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The Integration of Computational Chemistry Algorithms into a Multimedia Environment

by Richard T. Hyde, BSc MSc

Thesis submitted to the University of Nottingham
for the degree of Doctor of Philosophy, May 1996

DECLARATION

No portion of the work referred to in this thesis has been submitted in support of an application for another degree or qualification at this or any other university or other institute of learning.

Richard T. Hyde

As a decrepit father takes delight
To see his active child do deeds of youth,
So I, made lame by fortune's dearest spite,
Take all my comfort of thy worth and truth.

William Shakespeare
(1564 – 1616)

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ABSTRACT

Organic chemistry teaching involves the explanation of most phenomena in terms of atomic and molecular models. The main challenge for the student is the creation of mental three-dimensional images of molecules. Unfortunately, many students find the visualisation of the spatial arrangements of molecules a difficult task. For this reason, chemistry teaching has seen the introduction of many innovative teaching tools in an attempt to bring the subject to life for students. Until recently, the cost of computer hardware has prohibited the extensive use of computers within the undergraduate chemistry curriculum. However, the desktop computer has provided a cost-effective platform for developing integrated courseware that presents abstract concepts to the chemistry student.

This thesis begins with a review of the design and evaluation of computer-based learning, together with the integration of computers into chemistry education. Two studies then describe the design, implementation and evaluation of novel computer-aided learning material that combines computational chemistry tools and multimedia courseware. The first study assesses the feasibility of integrating interactive three-dimensional molecular modelling into tutorial instruction to provide a visualisation tool for undergraduate organic chemistry. A detailed evaluation has provided substantial evidence concerning the effectiveness of this technique. The second study involves the design of instructional courseware that combines interactive computational chemistry tools and 'talking head' video narration. An innovative training tool that allows medicinal chemists to study analytical chemistry techniques is described. The evaluation of a prototype package has revealed valuable information concerning the combination of dynamic and interactive media.

Emerging guidelines for the integration of computational chemistry tools and interactive molecular modelling into multimedia courseware and suggestions for further work are proposed.

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Chapter 1

A History of CAL Evaluation

"Failure to demonstrate the efficacy of CAI would make it more difficult to generate funding for computer labs and educational instruction. Nevertheless, software, or any other instructional tool, must be evaluated. Good intentions and hard work are not sufficient justification for its use."

(Nancy Duncan, 1993)

1.1 Introduction

Computer-aided learning (CAL) has been used in education for more than twenty years. Many advantages have been attributed to the use of CAL including self-paced learning, immediate response and knowledge of results, active learning, variety, ease of record keeping, flexibility, timeliness and reduced learning time [1-3]. Despite these benefits, computers have only recently gained widespread acceptance in higher education. Unfortunately, this endorsement has had more to do with advances in computer technology than with academic requirements or priorities [4].

The integration of multimedia into CAL is the main reason for the increased interest in educational software. Multimedia courseware does provide an outstanding new teaching opportunity since it has the potential to support the learning process as effectively as traditional teaching [5]. Even so, for CAL to be credited by educators as a reliable teaching resource it must be accompanied by rigorous evaluation, as for any novel teaching technology [6-8].

A large quantity of research has accumulated concerning the effectiveness of CAL and it has produced either inconclusive or slightly positive results [1, 8]. Recently, an increasing body of literature has begun to question the design and relevance of these studies. Together with the rapid advancements in computer technology, this has ensured that the systematic evaluation of courseware has lagged behind its development [7, 9, 10]. It is not surprising that the evaluation of instruction and learning has been called the most complicated problem anywhere in science today [11].

This chapter summarises the different strategies that have been used for the evaluation of instructional software. Emerging approaches, which may produce more reliable guidelines for the design of effective CAL and hasten its proper acceptance into higher education, are also introduced.

1.2 Media Comparison Research

Most of the traditional research on CAL effectiveness has compared CAL with conventional instruction, such as the traditional lecture, in so-called media comparison studies [2]. This approach is the recurring practice every time a new instructional technology is introduced [1].

Media comparison research has been criticised by several workers. For example, Bates (1981) says that in most comparative studies the media are assumed to be equivalent. Furthermore, unknown variables are often randomised between the experimental and control groups. This design often leads to more variation in learning within, rather than between, the media being studied [12]. Duncan (1993) is more specific, and considers non-random assignment of subjects to experimental and control groups to be a major threat to the internal validity of comparative research. For example, student characteristics such as age, sex, ability, computer anxiety, aptitude, motivation and prior knowledge may all influence the experimental outcome and must be carefully controlled [13].

Ransdell (1993) identifies the novelty effect as another user variable that can seriously affect the external validity of media comparison studies [7]. This effect is the most commonly cited problem related to CAL research [1]. It is caused by the experimental treatment in a study being seen as more effective because it is different from the traditional one. The novelty effect is a particular problem with multimedia courseware, which inexperienced users often rate too highly.

For the reasons above, most workers now accept that media comparison is the least productive method for CAL evaluation [6-8, 12-18]. Current research is turning away from the comparative approach. This is due to the difficulty of controlling the number of variables and also to the fact that CAL has proven to be relatively effective [1] (see Section 1.5).

1.3 Media Replication Research

An alternative to media comparison research which showed initial promise was media replication [19]. This approach investigates the relative effectiveness of one or more dimensions of CAL, for example, learner control, feedback or screen design. The evaluation process isolates the effectiveness of a single dimension or attribute of CAL (*e.g.* learner control) in comparison with an alternate attribute (*e.g.* program control). Media replication studies are supported by Clark (1989), who incorporates them into his prescriptive research recommendation (see Section 1.7.2) [20]. However, some workers, notably Reeves (1992), emphasise that replication studies have enjoyed only a little more success than media comparison research [21].

1.4 Aptitude-Treatment Interaction

In the late 1970s, the Aptitude-Treatment Interaction (ATI) approach to evaluation was devised [22]. This technique assumes that learning involves interactions between the task the learner performs, the learner and the characteristics of the media. Therefore, the optimal instructional method is seen to vary as a function of user attributes [13]. During this period, researchers began to focus on finding the relationships between these factors and their effect on learning outcomes.

Following the criticisms of other research approaches, ATI studies were often rigorously designed and implemented in controlled laboratory settings. Even so, the most common finding was the observation of no significant difference between the new and traditional media. Various criticisms have been aimed at ATI research, most of which are concerned with the highly controlled environment in which the studies are often carried out. For example, the relevance of the findings to classroom settings was raised by several workers [8]. For this and other reasons, ATI research has been superseded by other methods.

1.5 Metaanalytic Evaluation Studies

The technique of metaanalysis combines the effect sizes of individual studies (expressed as the average distance between experimental and control groups) into one common effect size. It has been particularly useful for assessing media comparison research (see Section 1.2), since the effects of multiple factors on learning can be separated for individual examination [7].

A metaanalysis by Jolicoeur and Berger (1986) highlighted a particular limitation of comparative research. These workers focused on studies that evaluated commercial products and conclude that most work has low reliability because it was not carried out in genuine classroom settings. Therefore, they stress the need for researchers to use realistic environments for the evaluation of instructional programs [23].

A summary of 16 metaanalyses and other reviews was published by Niemiec and Walberg (1987). The results of this synthesis suggest that the typical effect of CAL on student achievement is to raise outcome measures by 0.42 standard deviation units. These workers conclude that CAL is a moderately effective instructional intervention, but attention must be given to novelty effects in future work [24].

Kulik and Kulik have carried out a series of metaanalyses on studies comparing computerised and conventional courses. Their most recent analysis (1991) compared 254 controlled evaluation studies that met specific criteria. These specifications excluded work that did not take place in actual classrooms and experimental designs with methodological flaws. In keeping with earlier analyses, they found that the average CAL student outperformed conventionally taught students. They conclude that the exam scores for CAL students are raised by 0.3 standard deviation units, compared to non-CAL students. These workers also conclude that the effects of CAL are larger for published studies, for short duration evaluations and for studies where the teachers used for the CAL and non-CAL media classes were different [25].

The results of metaanalytic studies have highlighted weaknesses in many experimental designs. Nevertheless, studies that used specific criteria for the inclusion of published data report a moderate, positive effect of CAL. However, the critical factors causing these benefits remain unknown. Therefore, evaluation studies that emphasise obtaining statistical significance do not provide guidelines for future courseware development or use [13].

1.6 The Media or Method Debate

The controversy over traditional media comparison research led Richard Clark to initiate a debate in 1983 that continues in the literature. His argument was that media comparison problems are driven by the fact that media are merely delivery devices and it is the method or content that is introduced along with the medium that influences learning. In his paper of that year [5], Clark uses a now famous truck analogy, in which he states:

> "... [media] *are mere vehicles that deliver instruction but do not influence achievement any more than the truck that delivers our groceries causes changes in our nutrition."*

Clark has strongly supported his views recently (1994) by highlighting the lack of empirical support for media influences on learning [26].

The stance taken by Clark launched a wave of critical discussion. In a review of media research, Kozma (1991) takes issue with Clark and insists that some students can take advantage of a particular medium's characteristics to help them construct knowledge via mental model formation (see Section 2.5). Kozma calls for a continuation of media research, but with a focus on the effects of media on learners' mental representations and cognitive processes [27].

Recently, Kozma (1994) has again replied to Clark's remarks by declaring that media can work with methods collectively to influence learning. This makes it difficult, if not impossible, to isolate the effects of media and methods. Kozma uses the example of a molecular animation to teach chemical equilibrium. He questions whether it would be possible to use a different medium to convey the same message. Changing the medium would inevitably require a redesign of the method [28].

Another instructional technologist, Robert Reiser, is also an advocate of the influence of media on learning. He states that Clark is correct in insisting that methods are what cause learning to occur. However, Reiser notes that Clark overlooks the fact that media have certain attributes, and in certain situations those attributes are unique and not readily independent of methods [29].

Tennyson (1994) offers a useful overview of the current state of the media debate by summarising the positions of the authors involved. He considers the whole debate similar to a general problem in science, that is, those involved are trying to generalise their paradigm to a complex world. Tennyson suggests a more integrated solution to the issue, such that media do not influence learning unless they are linked to the method. Like Kozma, he believes that media are always embedded in a complex association with the instructional method, learner variables, content, context and risk. Therefore, researchers should remain flexible and embrace the complexity of media evaluation. Tennyson concludes that the central role of media in instructional design ensures that the media or method debate will continue for many years [30].

1.7 New Directions for CAL Evaluation

1.7.1 Introduction

The inadequacy of media comparison and replication studies highlighted by the media debate has prompted several other workers to propose more fruitful paths for the evaluation of CAL. These methods have been rarely used to date, but they promise to yield a sound scientific foundation for the design of instructional courseware [16].

1.7.2 Research Framework

In addition to criticising previous work, Clark has made suggestions for future developments in instructional technology research. He highlights the fact that many workers spend too little time reviewing the psychological literature preceding their research and too much time detailing the methods used in their studies. Clark suggests that workers should go beyond descriptive methods and adopt a prescriptive research methodology. In this way, the emphasis will shift from *what* was done in a study to *why* it was done. Only then will research lead to effective training methods for increasing achievement and motivation [20].

