness of the length to the subject matter;
(iii) accessibility of supporting material.

Teaching Introductory Chemistry using Concept Development Case Studies: Interactive and Inductive Learning

PAPER

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At Rice University, we have used an unusual approach to introducing fundamental chemical concepts in the introductory General Chemistry course. New concepts are developed through inductive reasoning in a series of case studies. These are designed to complement an interactive or "Socratic" classroom technique, in which the focus is on active intellectual engagement of students in a discussion of chemical concept development. The methods are described in detail, and results are presented which demonstrate the effectiveness of the approach in developing a deeper understanding of chemistry as well as critical thinking skills.

Introduction

The standard approach to teaching chemistry at the introductory college level has not changed significantly in decades. Material is introduced in lectures, which typically are expository and explanatory statements of concepts and applications. Homework assignments and exams are, in the main, skill tests requiring numerical or descriptive problem solving and factual recall. A glance at any of the many available General Chemistry texts reveals clearly the pervasiveness of the traditional approach.

The flaws in the standard approach are both familiar and well documented[1,2,3]. Students perceive it as boring and without purpose. Furthermore, even after instruction, students retain significant misconceptions about many fundamental chemical principles[4] including the meaning of an atomic view of nature[5], the nature and origin of bonding energies, the significance of the octet rule[6], and the differences between chemical and physical properties[7].

It has been established that most students learn much more effectively in active and cooperative learning environments[8] in which they develop new ideas logically from simple principles by a process which involves inductive reasoning[9-11]. By contrast, the lecture format is almost entirely passive, with students spending their class time simply transcribing the lecture, disengaged from the intellectual content[12]. New concepts are presented *fait accompli* which encourages students to accept ideas that they do not understand, and to commit challenging material to memory rather than try to understand it and integrate it with their existing knowledge.

The limitations of the traditional lecture have not gone unnoticed, of course. A number of approaches have been introduced to initiate what has been termed 'active learning'. These approaches include peer instruction[13], concept question discussion[12], discovery laboratories, team assignments, and 'minute' essays. Other innovations have focussed on methods for making the explanations easier or more illuminating, particularly in revealing challenging concepts such as the particulate model of nature. New textbooks typically focus on new problem solving approaches and examples. Computer animations of simulated molecular processes have certainly been found to help students understand particulate concepts. Video presentations make chemistry more visual and real. Computer tutorial programs provide more individualized instruction than is possible in the large lecture format. These are very important modifications to the traditional pedagogy and their widespread incorporation into chemistry instruction should be encouraged. However, in most cases these cannot fully address the fundamental problem, since they are superimposed on the basic structure of the traditional declamatory lecture.

We decided to go a stage further and devise a course in which the lecture itself was a truly interactive experience. This required the design of a suitable resource to support the student learning. We describe here the development and use of the resource which we developed for this purpose.

Preparation of Case Studies in Concept Development

Our initial analysis of the problems faced by students suggested that, although many chemical processes are familiar in everyday experience, the chemical concepts underlying these processes are themselves unfamiliar. This is because chemical models are inherently molecular, outside the range of everyday experience, and therefore models are far from intuitive. Our goal was to help our students to develop the chemical intuition which would allow them to bridge the gap between the familiar processes and the unfamiliar chemical concepts and models. We therefore used the same inductive reasoning method as was used originally by chemists to develop the chemical models in general use today. This means introducing each major chemical concept through discussion of relevant experimental observation, and logically developing a model to describe these observations.

The resource we developed had to be suitable for the General Chemistry course at Rice University which is taken by between 250 and 300 students in a single class section with a single instructor supported by Teaching Assistants. The class meets three times per week, 50 minutes per day, for 15 weeks in a semester. In addition, students meet once per week in small discussion sessions of 30-40 students. Most spend 5 – 9 hours per week of their own study time on this course including reading, homework, discussion, group review etc. In these regards, the course at Rice is similar to most General Chemistry courses in the USA.

With this in mind we prepared nine case studies of the development of chemical concepts. These are listed in Table 1 and they are provided in textbook format for the students[14] and are available via the web (see section on Availability). This is not the only text used by students on this course since it is concerned primarily with the development of the concepts. For applications, students rely on a more conventional text, 'Atoms, Molecules, and Reactions'[15]. Student surveys (see later) reveal an extremely strong preference for the 'Case Studies'. Each study introduces new concepts using a series of seven steps analogous to those typically used to develop any new concept in science. These are shown in Table 2.

The material in each of the nine case studies is completed in two or three of the 50 min slots. This leaves two or three other 50 min slots (which are devoted to appropriate applications and problem solving), one or two discussion sessions (devoted about half-and-half to review/discussion of the class material and to reviewing homework answers) and homework. Homework is assigned weekly, typically consisting of 5-8 essay questions covering the concept development studies, and an additional 5-8 standard objective problems to solve. It is due in at the Monday class; it is graded that afternoon by the teaching assistants, and returned that evening during discussion. The primary roles of homework are as a study guide and as practice in writing short paragraphs about chemical concepts.

The style and structure of the case studies is illustrated by a description of Case Study 3 'Periodicity and Valence'. The full text can be viewed on-line (see Availability).

In this case study, the aim is to develop the concepts of a valence shell and the octet rule as means of predicting atomic valence. These concepts form the basis of Lewis structures of molecules, perhaps the most significant of the chemist's theoretical models. The case study is designed both to bring meaning to these models and to encourage students to distinguish experimental facts from conceptual interpretation. It uses the experimental facts which were actually used to develop these concepts, and so introduces an historical perspective to their learning.

The Foundation (step 1 in table 2) is Case Study 1 (Atomic and Molecular Theory). Therefore it is assumed that students understand that relative atomic masses have been measured and the valences of the elements are known from molecular formulae. The principal Question (step 2) posed is what property of an atom determines the valence of the atom. The first Experimental Observations (step 3) of the properties of elements reveal the grouping of elements by physical and chemistry properties and from these groupings the Periodic Law is developed with emphasis on the periodicity in the principal valences of the main group elements (this is the Model Building of step 4 and leads to Further Questions).

In order to develop a model for periodicity, 'Further Observations' are needed. At this point the results of electroplating experiments are used to demonstrate that atoms contain particles of negative charge, i.e. electrons. This leads to the 'Further Question' of how these charges are arranged in an atom, a question which is answered by analysing Rutherford's observation of the scattering of alpha particles by gold atoms. Inductive reasoning leads to the familiar nuclear model of the atom.

The atomic model remains incomplete, however, until the number of electrons in each atom has been determined. Here we use the actual experimental evidence from Moseley's measurement of the atomic X-ray emission frequencies. The number of electrons shows that elements with the same

Table 1 List of case studies

The Atomic Molecular Theory – development of the theory from the Law of Definite Proportions, the Law of Multiple Proportions, the Law of Combining Volumes, and Avogadro's Hypothesis.

The Kinetic Molecular Theory – observation of the gas laws, derivation of the Ideal Gas Law, analysis of deviations from ideality, development of the postulates and conclusions of the Kinetic Molecular Theory, and interpretation of temperature in molecular terms.

Periodicity and Valence – this is discussed in the example above.

Chemical Bonding and Electron Pair Sharing – development of the Lewis structure model of chemical bonding from observations of molecular stability, bond lengths and bond strengths, development of the concept of resonance, observation and analysis of ionic versus covalent character, development of the concept of electronegativity.

Properties of Polyatomic Molecules – observation of molecular geometries, development of Valence Shell Electron Pair Repulsion model, observation and analysis of molecular dipole moments.

Atomic Structure and Valence – observation of quantum mechanical behavior in radiation and matter, development of postulates of quantum atomic theory, analysis of electron configurations, theoretical analysis of the Periodic Table and valence.

Chemical Bonding and Molecular Structure – development of quantum behaviour of electrons in molecules, observation and analysis of diatomic bond strengths, development of the molecular orbital energy level diagrams and the concepts of bond order and paramagnetism, analysis of molecular geometries, development of the concept of hybridization.

Energetics of Chemical Reactions – observation of specific heats of materials, observation of chemical reaction heats, development of Hess' Law and the concept of state functions, application of Hess' Law to formation energies and bond energies.

Spontaneity of Chemical Reactions – observation of spontaneous change, relationship of spontaneous change to probability via Boltzmann's equation, observation and analysis of absolute entropies in terms of Boltzmann's equation, development of the Second Law of Thermodynamics, observation of spontaneous phase separation in liquid mixtures, development of the concept of free energy.

Table 2 The process of concept development

Foundation: We first define a set of material on which the remaining observations and developments will be based. This directs the students to concentrate on relevant material.

Questions: The ideas presented in the foundation produce a group of open questions for discussion. These questions might arise from observations that are not fully explained by the foundation or that even appear to be inconsistent with the foundation. Or they might arise from a need to further clarify or detail a previously developed model.

Observations: Chemistry is inherently an empirical subject, based on actual observations of natural processes. This is most clearly revealed to students when they begin with the relevant experimental observations which lead to a model. In our concept development studies, we use (whenever possible) the actual experiments which were used historically to develop each chemical concept.

Model building: The appropriate scientific response to a new set of experimental observations is to begin assembling a model which is consistent with and accounts for the observations. "Occam's razor" is introduced in practice, as students are taught to seek the simplest model to account for the observations.

Further questions: As is familiar to research scientists, each new model often presents more new questions than it answers. A significant part of the utility of the new model, indeed, is to suggest directions for further experiments and observations.

Further observations: These might be logical extensions of the previous observations. They might also be, as often occurs in science, unrelated observations which, when combined with the tentative model, lead to further progress in developing a model which leads to deeper understanding.

Model modification: Additional observations permit us to refine a model, adding detail, removing ambiguity, or establishing limits of applicability. The process of questioning, observing, and model building is repeated iteratively until the original questions are satisfactorily answered.

valence show a periodic variation in their number of electrons. This quickly leads to the conclusion that the electrons in atoms are grouped into shells, including a valence shell which determines the chemical reactivity of the atom. The periodicity of the elements also permits determination of the number of electrons in the valence shell. Combining this with the known valences of the elements produces direct observation of the octet rule for main group elements.

This very brief description does no more than illustrate the Case Studies in Concept Development and demonstrate that both the experiments and the reasoning are within the grasp of introductory chemistry students.

Using the Case Studies

The students are introduced to the course 'rules' at the beginning of the course which are summarised in Table 3.

The main objective of the classroom sessions is to encourage students to verbalise in their own terms the reasoning which leads to the understanding of the concepts developed in the Case Studies. The application of the course rules (table 3) helps to ensure the involvement of the entire class. Other techniques are helpful too. Once per class session, rather than calling on a volunteer to answer, students are asked to answer the question to a neighbour. The buzz of noise which always accompanies this request is a testimony to its effectiveness. It gives everyone a chance to answer, particularly students who are too shy to speak in front of a large group and it lets students check their answers before volunteering to speak up. A further incentive to volunteer is that students receive extra credit for answering questions; even though each answer amounts to only about 0.15% of the credit for the course grade it appears to be sufficient to encourage participation. The real key is to make eye contact with the students to encourage them to attempt an answer. All answers are rewarded, even if incorrect, and no answer is ever ridiculed.

The question and answer format encourages active participation in the learning process and leads to genuine classroom discussion (even in a class of 250 students). Students frequently respond to an answer by correcting it (or providing a different answer), by clarifying each other's statements, or by extending each others' line of reasoning. In this way the formal presentation of the procedure of concept and model building given in the Case Study is transformed into an active learning process. The instructor leads the students through the steps, but they have the opportunity to develop their own understanding of each new concept in terms which make sense to them. This is a crucial step in the learning process according to the Constructivist Theory of learning[16].

In the seven years during which these case studies have been used it is rare to have less than 10 students raising their hands, and there has never been an occasion when none has offered an answer to a question. Typically, the first question posed in the course results in 40 – 50 volunteers keen to provide an answer. Throughout the course a typical number would be 20 or more. It is not possible in a class of 250 to ensure 100% participation. Our surveys tell us that about 1/3 of the students raise their hand every day or almost every day. About 60% of the students raise their hands at least occasionally. Only about 15% of the students say that they never participate at all.

The emphasis on active involvement and inductive

Table 3 Summary of the course rules.

Students study an assigned part of the case study (typically 1/3 to 1/2 of one of the Case Studies) before each class;

During each class the instructor guides inquiry and conclusions by asking appropriate questions;

Students are awarded marks for participation in class discussion;

Students wishing to answer a question must raise their hand and wait for the instructor to invite an answer;

Answers called out are ignored;

The instructor always leaves a gap of at least three seconds before selecting a student to give an answer;

reasoning are reinforced by the assignments given to students in both homework and examinations. If assignments follow the standard problem solving exercises, students rapidly learn to disregard 'extraneous' material about how the chemical concepts were derived. Therefore, questions on homework must challenge the students to explain the logical connections between experimental observations and theoretical models. Limitations of these models must be explored, and contrasting results must be considered to verify the limitations. Similarly, exams must ask for descriptions of relevant experiments along with logical reasoning leading to conceptual development, or must ask for rationalization of experimental observations on the basis of the models developed. Of considerable significance is that these homework assignments and exam questions challenge the students to write clearly, logically, and articulately about scientific concepts, which is a rare opportunity for most university students[17].

The mark for the course is based on examinations, on homework, and on student participation. There are three ninety-minute midterm examinations and a three-hour final examination each composed of about 2/3 concept development essay questions and 1/3 objective questions and problems to solve.

Student Feedback

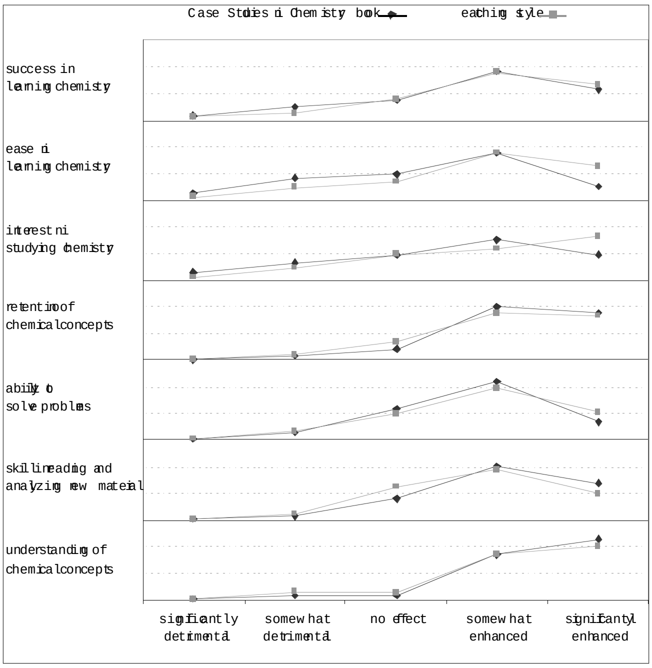
We have analysed the successes and failures of the interactive and inductive learning approach at Rice with a variety of instruments, including extensive end-of-semester surveys and comparisons of pre-instruction quiz with post-instruction exam. We also have anonymous testimonials from course evaluations and exit surveys[6,18].

The opinion surveys are strikingly positive. In each of the past seven years, we have asked students for the contribution of both the concept case study approach and the Socratic teaching approach to various elements of success in instruction. The results for the Fall semester of 1999, shown in Figure 1, are representative of these results over the years. For example, when asked for the contribution of the text 'Case Studies in Chemistry, to their understanding of chemical concepts, 51% of the students responded that their understanding was 'significantly enhanced', and an additional 39% said that their understanding was 'somewhat enhanced', a remarkable 90% positive reaction at the end of the semester. Figure 1 clearly reveals that the great majority of students feel that the case study approach with Socratic teaching enhances their retention of chemical concepts their skill in reading and analysing new material, their ease in studying chemistry, and their success in studying chemistry.

One might be concerned that the enhancement of understanding of chemical concepts comes at the cost of problem solving ability. However, Figure 1 shows that 65% of the students feel that their problem solving ability was enhanced by the concept study approach, presumably because it is easier to work problems about concepts which are understood clearly.

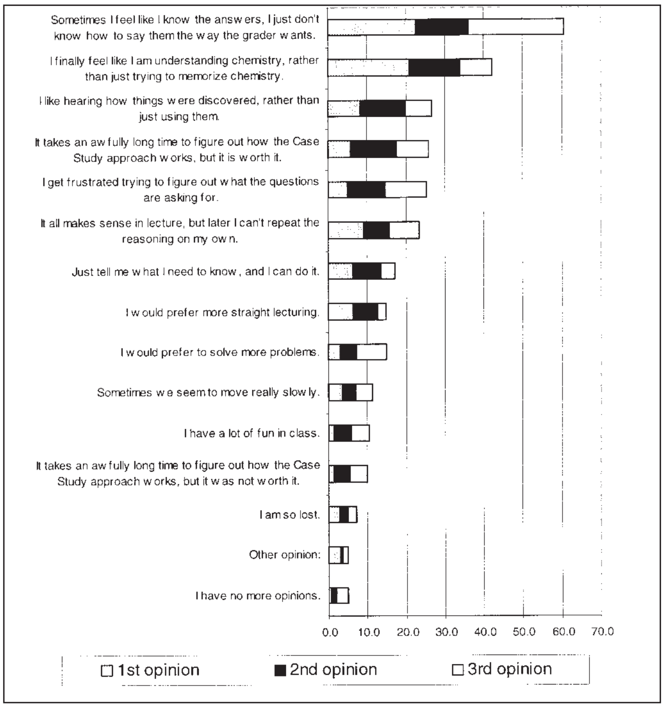
As a means of getting detailed and systematic opinion data about the concept development case study approach, we have

Figure 1



Exit survey results from General Chemistry (Chem 121) at Rice University for the Fall Semester of 1999. Students were asked to describe the contributions of both the Case Studies in Chemistry book and the Socratic teaching approach to their learning in the different categories on the vertical axis. In each category, the axis runs from 0 to 150 students, with grid lines at 50 and 100 students. The total number of students in the survey is 221.

Figure 2



Exit survey results from General Chemistry (Chem 121) at Rice University for the Fall Semester of 1999. Students were asked to select from the list of opinions on the left the three options with which they most strongly agreed. The horizontal axis is percentage of students selecting that opinion. The total number of students in the survey is 221.

offered students a list of 13 oft-quoted opinions, of which some are negative and some are positive. We then ask the students to identify the opinions with which they agree with most strongly, next most strongly, and third most strongly. The results for the Fall 1999 class are shown in Figure 2.