A further area for investigation is suggested by Ullmer (1994). He believes that interaction is the key learning process since it allows users control over their learning (see Section 2.8.3). Ullmer suggests that the research focus should shift from measuring a medium's efficiency in delivering content towards assessing how well students adapt to this freedom to apply their own learning styles [31].

Several recommendations have also been made to improve the basic design of CAL studies. In keeping with the conclusions from several metaanalyses (see Section 1.5), several workers highlight the fact that few CAL evaluations are conducted in realistic settings. Therefore, the ecological validity of most work is jeopardised [11, 32-35]. Yildiz and Atkins (1993) note that an authentic environment is essential to allow innovative media to be exploited to their full advantage. This increases the chance of novel learning benefits revealing themselves [8].

The short duration of evaluation studies has also been criticised. In particular, Reeves (1992) analysed study duration times and found the average to be around 30 minutes, which is far too short for learner attributes to take effect. Reeves concludes that CAL studies lasting many hours, extended over several days or even weeks are required to validate results [21].

An innovative direction for multimedia research is suggested by Reeves (1993). He suggests that qualitative methods, such as observations of user behaviour, are employed to redirect multimedia evaluation towards more meaningful outcomes. These observations could then be related to existing learning theory, which may highlight areas for later quantitative examination. However, Reeves warns researchers against applying qualitative methods as badly as quantitative techniques have been used in the past [36].

1.7.3 Triangulation

The concept of collecting quantitative and qualitative data in a study is taken further by Reeves (1994). He uses the term 'triangulation' to describe using multiple measures with the aim of converging more accurately on a variable associated with learning. For example, a multimedia designer wishing to find out about the motivation of learners using a product may use a combination of techniques such as, a questionnaire, an interview protocol and user observations to estimate motivation. Reeves notes that in the triangulation approach, errors in one type of measure are assumed to be cancelled out by errors in another measure [37].

A successful use of multiple measures for evaluating multimedia courseware is described by Barker and King (1993) (see Section 2.7.2). This study combined expert evaluations, user trials and verbal observations in the evaluation of 43 multimedia products. The subjectivity of the evaluation was carefully controlled to give validity to the exercise. The multi-facetted approach resulted in several innovative interface design features revealing themselves, which were not anticipated during the design of the study [38].

1.7.4 User Modelling

In an attempt to move research towards more prescriptive outcomes (see Section 1.7.2), Reeves (1992) suggests that the computer is used to model the user of interactive multimedia courseware. Reeves explains that the powerful data collection capabilities of CAL lend themselves particularly well to computer modelling, enabling researchers to embrace the complexity of a learning situation. In this way, a complex array of input variables and instructional treatments can be related to multiple outcomes. The derived relationships can then be used to help explain the effects of instructional software [21].

To illustrate his point, Reeves quotes a study by Gustafson *et al.* (1990) that adopted a user modelling approach to evaluation. In this investigation, data collection routines were incorporated into HyperCard [39] stacks which recorded student paths through the courseware, their selections, time spent in various learning tasks and responses to questions. Analysis of the data revealed unexpected insights into menu structure, student understanding of options and fluctuations in their motivation levels [18].

A more theoretical approach to user modelling is suggested by Jih and Reeves (1992). Since interactivity is a crucial component of CAL, these workers call for research on the mental models (see Section 2.5) that users form as they interact with such systems. Jih and Reeves suggest that mental models are assessed at appropriate points in the courseware, by asking users to provide reasons for their actions and to explain how certain parts of the program work. Research on mental models will identify important characteristics of cognitive processes and help in the development of guidelines for designing interactive learning systems [40].

1.8 Chapter Summary

In this chapter, the different strategies used for the evaluation of instructional software over the past twenty years have been discussed. The traditional techniques of media comparison, media replication and Aptitude-Treatment Interaction (ATI) research are widely criticised because of flaws in the theoretical approach or basic experimental design of almost all published work.

More recently, qualitative methods have been suggested as an alternative approach to evaluation. Several studies show that in combination with quantitative methods, a rich picture of courseware effectiveness will emerge. A more theoretical strategy of studying the mental models that users form during their use of CAL has also been proposed.

Twenty years of quantitative research on CAL has produced an inadequate basis to guide the development of interactive learning materials. If the recently described approaches are followed, interesting research and findings will undoubtedly result. This in turn will have an impact on future CAL developments and extend our knowledge of instructional theory. To achieve this, CAL researchers must pay attention to the organisation and clarity of their work, the internal and external validity of their experiments and they must avoid proven unfruitful research approaches.

Chapter 2

The Design of CAL

"Historical accident has kept programmers in control of a field in which most of them have no aptitude: the artistic integration of the mechanisms they work with... Learning to program has no more to do with designing interactive software than learning to touch-type has to do with writing poetry."
(Ted Nelson, 1990)

2.1 Introduction

Successful CAL programs require more than state of the art hardware, adequate content and effective student evaluation. The user-friendliness of software is also of concern to courseware designers [41]. If confusion is involved in using programs specifically designed for education and training, the effects on learning are especially detrimental [40]. Moreover, if the learner has to concentrate on using the interface, then attention will be drawn away from the domain being taught [42]. Since the student-computer interface provides an entry point to the content it must be carefully designed if it is not going to limit the quality of the interaction [41]. Therefore, a successful CAL interface is transparent and enables the user to interact directly with the content [43].

Until recently, interface design has been a neglected issue in educational software development [44, 45]. It is commonplace to see designs driven by the technology, with the user's needs being largely ignored. However, more powerful authoring systems and multimedia technology have greatly broadened the interactive capabilities and complexity of CAL. Consequently, the quality of the interface has become an important design issue [44, 46].

Design encompasses several separate issues in CAL development, principally interface design (*i.e.* the learning environment), instructional design (*i.e.* pedagogical aspects) and graphic design (*i.e.* visual quality). To ensure the production of a consistent, responsive and dependent teaching tool, attention must be given to all three of these issues during the authoring process.

This chapter describes the design of CAL, from the initial planning stages to the design of the interface and the instructional content. Issues related to the incorporation of multimedia into CAL are discussed separately as this has produced several unique problems for the courseware designer.

2.2 The User Interface Design Cycle

2.2.1 Introduction

The iterative design-test-modify cycle shown in Figure 1 is used for most software development and is universally recognised as the only reliable route to a successful interface [2, 47]. It is sufficiently adaptable to be used in many environments, including CAL development programmes. The user/task analysis takes place first. The requirements for the interface can then be specified, taking both the needs of the user and established interface design standards into account. Prototyping of the package takes place next, either as a paper storyboard or as a simplified working version. The prototype is evaluated with real users at various stages (see Chapter 3) until the usability of the system has been maximised and a satisfactory interface is produced. The components of this design cycle and their relevance to the design of CAL are described below.

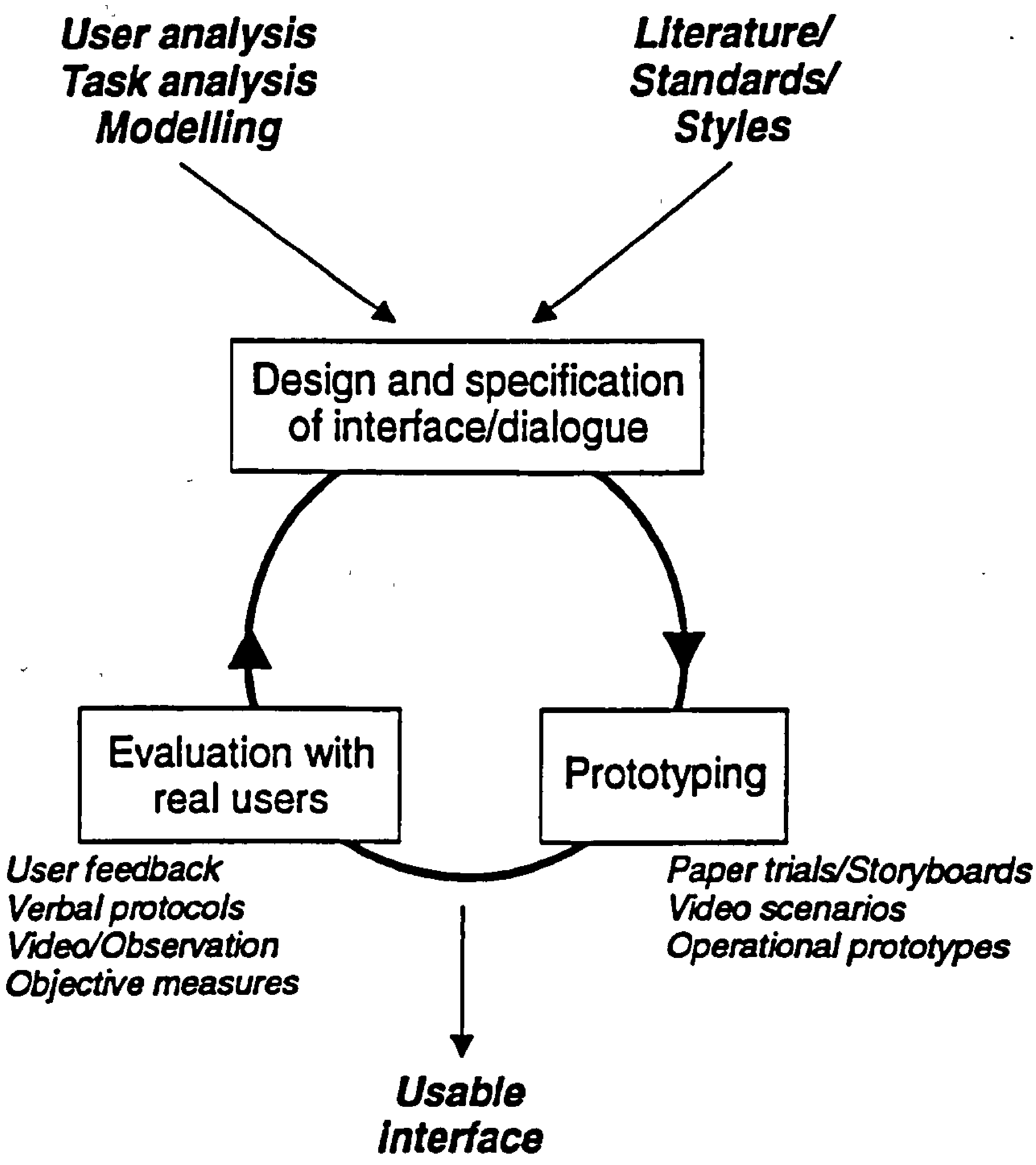

Figure 1 The *design-test-modify* interface design cycle

(modified from Waterworth, 1992) [61].

2.2.2 Task Analysis

Task analysis examines the needs of the user and their use of the present system in order to establish a set of functional requirements for the new system. It should therefore precede the design process. In the analysis, a set of questions are asked concerning what the users do now and exactly what the new system is expected to do for them. Who is the user? Where is the task performed? How is the task learned? How often do users perform the tasks? The answers to these questions provide an input to the design process by giving an in-depth knowledge of the user's needs.

In CAL design, the results from the task analysis should be combined with those gained from user modelling, which addresses amongst other things, the instructional design of the proposed courseware [43]. What teaching styles will the interface need to deliver? How much learning diversity will the interface need to accommodate? What activities will the users need to perform during their interactions (*e.g.* use a calculator, takes notes, use a glossary, etc.)? The answers to these and other questions are then combined with the technical requirements and limitations of the target hardware and software. The result is an accurate list of functional requirements for the new system.

2.2.3 Prototyping

Prototyping is the development of a visualisation of the user interface early in the development life-cycle. It allows the designer to be creative since it involves no theory or specific methodology [48]. Therefore, it is suitable for CAL development as an innovative interface may be required to allow a new media type or learning style to be incorporated. The evolving prototype should be a simplified version of the proposed software. Modern authoring systems make the prototyping of CAL relatively easy (see Section 2.3). Once accepted, the prototype can be further developed into the final deliverable.

2.3 Authoring Systems

Authoring systems are high level environments for generating interactive courseware. They are designed to enable programs to be produced quickly and without the need for low level programming [43]. This is often achieved through an object-based interface, using a set of icons to represent the required operations [49].

All of the available authoring programs have their particular strengths and weaknesses and the system of choice depends on the requirements of the proposed courseware. One important feature of modern authoring systems is their ability to execute external programs and low level code to extend their flexibility [43, 50]. On the Windows platform this includes the ability to load and run dynamic link libraries (DLLs). Another important consideration is the availability and legal status of a run-time environment for the authored courseware. Most authoring systems are distributed with a run-time version of the development package and this must be distributed with the courseware to enable it to be executed on remote systems.

The instructional design of courseware is still the realm of the author and not the authoring system. Furthermore, authoring systems are often criticised for not taking account of learning theories [35]. King (1994) proposes that future systems should include cognitive strategy tools to help the courseware designer produce material that follows established theories of learning [51].

2.4 Courseware Architecture

A frequent limitation of CAL systems is their lack of adaptability. Courseware is most often developed in a read-only form, such that it offers no opportunity for the teacher to amend or update the content. This inflexibility has been an important limitation and has reduced the acceptance of CAL in education.

The structure of CAL can be divided into functional units that, if separated at the design stage, provide more system adaptability. Park (1992) suggests that the content (*i.e.* the media) and instructional logic of hypermedia systems should be kept separate for this reason [52]. Tait (1993) goes further, by recognising that CAL systems have a four part architecture: content, presentation, interaction and control [53]. He proposes that the content should be expressed independently of the presentation and interaction (*i.e.* the interface). He explains that the content evolves rapidly but the user interface is only updated at intervals. By adopting this structure, teachers can concentrate on updating the content whereas the user interface can be revised independently by the designers. If CAL is modularised in this manner then the resultant courseware will be more reusable and less susceptible to what Khan (1995) calls software corrosion [35].

2.5 Mental Models

Successful users of CAL systems possess adequate 'mental models' of the form and function of the program's user interface [54]. Sein *et al.* (1993) explain that a mental model is the user's internal understanding of the structure and functionality of a system and it guides their interaction with the program [55]. Users are less likely to become disorientated with a CAL program if they understand how the system works [40]. Incorrect mental models, on the other hand, introduce confusion and focus the user's attention on the shortcomings of the interface rather than the content. Therefore, an accurate mental model is necessary for maximum performance, particularly in tasks that require extension of knowledge to new contexts.

Users can create their mental models by using the system (mapping via usage), by drawing analogies from other systems (mapping via analogy) and through training (mapping via training). Complex mental models can be created that use a combination of these mapping techniques [55].

An influential publication by Kozma (1991) discusses how the characteristics of media can effect the structure, formation and modification of mental models. Kozma suggests that computers can be used to symbolically represent entities that might help mental models to form. More importantly, instruction can be designed to illustrate abstract entities that novice users, in particular, do not usually incorporate into their mental models. For example, an arrow representing velocity can become longer or shorter depending on the direction of acceleration. By interacting with such abstract objects, novice users may become aware of any inaccuracies in their models. Through continued use, they are able to move to more accurate mental models of the phenomenon being taught [27].

Preece (1994) also observes that the mental models adopted by inexperienced computer users are often vague and incomplete. Furthermore, she suggests that it is hard to find empirical evidence for the existence of these models at all. However, Preece argues that interface designers should concentrate on those methods that will invoke appropriate mental models [56].

2.6 CAL Interface Design

A good interface is transparent to the user, but few actually achieve this. Many interface design guidelines exist, from the most general to the more specific. Most of the established guidelines for CAL interface design are common sense, but designers continue to ignore even the most basic principles [45, 57]. This is not helped by the fact that screen design guidelines have not kept pace with developments in computer technology [58].

Both Apple and Microsoft have published detailed design recommendations [59, 60]. It is widely recommended to follow such standards unless there is a good reason not to do so, since students will resent having to learn new conventions and procedures [43]. But within this framework there should still be room for innovation in interface development [61, 62]. This is supported by Staples (1993) who concludes that there are many unexplored opportunities in the visual design process [63]. In this section the full spectrum of CAL interface development is covered, from general principles of usability to the basic elements of screen design.

2.6.1 Usability Guidelines

To ensure that a usable system is developed, usability guidelines should be used in the design process. These guidelines are general purpose but those of relevance to the design of CAL are outlined below.

- *Consistency* [2, 41, 64, 65]

Consistency aids the learner decide where they are in the program and what they should do next. This includes all visual aspects, such as text style, techniques of erasure and the use of colour. Consistent screen layouts reduce the 'cognitive load' placed on the user, therefore reducing the burden on their short term memory.

- *Simplicity* [41, 43, 46]

The interface should be logically organised, uncluttered and pleasant to use.

- *Naturalness* [43, 65]

The system should be intuitive to use and allow the user to perform the required tasks with a minimum of confusion.

- *Learnability* [43]

The amount of training required to use the system should be minimal.

- *Supportiveness* [43, 46, 66]

An important feature of CAL is the availability of an appropriate set of end-user tools and services (*e.g.* note book, glossary, help, etc.) appropriate to the task that the user has to perform.

- *Relevance* [41, 46]

Only material of direct relevance to the current task should be displayed on the screen. Also, the availability of user services should be carefully controlled to reduce complexity.

- *Flexibility* [43, 44, 62, 67]

The courseware should be sufficiently flexible to be able to cater for different user learning styles, requirements and preferences.

2.6.2 Functional Areas

An intuitive technique for organising CAL displays is to divide the screen into several well-organised functional areas [68]. A comparative study by Aspillaga (1991) shows that displaying text at a consistent location, and of relevance to graphical information, facilitated learning [69]. Galitz (1993) further suggests that functional areas of related items can help users navigate through a program [64]. These functional groupings can be separated by shading, lines or boxes and may change in size throughout the courseware, but the basic layout should remain the same. In an instructional program this will help learners to focus on the content without constantly having to search for the options they require [2].

Any arrangement of functional areas may be used, but research has shown that some orientations are more desirable than others. For example, information that should be seen first must go on the left and/or top of the screen [2, 43, 64]. The centre of the screen is usually reserved for the content of the courseware, with navigation and orientation information positioned around it.

Heines (1984) identifies five standard components that should be present on a CAL screen [70]:

- *Orientation information*

The user needs to constantly know where they are in a lesson. This information can be supplied by putting the section and sub-sections headings at the top of the screen. The orientation information is generally for reference only, therefore it is best to display it subtly to highlight this fact.

- *Directions and learner responses*

Directions tell the user what to do next and therefore help with the response. Many displays are intuitive and will not require this component.

- *Error messages*

These should always be presented in the same area of the screen.

- *Student options*

These options consist of relevant tools to which the user may want access at any time during the course of the lesson (*e.g.* help, notebook). The selection of tools may vary throughout the lesson.

- *Text and graphic areas*

These are usually the largest areas on the screen with the others arranged around them.

2.6.3 Navigational Strategies

In CAL systems where navigation is under user control, such as hypermedia courseware [52], the problems of orientation in the information resource become particularly important [47]. Navigational aids are therefore required in these environments to provide orientation cues and to reduce the load on the short term memory (the cognitive load) of the user. The techniques used by designers to simplify user navigation include metaphorical interfaces, guides, maps, overviews, tables of contents, search and backtrack facilities and indexes [43, 47]. De Jong *et al.* (1993) warn against the over-provision of navigational tools, since this may distract the users from the content of the courseware. These workers suggest that the types of navigational aids incorporated into a package should be decided by its objectives, embedded media types and the user population [71].

The navigational strategies used in a CAL package have a major influence on the mental model (see Section 2.5) of the courseware held by the user [40]. Users automatically create mental models of the systems they interact with to make their interaction more efficient [43]. The navigational aids described below attempt to enhance the user's mental model of instructional courseware.

2.6.3.1 Interface Metaphors

An interface metaphor is a conceptual mapping between aspects of the user's mental model of a system and the real world [61]. This can be achieved in CAL by using familiar objects to represent the functionality of the program [72].

Common interface metaphors include a book, a library, a desktop and an encyclopedia. Metaphors based on such real world objects are extremely effective at reducing interface complexity by allowing users to capitalise on their existing knowledge [47, 73]. O'Malley (1990) emphasises the importance of consistency in the use of these metaphors as this will enable users to make correct predictions about the behaviour of the system and improve the effectiveness of their interaction [42].

The scope for interface metaphors has been increased with the introduction of multimedia systems. For example, the incorporation of sound into a metaphorical interface provides an unexplored opportunity for a mixed media metaphor [74].

The use of interface metaphors does have its problems and they should be chosen with great care, since badly chosen metaphors are counterproductive. In addition, Waterworth (1992) warns against over restrictive and cumbersome interface metaphors. Occasionally it may be necessary and even advisable to incorporate so-called 'magic' features that deviate from the metaphor model but provide extra and maybe vital power to the system. For example, a hypermedia system built around the metaphor of a map, which can be explored to navigate around information about a certain geographical region could be enhanced with such magic features as 'time cars'. This facility would allow abstract browsing, such as the comparison of features at different periods of history [61].

2.6.3.2 Maps

A graphical map of courseware structure is a particularly effective navigational tool [16, 75]. These maps are more effective than text-based spatial descriptions [62]. They can be used to show the current position in the system [46] and if correctly designed they can reinforce the system metaphor [43] (see Section 2.6.3.1). Within hypertext and hypermedia systems in particular, where navigation is non-linear and under user control, overview maps are an essential orientation aid [76].

Reeves and Harmon (1994) describe an extension to the map concept. This involved the recording on the map of those parts of the system that have already been visited. This technique can help to alleviate user-disorientation. They caution against providing too much information on the map, as this may result in more confusion [58].

Preece (1993) emphasises that our knowledge of effective map design for hypermedia is incomplete. As such systems grow larger and more complex, so the maps they contain must become more intuitive and flexible [47].

2.6.3.3 Guides

Guides, or intelligent agents, are another solution to the problems of hypermedia navigation [77]. The notion is that a computer-generated character can mediate between the computer and the user by giving overview tours of the system, providing context-sensitive advice, suggesting next moves or locating specific information [47]. In doing so, they increase user motivation and make the system more engaging [78]. Also, Park (1992) suggests that learners make better decisions with guidance [52].