The data show that there are two primary popularly held opinions about the approach. The most popular opinion is that "Sometimes I feel like I know the answers, I just don't know how to say them the way the grader wants". This apparently negative response is a potential cause of disquiet which we discuss in the next session.

The second most popular opinion is positive: "I finally feel like I am understanding chemistry, rather than just trying to memorise chemistry." This sentiment runs in parallel with the third and fourth most popular opinions, "I like hearing how things were discovered, rather than just using them," and "It takes an awfully long time to figure out how the Case Study approach works, but it is worth it." In our experience, then, the students appreciate the opportunity to see beneath the surface of chemical concepts and to participate in scientific reasoning, even if they are concerned about the impact that these discussions may have on their grades.

In the light of some known difficulties which students experience, we have begun a long-term systematic study of student learning in General Chemistry by comparing student performance on pre-instruction diagnostic quizzes ('pre-test') with performance on midterm and final exams ('post-test'). Some results for the pre-tests given in Fall 1998 are described elsewhere[6], and a full analysis of pre-test post-test correlation will be published. Here we cite two examples of improved student performance following instruction via the interactive inductive learning approach.

First, students often show confusion over whether the process of bond breaking requires the input of energy or results in the release of energy. We have found dramatic improvement in student understanding of bond energetics following interactive inductive learning. In a pre-test multiple choice question, 34.7% of students correctly said that "when breaking a bond, energy must be added", whereas 24.4% believe that "energy must be released" and 40.9% believe that "the energetics depend on the circumstances." After interactive case study instruction we found that 74% of our students correctly describe the energetics of bond breaking. Furthermore we found that 50.6% of our students can correctly or nearly correctly describe in detail the disposition of the absorbed energy in terms of changes in energies of the bonding electrons, thus demonstrating a depth of conceptual understanding of bond energy. In direct contrast, a recent study at the University of California demonstrated that traditional lecture instruction and problem solving has little if any effect on students' misconceptions about bond energetics. However, these researchers also found that interactive teaching in a control group did improve understanding significantly.

As a second example, students often apply the fundamental tenets of Valence Shell Electron Pair Repulsion theory incorrectly. For example, on pre-test quizzing, 35% of our students believe that NBr_3 molecules have trigonal planar geometry, and 37% attempted to predict the geometry by considering only the repulsion between N-Br bonds. (The question we asked was developed by Treagust and coworkers[19,20], who found similar poor performance amongst high school chemistry students on post-instruction quizzes.) By contrast, following instruction via the case study approach, 84.7% of our students could completely correct all of the errors in a given statement that "In Nitrogen Tribromide (NBr_3), the three N-Br bonds are identical. The three electron pairs in these bonds repel each other equally, resulting in a planar molecule with equal 120° bond angles."

These two pre-test post-test comparisons reflect a fraction of the data we have available, all of which lead to the same promising conclusions. Students learn chemical concepts very effectively when they are taught interactively using concept development case studies, and they are also able to apply these concepts in solving chemical problems.

Discussion

The approach described in this paper is based on two key principles. First, effective learning requires intellectual engagement of students in the instructional process. This requires an active learning environment, but it also requires textual materials which complement active learning, so that discussion of chemical concepts is possible. Second, students learn concepts far more effectively when these concepts are developed via observation and inductive reasoning, rather than in expository prose. This requires a textbook which presents the experimental basis and reasoning behind chemical concepts, rather than simply a statement of these concepts along with problem solving applications. After seven years of experience of interactive teaching, using our textbook of Case Studies in Concept Development as our main reference source, we believe that our principles have been vindicated. Furthermore, we believe that our approach goes some way towards meeting the point made by Kooser and Factor[21] that we have an obligation to give our students "*a more realistic picture of the scientific enterprise in all its ramifications*".

There are some challenges associated with teaching interactively as described here. Not surprisingly, we move through our material somewhat more slowly, so a smaller number of topics can be covered per semester. In our view, that price is well paid, in that we much prefer to have our students cover a smaller amount of material that is well understood than a larger amount of material that is not understood. We also note that the course as taught is more labour intensive than one taught with an emphasis on lectures and problem solving. Since homework and exams do not typically have objective answers, they cannot be graded electronically. As such, a great deal of effort is required by the teaching assistants to grade verbal answers to concept questions.

A major question for us when we started using this approach was whether the focus on chemical reasoning would compromise the student's ability to solve traditional problems. We have combined our exercises in chemical reasoning with traditional problem solving and descriptive chemistry, since these are also important components of a chemical foundation. Our conclusion based on our observation of the students and on their responses to our questionnaires is that teaching chemical reasoning is a very effective way to teach chemical problem solving.

As far as assessment is concerned, we recognise the problem of students feeling that they know the answer but not being sure what the grader wants. To some extent this reflects the fact that most students have come to expect that, in science, there is a single right answer, and producing that answer on an exam is a guarantee of a good grade. This is consistent with the dualist mentality (everything is right or wrong, black or white, etc) which is associated with the first stages of intellectual development described by Perry[9]. The approaches used at Rice run counter to this expectation and indeed are intended to help the students to progress to higher levels of development. The difficulty of achieving this is demonstrated by the frequency with which our students express discomfort about being graded subjectively on scientific material. Our response is to strive to both make our expectations clearer to the students, and to explain to them that science involves subjective judgements. In this connection we agree with Bailey's recent comment that " we should not be afraid to use our professional judgement in assessing skills which do not lend themselves to objective measurement"[22]. Every year we find that a few students attempt to memorise the case studies, but the approach works very poorly because of the style of exam question that we set.

The material presented in the Case Studies in Concept Development could be used within any standard course in General Chemistry, to reveal to students how the concepts they are learning were developed, and traditional teaching approaches could be used. However, a major advantage to presenting new material in an inductive reasoning approach is that it greatly facilitates active learning approaches in the classroom, and we recommend this approach strongly. Lecturing about the development of concepts may well be more illuminating to the students than simply describing the details of a concept, but ultimately it probably only shifts the focus of the student from memorising the concept to memorising the experiments. Rather, the goal of a chemistry course, and thus the goal of classroom activity, should be to stimulate independent critical thinking about chemical concepts under the guided instruction of the teacher.

We have found over the past seven years that the combination of interactive teaching and concept development studies has been both effective and well received by our students. A significant question is whether the approach is only effective at a highly selective institution like Rice University. We cannot currently answer that question directly, since the approach has not been employed anywhere other than Rice. However, we do get a broad profile of student backgrounds, particularly with regard to prior instruction in Chemistry. Our surveys demonstrate that the approaches described in this paper are more frequently perceived to be effective by our more poorly prepared Chemistry students than they are by our well prepared students. These data suggest that the interactive and inductive learning approach should find wide applicability.

We conclude with a few anonymous testimonials from our students, submitted during the Fall 1999 exit survey. Whether these are truly representative of the opinions of most students is open to question. But these are powerful statements about the impact on at least these two students.

"I feel that I have really learned chemistry. The way that it is presented in the case studies book simply forces you to pay more attention to the subject matter and to have an in depth understanding of the chemical phenomenon."

"I will admit, that at the beginning of this course, I was one frustrated person who couldn't stand the case studies, but as time progressed, I found myself actually grasping to certain concepts and ideas that I never cared for in high school. You see, in high school, I was just given the theories and laws and their respected formulas to memorize, and that's exactly what I did. But in this course, I actually knew why those theories existed; why they carried those certain formulas; I couldn't memorize anymore; I really had to understand what was going on…and that has been the most important lesson of all."

Availability

The complete text of 'Case Studies in Chemistry' is available on-line to educators by permission of the author at http://chemed.rice.edu/CaseStudies. Both html and pdf formats are available. Case Study 3 can be accessed without registration. The rest of the text requires registration on-line with the author.

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SolEq: Tools and tutorials for studying solution equilibria

PAPER

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SolEq (Solution Equilibria) is a CD-based package of tutorials designed for teaching equilibria to senior undergraduate students. Between them, they cover the principles and applications of acid-base, redox, solubility, and metal-ligand chemistry in both homogeneous and heterogeneous systems. It also provides the computational software for applying equilibrium principles to real systems (speciation programs, database, ionic strength and van't Hoff corrections *etc*.). The 29 tutorials and 8 computational packages are linked seamlessly *via* tool bar functions. SolEq has been used to support lecture and laboratory courses on environmental chemistry, coordination chemistry and analytical chemistry. It has also been used to create a customised refresher course for a graduate about to embark on a research programme in environmental chemistry.

Introduction

Equilibrium principles play a pivotal role in chemistry. For example, equilibrium processes are critical in the aquatic environment around us, and in the plasma and intracellular fluid within us. We recognise the importance of equilibrium by inclusion of topics such as solubility and acid-base theory in elementary chemistry courses, even though we may not cover them rigorously. However, these principles also underpin more complex systems and applications (*e.g.* environmental, industrial and biological processes, speciation and coordination chemistry).

In spite of the central role that this topic plays in chemistry, we were unable to locate suitable resources to support two undergraduate courses that we are required to teach. One is on 'the energetics of complex formation', an advanced inorganic chemistry course that involves an in-depth treatment of energetic (equilibrium) principles. The other is on aquatic chemistry, with emphasis on equilibrium reactions (metal ion speciation) and redox processes in environmental systems.

Our survey of available resources showed that excellent texts are available in specialist areas. Typically these adopt a chemical energetics (equilibrium) perspective against which to address issues in environmental chemistry[1,2], industrial chemistry[3], and aquatic chemistry[4]. These texts, because of their depth, rigour and specialisation, are not appropriate for courses to non-specialists or for a generic approach. In other areas, such as thermodynamic aspects of coordination chemistry and its applications in biological systems we have found a dearth of suitable teaching resources. We therefore determined to create a resource that would meet our requirements and be suitable for use by middle and advanced-level university undergraduates and by graduate students whose research involves any aspect of solution equilibria.

Such a resource would support a generic approach to solution equilibrium by drawing together redox, acid-base, metal-ligand and solubility equilibrium in one integrated package. It would also provide adequate, self-contained teaching resources in all of these areas, especially for metal-ligand systems. It was our premise that effective teaching of solution equilibrium should involve not only the conceptual and theoretical aspects of equilibrium, but also its application in a wide range of real systems. For this reason we wanted students to move seamlessly from theory to problem solving. This is not easy to achieve using a conventional text-book approach, since many of the problems relevant to equilibrium systems (*e.g.* speciation, buffer, and polyprotic acid calculations) involve complex calculations for which computational software is necessary. However, a CD could include the computational software necessary to effect calculations so that a single resource based on a CD would facilitate the integration of theory and problem solving. A CD would also allow us to include material which cannot be incorporated into text (*e.g.* titration simulations) and all the material would be readily accessible to tutors who wished to use it to enrich lectures and other classroom teaching. We also believe that this contemporary technology provides greater focus for the less well motivated student, and encourages exploration beyond the limits of any prescribed course.

For all these reasons it seemed appropriate to develop a CD rather than a text-book. In this paper we describe the resource, SolEq, which we developed to meet these needs. We report how the SolEq tutorials provide new generic resources for the teaching of solution equilibrium, how they use computational tools to quantitatively apply equilibrium principles to real systems, and how they have been applied in a number of teaching situations.

An overview of SolEq.

The SolEq package is available on CD and is Windows 95/98/NT compatible. It contains 29 tutorials which are listed in Table 1. They are designed to allow students to:

- work through the principles of solution equilibrium;
- facilitate application of equilibrium concepts to problems in multi-component real systems;
- effect relevant calculations and teach computational skills through use of provided software;
- develop student familiarity with equilibrium databases and speciation programs, with ionic strength corrections and use of the van't Hoff equation;
- provide explanation of background theory to the computational software in specific tutorials or Help files.

Some tutorials introduce the simulation packages and software. For example, tutorial 29 'Metal/Ligand Titration Simulations' instructs in the use of the program Metal/Ligand Titrations. This program can simulate the effect of the magnitude of log $K_1(M + L = ML)$ on the metal-ligand titration curve (specifically the effect of M^{z+} on the L/H_nL^{n+} buffer region, $M^{z+} + H_nL^{n+} = ML^{z+} + nH^+$). The shift in pH range for the buffer region and the change in metal or ligand speciation can be demonstrated simultaneously as the pK_a value(s) of H_nL^{n+} and/or log K_1 are varied.

The text incorporates many hypertext-active links; double-clicking on one of these activates a window with a linked file that contains additional information (*e.g.* derivation of equations) or illustrations. For example, tutorial 18 'Acid Rain' includes striking pictorial images of pristine and damaged environmental systems and graphs of acid or NO_x deposition in Europe. Some tutorials include simulations which allow the display of real-time changes in pH titration curves, buffer capacity plots, distribution curve plots *etc.* through varying the number and magnitude of pK_a values, the metal/ligand ratio, the ionic strength, or reagent concentrations.

As table 1 shows, there is an introductory tutorial and the remainder are divided into four main groups: Homogeneous Systems (Principles; Applications), and Heterogeneous Systems (Principles; Applications). Each tutorial is also graded according to difficulty: Level 1 tutorials are appropriate for years 1 and 2, Level 2 for year 3 (and the more capable year 2 students), Level 3 for years 3 and 4. Some of the topics (*e.g.* principles of metal-ligand equilibria in tutorials 10, 12 and 13) are covered in considerably more detail than in available textbooks. Each tutorial is structured as a series of tabbed 'book' pages; i.e. they have a 'softbook' format. Most pages have exercises and worked answers. Each tutorial commences with a list of Learning Objectives, and finishes with a Summary and List of References, and can be completed in 1 to 5 hours.

The tutorials are supported by two titration simulations and eight software packages (*e.g.* for speciation calculations). These can be used as stand-alone items (*e.g.* in conjunction with the teacher's own exercises) or accessed from the tutorial pages *via* tool bar icons.

Voice files that provide an introductory overview to the package in English, Swedish, Russian, German, French, and Japanese are incorporated into the package.

Student feedback on the use of SolEq has been obtained by exit questionnaires after laboratory applications, and from informal discussions with and observation of students using the package.

Examples of Use

Over a three year period, different parts of the package have been used by university chemistry students in several countries. The flexibility of the package is illustrated by the following examples of its use.

Computer-generated lecture demonstrations

Material from some tutorials has been selected and used to enrich lectures with visual displays and demonstrations. For example, one of the objectives of a lecture course on 'Inorganic Energetics' is that students should learn to use a database of stability constants (*viz.* ML-Database) and to carry out speciation calculations (using Species). We have used exercises from Tutorial 13 'Macrocyclics' and Tutorial 15 'Selectivity' to help students to learn these skills. Other examples of the incorporation of SolEq material into lectures include

- incorporation of pH titration and buffer capacity plots into lectures on polyprotic acids and buffers
- use of simulation packages to introduce complex topics and generate an initial overall appreciation of the concepts involved.

In all these examples we have introduced the relevant software at the appropriate time in a lecture to demonstrate key principles. In our experience this has been an effective way of encouraging the students to use the software in their own time (using Help files or a dedicated tutorial) and in this way improve their skills.

A lecture course on complex formation

For three years a course on complex formation for third year students at the University of Canterbury has been taught using, as the sole reference work, the four tutorials ‘Thermodynamics’ (number 10), ‘Chelates’ (number 12), ‘Macrocyclics’ (number 13) and ‘Selectivity’ (number 15). The course is nominally nine lectures long, but the directed use of the SolEq package has allowed us to adopt a more student-centred approach in which the students take more responsibility for their learning. The relevant tutorials and software packages in SolEq are demonstrated to the students by use of computer projection facilities in the first and second lectures. The remaining seven lecture slots are used to focus their personal study for which students have unlimited access to SolEq on computers in the departmental computer room, and in the students’ coffee room and in the library. The approach is rooted in the identification and exploration of the factors that control the formation of stable complexes.

Table 1: SolEq modules

Tutorials

Introduction
1. An introduction to solution equilibria (lg K, ΔG, ΔH and ΔS)

Principles –homogeneous:

Level 1*
2. Acids and bases (protonation, acid dissociation, base hydrolysis)
3. Buffers (properties, preparation and buffer capacity)
4. Introduction to metal-complex formation (basic principles)
5. Complex formation (mono- and poly-dentate ligands)
6. Stability constants (stepwise (K_n) and cumulative constants (β_n); use of $\beta_{p,q,r}$)

Level 2:
7. Polyprotic acids.
8. Redox equilibria (balancing equations, E, pε, Nernst equation)
9. Potentiometric titrations (redox titrations, *e.g.* Ce^{4+}/Fe^{2+})
10. Thermodynamics (ΔG, ΔH and ΔS; temperature and ionic strength effects)
11. Speciation (a primer on setting up calculations and interpreting curves)
12. Chelates (chelate effect; denticity; ring size; applications)
13. Macrocyclics (macrocylic effect; N and O, as well as N,O donors; cryptates and calixarenes)

Level 3
14. Electron activity (concepts; pε-pH, pε-log C; calculations)
15. Selectivity (thermodynamic basis of hard/soft, class A/B classifications)

Applications –homogeneous:

Level 2
16. Metal speciation in natural waters (modelling of Cu^{2+}, Zn^{2+} and Pb^{2+})
17. Metal speciation in seawater (iterative calculation methods)
18. Acid rain (quantitative analysis of acidity-generating equilibria)
19. Trace metals in blood plasma (low molecular mass ligands and proteins)
20. Chelation therapy (use of chelates to remove toxic metals)

Level 3:
21. Marine carbon dioxide system (solubility of CO_2, effect of pH)

Principles –heterogeneous:

Level 2:
22. Solubility and solubility products (molecular and ionic solutes)
23. Complexation and solubility (effect of complexation and pH on solubility)
24. Precipitation titrations (volumetric analysis)

Applications – heterogeneous:

Level 2:
25. Mineral solubility in complexing media (simulating soil weathering)
26. Treatment of metal-contaminated soil (chelates, electrokinetics)
27. Lake equilibria; Lake Baringo, Kenya (speciation of major and trace metals)

Titration simulations:

Level 2:
28. Acid/base titration simulations (with simultaneous speciation)
29. Metal/ligand titration simulations (with simultaneous speciation)

Software Packages:

ML-Database, a database of stability constants for 18,000 metal-ligand pairs, a selected subset from the IUPAC Stability Constants Database.
Buffers, for exploring buffer properties, buffer capacity and for calculations.
Species, for speciation calculations in multi-component, multi-phase systems.
Titration City, to simulate curves for acid-base, redox, and precipitation titrations.
Acid/Base Titrations, to create and display titration and speciation curves in real time.
Metal/Ligand Titrations, to create titration and speciation curves from stability constants.
KvI, to calculate the effect of ionic strength on K (Davies equation).
KvT, to calculate the effect of temperature on K (van’t Hoff equation).