A guide can be presented in any media format, but in a study by Austin (1994), a video of a 'talking head' was shown to elicit the greatest response from the user [79]. Austin concludes that the video was more authentic than just audio, or a still image with audio narration, since the users could watch the lips and expressions of the subject. Therefore, by exhibiting some of the multi-modal communication characteristics of its human source, the user saw the guide as more valuable. The disadvantage of such an attention-holding device is that users devote more of their time listening to what the guide has to say. This may disrupt their learning of the subject material in the program.

Conversely, guides can be used to aid the learning process by providing point of view on the information contained in the system. The use of multiple guides, with each one offering a different perspective, may be a valuable way to help users form new concepts and intuitions about information [80].

Laurel *et al.* (1990) suggest that guides may have a further benefit, by helping to alleviate the problems of media integration at the interface, particularly between dynamic media (such as video) and static media (such as text) [80]. They could achieve this by providing suggestions for next moves to any media type, for example, play a video clip then read some text, or read some text then interactively rotate a molecule.

The design of guides must be carefully controlled to ensure that they do not mislead users into performing inappropriate actions. In particular, Nass and Steuer (1993) show that different computer-generated personalities elicit variable responses from users. They postulate that gender, age, quality of voice, language and pictorial representation may also affect the user response [81].

2.6.4 Cursors

The shape of the pointing device or cursor on the visual display is often used within computer applications to show the current state of the program. This technique has been extended to interactive courseware since modern authoring systems, such as Authorware Professional, allow the cursor to be set to a system or user-defined shape [82]. For example, the cursor can be changed to a pointing hand to indicate that it is over a hypertext area and an hourglass cursor can be used during background activities that prevent interaction momentarily [64]. By changing the cursor to a shape relevant to the activity currently being performed, user confusion will be reduced with a resulting boost to their system confidence [38].

2.6.5 Colour

Software designers often lack the training and visual perception of the graphic designer or artist [83]. Consequently, the use of colour on the computer screen often causes difficulty for CAL designers. However, there are a number of guidelines gained from using colour on the printed page that are equally applicable to the computer screen.

Research into the effectiveness of colour in the learning process has produced mixed results but it is generally believed that colour enriches learning materials and helps with the retention of information [84]. Most of this work has focused on media other than the computer screen, but it is probable that the conclusions made will be transferable to the computer display [85]. Donahue (1973), for example, reports that college students judged colour films as more pleasing and significantly more interesting than black and white presentations [47]. Apart from being more visually engaging, research also suggests that colour is easier to discern than size or shape [86]. The use of colour for distinguishing between different types of information is therefore a recommended design technique.

Common meanings for colours should also be transported onto the CAL interface, since these meanings already exist in the world at large and users find them very difficult to unlearn. Galitz (1993) lists some common colour associations that should be considered during the CAL interface design process [64]:

- *Red* - Stop, fire, hot, danger.
- *Yellow* - Caution, slow, test.
- *Green* - Go, OK, clear, vegetation, safety.
- *Blue* - Cold, water, calm, sky, neutrality.
- *Grey* - Neutrality
- *White* - Neutrality
- *Warm colours* - Action, response required, spatial closeness.
- *Cool colours* - Status, background material, spatial remoteness.

As with other screen design elements, colour should be judiciously used in interactive courseware, as poor usage may impair performance [43]. Many studies show that the maximum number of colours a user can effectively distinguish is between four and ten, with emphasis on the lower numbers [64]. Clarke (1991) concludes that the use of more than seven colours on the CAL display is confusing and requires the user to spend more time decoding the information [87].

Besides the quantity of colours used, colour combinations are also an important consideration in courseware design. The basic principle is to aim for the best contrast between background and foreground colour. For example, extreme colour pairs such as red and blue or yellow and purple should be avoided. This will avoid frequent refocussing and visual fatigue. Colour blindness must also be taken into account, since between 7 and 10% of the population are colour blind. Certain colour combinations, for example, red and green should therefore be avoided [83]. An effective solution to the problems of visual handicap is to allow the user to select their preferred colour combinations.

2.6.6 Electronic Text

The presentation of text on computer screens has received a great deal of attention [46] but there are still few empirically-based guidelines for the design of text in ways that ease learning [68]. One distinction that has been made is the difference between screen and page-based text. For example, screen text can be dynamic and interactive [85] which creates new possibilities for the design of learning materials. A further consideration for CAL design is that users read screen text 20-30% more slowly than paper text, though comprehension remains the same [43].

The density of text is an important factor in determining the efficiency of reading from a computer screen. It is generally accepted that text on the screen should be well spaced and kept to a minimum [46, 68] and segmentation into logical blocks and the use of headings will improve comprehension [88]. In addition, lines of text should be no more than 40-60 characters in length and sentences should be less than 30 words long. If these guidelines are coupled with an active, personal writing style (as if addressing the user) then engagement will be maintained [64].

The characteristics of different fonts can also be used to improve the quality of CAL text. For example, sans serif fonts, such as Helvetica, are often used for titles and headings to make them stand out. However, serif fonts, such as Times Roman, are more readable for large blocks of text because the serifs help the eye to track across the page [43].

2.6.7 Static Graphics

In a review of the use of graphics in CAL, Siliauskas (1986) observes the shift from textual to graphic orientated courseware [89]. The instructional benefits of this illustrated courseware are observed by Kozma (1991) [27], and this view is held by most designers of CAL materials [45, 46, 85]. The broad 'band width' and the fact that different elements of an image can perform different functions may partly explain why pictorial communication is effective [72]. However, graphics are often used as an additional extra in courseware, which suggests that designers do not understand the principles of using illustrations to enhance learning [90].

A complete set of guidelines for using graphics in CAL are lacking but the assumption is that those derived from illustrations in printed materials are transferable to the computer screen.

Clarke (1992) brings together several recommendations for using graphics in computerised instruction. For example, it is generally accepted that graphics should be accompanied by explanatory captions and should be related to the main body of text or they will not enhance learning. In addition, pictures can sometimes be used as substitutes for words or as providers of non-verbal information [85].

2.7 Multimedia CAL

2.7.1 Introduction

Multimedia CAL uses more than one medium for the distribution of information to the user. The media used in such packages include a selection of sound, music, animation, text, narrative, video and images. Multimedia courseware has the potential to provide clear, error free communication. However, Tognazzini (1990) highlights that multimedia instruction also has the potential for causing utter confusion [91]. Every medium has its own instructional attributes and weaknesses [17] and when combined, they have the potential to reinforce or interfere with other media in the package [92].

Research suggests that multimedia packages are more engaging than other methods of instruction [93]. Hapeshi and Jones (1992) suggest that this is because multimedia courseware represents real life events to the user that they can relate to more easily than traditional text-based instruction [94].

It is also proposed that multimedia courseware results in better retention of information. The 'dual-coding' theory has been established to explain this observation. This theory was first put forward by Paivio (1979) who suggests that there are distinct verbal and visual models of material representation [95]. The theory predicts that learners will remember and transfer material (into long term memory) better if they encode the information both visually and verbally. Such a dual media representation will give users two separate ways of finding the information in memory [96-98]. The dual-coding theory of multimedia learning is illustrated diagrammatically in Figure 2.

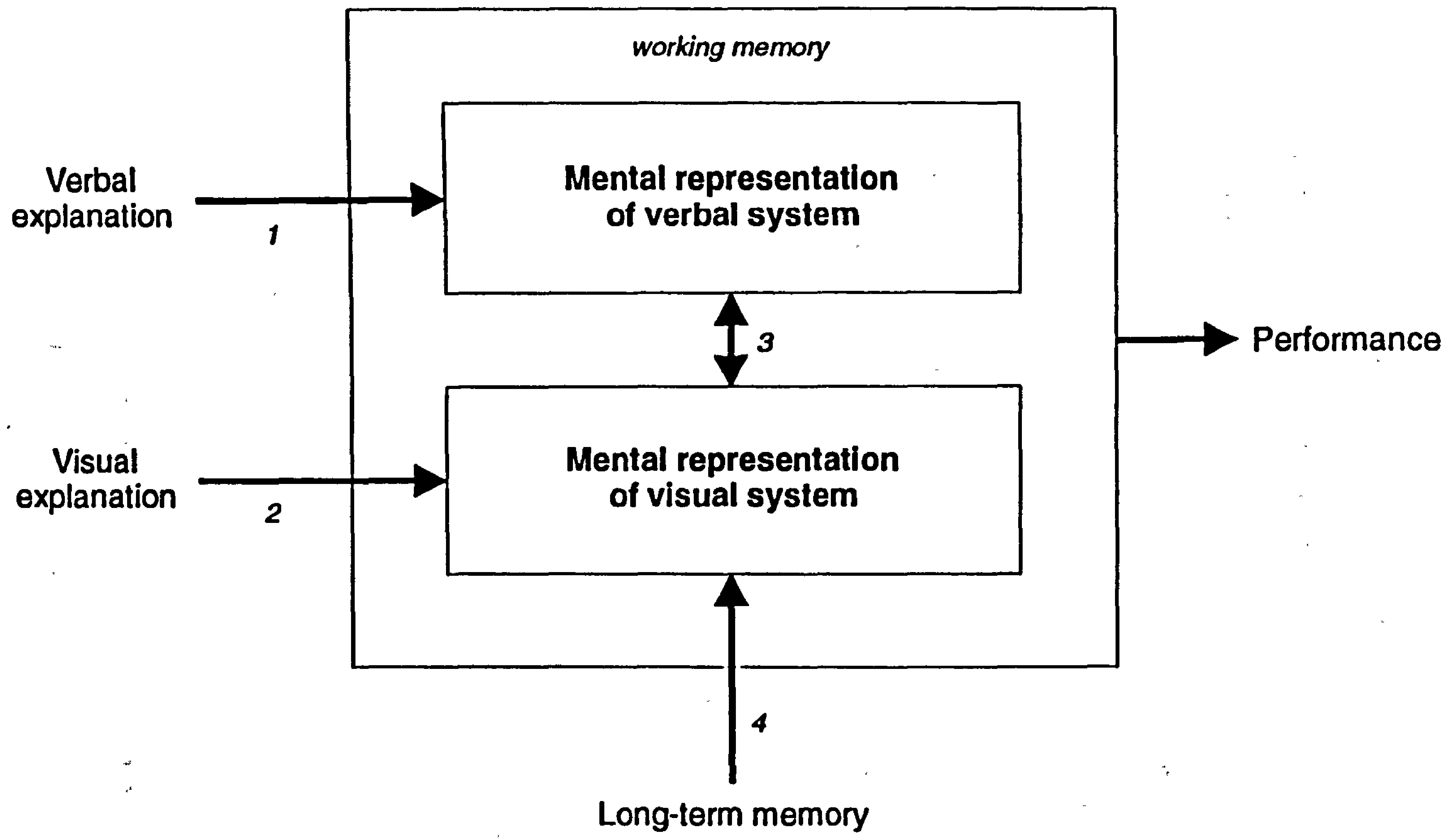

Figure 2 The 'dual-coding' theory of multimedia learning (after Mayer and Sims, 1994) [97]. 1) Building of verbal connections, 2) building of visual connections, 3) building referential connections, 4) retrieval from long-term memory.

More recently, the dual-coding theory has been extended to include learning from multimedia applications. For example, Park and Hopkins (1993) propose that verbal explanations of animations lead to more effective mental model formation [99]. Mayer and Anderson (1991) also examine the effects of narration on learning from animations. They showed that when animations were accompanied by narration, more creative solutions were created on problem solving tasks [100]. In a more recent study, Mayer and Sims (1994) suggest that spatial ability is a key factor in determining the ability of users to create referential connections between verbal and visual information in a multimedia package [97]. However, all possible combinations of media presentation have not been examined and designers still do not fully understand how people learn from words and pictures.

Reeves and Harmon (1994) observe that most currently available multimedia packages are limited to tri-media or even bi-media [58]. Though, as Kentish (1989) points out, the production of multimedia CAL is rapidly increasing as the technology for handling it improves and becomes more cost effective [101]. These technological limitations have left many unexplored media combinations, though it is not known whether all combinations stand to enhance the user learning experience. Research in this area has been hampered by the innovatory nature of multimedia packages, since it is generally not known how a new medium will work and therefore it is difficult to measure its effectiveness [102]. The production of quality multimedia courseware therefore continues to be an exploratory challenge for the instructional designer [65].

This section examines the qualities of dynamic media that should be considered during the CAL design process. The design of the multimedia user interface and the integration of media into instructionally effective courseware are also considered.

2.7.2 Multimedia Interface Design

The most important issue in the design of multimedia systems is the provision of intuitive and consistent access to the complexity of multimedia data. The emphasis is on enabling the user to browse through the courseware without getting lost in the information.

Research into multimedia interface design has addressed navigational issues and several guidelines have been proposed. Tognazzini (1990) suggests that user navigation should be reduced or eliminated by avoiding complex menus and by designing systems with a user-centred approach. In addition, users should be provided with clear, visual communication and central landmarks such as overview maps should be provided to help with navigation [91]. Further mechanisms to assist with multimedia navigation are described in Section 2.6.3.

Barker and King (1993) carried out an in depth analysis by evaluating 43 interactive multimedia products, and found many desirable interface features and novel ideas. High quality interactivity, navigation (*e.g.* maps), context-sensitive help and user support (*e.g.* glossaries) were found to increase the effectiveness of the packages. The use of an audio track to enhance text or graphics, spreading the user's cognitive load across another sense, was also very powerful. Software adaptability was another valuable feature, enabling the users to structure the data according to their chosen learning style [38].

The importance of allowing different learning styles in multimedia courseware is also stressed by Koumi (1994). There are several ways in which adaptability has been integrated into multimedia CAL. Some applications allow the interface to be prioritised towards text, video or sound [43, 103]. Austin (1994) describes another technique, which is to allow the user to disable the audio or visual components of a motion video clip independently [79].

2.7.3 Motion Video Design Issues

With the technological advances in computer hardware, the dynamic visual display has become a primary component of instructional courseware. In an extensive review of studies comparing the learning effect of static and dynamic visual displays, Park and Hannafin (1993) conclude that dynamic displays, such as motion video, are generally more effective than static visuals [99].

The broad band width of motion video is an important consideration for designers of instructional courseware, since it dramatically increases its social presence [104]. For example, Austin (1994) observes that users perceived 'talking head' video as more authentic since they could see the movement of the lips and variety of expression in the subject [79]. This realism makes motion video particularly suitable for social, dynamic or informal communication within CAL [104, 105].

Along with the advantages of motion video there are several undesirable features that the multimedia author must attempt to control. A consequence of the realistic presence that video can create is the possible humanisation of the computer by the user. Hapeshi and Jones (1992) explain that this may induce undesirable behavioural changes from the user [94]. This realism may also demand more of the user's time because of the complexity and engaging qualities of video material [79].

A further issue is highlighted in a study by Gustafson *et al.* (1990). They conclude that motion video can be distracting because of the attention that it demands from the user. These workers suggest that video incorporation be carefully restricted so that undesirable effects such as these do not occur [18]. Further issues related to the integration of video and other dynamic media into CAL are discussed in Section 2.7.5.

Another well-documented criticism of motion video is that most users adopt a passive stance towards it since they see it as a familiar medium [88, 106-109]. Consequently, they will invest less mental effort in processing the information it contains so reducing its effectiveness as a learning resource. A solution to this passivity is to make the video interactive and challenging by interspersing small clips with questions and tasks for the user to perform [106]. Cennamo (1993) calls for further investigation into the dominance and passive attitude of users towards motion video [108]. This is particularly important since multimedia designers are now incorporating other dynamic and interactive media into CAL.

2.7.4 Audio Design Issues

When compared to what is known about the visual aspects of instruction, not much is known about the use of audio in courseware [74, 110, 111]. Until recently, the use of sound at the interface has been restricted by computer hardware to providing alert and feedback information [56]. This may account for the absence of a proven set of guidelines for the incorporation of sound into instructional computer software.

As the multi-modal output of computers increases, the benefits of using audio to reduce interface complexity have become more attractive [56]. Sound demands more mental processing by the user than visual information [108, 112] and this can be used to good effect in the CAL design process. Brown *et al.* (1989), for example, suggest that auditory cues can be used to direct attention to certain areas of the visual display, therefore freeing screen space for other purposes [86]. Aarntzen (1993) supports this idea and further suggests that audio can be used to announce events, motivate the user and complement concurrently presented visual information [110].

To ensure that the most effective use is made of audio in CAL, the specific qualities of the auditory channel must also be considered during the design process. First, it is difficult for the user to pace themselves and backtrack through audio material because of its transient nature. This problem can be alleviated by using short sound clips [94] and by providing a repeat clip option [110]. The fact that audio is a serial medium is another limitation of this channel but, as Unnava *et al.* (1994) point out, it makes speech particularly effective for describing ordered events or sequences of instructions [113].

Another important quality of audio is its dynamic nature since, as Mayes (1992) suggests, this may lead to memory overload by the user [74]. This concern is also addressed by Alpert *et al.* (1995) [78]. Both researchers conclude that sound clips should be followed by a delay to give users time to process the audio information.

CAL designers should also consider the broad band width of audio. In a similar way to video, this attribute increases the social presence of the audio channel [105]. With careful design of audio material this effect can be used to help the learning process. For example, the mode of a voice may act as a handle to the information in memory. Though, as Aarntzen (1993) concludes, much more research is required on the effects of different voices and gender on learning from audio material [110].

A more practical concern regarding the increased use of audio in courseware is that of noise pollution. Control measures are required to solve this problem, which may include the use of headphones or quiet directional speakers [56, 94].

2.7.5 Media Integration and Selection

Among the most important issues for designers of multimedia CAL are how to combine the media and which media to use for presenting different kinds of information [47]. Prosser (1984) further emphasises that the way media are used and integrated into an instructional lesson is as important to its success as the quality of the media [114].

A recurring criticism of multimedia CAL is that the media appear to be tacked onto the interface and that, consequently, they disrupt rather than enhance the learning process. In addition, the most common practice has been to design packages based on technical or economic grounds and courseware objectives have often been invented to justify the use of a particular medium [17].

The coordination of multimedia materials to produce effective instruction is a difficult task [77]. However, Romiszowski (1993) suggests that the multimedia author should focus on instructional design issues and use the most appropriate media for the desired learning outcomes [115]. For example, if motion is required for a particular task, the medium that illustrates motion most effectively should be used [116]. Mayes (1992) considers attention holding to be the key aim of multimedia designers. He suggests that changing the modality (*i.e.* mixing the media) throughout a package will help to maintain the attention of the user [74].

The integration of multimedia into CAL presents several problems for the courseware designer. An important issue is how dynamic media, such as video, audio and animation are controlled by the user. The author must decide whether to make the controlling devices for these media (*i.e.* how the user interacts with them) compatible with those for static media such as text and images. A seamless integration of all media types through using a consistent interface is recommended [80], but this should not limit the introduction of innovatory control devices. In these cases some new media control device should be incorporated into the design of the user interface [61].

There are few definitive guidelines for the integration of multimedia into instructionally effective courseware [43]. However, research on learning from television has been extended to CAL to provide pointers for the combination of dynamic media such as video and audio.

It is generally accepted that if sound and vision are carefully combined in instructional material, they will work together to focus attention and aid comprehension [17, 27, 74, 110, 111, 117]. However, it is critical that the media correspond with each other (*i.e.* they embody the same message) to ensure the clarity of the information [88, 118]. For example, a study by Grimes (1990) shows that users who experienced the highest correspondence between audio and video exhibited the most efficient division of attention and the best memory scores following use of the courseware [112]. This recommendation is supported by other studies [94, 108].

The issue of media correspondence arises because of the relative dominance of the visual channel over the audio channel. This has been demonstrated in a study by Austin (1994) which shows that the audio component of a lesson is ignored if a different visual message is shown concurrently [79]. Grimes (1990) explains that visual messages do not require as much attention as audio to be decoded by the user. Consequently, in a complex audiovisual presentation, users will devote most attention to the visual channel [112]. Therefore, the instructional designer must be aware of the potential redundancy of the audio component in a package [17, 119].

The simultaneous presentation of visual and verbal narration is another factor that influences the instructional quality of CAL. Baggett (1987) suggests that the visual and verbal components in a lesson should ideally be in synchrony. However, if the lesson design prevents this, the visual component should always precede the verbal narration. This ordering of visual and audio components has been shown to result in the best retention for learning a procedure [120].

2.8 The Instructional Design of CAL

2.8.1 Introduction

Courseware produced by combining modern authoring systems with multimedia technology does not guarantee learning for the user [16, 121]. Computer software designed for instructional purposes should incorporate known principles of effective teaching and learning, such as those derived from classroom teaching, to maximise the quality of the user learning experience [122, 123]. Unfortunately, as Romiszowski (1993) observes, technology is currently leading the development of interactive multimedia courseware in non-pedagogically ideal directions [115].

Taking account of the concepts described in this section will help ensure that CAL maintains the instructional effectiveness of traditional teaching methodologies.

2.8.2 Designing for Learning

The basis for most of the principles of instructional design is the maintenance of user motivation throughout the lesson [124], where motivation is exhibited as a will to learn and curiosity about the learning material itself [125]. Kinzie and Berdel (1990) address this issue of so-called continuing motivation, and describe it as an important technique to encourage users to really explore computerised instruction and learn [126]. This group have also proposed several guidelines which will help to ensure that user motivation is maintained throughout a CAL lesson. The presentation of challenging situations via the use of graphics and animation will increase curiosity with the content, as will user control over the medium and the theme used to present the material [121].

The sequencing of the content in a CAL lesson is also an important consideration if user motivation is to be maintained. Jekovsek *et al.* (1989) note that learners prefer to apply what they have learnt soon after they have learnt it [127]. Users should therefore be given the opportunity to experiment, for example, enter data or manipulate objects, soon after having learnt about the concept they are studying. This is supported by Hooper and Hannafin (1991) who suggest that independent user practice should be distributed throughout instructional courseware [88].