* In the context of a three-year B.Sc., Level 1 tutorials are appropriate for years 1 and 2, Level 2 for year 3 (and the more capable year 2 students), Level 3 for years 3 and 4.

The course content is best illustrated by some of the questions that students are required to explore using the SolEq package:

- Is Cd^{2+} a Class A (Hard) or Class B (Soft) metal ion? Students discover the answer by calculating the speciation of Cd^{2+} as a function of pH in a solution containing Cd^{2+}, dithizone (diphenylthiocarbazone) and acetylacetone (2, 4 pentandione) at millimolar concentrations.
- Under what conditions can a negative chelate effect occur? (Students calculate the effect of total concentration on the speciation of Zn^{2+} in a Zn^{2+}-ethylenediamine-triethylenetetramine mixture).
- Establish that when Gd(DOTA) is used as a MRI reagent at the therapeutic dose, DOTA is not sequestered by plasma Ca.
- Establish that 1 mM cyclam is able to complex 1 mM Cu^{2+} quantitatively, even in a 1000-fold excess of triethylenetetramine.
- In an EDTA titration of Ca^{2+} in the presence of Zn^{2+} at pH 10.0, what is the minimum concentration of CN^- required to mask 1 mM Zn^{2+} in the presence of 1 mM Ca^{2+} and 1 mM EDTA?

The SolEq package makes this approach possible because it allows the students to move seamlessly between text, exercises, and supporting software such as 'Species' (for calculations) and 'ML-Database' (for information retrieval). For all exercises, the student has access to worked answers through hypertext links.

Laboratory application I: Speciation calculations

Tutorial 16 'Metal speciation in natural waters' has been used for 3 years with a third year Environmental/Analytical laboratory course at the University of Canterbury. This tutorial introduces the database of stability constants (ML-Database) and takes the student through methods for correcting stability constants for ionic strength effects (KvI software). Through links with the software package Species, students complete calculations on the speciation of Cu^{2+}, Zn^{2+} and Pb^{2+} and are thus shown that the speciation of each metal ion is distinctive and that its speciation in humic, fresh and sea waters is very different.

With this background, students are expected to be ready to work on their own problems. Alternatively they can choose, or the instructor can assign, one of the in-built projects. As an example, one of these is a project concerning the discharge of an aluminium-rich waste solution from a water treatment plant into a river; it illustrates the complexity of the problems that can be attempted.

'A factory discharge into a river contains 10^{-3} M Al^{3+}. The discharge is diluted 50-fold on merging with the river. The major ion composition in the river is $[Ca^{2+}]_T = 0.0006$ M, $[Mg^{2+}]_T = 0.00007$ M, $[F^-]_T = 0.00005$ M and $[SO_4^{2-}]_T = 0.0001$ M. The river also contains 15 ppm fulvic acid, which may be modelled as 7.5×10^{-6} M malonic acid. The river pH is 4.9. Al(malonate) complexes, Al-F complexes and the $AlSO_4^+$ complex are not toxic to fish, whereas the free Al^{3+} ion is. Determine whether the concentration of toxic Al exceeds the threshold of 5×10^{-6} M for survival of fish. Would the same conclusion be made if the river contained less fulvic acid (say 1.5 ppm)?

Use Mini-SCDatabase to obtain the stability constants for relevant Al complexes and use KvI to adjust them to the required ionic strength. Use the provided file MineAl.spc as a template to establish your Species input file'.

This and other problems have sometimes been set for students who have not previously used SolEq. In these cases, a 10 minute introduction from the instructor has been enough to enable the students to get started. The instructor also needs to interact with the students when they are ready to start the Species calculations and again when they start their project assignment. This tutorial plus assignment takes approximately 3.5 hours. Students (working individually or in pairs) frequently remain at the terminal for this length of time, without apparent loss of concentration. In conversation with them, it appears that they are enthused by the fact that after a comparatively short practical experience (plus background course work) they have access to, understanding of, and adequate competence with, software and databases that can facilitate answers to complex environmental questions.

Feedback from exit questionnaires has been uniformly positive.

Laboratory application II: A Food Technology course

The SolEq package has been used at the Moscow State University of Food Technology to support the laboratory course in Physical and Colloid Chemistry. These students are training to be Food Technologists in the bakery, beer, wine, sugar beet and plant oil based industries and do not have strong chemical backgrounds. For this reason the students are provided with a 14-page manual in Russian (written in-house) which includes instructions on how to use the selected software packages Acid/Base Titrations, Species and ML-Database.

The manual includes 10 exercises with questions focused on particular food-industry cases. For example, students use Acid/Base Titrations to calculate and print out the speciation curve for citric acid and so determine the optimal pH for crystallization of citric acid and crystallization of tripotassium citrate. Students follow up the experimental (conductivity) determination of pK_a for acetic acid by calculating the speciation curves. This demonstrates that acetic acid ($pK_a = 4.8$) exists only as CH_3COOH at $pH < 3$ and only as CH_3COO^- at $pH > 7$, whereas at $3 < pH < 7$ there is a mixture of both species!

Other questions which students investigate are

- the pH range over which glycine exists in the isoelectric state;
- whether Ca^{2+} will form complexes with glycine in blood plasma (at pH 7);
- the pH at which the Fe^{3+}-H^+ and Al^{3+}-H^+ systems best initiate coagulation of sols.

A refresher course and research tool

The SolEq programs have been used as a research tool at Queen's University, Belfast by a graduate commencing measurements on stability constants for ternary systems relevant to natural waters. This student was able to use selected tutorials (*e.g.*16 'Metal speciation in natural waters' and 29 'Metal/ligand titration simulations'), the extensive Help files (*e.g.* the definitions and standard reporting protocols for stability constants), together with the software package Species, to answer questions like

- what concentrations of metal and ligand will be needed to generate adequate end points?
- how many inflexions will the titration curve have?

The Species software allows distribution diagrams to be generated from the determined stability constants after following the appropriate tutorial (number 11, 'Speciation'). Since SolEq contains files for modelling trace metal complexation in various types of natural waters the ternary complexation data could be incorporated into these files thus making it possible to answer questions such as "Could ternary complexes contribute significantly to the speciation expected under typical natural water conditions?"

In this way the student designed her own refresher course through which she became proficient with the calculation and simulation programs, and used the SolEq package to aid experimental design.

Discussion

The examples of applications of SolEq illustrate that we have met our objective of creating a flexible resource. Student feedback has been largely formative and has led to improvements in the presentation and wording, to clarification of the learning objectives, and to an increase in the number of exercises embedded in the tutorials. Student feedback also led to the incorporation of the facility for students to download a hard copy of each Principles tutorial for personal records or study (this is non-interactive, but it has been so constructed to contain all text including hypertext-linked files, problems and worked answers to exercises).

Student responses on feedback questionnaires indicate that the package is technically satisfactory: analysis of the responses shows that most students find

- the instructions are adequate;
- the tool bar functions and hypertext links are easy to operate and are valuable;
- the pictorial and graphical representations are well conceived and informative;
- the tutorials are of appropriate length and challenge;
- the learning environment is to their liking.

Students whose first language is not English have commented favourably on the use of the voice files giving an introductory overview.

We have observed a high level of commitment from students to the set assignments and we have noted that students make frequent use of the tutorials in their own time. We conclude from these observations that the package is motivating. We suggest that one reason for this is that SolEq provides bridges between the teaching of theory and its application to problems in real systems. We believe that this is a benefit of an integrated text/computational system that cannot be provided as comprehensively or in such a focussed manner by a textbook.

Our experience with the SolEq package has convinced us of the value of a CD that has allowed us to combine in a single resource the key qualities of a textbook with the interactive computational and graphing facilities of software.

Availability

Demonstration tutorials and the programme Species can be downloaded from the SolEq web site at www.acadsoft.co.uk. The demonstration tutorials cover each level, with examples from both Principles and Applications modules. The web site also features an enquiry form for additional information and a downloadable or email order form.

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Introducing first-year students to some skills of investigatory laboratory work

PAPER

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In order to introduce students to some of the skills involved in carrying out an analytical investigation, we devote the final three weeks of our first year laboratory course to the analysis of some common household products. Students, working in pairs, are allocated a specific problem and are given complete responsibility for investigating it. This involves planning the procedure, carrying it out, and interpreting the results. The procedures involved are simple titrimetric ones, but the application is non-trivial for these students. Our experience with this approach has highlighted for us some of the limitations of the recipe laboratories, and is regarded by both students and demonstrators as an effective learning experience.

Introduction

A great deal of the laboratory work carried out by chemistry undergraduates falls into the category described by Meester and Maskill[1] as ‘controlled’ experiments – those in which the answer is known in advance. Typically, these experiments involve following recipes and, as Bennett and O’Neal[2] argue, are more properly regarded as ‘exercises’ rather than ‘experiments’.

There are good reasons for this as discussed by Clow[3], who argues that well-researched laboratory exercises maximise the breadth of practical experience to which students can be exposed and the quality of the results they obtain. An unfortunate consequence is that many students follow the recipes line by line without questioning or seeking to understand the exercise in a broader context[4]. Almost certainly this strategy is forced on them by the limited availability of ‘working space’ of the mind[5]. This can easily become overloaded by the need to manipulate theory, manual dexterity and lab management all at the same time, and overload leads to a shutting down of the mental processes with the prevention of learning[6].

A major limitation of following a prescribed protocol is that this represents only a small part of the whole process of experimental science[7]. The recipe lab omits the stages of planning and design, and it encourages ‘data processing’ rather than ‘data interpretation’. Verdonk[8] has coined the word ‘bookification’ to describe the resulting move from ‘fact making’ to ‘fact learning’; he described an investigation of ester synthesis designed to provide students with some insights into the process of scientific research. This particular exercise would not fit well in the context of our first year laboratory work. However, we saw other opportunities for introducing aspects of experimental design (fact making) using the simple procedures introduced and practised by our students during the first year of their course.

We describe here our approach to introducing our first year students to some basic features of an analytical investigation.

Planning the Investigations

The first year chemistry class consists of 20 – 25 students. Typically, these will have taken Scottish Highers (including chemistry) and some will have studied chemistry at the more advanced level needed for the Certificate of Sixth Year Studies (CSYS). The present Higher syllabus does not have a practical requirement and therefore many undergraduates enter university having only carried out test tube experiments throughout their time at school.

The practical module for the first semester needs, therefore, to place great emphasis on learning and revising practical techniques such as titrimetric analysis, purification, and identification of organic molecules. The second semester module builds on these practical techniques. At the beginning of the practical course, students are provided with a booklet entitled “Laboratory Practice/Data Handling Handbook”. This contains guidelines for writing a lab diary and a formal report, together with other useful information such as units, errors, and how to draw graphs. This booklet is used as the basis for two tutorials (of 2 hour length) held in the two weeks preceeding the start of laboratory classes. During these tutorials, students discuss with the tutor all important aspects of laboratory classes including practice in drawing graphs, recording data, and writing up experiments.

During the course there is one three-hour laboratory session each week, but students are required to spend time outside the laboratory processing their data for completion of their Lab Diary. The set exercises as are not written up as a formal report, but in a lab diary or record as described in the booklet. This should contain detailed accounts of all laboratory work, including title, date, aims and objectives, results/data recorded, any necessary graphs or calculations, a discussion of errors (if relevant) and conclusions. It does not need to contain information already provided in the laboratory manual and extreme neatness is not expected since entries are made whilst the experiments are performed. However the content must be adequately detailed and the report sufficiently well-ordered and neat to allow a detailed formal report to be written at a later stage. The lab diaries are marked every week, and written and verbal feedback is provided with the result that detectable improvement is observed during the year.

The demonstrating is shared between a member of the academic staff and a post-graduate student, both of whom are present throughout the laboratory sessions.

When we decided to introduce the investigation we planned it according to the following principles:

- there must be a range of things to investigate so that not more than two pairs of students were tackling the same problem at the same time;
- each investigation must be simple enough for a pair of students to reach a successful conclusion within the two week period;
- it must motivate the students (be seen to be relevant);
- the procedures must be safe.

Using these principles, we decided that each investigation should be an analysis of some constituent(s) of a household product which could be satisfactorily carried out using a titrimetric procedure. Table 1 shows the information given to students for four of the investigations currently in use, other investigations involve analysis of the amount of iron in iron tablets, and of vitamin C in vitamin C tablets. Note that full information is not given, and so students have to make their own decisions and evaluate the likely errors in the procedures they adopt. For example, most choose to determine the water content of margarine by evaporating it to dryness and measuring the weight loss; this is a simple procedure, but one which creates opportunities to discuss the problems of removing all the water from an emulsion. Similarly, the determination of citric acid by titration leads to discussions of the assumption that other organic acids are present in negligible amounts, and it raises the importance of using appropriate controls and standards to take account of the fact that citric acid has three titratable groups.

The investigation is introduced to the students at the end of the last of the lab sessions in which they carry out set exercises. Students work in pairs, usually of their own choosing, which normally means that both members of the pair are of similar ability. Each pair of students is allocated a particular investigation and they are told that they have one week in which to plan their investigation. We recognise that not all of the investigations are of equal difficulty. We assign the more challenging ones to students who have demonstrated higher ability during the earlier part of the course. This helps to ensure that students of different ability are equally stretched by the investigation. They are reminded that, in many cases, they have carried out similar analyses earlier in the year, and their attention is drawn to useful reference books in the laboratory and the library. These provide sufficient information to allow them to plan these simple investigations. A week later the students return to discuss their proposals with one of the demonstrators. When the supervisor is satisfied that a pair of students have a sensible plan, they are allowed to proceed with the experiment. This means that they have the remainder of that session and two more full sessions in which to complete their investigation and prepare their formal report.

30 marks out of a possible 130 for the semester are allocated to the investigation. 10 of these are allocated for the quality of the planning work and discussion with the supervisor, and the other 20 for the quality of the report.

Investigations in Practice

Initial Discussions

With the relatively small numbers of students on this course, we have not found it necessary to instigate a formal timetable for the initial discussions with students. Pairs of students are dealt with on a first-come, first-served basis. Since not all the students time their arrival for the start of the lab session, most have only a short wait before a supervisor is free. Those waiting can usefully spend their time collecting (with the help of the lab technician) equipment and apparatus they plan to use, and preparing their lab manual.

Table 1: Examples of briefing statements for investigations

	Title	Aim	Background Information
1.	Purity of Baking Powder	To determine the purity of baking powder	Pure baking powder should be 100% $NaHCO_3$. It should be possible to determine the percentage by weight of $NaHCO_3$ in baking soda using a simple acid-base titration.
2.	Analysis of Margarines	To determine the salt content of margarines/butter. To investigate the relationship between salt and water content.	The salt content of margarine/butter may be determined via a precipitation titration using standard $AgNO_3$ as the reagent
3.	Citric Acid Content of Fruit Squashes and Fruit Juices.	To determine the citric acid content in fruit squashes and juices.	Determine the mass of citric acid present in fruit squash and juice using acid-base titrations. Suggest using lemon squash and grapefruit or pineapple juice.
4.	Analysis of White Vinegar	To determine the percentage of ethanoic acid (acetic acid) in white vinegar.	Vinegar should contain no less than 4% by volume of ethanoic acid. It should be possible to determine the amount of ethanoic acid in the vinegar using a simple acid-base titration.

Student preparation for the discussions is variable. Some have thought clearly about the procedures they will use and come with extensive notes. Usually discussion with such students takes only 5 – 10 minutes. Longer discussions are usually needed for students who are less well prepared. The discussions focus on the procedure. For example, for the analysis of vinegar, the supervisor needs to check that the students have selected a suitable indicator and concentration of NaOH with which to carry out the titration, and that they have a suitable strategy for determining what is an appropriate sample of vinegar. Standardisation of reagents is also discussed at this stage: students are reminded that the concentration of some solutions (for example of NaOH) is known approximately, but must be standardised. Normally, there is no discussion of apparatus and equipment; it is assumed (often wrongly!) that students have learned through experience the correct use of standard laboratory glassware.

Laboratory Work

When the students start their laboratory work they are, for the first time, following a recipe of their own design. Their response highlights the problem that their previous experience of following established recipes has not always prepared them effectively for this responsibility. For example, we have occasionally observed students making up solutions of primary standards in a beaker or a conical flask instead of in a volumetric flask. Apparently they have been following recipes so uncritically that they have not learned elementary lessons about accuracy and appropriate glassware. These kinds of mistakes lead to valuable discussions with a supervisor the key lessons of which are reinforced by the need to start again.

As well as providing students with opportunities to learn from their mistakes, these investigations also introduce other important aspects of real science. Students discover that analysis involves samples which are less amenable than laboratory solutions to which they have become accustomed. For example, grapefruit juice is sticky, and not easy to pipette; vinegar needs diluting before it can be titrated with 0.1M NaOH.

The nature of an investigation is that even the best prepared students need to make some exploratory measurements to establish that their reagents and samples are of appropriate concentration. In spite of this, and the fact that some students make basic mistakes which force them to start again, the basic procedures are sufficiently simple that all students are able to complete the laboratory work within two 3 hour laboratory sessions. Some will complete theirs within a single 3 hour period.

Student Report

These investigations into simple household products are used to provide the students with their first opportunity to put into practice the conversion of their lab record into a formal report. The booklet provided at the beginning of the course includes detailed help on how to do this. Some students will seek further help from the laboratory supervisors. A key feature of the report is that students are expected to evaluate the procedures they used. As described in the section on Planning the Investigations, this is not a trivial problem. The final report is expected to be produced on a word processor. Thus it offers an opportunity for students to practice their IT skills, their writing skills, and referencing skills, in all of which they have had instruction in the previous semester. Feedback (both written and verbal) is given on their performance in order to help to prepare them for formal reports which are expected in later years.

Discussion

Feedback from students has been obtained through semi-structured informal discussions. It is clear from these that the use of household substances helps the students to appreciate that chemistry has relevance and that the standard practical skills they have been learning and practising are not just academic exercises. These are key factors in the motivation of students. They find it challenging but also satisfying to take responsibility for their own procedure, and they enjoy the opportunity to work at their own pace. The overall impression from the students' comments is that they are motivated by the experience.

The supervisors are similarly enthusiastic. The quality of the interaction with the students is rewarding. Even when this results in throwing some of their freshly made solutions down the sink, the discussion itself concerns their own decisions (and the reasons why these could be improved) instead of the more usual situations in which interaction with students is largely limited to interpretation of the lab book. Like the students, the supervisors find that these lab sessions are refreshingly unpredictable and enjoyable.