Motivating instruction promotes deep processing of the content [88], which leads to more understanding and retention of the information. Multimedia technology does provide opportunities for more motivating courseware [88], but these features must still be consciously designed into the software [128].

A set of guidelines are put forward by Shuell and Schueckler (1989), and they provide a basis for the instructional design of effective CAL [123]. Several of these principles are supported by other studies:

- Students should be informed of the instructional goals and objectives of the lesson within an easily understandable network [88].
- A check should be made to detect if a student has the prerequisite knowledge to use the courseware.
- The program should re-teach any information that the user is lacking.
- Material should be presented in steps or blocks appropriate for the subject matter and grade level [46, 51].
- The instructional portion of the program should be consistent with the stated objectives.
- The organisation and structure of the material being learned should be made clear to the learner [51].
- Appropriate examples should be made for guided practice [117].
- A check should be made to see if the student understands the material being learned.

- The learner should be provided with feedback on the adequacy of his or her performance [129].
- Re-teaching should occur in those areas where the learner is making numerous errors.
- Opportunity should be made for independent practice.
- The program should provide for closure, via a summary or review of important points of the lesson at the end.
- A profile of the student's strengths and weaknesses should be maintained for later review by the teacher.

2.8.3 Interactivity

Interactivity is probably the most important component of effective CAL [15, 31, 40, 66, 109, 123]. Interactive courseware promotes higher cognitive processes than passive courseware, such as, composition, analysis, synthesis, self-assessment and review, these being key qualities of effective learning material. Moreover, interactive instruction has been shown to result in more learning than passive instruction [2].

Emerging technologies, such as multimedia and modern authoring tools, offer more opportunities for interactive instruction, but they do not inherently induce more interaction than traditional media [88]. Effective interaction must be consciously designed into all instructional materials. Unfortunately, there is still little agreement about what constitutes meaningful interaction, but Bork (1987) suggests that the ideal human-computer interaction would be similar to a typical interaction between humans [130].

Interactivity must be carefully designed to avoid disrupting the learning process. To prevent this, both the mode and style of the interaction should be intuitive to the user [66]. In addition, the degree of interactivity integrated into CAL is subject to the constraints of user understanding, since if too much is provided, the mental capability (or cognitive load) of the learner may be exceeded. The degree of interaction incorporated should depend on the goal of the activity and the complexity of the concepts to be learnt [131].

Different levels of interactivity have been described that allow varying degrees of user control within computerised instruction. Goforth (1992) specifies two types of interactive control applicable to CAL, namely extrinsic and intrinsic control. For example, a student has *access* to recorded images (extrinsic control) but can *interact* with simulations (intrinsic control). Access control is extrinsic, since the features the learner manipulates in exploring the content are essentially independent of the content, as in searching through text. Interactive control is intrinsic in that the learner manipulates features of the content directly. Goforth suggests that the intrinsic control of interactivity offers the greatest potential for CAL [131].

Computer simulations and interactive graphics are possibly the most effective ways to give users interactive control over the content of CAL displays [99, 132]. These simulations of processes or objects allow learners to use their own learning style to explore and reason with the information presented. This active exploration is often a preferred learning mode [133]. King and Barker (1992) suggest that the most effective simulations allow learners to change variables and observe the results. Conversely, fixing variables and restricting the interaction to moving a slider or pressing buttons reduces the quality of the simulation and may turn learning into a passive process [66].

Besides interactive features of the courseware itself, the physical operations involved in manipulating computer input devices have an important role to play in the directness of an interface. For example, O'Malley (1990) explains that the act of holding a mouse button down and dragging to perform an action is a positive and engaging operation. The tension in the finger gives constant feedback about the mode the user is in [42]. A variety of mouse clicking and dragging operations can be incorporated into CAL to maintain the attention and interest of the user.

2.8.4 Situated Learning

Long term memories of events and facts often include the context or environment in which the learning took place [134]. Educationalists call this 'situated learning' and it is based on the assumption that learning is most effective when it is in the context of some meaningful, real-world task [16, 62, 135, 136]. CAL can be designed to take advantage of this human quality by creating visual or social contexts for the presentation of information. This will increase the chance of prior knowledge being activated and encourage the creation of a meaningful and memorable experience [104].

2.8.5 Learner Differences

As with traditional teaching, it is important to recognise that users of CAL differ not only in their abilities but also in their learning styles [137]. Groat and Musson (1995) observe that learning style differences have implications for the degree of success or failure experienced by users of software [138]. Courseware designers must therefore take account of individual learner differences in the design process [139]. All user differences cannot be addressed with a computer [137], but by incorporating flexibility and adaptability into CAL (see Section 2.4), it can be made more accessible to a wider variety of users.

Jih and Reeves (1992) suggest that prior experience is an important factor in determining the learning style adopted by users [40]. These workers also comment that the quality of the user's mental model of the system will decide the learning style that they adopt. To account for this variety, courseware should be designed for novice and expert learners by incorporating several levels of difficulty [117]. This facility can help to prevent novice users being overwhelmed by over-abundant options and subject complexity.

2.8.6 Feedback

The provision of informative feedback in instructional courseware is a key element in determining the success of the program [61, 140, 141]. Users need to know what the consequences of their actions are, since they cannot make sensible decisions if this information is hidden or delayed. Effective feedback encourages learners to reflect on their actions [142] and it should therefore be in context and not require further explanation [125].

2.9 Chapter Summary

This chapter has examined the research relating to the CAL design process, from the initial planning stages to the design of the user interface and the instructional content.

The recurring theme throughout this discussion has been the importance of identifying the characteristics of the user and designing courseware that meets their requirements. It is particularly important that computer programs designed for instruction have intuitive user interfaces. Learners will then focus on the information in the package and not on the complexities of the interface.

The incorporation of multimedia into CAL has been facilitated by more powerful and cost-effective computer hardware. As discussed in this chapter, multimedia courseware is an effective instructional tool but its use presents several novel problems for the instructional designer. These issues are brought about by the potential complexity and broad band width of multimedia information. Definitive guidelines for the design and integration of multimedia into CAL are still lacking, but the extension of work on learning from television and other media has provided a starting point. Principles of instructional design derived from traditional teaching have also been extended to include multimedia courseware design. The conclusions from this work also emphasise that the user should be the focus of the design process. The maintenance of user motivation and high quality interactivity must be considered foremost to ensure the design of instructionally effective courseware.

Chapter 3

CAL Evaluation Methodologies

"Is software accurate? Does it match curricular objectives? Is it instructionally sound? Is it technically adequate? These are questions generally used to evaluate instructional software. But an even more important question is often ignored: Do students learn the skills that the program is designed to teach?"

(Zahner *et al.*, 1992)

3.1 Introduction

Evaluation of computer software is concerned with the measurement of usability. Usability has been described as a function of efficiency, low error rates and user satisfaction [143].

The evaluation of CAL takes account of usability measures and pedagogical issues such as, whether the lesson objectives have been met, identification of the reasons for the observed performance and specification of those parts of the instruction where modification is required [2]. Therefore, the aim of CAL evaluation is to show that a package benefits learning, or as Anderson and Draper (1991) put it, to show that there is no better substitute for the computer [11].

There are many measures that can be applied to assess the usability of CAL [61]. The methods of choice are determined by the kind of results required, but the resources available (*i.e.* funding, expertise and time) and the stage in the software development process are also important considerations.

This chapter begins with a discussion of the rationale behind the evaluation of CAL. The various methodologies developed for software evaluation are then described, including their advantages, disadvantages and their application to CAL evaluation.

3.2 Evaluation Rationale

CAL evaluation is an on-going practice that takes place throughout the design process. Evaluation carried out while a program is under development is known as 'formative evaluation'. This stage of an evaluation is part of the design-test-modify interface design cycle (see Section 2.2.1). It is focused on the improvement of the courseware through making small modifications to the program [37]. Following the implementation of the product, a 'summative evaluation' takes place. The aim of this stage is to test the success of the software and investigate the contextual conditions that achieve the best results. Laurillard (1994) highlights that the pressure to release CAL materials can lead to the merging of the formative and summative evaluation phases [4].

The approach taken to usability evaluation is another important consideration for the evaluator. Maguire and Sweeney (1989) distinguish between three general approaches to usability evaluation [144]:

- those assessing the user's performance while using the system,
- those that apply theoretical models of task performance and
- those based on an expert's judgement.

Maguire and Sweeney explain that each of these approaches to evaluation have their own characteristics which determine when they should be applied. The user-based approach directly involves the user and is concerned with measures relating to user performance (*e.g.* accuracy), psychophysiology (*e.g.* stress), behaviour (*e.g.* gestures), attitude (*e.g.* opinions) and cognition (*e.g.* understanding). The theoretical approach does not involve users and allows predictions to be made about the learning of the system. Finally, the expert-based approach employs human-computer interaction (HCI) specialists to assess the level of conformance to guidelines or standards.

The attainment by the learners of the required lesson objectives is the main consideration in a CAL evaluation and so the user-based approach is the most commonly applied methodology. The user approach enables the evaluator to determine exactly what happened during a user session. This information can then be used to modify either the interface or the instructional content, as necessary [2].

For a comprehensive evaluation of software usability, it is recommended to use more than one evaluation method in a study (see Section 1.7.3). For example, Macleod (1992) suggests that an observational method (*e.g.* interaction monitoring) can be combined with a survey method (*e.g.* a questionnaire). This allows both user performance and satisfaction to be used in the assessment of the usability of a system [145]. This technique is also supported by Maguire and Sweeney (1989) who suggest that combining evaluation techniques in this simple fashion may be sufficient to enable more valid conclusions to be made [144].

3.3 Observational Evaluation

3.3.1 Introduction

Observational evaluations require a population of users who actively use the system being studied. The users are given a set of tasks to perform that are recorded for later analysis. These techniques have the benefit that the designers of the system can be involved, allowing them to see any flaws in the design directly [145]. Observation of users is a time-consuming operation. It can range from one-to-one observations, to the use of video cameras and computers to record user interactions [37].

This section describes the techniques of observational evaluation employed to evaluate CAL (see Table 1 for a summary).

3.3.2 Direct Observation

Direct observation is the simplest observational method and involves someone familiar with usability issues watching individual users performing tasks with the system [145]. Objective details are recorded by the evaluator that may include; time taken to complete certain tasks, frequency of errors and relevant events. Direct observation provides first hand feedback of user interaction, which helps in the interpretation of the results. Disadvantages of this method are that there is no permanent record of the interaction and the intrusive presence of the evaluator may affect the behaviour of the user [118, 146].

3.3.3 Interaction Monitoring

Interaction monitoring, or software logging, involves the collection of user interaction data during their use of a system and it may operate in several ways. For example, all user inputs (*e.g.* keystrokes and mouse movements) can be recorded, or screen outputs can be captured at specific points in a session [144].

The main advantages of system monitoring are that it is non-invasive, objective and does not require the evaluator to be present. Also, unlike direct observation of the user it provides a permanent record of the session. However, the interpretation of large quantities of interaction data is a major undertaking. This problem can be eased by clearly defining the purpose of the evaluation and having software tools to aid the analysis. In this way a specific set of relevant parameters can be analysed in depth. For example, Maguire and Sweeney (1989) suggest that categorisation of monitoring data will help to reveal patterns in the users' interactions. The evaluator can then explain these patterns in terms of cause and effect, and make any necessary improvements to the software [144].