The formal reports follow the guidelines provided in the Laboratory Practice/Data Handling Handbook. The standard is, as would be expected, variable, but on average the reports are sound, and the best are very good. We are satisfied that the experience provides a useful foundation on which future courses can build.

One useful feature of these investigations is that they are very appropriate for our HND students. These students are not given marks, but have to achieve the performance criteria:

(a) the proposed methodology is valid and feasible and consistent with the aims of the experiment.
(b) the experimental procedure carried out is correct in terms of safe working practice and practical skills.
(c) the report produced is clear and concise and correct in terms of the experiment outcome.

The structure of these investigations makes it very easy to assess whether HND students can be given a pass for each of these criteria, and thus whether they have passed outcome 3 of the Basic Laboratory Skills Unit.

In conclusion, we believe that the virtue of our investigations is that they involve the application of simple procedures to tackle investigations which (at least for first year students) are not trivial. This combination makes them educationally rewarding and enjoyable.

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Evaluation of teaching and learning: matching knowledge with confidence

COMMUNICATION

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We have used a two-part questionnaire to obtain feedback from students immediately before, immediately after, and six weeks after carrying out a computer-based simulation. The simulation is intended to help students to develop investigative skills. The first part of the questionnaire tests knowledge by means of multi-choice questions. The second part asks students to assess their confidence in their understanding or in their ability to apply knowledge. The use of this evaluation strategy has allowed us to formulate hypotheses about ways to improve the student learning experience in future years. We conclude that this evaluation strategy can be a valuable and generally applicable way of identifying whether a particular learning experience helps students to develop an appropriate balance of knowledge, understanding and ability to apply knowledge.

Introduction

"Most British people, most educators and most students now believe that it is one of higher education's purposes to prepare students well for working life"[1].This sentiment is reflected in a number of recent reports which emphasise the need for degree courses generally[2] or specifically in chemistry[3,4] to adopt a more student-centred approach to teaching so that students develop a range of personal and professional skills appropriate to a scientific education.

Many individual teaching and learning strategies have been developed to bring about more active student participation in their education[e.g. 5–8]. One largely unsolved problem is evaluation of the effectiveness of such innovations. Their aim is rarely limited to that of helping students to achieve a higher mark in a conventional examination, and therefore it is not appropriate to evaluate them by attempting to measure a change in examination performance. Bodner et al have discussed the different reasons why this is inappropriate[9]. They argue that the main purpose of evaluation of any new teaching initiative is to discover what modifications to make which will maximise the positive effects and minimise the negative ones (since we should take for granted that any significant change will have some effect). We were faced with the problem of choosing an appropriate strategy for evaluating the success of introducing one of the eLABorate computer simulations[10] to a class of first-year biochemistry students. The particular simulation is enzymeLAB[11,12,13]. This simulation allows students to investigate the effect of substrate concentration, enzyme concentration and pH on the rate of an enzyme catalysed reaction. It is designed to build on (and hence consolidate) basic knowledge of enzyme kinetics, and to develop an understanding of how this knowledge is applied in the design of an investigation.

We were attracted by the strategy recommended by Draper for evaluating interventions in the classroom[14,15]. This involves two interesting features which we have not used previously. First he recommends the use of the same questionnaire as a pre-test, a post-test, and a delayed post-test (follow-up). Second he recommends that the questionnaire should be designed to make a dual evaluation by using *"a measure of the student's confidence in fulfilling the learning objectives, and a knowledge quiz."* We therefore decided to devise a two-part questionnaire. The first part was designed to be a knowledge quiz testing aspects of knowledge of enzymes which would be useful in planning a real investigation of an enzyme. The second part would seek information about their confidence in their understanding of concepts or in their ability to apply knowledge.

We report here the results of using our two-part questionnaire with a group of 23 first year biochemistry students. The number of students is too small for us to draw firm conclusions about the effectiveness of the simulation as a teaching aid. However, we believe that the results demonstrate that the evaluation strategy is a useful one, and could be used to advantage to evaluate a wide range of learning experiences.

Methods

The Simulation

The simulation deals with an enzyme which obeys Michaelis Menten Kinetics; that is, the rate of the enzyme catalysed reaction (v) is determined by the equation

$$v = \frac{V_{max}S}{K_m + S}$$

Where S is the concentration of substrate
K_M is a constant at constant pH (but may vary with pH)
V_{max} is a constant at constant pH and enzyme concentration (but may vary with pH and, at given pH, is proportional to enzyme concentration).

The key features are:

- the program selects the parameters (V_{max}, K_M, and their sensitivity to pH) so that each student is given a different enzyme;
- the user selects values for the pH and the concentration of enzyme and substrate at which the rate of the reaction is to be measured;
- the resulting value of v which is displayed has a realistic experimental error with a standard deviation of 5% of the correctly calculated value.

Aspects of the enzymeLAB program have been described elsewhere[8,11,12,13].

The Context

The first year cohort of Biochemistry students at York consists of about 25 students. This exercise forms part of a nine week module ‘Biochemical skills’. In this module, students perform a variety of tasks, usually working in teams. Examples include designing, carrying out, and interpreting biochemical investigations. The module is based on a workload of one day a week for eight weeks with an assumption of a small amount of additional private study.

The enzymeLAB exercise forms the practical component of one day of the course. The students are required to determine the value of K_M and V_{max} for their enzyme at pH 7, and to investigate whether the optimum pH of the enzyme is affected by the concentration of substrate. The precise wording of the task, as given in the student worksheet is as follows:

You have four tasks

(i) Show that the kinetics of your enzyme are consistent with Michaelis Menten Kinetics.
(ii) Find the value for V_{max} and K_M at pH 7.
(iii) Find the optimum pH of your enzyme.
(iv) Find out whether the optimum pH varies with the concentration of substrate.

First year students have little or no experience with this kind of problem which essentially involves recalling factual knowledge and applying it to a problem which cannot be solved by applying a fixed algorithm. The class therefore starts with a discussion designed both to bring key knowledge to the forefront of their minds and to help them to develop their own strategy for approaching the problem. The discussion lasts for 60 – 90 minutes. Students are then given access to the computers. They work on their own with one or two tutors available to answer questions and to provide support and guidance as necessary. About 45 – 60 minutes before the end of the session, the students are called together to discuss their findings.

Evaluation

For reasons outlined in the introduction, we aimed to evaluate the effectiveness of the exercise by a two part questionnaire. The same questionnaire was completed by the students before the start of the introductory session, after the end of the final discussion, and (without warning) in the final session of the course which is about six weeks later.

In 1998-99 we used six multiple choice questions, listed in Table 1 to test key aspects of the students’ knowledge of enzymes. Each question was provided with a correct answer, three distracters, and ‘don’t know’. In the interests of space, neither the correct answer nor the distracters are shown in Table1. The questionnaire was completed anonymously, and we emphasised that it was not a test, so that students should answer “don’t know” rather than guess at the correct answer.

The second part of the questionnaire, designed to establish the students’ confidence in their understanding and in their ability to apply knowledge, is shown in Table 2.

No time limit was set for the completion of the questionnaire, but students were encouraged not to spend time puzzling about their answers. All students completed both parts of the questionnaire in less than 10 minutes.

Results

The results obtained for 1998-99 from the multi-choice questions are summarised in Table 1. We have not distinguished between the different incorrect responses, though we recognise that further information about misconceptions might in principle be obtained from an analysis of the frequency of different incorrect responses. In this case, we decided that the number of students was too small to justify analysis at this level of detail. In general the completion of the exercise resulted in an increase in the number of correct responses, but for all questions except 5 it reverted somewhat towards the pre-exercise level after six weeks. The major difference between the pre-exercise and the follow-up responses is the smaller number of ‘don’t knows’ in the latter.

The responses to the second section of the questionnaire related to student confidence are shown in Table 2. As with the first part of the questionnaire, student confidence in their

Table 1: Student responses to questions in Section 1.

Number of students giving correct, don't know or incorrect responses in the pre-exercise test, the post-exercise test, and the follow-up test (six weeks later).

Note that all 23 students in the class completed the pre-exercise questionnaire; three were given permission to leave early and did not complete the post-exercise questionnaire; two students were absent from the final session when the follow-up questionnaire was completed.

		Number of student responses		
		Pre	**Post**	**Follow-up**
1. Which of these is the Michaelis-Menten equation, used in enzyme kinetics?	Right	13	20	15
	Don't know	2	0	0
	Wrong	8	0	6
2. Between what ranges of values would you expect the K_M of most enzymes to lie?	Right	6	16	14
	Don't know	12	0	1
	Wrong	5	4	6
3. Which one of the following *best* describes the conditions required for v to be near to V_{max}?	Right	13	16	11
	Don't know	5	0	1
	Wrong	5	4	9
4. Which one of the following is the best range of values of [S] to use to calculate K_M and V_{max}?	Right	2	6	4
	Don't know	10	2	1
	Wrong	11	12	16
5. Which one of the following *best* describes what effect changing the pH from the optimum would have on an enzyme's kinetic constants?	Right	7	11	16
	Don't know	7	3	2
	Wrong	9	6	3
6. Which one of the following is the most appropriate statement about the optimum pH of an enzyme?	Right	2	9	4
	Don't know	8	1	5
	Wrong	13	10	12
Overall Percentage	Right	31%	65%	51%
	Don't know	32%	5%	8%
	Wrong	37%	30%	41%

Table 2: Student responses to questions in Section 2.

Responses were awarded a score of 1 – 5 according to whether they responded 'no confidence', 'little confidence', 'some confidence', 'confident', 'very confident'. The number shown is the mean of these scores.

How confident are you that you ….	**Average Score**		
	Pre	**Post**	**Follow-up**
1. know what the Michaelis-Menten equation is, what it means, and how to use it?	3.17	4.30	3.29
2. understand what K_M and V_{max} are, what they mean, and the effect they have on the rates of enzyme-catalysed reactions?	3.44	4.10	3.43
3. have a good feel for the ways in which pH can affect K_M and V_{max}?	2.30	3.44	2.57
4. understand what it means for an enzyme to be saturated?	4.09	4.05	4.14
5. could plan a series of experiments to determine the K_M and V_{max} of an enzyme at a given pH?	3.35	3.75	3.33

understanding and in their ability to use knowledge shows an immediate increase as a result of completing the exercise, but appears to revert to the pre-exercise level after 6 weeks.

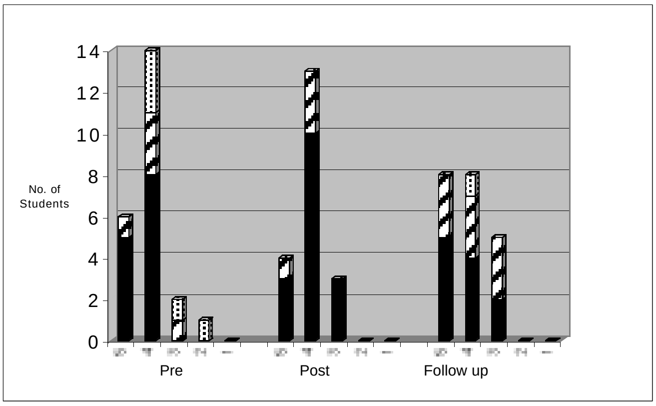
We examined the match between student knowledge (correct answers to questions in Section 1) and student confidence (Section 2). We illustrate our approach to this with questions 4 and 5 in Section 2. Question 4 asks "How confident are you that you understand what it means for an enzyme to be saturated?" In our view, for this confidence to be justified, the student must know that the observed rate of the enzyme-catalysed reaction (v) approaches the maximum rate (V_{max}) when the concentration of substrate is several times greater than the enzyme's K_M (which is the subject of Question 3 in Section 1 of the questionnaire).

Question 5 (Section 2) asks "How confident are you that you can plan a series of experiments to determine the K_M and

V_{max} of an enzyme at given pH?" This planning requires the selection of values of substrate concentration at which to measure the rate of the enzyme catalysed reaction; it is important to select values of substrate concentration which range on both sides of K_M and have a reasonable spread (say between 0.2 and $2K_M$). This knowledge is tested by question 4 in Section 1 of the questionnaire.

We have prepared histograms to show the data obtained from the questionnaires for these two confidence questions. These are shown as Figures 1 and 2. There are separate histograms for the data obtained pre-exercise, post-exercise and at the follow-up stage. The histograms show, for each level of confidence (very to none) the number of students responding correctly, incorrectly or don't know to the relevant question in Section 1. These histograms show that student knowledge (or lack of it) does not correlate well with their confidence in their understanding or their ability to apply their knowledge.

Figure 1 Student confidence in understanding of enzyme saturation.

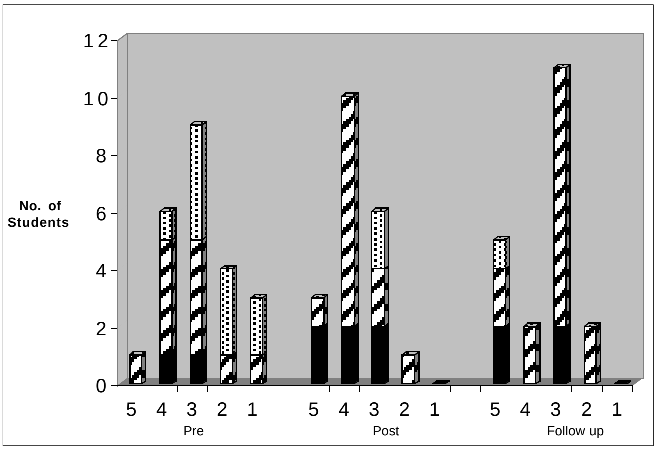


Histograms show numbers of students responding 'very confident' (5), 'confident' (4), 'some confidence' (3), 'little confidence' (2) and 'no confidence' (1) to Question 4 in Figure 2. These are correlated with answers to Question 3 in Figure 1:

■ correct; ▨ don't know; ▦ incorrect.

Data are shown for the Pre-exercise (PRE), Post-exercise (POST), and FOLLOW-UP responses.

Figure 2 Student confidence in ability to plan experiments to determine K_M and V_{MAX}



Histograms show equivalent data to Figure 1 for question 5 in Table 2 correlated with answers to Question 4 in Table 1.

Discussion

Our primary purpose in writing this paper is to present a critical retrospective analysis of the design of our questionnaire, in the belief that this will encourage others both to adopt the general approach, and also to avoid making some mistakes. This discussion is therefore in two parts. First, we make some interpretations of the data we obtained from the questionnaire. Secondly, we evaluate the questionnaire critically with a view to identifying specific ways of improving this particular questionnaire and also general features which we believe are important in other questionnaires of this kind.

Interpretation of Data

This analysis is designed to illustrate the sort of conclusions that can be drawn from the two-part questionnaires used pre-post-, and as a follow-up to the simulation exercise. Table 1 shows encouraging improvement in the number of correct answers to Section 1 of the questionnaire immediately after completing the exercise. Six weeks later it is encouraging that the proportion of correct answers is substantially higher than at the pre-exercise stage. We are not particularly surprised that there has been some reversion to the pre-exercise level six weeks later; we believe it would be unreasonable to expect a single exercise of this kind to reconfigure the long-term memory in such a way as to make this detailed factual information immediately available.

What is particularly notable is that the percentage of 'don't know' responses falls dramatically in the post-exercise questionnaire and stays low in the follow-up questionnaire. Questions 2 and 4 elicited the highest number of don't know responses in the pre-exercise questionnaire. This is not surprising since it is unlikely that answers to these questions would have been emphasised in first year lectures on enzyme kinetics. In the follow-up questionnaire, students rarely answered 'don't know' to either question. Unfortunately, for question 4, this resulted mainly in students giving incorrect answers! Question 6 is of interest in that it provided half of the 'don't know' answers in the follow-up questionnaire, even though we had hoped that the exercise would help the students to understand the effect of pH on enzymes. A possible conclusion is that, because different enzymes respond differently to pH change, students could not explore the possible range of effects by studying a single enzyme, and the class discussion did not bring this out sufficiently.

In contrast to the apparently improved knowledge-base demonstrated in table 1, the students' confidence appears to rise immediately after the exercise but reverts almost exactly to the pre-exercise level six weeks later. Bailey[16] has noted a fall in students' confidence in their skills after participating in exercises designed to improve these skills[17]. He attributes this to the students making a more realistic assessment of their skills when they understand better what is involved. It may be that a similar phenomenon is occurring here.

For reasons given in the next section, we limit our detailed discussion of the questions of confidence to questions 4 and 5, data from which are shown in Figures 1 and 2. Question 4 (Figure 1) is concerned with student *understanding*. In contrast, question 5 (Figure 2) deals with confidence in *ability to apply knowledge*. Figure 1 shows a high level of confidence in understanding of the meaning of enzyme saturation. This high level of confidence appears to be largely justified by the student knowledge of the conditions which would lead to saturation. The situation illustrated by Figure 2 is less satisfactory: here the confidence levels (though lower than those shown in Figure 1) are still reasonable, but this is not well-founded as is shown by their ignorance of one of the key facts which would allow them to design an investigation to determine K_M and V_{max}. If this truly reflects the student attitude it may show that they are not good at recognising the factors that need to be taken into account in designing an investigation. This may be evidence of a need for more opportunities to play a more active role in the design of experiments.

The Questionnaire

All the questions in Table 1 (if rewritten in free-response format) would have to be considered by anyone planning an investigation of a hitherto uncharacterised enzyme. Well-designed investigations are therefore likely to be planned by investigators who either can provide good answers to these questions or recognise their ignorance so that they can look up background theory before they start.

The questionnaires were completed anonymously. A disadvantage of this is that the potential to trace the development of an individual student's understanding is lost because we are not able to assign each questionnaire to a specific student. It is worth considering whether anonymity is sufficiently important to the student to require that it be maintained.

In evaluating responses to questions 1-3 of section 2 it became clear that the precise wording of the confidence questions is especially important: we cannot be sure how students would interpret questions which ask what is 'meant by' the Michaelis Menten equation, K_M or V_{max}, or what they would understand by 'having a good feel' for the effect of pH. Our rule for setting these confidence questions in future is that they should be of two types. One type would be worded "how confident are you that you *understand* (some well defined concept)", and a necessary condition for including it would be that we could write down a clear statement which we could accept as demonstrating understanding of the concept as described in the question. The second type would be worded "how confident are you that you can (carry out some task involving application of knowledge)", and a necessary condition for including it would be that we could write down a clear protocol for carrying out the task together with basic knowledge on which the protocol is based. Our suggested written statements on the confidence questions would serve two purposes. They would ensure that the questions were worded in a way which could be usefully interpreted by students. They would also emphasise the knowledge which should underpin the understanding and the application of knowledge. This would provide effective guidance on appropriate test questions (and relevant distractor answers) for Section 1.