Computer logging of user interaction is widely recommended for the evaluation of CAL [27, 104, 147, 148] and has been successfully used in many evaluation studies [92, 149-153].

A particularly valuable study, which employed computer logging was carried out by Gustafson *et al.* (1990) [18]. These workers looked at the design and implementation of an interactive videodisc training system entitled, 'Macintosh Fundamentals and Beyond'. On-line tracking of student paths and time spent in various parts of the course were facilitated by specially written routines. Analysis of the data revealed several insights into the design of the instructional material, some of which are outlined below:

- A large variance in completion times was noted, which indicates that the package is a truly self-paced system.
- The video material was largely ignored, possibly because users found it distracting.
- Most options were generally chosen in the order that they were presented on the menu, which highlights the importance of sequencing of menu options.

Tracking programs can also be used to study the mental models that users form when using interactive courseware (see Section 2.5). For example, Jih and Reeves (1992) suggest that user navigation through courseware and their use of various features is time-stamped. Inaccuracies in the users' mental models of the interface will be highlighted by any confusion that is apparent following analysis of the monitoring data. The patterns that may emerge include repeated operations and backtracking through the information structure [40].

	Analytic	**Expert**	**Observation**	**Survey**	**Controlled experiment**
Timing of use	Early	Any	Prototype or late	Prototype or late	Any
User-based	No	No	Yes	Yes	Yes
Type of data:					
Quantitative	Yes	No	Yes	Yes	Yes
Qualitative	No	Yes	Yes	Yes	Yes
Diagnostic	Narrowly	Yes	Yes	Yes	Narrowly
Costs:					
Time	Medium	Low	Medium	Low/medium	High
Money	Low/medium	Low	Medium	Low/medium	High
Main advantages	Used early in design Fairly low cost	Low cost Quick Diagnostic Broad scope	User-based Diagnostic Broad scope	Fairly quick User-based Users' views Diagnostic Broad scope	User-based Rigorous
Main disadvantages	Narrow scope Not user-based	Not user-based Reliability problems	Less effective early in the design cycle	Less effective early in the design cycle	Narrow scope High cost

Table 1 Evaluation methodologies for computer software (Macleod, 1992)

3.3.4 Video Recording

A video recording of user interaction with a system is the most detailed observational record that is available. However, these studies are costly and detailed analysis of the video material is extremely time consuming. In addition, the evaluation usually takes place in a usability laboratory, which reduces the authenticity of the data [145]. Therefore, video recording is mainly used when a highly controlled environment is required, such as for the evaluation of a specific feature of a commercial product. The high cost and lack of authenticity have prevented it from being used extensively for the evaluation of CAL.

3.4 Survey Evaluation

3.4.1 Introduction

The evaluation methods described so far have ignored the users' opinions about the system. Incorporating user attitudes into an evaluation can have a substantial influence on the design of the final product. In common with observational methods, survey evaluation techniques also involve real users, but they contribute information after rather than during their use of the system. Measuring attitudes in this way involves assessing the users' perception of reality, and so these techniques are subjective and do not always correlate with more quantitative observational measures.

A critical consideration in the design of a survey is the selection of subjects for the study. In a CAL evaluation, the subjects must represent a subset of the target population to give ecological validity to the results. Ensuring that the users have an appropriate level of experience with both the subject material and computer systems will produce more reliable data [92, 154]. For example, Whitnell *et al.* (1994) used a questionnaire to evaluate a series of multimedia chemistry lectures (see also Section 4.3.3). The results were validated by the first two questions on the questionnaire, which determined the students' molecular chemistry and computer experience [155].

This section describes the techniques of survey evaluation used for the evaluation of CAL (see Table 1 for a summary).

3.4.2 Questionnaires

Questionnaires are widely used in software evaluation. They offer advantages over other methods, since they collect information from the actual users of the software. The data are gathered following a realistic implementation of the program which means that questionnaires are particularly useful for CAL evaluation where an authentic environment is a prerequisite (see Section 1.7.2).

The subjective nature of questionnaires means that they are harder to interpret than observational measures. Rubinstein and Hersh (1984) put forward three potential biases which may explain this:

- *Halo effect* — the tendency of some people to respond positively (or negatively) to all questions in a set.
- *Acquiescence* — the tendency of some people to respond in an agreeable, positive way to all questions.
- *Cognitive dissonance* — the tendency of everyone not to admit being biased, illogical or inconsistent as the result of external influences.

Most of these effects can be neutralised by phrasing some questions positively and some negatively on the attitude scale [149, 156]. In addition, Maguire and Sweeney (1989) suggest that ambiguous statements are avoided on a questionnaire [144].

The benefits of careful questionnaire design were demonstrated by Hutchings *et al.* (1993). These workers evaluated a hypermedia system using a questionnaire containing statements most likely to produce a strong response from the users. Consequently, the study produced significant results concerning the effectiveness of specific parts of the system [149].

Preece (1994) describes two types of question structure that can be used on a questionnaire; 'closed questions', where the respondent is asked to select an answer from a choice of alternate replies and 'open questions', where the respondent is free to provide their own answer. Closed questions are usually incorporated into a rating scale [56].

The Likert scale [157] is a multi-point rating scale that has been successfully used for the evaluation of many CAL products [4, 92, 155, 158]. It allows the strength of agreement with a set of clear statements to be measured (see Appendix 4).

A carefully designed rating scale was used by King and Barker (1992) to examine the effectiveness of 43 interactive multimedia products (see also Section 2.7.2). The scale was designed so that innovation or good practice in the courseware would be revealed. A category based approach was chosen, with groups of questions being assigned to each of the categories concerning, for example, quality of interaction, motivation and interactivity. Key 'pointer' questions were used within each category to gain specific, pre-determined information from the evaluation. This approach enabled the researchers to decide whether a package exhibited a desired property or not. In addition, the use of open-ended text entry questions allowed casual observations on innovative and undesirable features to be captured. The results from the study revealed several interesting and exceptional features concerning the design and structuring of multimedia learning materials. These included observations on the role of different media and engagement, the relationship between interactivity and learning and the effectiveness of user support facilities [66].

3.4.3 Interviews

Interviews are one of the most time consuming of software evaluation techniques. They require a skilled interviewer and HCI expert. In addition, the questions to be asked must be carefully selected so that they cover all the relevant topics and leading questions must be avoided [56]. If the data resulting from an interview are to be statistically analysed, a pre-determined set of precisely phrased questions must be prepared before the evaluation.

The audio recording of interviews is effective if exact quotes are required to convince decision makers of the effectiveness of a package. Furthermore, interviewing users face-to-face can provide revealing and precise insights into the effectiveness of a system [145].

3.5 Chapter Summary

In this chapter, the rationale behind the evaluation of computer software has been discussed. The aim is to focus on some measure of usability in order to assess the effectiveness of a program. The concept of usability is especially important for CAL, since the underlying goal of these systems is learning and anything that hinders learning will severely affect the quality of the interaction.

To assess pedagogical quality, CAL evaluation should also involve the collection of performance data to determine the extent to which students learn the skills the software is designed to teach. In addition, the importance of user attitudes should not be underestimated for obtaining more casual observations on software quality. In fact, the combination of both observational and survey methodologies in a study is widely recommended to obtain the richest picture of courseware quality.

Multimedia technology has introduced new problems for the CAL evaluator. Evaluation techniques may have to be modified to meet the challenge of these new forms of instruction, but the assessment of student learning will remain the most important objective.

Chapter 4

Computers and Chemistry Education

"How abstract questions are translated into images is a problem of staggering depth. How was it, for example, that Kekulé imagined a snake swallowing its own tail just prior to realizing that the benzene molecule was structured like a ring."

(Pinker and Kosslyn, 1978)

4.1 Introduction

Undergraduate chemistry is a particularly challenging subject for the teacher since it is rich in analogies, models and complex ideas spanning mathematics, physics and chemistry itself [159]. In organic chemistry teaching this means that most phenomena must be explained in terms of atomic and molecular models [98]. Therefore, the main challenge for the student is the creation of mental three-dimensional (3-D) images of molecules [160]. However, many students find the visualisation of the spatial arrangements of molecules a difficult task [161, 162]. This is a major shortcoming, since students must develop insights into spatial and quantitative concepts to take more advanced courses or undertake research. For these reasons, chemistry teaching has seen the introduction of many innovative teaching tools in an attempt to bring the subject to life for students [159].

The computer has been used in chemistry research for many years. The arrival of more powerful machines with larger storage capacities has meant that increasingly large chemical systems can be studied, using more accurate calculations. In addition, high resolution computer graphics have allowed the visualisation of larger chemical structures and phenomena with ever increasing realism [163].

Until recently, the cost of computer hardware has prohibited the extensive use of computers within the undergraduate chemistry curriculum [161].

However, the modern desktop computer provides a cost-effective platform for presenting abstract concepts to the chemistry student [164]. The integration of computational chemistry tools into the curriculum has recently provided the student with powerful tools to help them understand molecular chemistry [165]. For example, molecular modelling is now a well established teaching aid, available to nearly all educational institutions [164].

This chapter begins with a description of the pedagogical and spatial aspects of chemistry education. There follows an overview of computers in the undergraduate chemistry teaching, including the integration of molecular modelling and multimedia into the curriculum.

4.2 The Process of Learning Chemistry

Chemistry is one of the most symbolically based of the academic disciplines [165]. This is a consequence of the abstract nature of most chemical processes. Success in learning chemistry is therefore dependent on the application of mental skills, such as, reasoning ability, spatial ability and specific knowledge [166]. Research has recently begun to focus on cognitive psychology in an attempt to understand how these skills are used in the learning process.

In a review of studies on chemistry learning, Janiuk (1993) concludes that concept formation is the most important element of chemistry knowledge, with other factors being knowledge structure, short-term memory capacity, development of cognitive abilities and the solution of problems [167]. Janiuk suggests that concepts can be split into two groups. Concrete-operational concepts are developed from first hand experience with objects or events and include objects such as, beaker, flame or metal. Formal-operational concepts, on the other hand, are more abstract and include concepts such as mole, chemical equilibrium or oxidation. The process of learning formal-operational concepts is more difficult and Janiuk concludes that most work has focused on this group, with the aim of finding the most effective teaching methods.

The path to understanding chemistry was also investigated by Kleinman (1987), who highlights the importance of mental imagery in this process. Kleinman suggests there is an increase in the degree of abstraction as a student becomes familiar with a chemical concept. For example, an experienced student may visualise the term 'equilibrium' as a seesaw rather than as a simple word association. However, if students form incorrect mental images of chemical concepts then abstract thought will be disrupted [168].

The process of learning chemistry is still not fully understood, but it is important for teachers to be aware of the principles involved so that they can justify their choice of instructional methods.