Our view is that only questions 4 and 5 in Section 2 of our questionnaire meet these criteria, and that questions 3 and 4 in Section 1 are suitable complementary questions. It is perfectly possible to use more than one question in Section 1 to test knowledge on which confidence questions in Section 2 should be based. However this would lengthen the questionnaire. A key feature of the questionnaire is that the students should not recognise that the questions in the two sections of the questionnaire are intentionally correlated; this helps to give a clearer impression of any mismatch between their confidence and the knowledge on which this should properly be based.

This evaluation strategy has suggested to us ways of modifying the exercise to improve the student learning experience. In particular, our data indicates the importance of helping the students to recognise the logic behind the design of the investigation which they carry out. Similarly, the responses to Question 3 in Section 2 suggest that it would be worth emphasising the opportunity to gain more understanding of the effect of pH on enzyme activity. Thus we have at least partially achieved our primary objective of evaluating the exercise with a view to improving the student learning experience in future years. The combination of knowledge-based questions and questions of confidence has provided more useful information than we would have obtained by leaving out either part.

Our experience illustrates some ways in which carefully constructed questions related to self-assessed confidence and objective knowledge can together be an effective way of collecting feedback. We conclude that this evaluation strategy can be a powerful tool for testing the effectiveness of innovations in teaching, providing that the questionnaire is designed using the principles we have described. We recognise that the same strategy could be used in a more general context, without the need for repeated exposure to the same questionnaire, to evaluate whether students have a balance of knowledge, understanding and ability to apply knowledge.

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http://www.york.ac.uk/depts/chem/staff/elaborate/

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Variety in Chemistry Teaching 1999

The following three papers were presented at the Variety in Chemistry Teaching meeting held at Heriot Watt University on 6 and 7 Sept 1999, and organised by the Tertiary Education Group of the Royal Society of Chemistry in conjunction with the Education Research Group.

The Proceedings of the meeting include abstracts of
- Discussion Forum on Incorporating Skills in the Chemistry Curriculum,
- four keynote talks,
- 17 posters
- 7 demonstrations of software
- 4 parallel sessions.

Copies of the Proceedings can be obtained from the Editor of UChemEd; cost £5.00.

The full papers reproduced here are

The Tertiary Education Group Lectures:
George Bodner (Purdue)
Mental models: the role of representation in the teaching and learning of chemistry.

The Education Research Group Lectures:
Onno de Jong (Utrecht)
Crossing the borders: chemical education research and teaching practice.

Alex Johnstone (Glasgow)
Chemical education research: where from here.

Mental Models: The Role of Representations in Problem Solving in Chemistry

PROCEEDINGS

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A combination of techniques including field notes collected in operating classrooms, informal interviews with students in a tutorial environment, and formal structured interviews have been applied to study problem solving in chemistry among groups ranging from freshman enrolled in general chemistry through 6th-year graduate students within a variety of content domains including general, organic, inorganic, and physical chemistry. Regardless of the level of the students from whom data have been collected or the content domain in which the data were obtained we have found that one of the characteristic differences between successful and unsuccessful problem solvers is the number and kinds of representations they bring to the problem.

Introduction to Research on Problem Solving in Chemistry

For over 15 years, we have been interested in bridging the gap between theory and practice within the domain of problem solving in chemistry; a gap that results from fundamental differences between what chemists do when they solve problems and what they tell students to do when they teach problem solving, regardless of whether they are teaching secondary school students how to work stoichiometry problems or advanced graduate students how to synthesize natural products.

Any discussion of problem solving has to begin with a definition of the term ‘problem’,

Whenever there is a gap between where you are now and where you want to be, and you don’t know how to find a way to cross that gap, you have a problem.[1]

and the term ‘problem solving’.

Problem solving is what you do, when you don’t know what to do.[2]

These definitions have a logical consequence: there is a fundamental difference between tasks that are *routine exercises* and those that are *novel problems*. Some would argue that problems are more difficult, or more complex, than exercises. If they are right, it should be possible to devise a task that is intrinsically an exercise, or intrinsically a problem. Our work suggests they are wrong. The difference between an exercise and a problem is the result of differences in the level of familiarity with similar tasks the individual brings to a given task. Consider the following question, for example.

What weight of oxygen is required to burn 10.0 grams of magnesium?

$$2\,Mg(s) + O_2(g) \rightarrow 2\,MgO(s)$$

This question is a *routine exercise* for most chemists, who have done hundreds, if not thousands, of similar tasks. But it is a *novel problem* for beginning chemistry students.

More than 50 years ago, Polya proposed a model of problem solving that consists of four steps or stages.[3]

- Understand the problem
- Devise a plan
- Carry out the plan
- Look back

Our work suggests that this may be a model of what content specialists do when they work an *exercise* in their area of expertise; but it is not a model of the way people solve real problems. To probe this hypothesis, consider the following question set in a textbook[4].

A sample of a compound of xenon and fluorine was contained in a bulb with a pressure of 24 torr. Hydrogen was added to the bulb until the pressure was 96 torr. Passage of an electric spark through the mixture produced Xe and HF. After the HF was removed by reaction with solid KOH, the final pressure of xenon and unreacted hydrogen in the bulb was 48 torr. What is the empirical formula of the xenon fluoride in the original sample?

When this problem is given to practicing chemists using a think-aloud protocol, it is clear that they do not follow Polya’s model by first understanding the problem, then devising a plan, and so on. The best evidence of this is the frequency with which they obtain an answer and then say: “Oh,... this is an empirical formula problem!” In other words, they only really understand the problem once it has been solved.

Several years ago, a more realistic model of problem solving was proposed by Grayson Wheatley. It consists of the following steps[5].

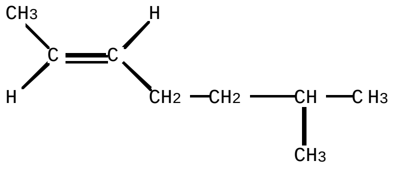
- Read the problem
- Now read the problem again
- Write down what you hope is the relevant information
- Draw a picture, make a list, or write an equation or formula to help you begin to understand the problem
- Try something
- Try something else
- See where this gets you
- Read the problem again
- Try something else
- See where this gets you
- Test intermediate results to see whether you are making any progress toward an answer

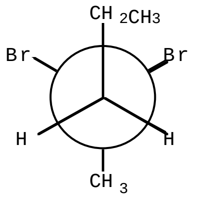
- Read the problem again
- When appropriate, strike your forehead and say, “son of a...”
- Write down ‘an’ answer (not necessarily ‘the’ answer)
- Test the answer to see if it makes sense
- Start over if you have to, celebrate if you don’t

Whereas exercises are worked in a linear, forward-chaining, rational manner, this model of problem solving is cyclic, reflective, and might appear irrational to someone watching us because it differs so much from the approach a subject matter expert would take to the task. The expert might be tempted to intervene, to show the ‘correct’ way of obtaining the answer. While this might make the expert feel good, it does not necessarily help the individual struggling with the problem.

Problem Solving in Non-mathematical Domains

Several years ago, students in the first-semester of an organic chemistry course for non-majors were given an exam in which they were asked to provide the systematic (IUPAC-approved) names of the following compounds:

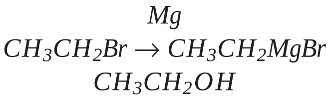




Most of the students successfully named the compound on the left, but not the one on the right. The students were not much more successful at naming this compound when this part of the question was repeated on the next exam, or when it appeared on the final exam. The students’ success (or lack thereof) is not as interesting as their response to this question when they were interviewed after the exam. Time and time again, they complained that this part of the question was not ‘fair’.

A similar phenomenon was observed when the following question appeared on an hour exam for the second-semester course.

A graduate student once tried to run the following reaction to prepare a Grignard reagent. Explain what he did wrong, why the yield of the desired product was zero, and predict the product he obtained.



$$CH_3CH_2Br \xrightarrow[CH_3CH_2OH]{Mg} CH_3CH_2MgBr$$

When he set the exam, the instructor (GMB) was convinced that this was a relatively easy question. (There is nothing wrong with the starting material, a common reagent used to prepare Grignard reagents. There is nothing wrong with the product of the reaction or with using magnesium metal to prepare this reagent. The only possible source of error was the solvent: CH_3CH_2OH.) He therefore used this item as the first question on the exam – to build the students’ confidence. When the exam was graded, he found that some of the students recognized that the solvent was a potential source of H^+ ions that would destroy the Grignard reagent produced in this reaction, but many of them were unable to answer the question. When these students were interviewed after the exam, they frequently expressed the opinion that this was not a ‘fair’ question.

The reaction of methylcyclopentane with bromine provides a third example of a non-mathematical problem which students found difficult. The students were asked to predict the major products of the reaction, to estimate the ratio of these products that would be formed if bromine radicals were just as likely to attack one hydrogen atom as another, and to use the relative stability of alkyl radicals to predict which product was likely to occur more often than expected from simple statistics.

Most of the more than 200 students in this course predicted that the reaction would give three products, with a relative abundance of 3:2:2, as shown in Figure 1(a).

During interviews held with these students after the exam, we found that they recognized that attack by a bromine atom at any of the three hydrogen atoms in the CH_3 group would give the first product. They also recognized that the molecule is symmetric, and it therefore doesn’t matter whether reaction occurs on the right or left side of the molecule when the second and third products are formed.

Some of the students recognized that there are *two* hydrogen atoms on each of the carbon atoms at which attack occurs to give the second and third products in Figure 1(a). These students therefore recognized that simple statistics predicts a 3:4:4 ratio for these products. Without exception, these students recognized that the reaction actually gives four products, in a 3:4:4:1 ratio, as shown in Figure 1(b).

Every one of these students came to the correct conclusion that it is the fourth product – the one their colleagues missed – that is the most likely product of this reaction because of the stability of the tertiary radical formed when the bromine atom attacks this carbon atom.

For our purposes, however, the most important observation revolved around the difference between the behaviour of students who were successful on this question and those who were not. Every one of the students who gave the answer in Figure 1(b) did exactly the same thing: they translated the line drawing for the starting material into a drawing that showed the positions of all the hydrogen atoms in this compound, as shown in Figure 1(c). None of the students who gave the incorrect answer in Figure 1(a) did this.

Our colleagues who practice and teach organic chemistry would have no difficulty with these questions; they would treat them as routine exercises, whereas it is clear that for the students they are problems[6]. We suggest that what all three examples have in common is that the representations presented to the students do not contain sufficient information for the students to solve the problem. Students (and many professional chemists) are more familiar with line structures of molecules than with Newman projections. For this reason the first step in providing the systematic name for the molecule in Newman projection is to transform it into a line structure – a step which the experienced organic chemist finds unnecessary.

Figure 1a

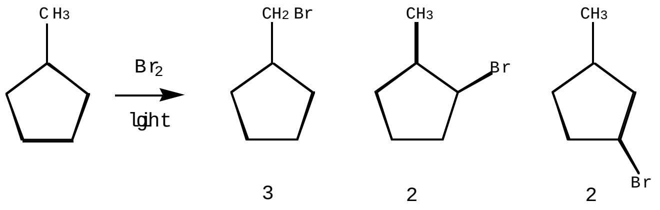


Figure 1b

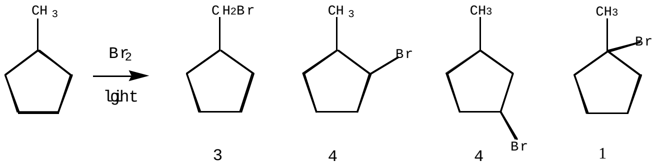
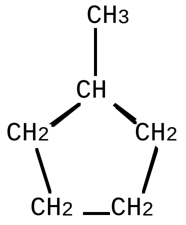


Figure 1c



The question based on the synthesis of a Grignard reagent causes no problems for our organic chemistry colleagues because the -OH group on the solvent would be a symbolic representation that would evoke images of protic solvents that would react rapidly (and perhaps violently) with the carbanion clearly evoked by the symbols 'CH_3CH_2MgBr'. The same is not true of students who either cannot or will not handle these letters and numbers as symbols for molecules or molecular fragments that can (and indeed will) undergo chemical reactions. Correct solutions to the third question, based on the reaction between methylcyclopentane and bromine, invariably involved the students in transforming the given representation as shown in Figure 1(c). This is a step which most experienced chemists would take automatically (either in their minds or on paper).

These examples hint that successful problem solving may involve the creation of appropriate representations. This suggestion requires more rigorous research and analysis. In order to do this we need to decide how the problem solving ability of various individuals should be compared and we need to define the term 'representation'.

Successful versus unsuccessful problem solvers

Efforts to understand the cognitive processes involved in problem solving have been underway for at least 100 years[7]. One approach has focused on differences between 'expert' and 'novice' problem solvers[8-10]. Smith[11] has criticized this expert-novice dichotomy as unjustly equating expertise with success. He argued that "*'successful' problem solvers often share more procedural characteristics that distinguish them from 'unsuccessful' subjects than do experts when compared to novices.*"

We agree that research on problem solving should focus on the differences between successful and unsuccessful problem solvers[12,13]. Our goal is to achieve a better understanding of the process by which individuals disembed relevant information from the statement of a problem and transform the problem into one they understand – in other words, how they build and manipulate the 'representation' they construct of the problem. We have therefore analyzed differences between both the number and the kind of representations built by successful and unsuccessful problem solvers in order to understand the role that representations play in determining the success or failure of the problem-solving process. The first step involves building an adequate definition of what we mean by the term 'representation'.

Simon[14] uses the term representation in the sense of an 'internal representation' – information that has been encoded, modified, and stored in the brain. Martin[15] uses the term in the same sense when he says that representations "*signify our imperfect conceptions of the world*." Estes[16] reminds us that "a *representation stands for but does not fully depict an item or event*." He notes that representations are attempts the brain makes to encode experiences. Thus, a representation is very different from a photograph, which preserves all of the information in the scene. Within the context of problem solving, it is useful to distinguish between internal and external representations. An operational definition of an internal representation is that it is the way in which the problem solver stores the internal components of the problem in his or her mind. In contrast to internal representations, 'external representations' are physical manifestations of this information. An external representation may be a sequence of words used to describe an internal representation, it may be a drawing or a list of information that captures particular elements of an internal representation, or (within the context of problem solving in chemistry) it can include the equation which shapes the way information is processed in subsequent steps in the problem-solving process – such as $PV = nRT$ or $E = E^{\circ} - RT/nF \ln Q$

Understanding the problem: The early stages in problem solving

Fifteen years ago, we began a series of experiments to study whether spatial ability is correlated with students' performance in the hour exams they took while enrolled in college-level chemistry courses[17]. Subsequent experiments with students in both general chemistry[18] and organic chemistry[19] showed that correlations with tests of spatial ability were strongest for exam questions that differed significantly from those the students had seen previously. Regardless of the type of question that was asked, the tests of spatial ability correlated best with the students' performance on *novel problems*, rather than *routine exercises*[6].

The tests of spatial ability used in these experiments were tests of disembedding and cognitive restructuring in the spatial domain. We therefore concluded that the preliminary stages in the problem-solving process that involved disembedding the relevant information from the statement of the problem and restructuring or transforming the problem into one the individual understands are particularly important in determining the success or failure of the problem-solving process. We described the goal of the early stages of the problem-solving process as trying to *understand the problem* or to *find the problem*. Larkin[20] reached similar conclusions when she concluded:

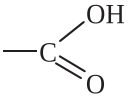
> *"To work on the problem, the solver must convert the string of words with which he is presented into some internal mental representation that can be manipulated in efforts to solve the problem. Understanding the problem then means constructing for it one of these internal representations."*

The preliminary stages in the problem-solving process in which students begin to understand the problem can therefore be thought of as stages in which the first step is taken toward building an internal (or mental) representation of the problem.

Our study of the relationship between spatial ability and student performance in organic chemistry involved the analysis of answers to free-response questions, such as predicting the product of the following reaction[18].

$$PhCOOH + SOCl_2 \rightarrow$$

Students who scored well on the tests of spatial ability were more likely to draw preliminary structures in which the Ph or phenyl group was represented by a six-member ring and the carboxylic acid group was represented by



They were also more likely to score well on this question.

Students with low scores on the spatial tests were less likely to do well in the course and they were more likely to write equations such as:

$$PhCOOH + SOCl_2 \rightarrow PhCl + SO_2 + HCl$$

or:

$$PhCOOH + SOCl_2 \rightarrow PhCOOCl + SO_2 + HCl$$

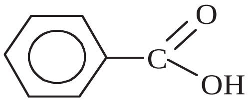
When these equations are shown to individuals who have many years of experience teaching general chemistry, they often note that the equations are not balanced. While this is true, it is not their most important characteristic (organic chemists are notorious for writing equations that are not balanced). For our purposes, the important characteristic of these equations is the fact that they are 'absurd' – there is no way to transform the starting materials into the products of these equations by the making and breaking of chemical bonds.

The correlation of success with spatial ability is consistent with our observations summarised earlier in this paper. We conclude that no matter how or where we collect data, we find that a significant difference between students who are successful in organic chemistry and those who are not is the students' ability to switch from one representation system to another.

Interviews with students who do poorly in organic chemistry have shown that they often have difficulty escaping verbal/linguistic representation systems. They tend to handle chemical formulas and equations that involve these formulas in terms of letters and lines and numbers that cannot correctly be called symbols because they do not represent or symbolize anything that has physical reality. Thus, they see nothing wrong with transforming PhCOOH into PhCl. We believe this result is linked to previous work on students' inability or unwillingness to think of chemical systems in terms of the particulate nature of matter[21-29].

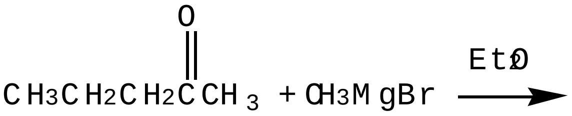
We have found that students locked in a verbal/linguistic representation system can recognize that the verbal/linguistic representation on the left and the symbolic representation on the right (below) describe the same compound.

PhCOOH



But they are unlikely to spontaneously switch from the representation on the left to the one on the right, or vice versa. Interviews with other students – who tend to do better in the course – have shown they switch back and forth between these representation systems as needed.

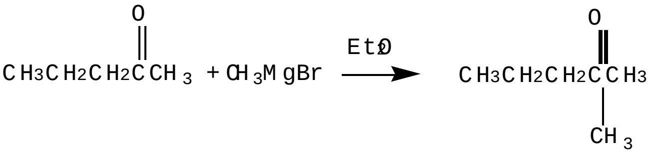
If this hypothesis is correct, similar *external representations* might be written by individuals with very different *internal representations*. Consider the following reaction, for example.



$$CH_3CH_2CH_2\overset{\overset{O}{\|}}{C}CH_3 + CH_3MgBr \xrightarrow{Et_2O}$$

When they write this equation in their notebooks, students believe it is a direct copy of what the instructor writes on the blackboard. An objective observer, comparing the two, would conclude that the students' notes seem to be direct copies of what the instructor wrote. In spite of the apparent similarity, there is a fundamental difference between what the instructor and many of the students write. The instructor writes *symbols,* which represent a physical reality. All too often, students write *letters and numbers and lines,* which have no physical meaning to them.

Interviews with students for whom chemical formulas are examples of a verbal/linguistic representation system showed that they are more likely to write 'absurd' formulas, such as the product shown in the following equation.



$$CH_3CH_2CH_2\overset{\overset{O}{\|}}{C}CH_3 + CH_3MgBr \xrightarrow{Et_2O} CH_3CH_2CH_2\overset{\overset{O}{\|}}{C}\underset{\underset{CH_3}{|}}{C}H_3$$

Only when the letters, numbers, and lines used to write these equations become symbols, representing a physical reality, do students recognize why this answer is absurd or recognize the flaw in the equation used to describe the graduate student's approach to the synthesis of a Grignard reagent described in the introduction.

The number and kind of representations constructed during problem solving

As we have seen, an essential component of an individual's problem-solving behaviour is the construction of a mental representation of the problem that can contain elements of more than one representation system. We have therefore studied differences in both the number and types of representations constructed by successful and unsuccessful problem solvers among a population of 1st and 2nd year graduate students faced with questions that dealt with aspects of the FT-NMR experiment known as two-dimensional nuclear magnetic resonance spectroscopy[30].

FT-NMR experiments involve irradiating the sample with a burst of RF energy, which is equivalent to exciting all the possible spin-state transitions at the same time. A detector then measures the change in the magnetization of the sample as it decays from saturation back to an equilibrium distribution of spin states. The signal collected from this experiment is subjected to a Fourier analysis. This transforms the signal from the time domain – in which it is collected – to a frequency domain spectrum identical to the result of the original NMR experiment.

2D-NMR is a two-dimensional NMR experiment that plays an important role in the process by which the individual peaks in the spectrum of a complex molecule are assigned to specific environments within the molecule. This content domain was chosen because multiple representations not only can but must be used to understand the 2D-NMR experiment.

The data obtained in our study of students' success or failure at utilizing information in a computer tutorial on 2D-NMR were consistent with the notion that the ability to switch between representations or representation systems plays an important role in determining success or failure in problem solving in chemistry[30]. Successful problem solvers constructed an average of about two representations per problem, while those who were unsuccessful constructed an average of just more than one representation per problem, a difference which is statistically significant.

The two groups also differed in the nature of the representations they constructed. Among the successful problem solvers, the most common representations were those that are best described as *symbolic*. These representations were characterized by a reliance on symbols or highly symbolic equations that might include fragments of a phrase or sentence. The most common representations constructed by the unsuccessful problem solvers were those best described as *verbal*. These representations, which were expressed either orally or in writing, contained intact sentences or phrases, such as: "the number of spin orientations of a spin-active nucleus is equal to two times the spin-quantum number plus one."

A possible explanation for the difference between successful and unsuccessful problem solvers, which might provide insight into the role of mental representations in problem solving, can be found in the schema theory of cognitive structures. Schema theory views cognitive structure as a general knowledge structure used for understanding[31]. Schema, also referred to as frames[32] or scripts[33], relate to one's general knowledge about the world. Schema are activated or triggered from an individual's perceptions of his or her environment and they provide the context on which general behaviors are based. Because they do not include information about any exact situation, the understanding of a situation they generate is incomplete. But, by including both facts about a *type of situation* and the *relationship* between these facts, they provide a structure that allows one to make inferences[34].

Within a given context, problem solving requires the activation of an appropriate schema that contains an algorithm or heuristic that guides the individual to the correct solution to the problem. The construction of the first representation is an effort by the individual to activate the appropriate schema. Thus, the first representation establishes a context for understanding the statement of the problem. In some cases, this representation contains enough information to both provide a context for the problem and to generate a solution to the problem. In other cases, additional representations may be needed since the solution may require more than one algorithm or heuristic. But the first representation provides the context on which the other representations are built.

Unsuccessful problem solvers seem to construct initial representations that activate an inappropriate schema for the problem. This can have three different consequences, each of which leads to an unsuccessful outcome.

- The initial representation does not possess enough information to generate additional representations that contain algorithms or heuristics that might lead to the solution, and the individual gives up.
- The initial representation leads to the construction of additional representations, but these representations activate inappropriate algorithms or heuristics and eventually lead to an incorrect solution to the problem.
- The unsuccessful problem solver may never actually achieve an understanding of the problem, in spite of the number of representations that were constructed in an effort to establish a context for the problem.

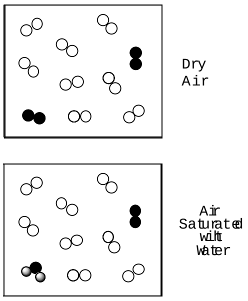
Implications for the teaching of chemistry

We have not yet completed a systematic study of what happens when our hypothesis about the role of multiple representations and multiple representation systems is used to change the way organic chemistry is taught in an operating classroom. We have, however, found that individual students, with whom we have worked in a one-to-one tutorial environment, can become more successful if we can convince them of the limitations of being trapped in a verbal/linguistic representation system.

Although most of our discussion of representations and representation systems so far has focused on organic chemistry, a similar phenomenon exists in general chemistry. Perhaps the best way to illustrate this is to ask the reader to consider the following question. *Which weighs more, a litre of dry air at 25ºC and 1 atm, or a litre of air at this temperature and pressure that is saturated with water vapour? (Assume that the average molecular weight of air is 29.0 g/mol.)*

Most students (and many of their instructors) are convinced that air saturated with water weighs more than dry air. (It seems reasonable that adding water vapour to air must increase its weight.) We have found, however, that many of these individuals change their mind when they are confronted with Figure 2.

Figure 2



Encouraging students to use different representations when solving a problem might therefore simply be a way of helping them recognize what information is important in generating the answer to this question. The symbolic/pictorial representation in Figure 2 prompts us to consider the implications of Avogadro's hypothesis, which assumes that equal volumes of different gases at the same temperature and pressure contain the same number of particles. Because the molecular weight of water (18.015 g/mol) is significantly smaller than the average molecular weight of air (29.0 g/mol), water that has been saturated with air actually weighs less than dry air.

Another illustration of the implications of this research for changes that might be made in the way we teach chemistry is provided by the following question which a typical beginning chemistry teacher might put to a class:

What is the pH of 100 cm³ of water to which one drop of 2 M HCl has been added?

The first author's work with almost 1000 teaching assistants at the University of Illinois or Purdue University suggests that relatively few of these individuals would instinctively focus their approach to this problem around the drawing in Figure 3. This is important, because these individuals invariably focus their approach around a drawing when they encounter problems from other domains, such as the following question from a placement exam given to students in the School of Science at Purdue University.

Two trains are stopped on adjacent tracks. The engine of one train is 1000 yards ahead of the engine of the other. The end of the caboose of the first train is 400 yards ahead of the end of the caboose of the other. The first train is three times as long as the second. How long are the trains?

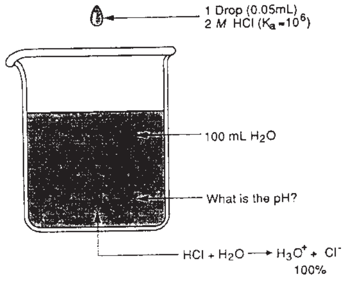
It is important to recognise that Figure 3 is not a drawing created *before* the problem is solved, but a drawing around which the solution of the problem is constructed. Each time more information is obtained – such as noting that a drop of this solution is about 0.05 cm³ or that HCl is a strong acid ($K_a \approx 10^6$) – it is incorporated into the drawing. Most of those who read this paper will not be surprised to note that we have found student performance on problem-solving tasks improves when drawings of this nature are used when the instructor solves problem in class. They might be surprised, however, by another implication of the research described in this paper.

Imagine that you were trying to balance the following equation in class.

$$I_3^-(aq) + S_2O_3^{2-}(aq) \rightarrow I^-(aq) + S_4O_6^{2-}(aq)$$

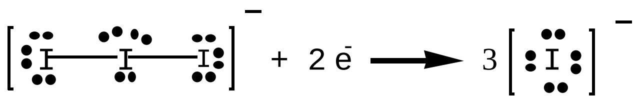
Chemists have historically approached this task by separating the reaction into two components, balancing each half-reaction, and then combining the half-reactions.

Figure 3

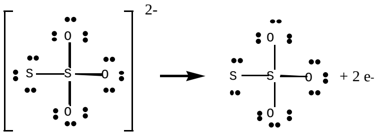


When you listen to them talk about this reaction in class, they utter statements such as: "two electrons are added to the starting materials in the reduction half-reaction *to balance charge*."

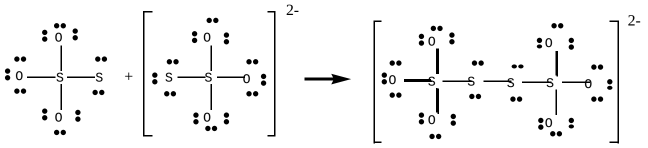
Recently, we have been teaching general chemistry by approaching reactions such as this in terms of Lewis structures. When this is done, two electrons are no longer added 'to balance charge'. They are added because two electrons are needed to transform the starting material into three iodide ions with filled octets of valence electrons.



These electrons obviously have to come from the thiosulfate ion. And they are more likely to come from the less electronegative terminal sulfur atom than one of the more electronegative oxygen atoms.



The neutral S_2O_3 molecule formed in this reaction combines with an $S_2O_3^{2-}$ ion to form the $S_4O_6^{2-}$ ion.



No one would argue that beginning students can use Lewis structures to *predict* the product of the reaction between the iodide ion and thiosulfate. We have preliminary evidence, however, that these students can understand how Lewis structures can be used to *explain* the products of this reaction. We also have evidence to suggest that students who have seen their instructor use this approach to balancing redox equations are more successful at similar tasks and more likely to understand what they are doing when they balance one of these equations. In many ways, this is nothing more than adding a symbolic representation – which carries different information – to the verbal/linguistic representation the students build when they read the equation they are being asked to balance. Our goal is to develop an approach to descriptive chemistry that would enable at least some of the students who take general chemistry to *predict* the product of the reaction between ammonia and the hypochlorite ion, rather than memorizing that the Raschig process produces hydrazine.

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Crossing the borders: Chemical education research and teaching practice

PROCEEDINGS

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1. Crises in current chemistry education

In many European countries, chemistry education faces a number of important recurrent difficulties. At the *secondary school level*, many students have a rather negative view of chemistry. They think of it as a rather dirty discipline and they experience difficulties in understanding key concepts and rules. Common student complaints are of the kind 'I know this chemistry formula by heart, but I do not understand its meaning'. Many teachers complain that repeated explanation and demonstration are not very effective and frustrate the teachers as well as the students. Coupled with this negative attitude, students' interest in chemistry as one of the chosen final examination subjects has decreased to a rather low level.

At *university level*, the number of first-year chemistry students is also decreasing. Students complain that laboratory courses involve many boring 'cookbook' problems instead of challenging tasks to explore new areas of chemistry. However, lecturers complain that many students are not able to connect lecture courses with laboratory courses and, for that reason, cannot apply (theoretical) knowledge of chemistry in the context of practical work.

Another category of problems concerns the *chemistry curriculum*. Well-known complaints involve the overload with factual material, the vague course structure and a lack of modern topics. Furthermore, the connection between the chemistry curriculum at secondary level and at tertiary level is rather weak.

Tackling the current crisis requires, among other measures, *the use of research*[1]. Unfortunately, many teachers and researchers point out that there is a gap between chemical education research and the implementation of the research findings in college and classroom teaching.

2. A gap between research and teaching

Those teaching chemistry, whether at university or at school, often feel dissatisfied with chemical education research. Their complaints can be summarised as 'much chemical education is not readily accessible to the teaching practitioners and, in any case, research outcomes seem to be either not very useful or are difficult to translate into useful teaching and learning activities for college and classroom practice'. However, chemical education researchers also complain about a gap between research and teaching. I suggest that there are three main reasons for the origin of these complaints.

First of all, an important cause of such complaints might be mere *survival*. Chemistry lecturers, as well as school teachers have to survive, which means that they cannot find time for reading research articles because they are already too busy with their existing teaching. Even if they have time for reading, they need extra time to translate and integrate the content into their teaching practice, and this is a skill they may not have been able to develop well during their period of teacher training or their career. Chemical education researchers also have to survive, which means that they have to publish in high-ranked journals read by only a few lecturers and teachers. Of course, researchers are free to publish in journals intended for university lecturers and school teachers, and indeed some of them do. However that does not provide rewards in terms of 'research' output.

A second reason might be the *differences in expectations*. Lecturers and teachers might be inclined to think that research ought to provide them with solutions for their teaching difficulties. Researchers might be inclined to believe that teachers are able to transform the reported research outcomes into useful ideas for teaching at college and school level. Unfortunately, both expectations are too high and not very realistic.

Finally, the gap may result from the choice of the *research paradigm* that is used. For many years (including the present), the (theoretical) frameworks of chemistry education research have been strongly influenced by general psychological theories about teaching and learning. Some decades ago, the leading theory was called 'descriptive behaviourism', which includes stimulus-response models about shaping behaviour by operant conditioning (a very common method for training dogs!). This perspective promoted an interest in the use of programmed instruction in chemistry courses (i.e. teaching which involves providing a series of tasks with direct feedback to the answers of individual learners). In the last two decades, another leading theory arose, called cognitive psychology. This approach stimulated an interest in chemistry courses based, for example, on theories about guided discovery learning and theories about conditions of learning. In my opinion, the value of both approaches for improving chemistry teaching and learning is restricted. The conclusions of research which has been carried out in the context of such psychological theories tend to be too general to be helpful for designing courses in specific chemistry topics. The weak relationship between general educational theories and specific teaching practices can also be explained as follows. Course developers use (often implicitly) basic conceptions of chemistry and chemistry education during the process of designing new teaching strategies. Their specific preconceptions of teaching a particular chemistry topic will often be more influential than their knowledge of rather general models of teaching and learning.

In conclusion, much research has focussed on aspects of teaching and learning which are essentially 'content-free' and refer to general problems of teaching and learning. However, teachers are faced with content-related difficulties in teaching and learning. They want to understand the reasons why these specific problems arise. But much research is not concerned with content-related information, and therefore does not help to bridge the gap between theory and practice. We need research which specifically takes content into account. In the language of educational researchers, such studies will have a strong 'domain-specific character.[2]

3. The line of domain-specific research

During the last decade, there has been increased interest in studies of the teaching and learning of specific chemistry topics. This domain-specific research is strongly stimulated by the current leading theory of knowledge acquisition: *constructivism*. According to this perspective (see e.g. Bodner,[3]), learning is a dynamic and social process in which learners actively construct meaning from their actual experiences in connection with their prior understandings and the social setting. Knowledge and learning are considered to be dependent on the situation. Cognition is in part a product of the activity, the context and the culture in which it is developed and used. A major implication for chemistry teaching is the idea that chemistry teachers should have an insight into students' (pre)conceptions of chemistry topics and should facilitate chemistry learning by creating conditions enabling conceptual change[4].

Many *domain-specific studies* were focused on students' conceptions of chemistry concepts and rules[5]. These studies often involve qualitative methods for collecting and analysing research data. This often involves analysing records of interviews, think-aloud monologues or classroom discussions. Think aloud monologues can be stimulated by inviting students to say what they think while they are performing a certain task (introspection), or by asking them (after finishing the task) to describe what they were thinking during the task (retrospection). An interesting example of the think-aloud method is presented by Osborne and Gilbert[6]. Their approach involved interviewing students who were presented with a set of simple line-drawings on cards depicting instances or non-instances of a particular science concept. Students were asked to categorise the picture on each card and then asked to explain their reasons. It appeared to be possible to explore students' *understanding* of a particular science concept beyond their *knowledge* of its formal definition.

In my opinion, domain-specific research is a very important tool for improving chemistry education. However, its value depends on the nature of the research instruments. Records of interviews and think-aloud monologues can be used before or after classroom instructions, but they are not very fruitful for investigating the teaching and learning of chemistry as it actually takes place in the laboratory or classroom. For that kind of research, it is particularly useful to produce records of discussions between students and their teachers in educational situations.

It is important to recognise that the quality of any final record is influenced both by the audiotaping of the original discussion and by its transcription.

The *audiotaping* of students and their teacher requires the presence of one or more tape recorders in the laboratory or classroom. One can be placed on the teacher's desk. Others can be placed on students' desks, especially when students have to work on tasks in small independent groups. If the teacher has the habit of walking around the room a lot, a portable tape recorder can be very useful. In all cases, it is important that the presence of recorders does not influence the behaviour of students or teacher. Only then, is it possible to record spontaneous discussions. It is my experience that students and their teacher quickly accept the presence of recorders and, after one or two sessions, ignore the equipment entirely.

Once the audiotape has been made, it must be transcribed into a record. One method consists of transcribing all recorded statements. Although this approach takes a lot of time, all statements are on paper. A second method consists of selecting a number of episodes for transcription, after first scanning the discussions on the tape. The selection involves making judgements about which episodes are most relevant to the formulated research questions. Although this approach saves time by reducing the length of the record, there is a certain risk of missing out on important information. In my experience, the most productive method is somewhere between the two: analysis of the first selection of episodes leads to the recognition of the need for an additional selection.

Domain specific research of this nature is often small-scale because of the time consuming methods of analysis. However, records of laboratory/ classroom discussions can be a rich source of information. It can be very useful for teachers to produce their own records for analysing their teaching activities as well as the conceptual difficulties of their students. This is illustrated by the following two examples. Both are concerned with the teaching of electrochemistry to upper secondary school students.

4. Examples

In the first example, the teacher introduces and discusses a specific electrochemical cell: the zinc-copper galvanic cell (Daniell cell). The teacher explains this cell and uses expressions like 'the zinc is negative' and 'the copper is positive'. The teacher goes on to explain that the copper bar becomes heavier because copper has been deposited on it by the following half-reaction:

$$Cu^{2+} + 2e^- \rightarrow Cu$$

It is important to note that the teacher does not use the expressions 'the zinc electrode is negative' and 'the copper electrode is positive', although these phrases are given in the students' textbook. (As a matter of fact, the terms 'negative' and 'positive' do not refer to the sign of charge of the electrodes but to the whole half cell under consideration. The signs are relative and depend on the particular combination of half cells. The sign of charges can be determined by electrical measuring methods including the use of a voltmeter or an ammeter).

The following discussion between two students was recorded.

Student 1:

According to this half-reaction, the copper ions get electrons by moving to that bar. But that electrode is positive. How comes that positive ions move to that positive electrode? We have learnt that entities with the same sign of charge will repulse each other, isn't it?

Student 2:

Yes! I do not understand it either. But this is chemistry, you know …

Note that Student 1 uses the term 'bar' as well as 'electrode'. The first term refers to an object, the second one to an (electrochemical) function of the object. However, the student does not consider the whole electrochemical context but only interprets the situation as a local one. He wants to use Coulombs' Law of electrical attraction and repulsion. But its use cannot explain the moving of copper ions towards the copper bar (copper electrode). In conclusion, the teacher's choice of words in providing explanations appears to have caused a big cognitive conflict amongst the students. The teacher has reasoned from a measurement point of view, in the sense that his expression 'copper is positive' implicitly refers to the sign of charge on the 'copper' half cell in relation to the 'zinc' half cell. However, the students are reasoning from another context, viz that of an electrical particle. If the teacher analyses this record of the students' discussion, he should become aware of students' conceptual difficulties and this should help him to develop other ways of explaining the zinc-copper galvanic cell.

In the second example, the teacher has demonstrated the electrolysis of a KBr solution between carbon electrodes. After the students have observed what happens they are asked to describe the electrode reactions.

It is important to know that the students had already been taught to predict electrode reactions by consulting a table of half reactions and the accompanying standard electrode potentials. That table shows that the standard electrode potential for the H_2O/H_2 couple (- 0.83V) is higher than for the K^+/K couple (- 2.92V). Students are supposed to conclude that H_2O is a better oxidising agent than K^+, and for that reason is involved exclusively in the electrode half reaction. However, this way of reasoning is not clear to every student as the following record of a classroom discussion shows.

Teacher: *In this case, what is the best oxidizing agent?*

Student *K^+ … uh, uh,... 2 H_2O …*

Teacher: *Water is the best oxidizing agent (…) The minus electrode, water produces... H_2...so, the gas you saw was hydrogen …*

Student: *But that potassium plus is attracted and water is not …*

Teacher: *(…) It is sufficient to take water, quite common according to the rules*

In the recorded episode, the student does not feel the necessity to accept a new chemistry rule from the teacher who said "it is sufficient to take water, quite according to the rules". However, the student prefers to use an existing physics rule which is more plausible to him, saying "but that potassium plus is attracted and water is not". In other words, the teacher reasons from a chemistry context, while the student reasons from a physics context.

Both examples show that one of the barriers to student understanding of (electrochemical) concepts and rules was the fact that teacher and student were reasoning in different contexts. The examples illustrate how records can bring to light, not only student misconceptions, but also communication difficulties between teacher (lecturer) and student which arise (for example) when both assume different contexts. Other records of laboratory or classroom discussions can also be used to investigate teachers' conceptions and actions.

5. Establishing closer links between research and teaching

Teachers, whether at school or university level are one of the most important 'actors' in the process of improving chemistry education. In that process, they can play different roles. They can be consumers of results of research and development projects (providing that the gap between 'theory' and 'practice' is not too big); they can be producers of new teaching materials and strategies. They can also act as researchers in their own classroom.

The motivation for this research is likely to be the recognition that students (or the teacher) are experiencing difficulties, and that there is room for improvement in the teaching. Having identified some specific learning difficulties, it is necessary to postulate reasons to explain the observed difficulties and then to devise teaching activities which will remedy the problem. These two steps are best based on research data which may be collected (as described above) by collecting audio records in the classroom and transcribing and analysing them. On the basis of the analysis the teacher can start to reconstruct his or her teaching practice based on a firm understanding of the problems experienced by the students. This individual approach means that the teachers address the problems which are personal to themselves. The lessons they learn can be made more widely available by sharing them with colleagues from the same institute or school and by inviting colleagues to discuss the results, and to use the same approach. Well analysed data which leads to useful conclusions can form the basis of a professional publication in an educational journal, thus emphasising the role of teacher as researcher and helping to establish closer links between research and teaching.

In doing this kind of research it is useful to remember that it is only a first step to introducing a change in teaching based on the analysis of a record. It is usually necessary to repeat the cycle which Lijnse[7] has referred to as the *'developmental* *research'* approach. In this approach, a small-scale curriculum development is linked to in-depth research on social, content and context specific teaching and learning processes. The structure of the research activities involves repeated cycles (a spiral) of activities, in which each cycle includes the following stages

- an evaluation of a current educational situations;
- formulation of research questions in conjunction with reflection on chemistry and chemistry education;
- development and implementation of new teaching strategies and materials;
- investigation of teaching and learning processes during classroom and laboratory sessions (important research instruments are audio/video-tapes for producing records of laboratory /classroom discussions);
- repetition of the cycle.

The cyclical approach is crucial to the individual teacher and can be used by professional research teams. It allows practitioners to link small-scale curriculum development to more in-depth research. Furthermore, if developmental research is carried out and published by practitioners at secondary level as well as at university level, the results can also help to bridge the gap between chemical education at this interface.

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Chemical Education Research: Where from Here?

PROCEEDINGS

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Introduction

I should like to begin by recording a number of depressing facts about Chemical Education over the past forty years. When we have cleared that ground the remainder of the paper will be a positive attempt to address some of the unpleasant observations.

- Students are not flocking into chemistry thirsting for knowledge. Almost everywhere students are opting out of chemistry.
- Since the early 1960's we have been inundated with chemistry schemes and courses full of promise, most of which have come and gone, leaving the promise unfulfilled. Examples are: Chem. Study and ChemBond from U.S.A., Nuffield and Salters from England, Science for the 70's and Alternative Chemistry from Scotland, ReCoDiC from France and many others.
- As researchers we have solved almost none of the reported problems in chemistry teaching: the mole, bonding misconceptions, misunderstandings about the nature of matter, equilibrium, free energy and many more.
- Research literature has been dominated by work on misconceptions, but little has as yet appeared about how to reverse these or to avoid them altogether.
- Most countries are struggling to find well qualified and competent teachers.
- We are deluding ourselves if we imagine that the general public are taking an increasing interest in chemistry. For normal daily living most people believe that they need no knowledge of chemistry, and maybe they are right.
- A sure way to kill conversation at a party is to confess that you are a chemist. You might as well be a tax-collector or a priest! Your fellow guests say things like:

"I was never any good at chemistry"
"I never understood atoms and molecules"
"I enjoyed splashing about in the laboratory, but I did not understand what I was doing".

All of this is a very pessimistic, but realistic view of the current situation in Chemical Education. Things have gone badly wrong over the past 40 years at some fundamental level.

This period has been characterised by much development activity in the field of Chemical Education. Much has been done to design demonstrations, microchemistry, computer assisted learning, CD ROMs, units on societal issues and a plethora of textbooks. However, most of these laudable activities have been devoted to the transmission of chemical knowledge rather than to any consideration of the nature and desirability of the content or to the nature of the learning process. In other words, we have been emphasising the '*how*' rather than the '*what*'.

The Chemical Education research which has been done has tended to be distorted by the few journals which would accept such material. The Journal of Chemical Education has largely ignored research with less than 2.5% of its articles devoted to it in the issues of 1996-97. The International Journal of Science Education has devoted over a third of its space to work on 'Alternative Frameworks' and this has tended to encourage an approach to research which was negative and offered few solutions to the problems exposed.

The more I have studied chemistry, chemical education and the psychology of learning, the more I have become aware that we are trying to share our beautiful subject with young people in an apparently 'logical' way and, at the same time, conflicting with what we know about the way people learn ('psychological').

I want to spend the rest of this paper attempting to harmonise a *logical* approach to our subject with a *psychological* approach to the teaching of our subject so that young people will catch our enthusiasm and enjoy the intellectual stimulus which our subject can, and should, offer.

Models to help our thinking

Most of my research has been based around two models. The first, *information processing*[1] is an attempt to suggest mechanisms for learning arising from a number of psychological schools. It reminds us that *perception* (how we take a first view of something) is controlled by what we already know and believe. Perception is what we use to select some stimuli for special attention and to filter out others. We look for things which are familiar or which 'make sense' and, if a stimulus does not accord with this, we see it as a surprise or even as something to be avoided or feared. What we already know, enjoy and recognise controls, to a large extent, what we admit through this filter.

The filtered material is admitted into the conscious part of our mind (Working Space) for further processing. Here it is matched with things we know, or modified into a form with which we are happy and then we decide, consciously or otherwise, to store or reject the information.

If we decide to store it, we look for clear attachments in our Long Term Memory[2] on which to fix our new knowledge or experience. In so doing we enrich our large interconnected network of knowledge, experience, belief, preference and prejudice. This new corpus becomes the controller of our next perceptual experience and so the cycle repeats itself. This model exposes some problems which students have with effective learning.

The first of these is that Working Space[3,4] is limited and we can consciously handle only a limited amount of information in a given time. If we try to manipulate too much at once, learning can become faulty or not take place at all, because we just overload and shut down.

A second problem is that if we try to store material in Long Term Memory and cannot find existing knowledge with which to link it, we either 'bend' the knowledge to fit somewhere (maybe completely wrongly) or we try to store it unattached[5]. The 'bending' process leads to Alternative Frameworks[6] or to what is euphemistically called Children's Science. The unattached (or rote) learning is easily lost because it has not been inserted into our mental filing system.

This model can be useful in helping us to think of ways to overcome some of the difficulties we mentioned at the beginning.

My second model has to do with the nature of chemistry. I believe that it exists in three forms which can be thought of as corners of a triangle[7]. No one form is superior to another, but each one complements the other. These forms of the subject are

- the *macro* and tangible: what can be seen, touched and smelt;
- the *submacro*: atoms, molecules, ions and structures; and
- the *representational*: symbols, formulae, equations, molarity, mathematical manipulation and graphs.

Most things which we encounter in the world, and on which we form many of our concepts, are *macro* in nature. We look for regularities and patterns by which to form concepts, but few such tangible observations and patterns exist in chemistry. Even the more abstract ideas such as 'love' or 'justice' are made more tangible by reference to actual examples. On the *macro* level, chemistry is what you do in the laboratory or in the kitchen or the hobby club. This is the experiential situation to which we are accustomed in most aspects of life.

But chemistry, to be more fully understood, has to move to the *submicro* situation where the behaviour of substances is interpreted in terms of the unseen and molecular and recorded in some *representational* language and notation. This is at once the strength of our subject as an intellectual pursuit, and the weakness of our subject when we try to teach it, or more importantly, when beginners (students) try to learn it.

First of all, the simultaneous introduction of all three aspects is a sure recipe for overloading Working Space. Experienced chemists can manipulate all three, but this is not so for the learner. Secondly, when the learner tries to store this triple layer sandwich of information, it is unlikely that he is going to find useful or usable points of attachment in Long Term Memory and so there is an attempt to 'bend' or 'manipulate' the information into a more tangible form and yet another Alternative Framework is born!

Example:

A teacher is trying to show that gases expand on heating and tries to introduce a kinetic picture and even some simple maths. The student remembers that things in general expand on heating, ignores the kinetics and rationalises the experiment by assuming that the atoms have expanded!!

The remainder of this Paper will attempt to show how these two models – *Information Processing* and the *Chemistry Triangle*, can be used to help our teaching by making the logical and psychological coincide. On the way along, we will have to think about the content. What may be logical to us in retrospect, may not be so for the learner. I would like the emphasis to be on *learning* and for teaching to be seen as the means of facilitating the learning process. I suspect that too often 'clever teaching methods' have given more pleasure and insight to the developer than to the learner. In this respect, I must plead guilty, having spent a great deal of time in methodology pursuits without fully understanding the learning process. It is so easy for teachers to confuse their own enthusiasms with that which will enthuse their students.

It is possible, even likely, that as we are devising new methodologies, we are learning something about chemistry for the first time ourselves. But this is learning by someone who is already an expert, not a novice. The insight which has broken through to us may be too 'rich' for a novice to digest.

The use of new technologies in teaching and learning may not be capable of being directly grafted on to our normal education provision without the exploration of the new psychological skills which we and the students have to develop. The television screen is associated, in the mind of students, with the rapid provision of informational 'soundbites' which do not demand deep thought or study. But we are trying to use it to generate what we hope is deep and lasting learning. It is no wonder that so many Computer Assisted Learning packages have proved to be ineffective and unpopular. One time enthusiasts like Norman[8] are now having second thoughts. CAL exponents would do well to read his book before going further. The development of our understanding of these processes (rather than the development of more programs) may be a fertile field for research for some time to come.

I should now like to turn to some actual examples of how we might use the models I mentioned above to help us to take a new view of our research and where it might lead in the future.

Using research to shape the curriculum

Syllabus Order

"Begin where the students are" is an idea as old as time. From an Information Processing point of view, begin with things that they will perceive as interesting and familiar so that there are already concepts in mind to activate the perceptive filter and provide anchorages in their Long Term Memory on which to attach the new knowledge.

Should we begin in the traditional way with salt, sodium carbonate, silver nitrate and barium chloride? Most of these substances are about as real as 'moon dust' to our students and do not provide the psychological framework they need to make sense of what we are trying to teach. This inevitably results in rote learning of undigested material and provides the raw material for the growth of alternative frameworks. They have traditionally been taught first because they are 'simple substances', but are they so simple? Their bonding is not simple either between ions or within ions. Their structures are not simple and they form molecules only in the gas phase or as figments of imagination! The binary compounds also perpetuate, in traditional teaching, the crazy ideas that metals are 'anxious' to lose electrons and non-metals are 'bursting' to accept them. A cursory glance at a table of Ionisation Energies or Electron Affinities shows how crazy this is. These false ideas, which may be alternative frameworks for teachers as well as students, are almost impossible to eradicate later!!

Should we begin with petrol, camping gas, plastics and foods? Organic chemistry has traditionally been thought of as too difficult for beginners, but a moment's thought will show that it is not necessarily so. We are beginning with the *macro* and can afford to take in some *submacro*. Students will accept that hydrogen forms one bond, oxygen two, nitrogen three and carbon four and this is not likely to become an alternative framework which has to be untaught. With this simple idea, you can go a long way in deriving molecular structures. Both corners of the triangle are 'visualisable' and can be made concrete with models. From this, simple formulae arise because the students can count the 'atoms'. There is no need for multipliers and awkward brackets (as in a compound like $Pb(NO_3)_2$). With only these simple submicro and representational ideas you can go a long way through hydrocarbons, alcohols, aldehydes, ketones, esters, carbohydrates, fats, proteins and plastics. Only when we meet carboxylic acids do we have to think about any change in bonding type.

Structures

Intelligent use of models as outlined above leads us into shapes. Some primary school children in Scotland do this as a fun part of their science lessons! (The submicro has become tangible to them, but I have yet to see evidence of the accompanying understanding which the enthusiasts claim).

To help students to rationalise these shapes, we need a new idea, which is easy to make visual, that bonds take up the orientation of minimum repulsion (VSEPR). One bond can point in any direction; two are directly opposite, three form a triangle and four a tetrahedron. This is easily shown by using long balloons to represent the bonds and seeing how they repel each other to form linear, trigonal, tetrahedral or octahedral arrangements. This is more intellectually rigorous than talking about tetrahedra arising from sp3 hybrids. To use the 'unreality' of atomic electronic configurations (isolated atoms in the gas phase) and try to create the reality of molecular structure from them, is intellectually suspect. Without an understanding of the mathematics (which I suspect few chemists have), sp3 or any other hybridisation label, is just mumbo jumbo. It is simply saying that, if you combine one s orbital with three p orbitals, you get a tetrahedral arrangement of orbitals, leading to bonds which point to the corners of a tetrahedron. Pasteur knew this long before orbitals were thought of!!

The Dreaded Mole

The mole concept is perfectly capable of being made tangible provided we do not dissolve it in water and talk about molarity. Kept as an extensive property of matter rather than an intensive property of solution, the mole is not a formidable idea. Students can see that 100 large balls will take up more space that 100 small balls. The idea of comparing like with like is well within their grasp. When this is applied to molecules, the relative volumes of moles of different substances allow us to 'see' the relative volumes of molecules. This holds well as a first approximation, since packing plays a relatively minor role. Measure out moles of an homologous series of alcohols (or other compounds) and set them side by side. The increase in volume between adjacent members in a series is a constant (19 cm^3). Students soon 'see' that the increase must be the addition of one mole of $-CH_2$. There are many more examples of where the mole allows like to be compared with like. Try weighing out equimolar masses of NaCl, NaBr and NaI and pack them into tubes of the same internal bore. It soon becomes evident that the size of Cl^- is less than Br^- and much less than I^-.

Physicists compare things by the kilogram or by unit volume to look for differences such as Specific Heat Capacity and Density. Chemists compare things by the Mole to look for patterns, often constants. Molar Heat Capacities for solid metals are almost constant (the Law of Dulong and Petit) because the same amount of heat energy is supplied to the same number of atoms to change their vibrational energy. If one converts gas densities from g dm^{-3} into the equivalent volume per gram mole we get a constant again. It is instructive to compare the volume of a mole of liquid water (18cm^3) with the volume of a mole of water vapour (22.4 dm^3) to get some idea of empty space in a gas. A test-tube with 18 cm^3 of water alongside a 20 dm^3 drum makes a visual impact! All of this keeps the mole tangible and visualisable.

As you can see, we have tended to remain with only two corners of our chemical triangle at a time, trying to keep new concepts as concrete and visualisable as possible.

We have gone a long way with simple formulae related to reactivity and structure. Nowhere have we balanced an equation or done a volumetric calculation. They have just not been necessary to do good chemistry and good science. The concepts have been kept in a form which tends to avoid Alternative Frameworks.

Moving Towards Inorganic

The *macro* place to start is with metals and their uses. Salts are mostly not within the experience of students and so they have no obvious anchor points within Long Term Memory. Salts arise out of acids and bases and now we have to admit the idea of ions. Many of the wrong ideas that students have, start with ions and salts. Most of the literature on Alternative Frameworks[6] in chemistry is concentrated here and this is not really surprising.

Neutralisation introduced as the formation of water, a familiar substance, might be the place to start before trying to sort out salts. Some very elegant two layer experiments for neutralisation show this well. If a volume of a base weighted with sugar is placed in a beaker, and the same volume of an acid of the same basicity and molarity is floated on top of it, interesting observations can be made. If two long electrodes attached to a battery and meter (or lamp) are lowered just to the interface, a reading is obtained. If the electrodes are pushed to the bottom through the two layers, the reading doubles. If the layers are now mixed completely, the reading drops by a half, indicating that two species of ions are no longer available for conducting current. Where have they gone and what is left still to conduct? Once again we are trying to make visual something which is usually treated abstractly or 'shown' by equations.

It may be that inorganic chemistry and the emphasis on acid/base titrations are historical artifacts of the time when chemistry was almost all analytical. One could be cynical and say that we keep stoichiometry in a prominent position because it is easy to set exam questions on it and easy for students to fail! A large number (maybe the majority) of practicing chemists never balance an equation or do a titration. We know that these operations cause all kinds of trouble for students. Why do we persist with them and cause students such anguish?

However, if we must deal with the mole in solution, our models should be able to help us to arrive at a method less likely to cause trouble.

The traditional way to do an acid/base mole calculation involves a number of steps which are likely to overwhelm Working Memory Space.

- Write formulae for the acid, the base and the products.
- Insert these into an equation and balance it.
- Establish the stoichiometric relationship between the acid and the base.
- Calculate the number of moles of the acid in the given solution and hence the number of moles of base needed for neutralisation.
- Convert the number of moles of base into a volume (if molarity is given) or into a molarity (if volume is given).

Another approach

Now let us apply our models to try to make the process tangible (*macro*) and to reduce the load on Working Space by splitting the problem into three simple steps.

The problem is:

What is the molarity of a solution of sodium hydroxide when 80 ml of it can exactly neutralise 50 ml of 0.1 molar sulphuric acid?

The more tangible steps towards solving it are

- Visualise the beaker containing the acid.
  How many moles of H^+ are in it?
  Molarity × volume in litres × no. of H^+ per formula of H_2SO_4
  $= 0.1 \times 50/1000 \times 2 = 0.01$ moles H^+
- Now visualise the beaker containing the base.
  How many moles OH- are in it?
  Molarity × volume in litres × no. of OH- per formula of NaOH
  $= z \times 80/1000 \times 1 = 0.08\,z$ moles OH-
- At neutralisation number of H^+ = the number of OH-
  $0.01 = 0.08\,z$
  $z = 0.01/0.08$ molar
  $= 0.125$ molar

The reader will notice that no chemical equation and no balancing was necessary.

It is really the old *normality* disguised, but is not the blind $V_1N_1 = V_2N_2$ which was criticised in the past.

A supposed justification for the balanced equation and calculations is that we can calculate yields, but this is only useful if the reaction goes to completion. Industrially, few reactions go, or are allowed to go, to completion and so this argument is doubtful. To use it to calculate percentage yields is another academic exercise. This now leads us to the idea of equilibrium.

Equilibrium

This is another area for Alternative Frameworks and the reasons are obvious from our models. In Long Term Memory there already exists a wealth of knowledge and experience of equilibrium, but not in the chemical sense. However, the language used for both static and dynamic equilibrium is very similar. When the chemist presents equilibrium ideas they easily find points of attachment in Long Term Memory, but almost all are wrong, giving rise to Alternative Frameworks.

Everyday equilibrium ideas have the following features:

- Equal masses (or equal moments) on each side
- Addition to the left makes the system tilt to the left.

Students know this from shopping, riding bicycles, carrying suitcases or walking along a mountain ridge.

Chemical equilibrium does not conform to these ideas, but chemistry students write in exam papers things such as:

"Equilibrium is achieved when the concentration of the products is equal to the concentration of the reactants".

"Apply pressure to the reactants", as if there were a reactants side and a products side.

"Addition of extra reactants changes the equilibrium". What does this mean?

There are quite good analogues available to make this visualisable, but most of them suffer from being 'two-sided' and so can perpetuate a wrong idea in which students forget that reactants and products exist in the same vessel at equilibrium.

Conclusion

In the short compass of a paper it is impossible to set out a whole curriculum for chemistry based on research, but I hope that I have indicated how research can influence our thinking and lead to better teaching and learning. The author is not a reactionary looking backward, but a researcher looking forward by applying research findings to real teaching situations. There is little justification for research for its own sake, but if it can affect practice and bring about benefit, it has a valuable role. I believe that our research has gone far enough already to be able to revolutionise the teaching of our science and other sciences, by bringing the logical and psychological together and so admit many more young people into an appreciation and enjoyment of chemistry.

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Letters

Assessment of Chemistry Degrees

From Professor Jon Williams
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I read with interest Professor Bailey's perspective on the assessment of chemistry degrees within the UK. I believe that it is unfair to say that, to a large extent, we do not use appropriate methods for awarding and classifying degrees in chemistry.

The formal examination, if it is correctly structured, can be a very effective method for judging the depth of a student's knowledge, as well as their ability to solve problems.

I am certainly not against the other forms of assessment noted in the article (e.g. collaborative project work, poster displays, essays, etc). Indeed, we assess these activities in our teaching programme at Bath, as do most other UK chemistry departments. What does concern me is that we keep the balance of assessment methods about right. I suspect that most chemistry academics are more competent to assess examination scripts accurately (including answers to discursive topics) than they are to assess, for example, collaborative project work. In my experience, examination marks offer a better representation of a student's ability than any other single method of assessment.

Professor Bailey urges us to use more opportunities for assessment, and to ensure that we only assess those skills which we would like our students to develop. Fine. But let's not abolish the formal (well-structured) examination in the process.

Professor Pat Bailey replies

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I do not disagree with the views of Jonathan Williams – formal exams do indeed test many important skills, and are undoubtedly the assessment method in which we have greatest confidence. Exams can assess (amongst other things) knowledge base, problem solving, critical thinking, reasoned argument, and essay writing skills. But I think that exams are often rather more limited in their scope because:

a) we set too many of them, leading to rather predictable and mundane questions;
b) exams are rarely designed with the explicit intention of rewarding a set of pre-defined skills.

From my perception of chemistry exams throughout the UK, I feel that students can often simply revise and learn the material for a specific modular exam and then forget it; and when asked for "explanation" type answers, they obtain good marks primarily for flagging up the key facts in their answers (i.e. getting the right tick list), rather than for being able to construct a well-reasoned, well-written argument. So the feedback (i.e. marks) students receive suggests "learn your facts, regurgitate them, then forget them, and you'll do well". This is, of course, absolutely fine if this is what is expected of graduates with a good chemistry degree. Nevertheless, many of our brighter and keener students obtain a much deeper understanding of their subject, although I fear that our assessment methods do not reward this adequately.

Conversely, most of the so-called "key skills" are flagged up by us as REALLY IMPORTANT, but are actually rewarded with a nominal percentage of the marks for a degree, particularly if one considers that such marks often show poor discrimination between students. With so much testing/examining elsewhere in the course, small wonder that students see straight through our words... and conclude that key skills are not very important at all!

Nevertheless, I'm not necessarily advocating that (say) 30% of degree marks should be allotted to generic transferable skills. But I simply point out that TEACHING such skills as part of a course, without giving serious marks for them, will inevitably produce many graduates who are not skilled in this way. Similarly, if we state in our course descriptors that we are addressing the key skills identified in the Dearing Report and Chemistry Benchmarking Document, we must be able to demonstrate that our degree classifications genuinely include these skills. If they do not, I would expect TQA to identify this as a deficiency, and it would be small wonder if employers continued to bemoan the poor level of generic skills in chemistry graduates.

Some Thoughts Following 'Crossing The Borders'

From Dr Alan Goodwin
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I was privileged to hear Onno de Jong's presentation at the Chemical Education Research Group lecture at Variety in Chemistry Teaching 1999, as well as to read the paper in its pre-publication format. I wholeheartedly agree with him about the importance of getting 'domain specific' aspects of teaching and learning back at the top of our agenda. Indeed, it seems axiomatic that the main focus of chemical education should be the understanding of chemistry, and yet this often seems to be eclipsed in interchanges with HEFCE and OFSTED by concerns for management, assessment, resources, cross-course policies etc. It seems that the actual learning of chemistry is considered to be unproblematic.

Overall I agree with de Jong that there are important lessons to be learned by paying close attention to the interactions which take place during learning. However, I am not convinced that recording and applying protocols is the only place to start – especially for academics who are more concerned with improving their teaching than with doing educational research.

The paper provides evidence that interesting insights can be gained by recording interactions in a classroom and transcribing the result – and then analysing the resulting transcript. Unfortunately, as de Jong agrees, this is a very time-consuming process and it seems a very expensive way of collecting data. I am particularly concerned that attempting to engage practising teachers in such activities would simply increase the bureaucratic pressure on them and alienate them further from educational research. This is not to undermine the importance of focusing on the teaching and on classroom interactions, but to suggest that such data could more efficiently and more naturally be obtained by the teacher noting ‘critical incidents’ which occur during interaction with students during classes. These can be backed up with information from students’ written work (including examination scripts) and through reflection on their own learning.

Most academics teaching chemistry have a wealth of experience of this sort, which is a really rich vein of information about the learning of chemistry. A little time spent analysing and reflecting on this experience can generate domain-specific ideas which are worth sharing with others (through discussions, letters etc) or which could form the basis of further investigations at the practitioner level.

de Jong’s description of the students’ conceptual difficulties with the Daniell cell is a good example of a problem which can be revealed by reflecting on observation and experience. I would speculate that Student 2’s response “Yes! I do not understand it either” could equally well be that of the teacher. It was certainly mine when a student first pointed out the problem to me. A key step in understanding how student misconceptions arise is the recognition that we academics cannot know everything, and that we are still learning[1]. Individual experiences provide important research data, the application of which can lead to improved learning. We are all researchers in chemical education when we document, reflect on, and share our experiences. Let’s keep this high on our agenda.

1. Goodwin A J, ‘The Teaching of Chemistry: Who is the Learner?’ Chemistry Education, Research and Practice in Europe, 2000, 1(1) Published on www at: http://www.uoi.gr/conf_sem/cerapie/

Key Skills Development Support from Central Services

From Sara Shinton
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Recent articles in this journal[1,2] illustrate the growing expectations on Higher Education Institutions (HEIs) to provide an environment which develops key skills as well as subject expertise. The introduction of an employability performance indicator[3] for HEIs and the pressure from students who are contributing financially to their education have brought key skills onto the agenda of all academic disciplines. The problem for hard-pressed academics is how to incorporate the teaching of these skills into an already overcrowded curriculum. There is a growing opportunity for central services to support academics in this role.

After discussing these problems with interested academics at the recent Variety in Chemistry Teaching meeting[4], I was encouraged to explain how this support is provided at the University of Newcastle upon Tyne in the hope that it may encourage chemists to seek the support of equivalent units in their own university.

The Academic Development Unit within the Careers Service aims to advance the embedding of key skills within academic curricula and provides a range of support activities. Many of our current projects stipulate that we work with academic departments and some enable us to buy the time required for academic staff to develop suitable resources. Our activities include:

- Keeping a database of effective practice, including materials which can be adapted by interested colleagues
- Disseminating effective practice by means of a website[5] and internal mailbase
- Providing an environment for the exchange of ideas and sharing of concerns across disciplines, through the mailbase and staff training seminars and presentations
- Identifying sources of external funding for development activities and supporting academic colleagues in the bidding process
- Developing and delivering materials and workshops to develop key skills in the student body

We are currently working closely with our Chemistry Department to develop support for students taking a sandwich year. In addition to subject specific sources, such as those developed by Drs. Wallace and Murray at Nottingham Trent University[6], we have been able to offer substantial support and delivery through external funding (from the DfEE Innovations fund) which has paid for all involvement from the ADU. This project funded the development of a reflective workbook and a series of workshops to improve students’ learning from their industrial training.

Our response to many requests for assistance from academics is to disseminate existing good practice. The materials developed by Bailey[7] have inspired similar activities in departments from Archaeology to Microbiology. In the last week I have directed a colleague in Ecological Resource Management to “A Question of Chemistry”[8] and sent details of Roger Maskill and Imelda Race’s[9] work to an academic in Marine Biology – both were impressed and relieved to discover materials that they could easily adapt for use in their own subjects.

These types of activities are not unusual to Newcastle. Like other active central support units, we are brought into frequent contact with academics, students bodies, employers, learned societies and other support units giving them many opportunities to identify, support and disseminate effective practice. Wherever they are found, a central support unit can act as a communication channel between you and other innovators. You can help them by introducing them to resources like UChemEd, which I find useful even outside chemistry. They can help you by providing you with the same kind of stimulation from colleagues of other disciplines that you enjoy when mixing with other chemists at Variety.

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5. See http://www.careers.ncl.ac.uk/academics
6. Murray R and Wallace R 1999 Good Practice in Industrial Work Placement (Project Improve)
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Future Arrangements for University Chemistry Education

From 1 Jan 2001 there will be significant changes in the organisation

Professor M J Pilling (Leeds) continues as Chair of the Editorial Board.
Professor P D Bailey (Heriot Watt) and Dr S W Breuer (Lancaster) become Co-Editors.
Dr C J Garratt becomes Editorial Consultant.

Volume 5 will be an electronic only journal, and will be accessible free of charge using acrobat reader software (obtainable *via* http://www.adobe.com).
The web page for U Chem Ed is accessible via the RSC Tertiary Education Group homepage at www.rsc.org/lap/rsccom/dab/educ005.htm

The URL for the UChemEd homepage is www.rsc.org/uchemed/echemed.htm

An Email list has been set up – subscribers to this list will receive Email alerts when new issues or papers are available.
You are advised to register with this list now.
To do this
either send the following email message to listserver@list.rsc.org
join uchemed-inf youremailaddress
or use the registration form on the U Chem Ed homepage

Back numbers (except for Vol 1) will also be available from the same web address and at no charge.
Both the April and September issues of Vol 4 will also be available in the same way.
Please draw this to the attention of colleagues who do not receive hard copies of the journal.

Submission of Manuscripts.

Small changes have been introduced to the Guidelines for Authors (inside back cover)
Would authors please read these carefully and comply as closely as possible with the guidelines. Please note especially that the preferred method of submission of manuscripts is by email as an attached Word file.

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Variety in Chemistry Teaching 2000

Variety in Chemistry Teaching, now in its 9th year, provides a forum for the exchange of teaching practises and of ideas about the learning and teaching of chemistry at degree level.

The meeting will provide opportunities for the sharing and discussion of experiences with and ideas about the learning and teaching of chemistry.

Our students need to develop an understanding of chemical principles and an ability to apply their knowledge in unfamiliar situations. We can help them by increasing the variety of teaching methods we use. Many individuals have developed interesting ways of teaching, but have had little opportunity to discuss their ideas with others. Variety in Chemistry Teaching offers that opportunity for colleagues developing their own approaches to improvements in their teaching.

Further information and registration details can be obtained from the organisers,

Stephen Breuer, Lancaster University	*s.breuer@lancaster.ac.uk*
Tina Overton, University of Hull	*t.l.overton@chem.hull.ac.uk*
Ray Wallace, Nottingham Trent University	*ray.wallace@ntu.ac.uk*

or can be found at

http://science.ntu.ac.uk/chph/netchemteach/homepage/html

Guidelines for Authors

1. The preferred method of submission is by e-mail as on attached document, preferably in Word. A disk copy in Word is also acceptable. In either case, tables and figures must not be incorporated into the Word file but submitted as separate file documents.

   John Garratt, e-mail cjg2@york.ac.uk
   Department of Chemistry, University of York, Heslington, York, YO1 5DD.

2. Full papers are normally between 3,000 and 5,000 words;

   communications should be less than 2,500 words.

   A word count (excluding references, tables, legends etc) should be included at the end of the document.

3. Presentation should be uniform throughout the article.

   Text should be typed in 12pt Times Roman, on single-sided A4 paper with 1" margins, double-spaced, unjustified, ranged left and not hyphenated.

   Always use an appropriate mix of upper and lower case letters: do not type words in uppercase letters either in the text or in headings (see 6). **Bold** or *italic* text and not upper case letters should be used for emphasis.

   All units should comply with IUPAC conventions.

   Tables and figures should be numbered consecutively as referred to in the text (use a separate sequence of numbers for tables and for figures). Each should have an informative title and may have a legend. Each table and figure must be provided on a separate page, and not incorporated into the text.

   Structures should normally be treated as a figure but small structures may be appropriately incorporated in the text.

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

   All pages should be numbered.

4. A title page must be provided consisting of:

   – informative title;

   – author '(s') names and affiliation, full postal address and email; (in the case of multi-authored papers, use an asterisk to indicate one author for correspondence, and superscript a, b, etc. to indicate the associated addresses);

   – an abstract of not more than 200 words.

5. Wherever possible articles should be subsectioned with headings, subheadings and sub-sub-headings. Do *not* go lower than sub-sub-headings. Sections should not be numbered. Headings should be no more than 40 characters in length and subheadings and sub-sub-headings no more than 30.

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

   Suggestions about other sections are made in "Editorial Policy".

   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.

   All references must be designated by a number in enclosed parentheses, NOT as superscript.

   Footnotes should not be used, but important additional information may be referenced, and included in the reference list.

6. Literature references are to be assembled, arranged numerically in order of first appearance in the text, and placed at the end of the article under References.

   Reference numbers should be followed by a period rather than being placed within parentheses and are placed flush with the margin.

   References exceeding one line should *not* be indented.

   The list of references should be typed double-spaced using the bibliographic style shown below.

   Titles of articles in journals should be included.

   Books and special publications:

   - Perry WG 1979 *Forms of intellectual and ethical development in college years: a scheme* (Holt, Rinehart and Winston, New York)
   - McCloskey M 1983, in: *Mental models* (eds. D Gentner and AL Stevens) (Lawrence Erlbaum, New Jersey)

   Journal articles:

   - Finster DC 1989 Developmental instruction I *J. Chem. Ed.* 66 659-661
   - Johnstone AH and Letton KM 1990 Investigating undergraduate laboratory work *Educ. Chem.* 27 9-11

7. All contributions submitted will be reviewed anonymously by members of the Editorial Board or Editorial Consultants. The decision of the Editor on the acceptance of articles is final.

8. Authors grant U Chem Ed the exclusive right to publish articles. They undertake that their article is their original work, and does not infringe the copyright of any other person, or otherwise break any obligation to, or interfere with the rights of such a person, and that it contains nothing defamatory.

9. No reprints are provided, but two free copies of the issue will be provided to the corresponding authors.

10. Papers will be printed direct from disk supplied by the authors *after* they have been informed that the paper has been accepted for publication.