4.2.1 Spatial Ability

Studies on the psychology of learning show that spatial ability is a primary parameter of intelligence [169]. Psychologists propose that mental images are created and manipulated in a 3-D 'work space', though more research is required to determine the nature of these 3-D mental images [170]. Spatial skills are particularly important when learning involves the use of visual materials, so success in chemistry is particularly dependent on this ability. Most of the research on spatial visualisation highlights the importance of individual differences and the need to consider these in the design of any instructional material [97, 166].

The effect of individual differences in spatial ability on the mental rotation of 3-D objects was investigated by McGee (1978). This study supports earlier work by highlighting a gender difference, in that males have better spatial abilities than females of the same age. A further observation is that spatial ability appears to be positively correlated with how ambidextrous an individual is [171].

A common conceptual problem for students of chemistry is the mental transformation from a two-dimensional (2-D) representation of a molecule (*e.g.* a Fischer representation) to its 3-D equivalent (*e.g.* a ball and stick model on a computer screen). In particular, research has shown that a high percentage of students cannot visualise molecules in 3-D [162]. Barke (1993) looked specifically at this problem and posed the question, "At what age is the spatial ability of students sufficient to be able to see spatial relations in two-dimensional illustrations?". He concludes that this ability develops by the age of 14 and by using appropriate imagery in the classroom, the spatial abilities of both males and females can be improved. Barke also observes that females tend not to use models as actively as males and consequently, their spatial abilities are less well developed. However, if a teacher ensures that females make intense use of models, their spatial abilities will develop to the same degree as males [169].

Spatial ability is also a strong predictor of user success in learning how to use computer systems. For example, a study by Sein *et al.* (1993) concludes that highly visual learners form mental models (see Section 2.5) of computer software more easily and can use these to guide their interactions [55]. The importance of spatial ability in learning to use computer systems has been highlighted by other workers [97, 172]. This ability is particularly important for effective use of molecular modelling packages, which require the visualisation of 3-D structure from 2-D computer screens.

4.3 Integration of Computers into the Chemistry Curriculum

4.3.1 Introduction

The reduction in funding to Universities has led to a greater student to staff ratio and to a reduction in the amount of practical work carried out by students [173]. Consequently, CAL is well placed to support the teaching of both lecture and practical chemistry courses.

Computers have brought several advantages to the teaching of undergraduate chemistry courses. Mottram (1994) suggests that CAL is ideal for enabling students to experience experimental situations that would be otherwise unavailable to them. However, Mottram warns against the over reliance on CAL as a teaching medium and supports the replacement of practicals with CAL programs only where there is a real requirement. A certain amount of hands-on experience is essential for students to gain an insight into real experimentation [174].

This section describes the integration of molecular modelling and multimedia technology into chemistry education. These tools have the potential to change the present approach to undergraduate chemistry education.

4.3.2 Molecular Modelling

Molecular modelling applications are powerful tools for building, visualising, analysing and storing models of complex molecular systems [163]. The rapid advancements in computer hardware have recently brought molecular modelling to the desktop personal computer. This has given students access to powerful visualisation tools to aid their understanding of abstract molecular chemistry concepts [175].

Several studies show that the use of molecular modelling makes a positive difference in the learning of chemistry. A study by Barnea (1995) collected information from chemistry teachers concerning the advantages of using computerised molecular modelling rather than plastic model building kits in chemistry classes. The main conclusions from this work are summarised below:

- A student can build molecules very quickly using a computer and display them in any representation (*e.g.* stick or space fill).
- Atom labels can be added or removed from a computer model to aid understanding.
- The energy minimisation capabilities of modern molecular modelling packages allow accurate 3-D structures to be presented.

An important feature of molecular modelling packages that emerged from this study was the provision of more than one representation for the display of molecules. This ensures students realise that different representations are merely alternate ways of showing the same structure.

Barnea did discover several disadvantages of using computer modelling applications from her study. In particular, the cost of molecular modelling packages often prohibits their use in schools and teachers may have to spend valuable time getting acquainted with the software. However, the general attitude of the teachers towards molecular modelling in the curriculum was favourable [84].

Other workers have suggested further advantages of incorporating modelling software into the chemistry curriculum. For example, the complexity of structures that can be built using modelling applications is highlighted by Bays (1992) [175]. Complex molecular structures are inherently more visually appealing and this increases the engagement of molecular modelling as an instructional tool. Another capability of modelling packages is their ability to simultaneously display two or more molecules with common features. Henkel (1990) sees this as a major advantage, since it allows drug molecules to be compared and it enables drug-receptor interactions to be studied in 3-D [161].

Unfortunately, the lack of quality software with the required functionality has delayed the integration of molecular modelling into the undergraduate curriculum [175]. One reason for this is that the guidelines for interface design have not kept pace with developments in the computational area [160]. For example, Cohen (1990) highlights the fact that most software development has concentrated on the integration of computational chemistry (*e.g.* molecular mechanics or dynamics) at the expense of providing intuitive graphical user interfaces [163].

Despite these criticisms, several guidelines for integrating molecular modelling into the chemistry curriculum have emerged. DeKock *et al.* (1993) suggest that computational chemistry tools should be presented in a context of actual use [160]. This is in keeping with the principle of situated learning (see Section 2.8.4) and could involve constructing a CAL lesson as a simulation or in a case study format.

Several other workers have investigated features that enhance the ability of users to visualise objects in 3-D on the computer screen. These guidelines are applicable to the design of molecular modelling packages and several have been incorporated into desktop applications. For example, the use of colour and depth cueing for portraying 3-D objects on the computer screen has been recommended [153, 176].

Attention has also been given to the design of devices that enable users to manipulate objects in 3-D space on the computer screen. Several of these devices, for example, rotating dials and joysticks have been used in the design of molecular modelling applications [163]. An additional device called the 'virtual sphere' was investigated by Chen (1988). This controller uses the mouse to simulate the mechanics of a physical 3-D trackball. To effectively use this device, the user must imagine the rotating object being encased in a glass sphere. Chen compared the virtual sphere to traditional rotational devices (*e.g.* sliders and buttons) and discovered that users found it more natural and faster to use than any other device [147]. The virtual sphere has been successfully incorporated into several molecular modelling applications [177, 178].

Due to the deficiencies in current teaching methodologies, the 3-D representation of molecules on the computer screen has great potential as an educational tool in chemistry [179]. However, the effective integration of interactive molecular modelling into chemistry courses remains a daunting problem for the chemistry teacher [160].

4.3.3 Multimedia

Recently there has been an interest in the use of multimedia in chemistry lectures and laboratories. For example, Illman (1994) suggests that the multimedia approach may work well for subject matter involving motion, change, dynamics, graphics and 3-D concepts and instrumentation [180].

The advantages of using multimedia for chemistry teaching have been well documented and include increased student interest, more retention of the subject material and the ability to illustrate concepts in ways not previously available. To test these ideas, Whitnell *et al.* (1994) evaluated the feasibility of replacing part of a physical chemistry lecture course with a set of multimedia presentations. These workers used an overhead LCD panel to present aspects of the course difficult to describe in a traditional lecture format, for example, dynamic or 3-D concepts. Following student evaluation, multimedia instruction was clearly most successful in illustrating concepts through animation and least successful when applied to the derivation of equations. In addition, there was a tendency for students to watch the multimedia lectures passively without taking notes. In conclusion, Whitnell and co-workers suggest that a balance is maintained in a multimedia lecture. This should be based on providing enough information for maintaining concentration, but not too much to discourage note taking [155].

As with any teaching technology, multimedia courseware will work well for some students but others will not perform as well. In particular, Illman (1994) suggests that a multimedia presentation will only be effective for 60 to 70% of students, perhaps because of the variety in learning styles [180].

4.4 Chapter Summary

In this chapter, the pedagogical and spatial aspects of chemistry education have been considered. Clearly, an understanding of the issues involved in learning abstract chemistry concepts is essential to enable the most effective instructional methods to be chosen.

The recent integration of molecular modelling into the curriculum has given students access to a variety of computational chemistry tools traditionally used for research. These include energy minimisation, molecular mechanics, *ab initio* calculations and electron density plots. In addition, multimedia technology has provided chemistry teachers with the tools to demonstrate dynamic concepts such as, reaction mechanisms, that were extremely hard to describe in a traditional lecture format.

The potential for more effective instruction through the integration of modern technology into undergraduate courses has therefore dramatically increased. It is now left to teachers to review the traditional lecture approach and introduce these new techniques into the chemistry curriculum where appropriate.

Chapter 5

Design of a CAL Package Integrating Molecular Modelling with Tutorial Courseware

"Among the most difficult aspects of medicinal chemistry for a student to master are the 3-D nature of drug substances and their interactions with 3-D biological targets."

(James Henkel, 1991)

5.1 Introduction

Probably the most difficult skill a student of chemistry has to accomplish is the visualisation of 3-D arrangements of molecules [161]. Compounding this problem is the observation that the perception of 3-D structure is very difficult to teach in a traditional lesson format. Consequently, many students are not able to visualise 3-D structures [162]. Spatial ability is a prerequisite to the understanding of a diverse range of molecular topics, from the stereochemistry of organic compounds to receptor-ligand interaction. Moreover, research has shown that high spatial ability leads to a deeper understanding of the mechanisms underlying most chemical processes [171] (see Section 4.2.1).

As discussed in Section 4.1, molecular modelling systems have been used for many years in the research environment to study 3-D molecular structure and interactions. Such systems have found limited use, however, on PC platforms due to the hardware requirements imposed by high resolution graphics [161]. As such, these valuable tools have been largely inaccessible to undergraduates to help them understand the spatial arrangements of molecules. Today, cheaper hardware and more powerful modelling software are providing opportunities for the integration of molecular modelling into CAL teaching tools [163].

Besides molecular modelling software, there are now many applications commercially available for authoring CAL material on PC platforms [50].

Most authoring systems allow the incorporation of hypertext and multimedia and they can communicate with external programs (see Section 2.3). Such authoring tools also enable courseware to be designed which encourages a high degree of student interaction.

Research has shown interactivity to be a key feature of effective CAL in that it increases engagement and maintains motivation [38, 40] (see Section 2.8.3). Molecular modelling packages employ a high degree of real-time manipulation of structures, making them ideal candidates for an interactive learning environment. In particular, using a mouse to rotate and change the representation of molecules is a visually rewarding process. It is likely that such on-screen manipulation would give students enhanced control over the learning process in an instructional situation. The visualisation of molecules too complex to be built using traditional model building kits would increase engagement further [175] (see Section 4.3.2).

This chapter describes the development of an integrated CAL package within the Microsoft Windows[1] environment. It combines tutorial courseware with the interactive 3-D molecular graphics extracted from a commercial modelling application. This is a novel approach for the teaching of spatial chemistry concepts.

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[1] Microsoft Corporation, One Microsoft Way, Redmond, WA 98052-6399, USA.

5.2 Aim

The aim of this study was to demonstrate the feasibility of integrating authored courseware with molecular modelling algorithms. The emphasis was to combine the instruction and modelling tools to create an engaging and intuitive learning environment.

5.3 Hardware and Software

An Opus PC486 33 MHz microcomputer with 8 MB of memory was used for all the programming work. The machine was installed with Windows 3.1 and MS-DOS 5.0. The minimum hardware requirements for the program are an 80386SX microprocessor and 4 MB of RAM. This combination gives acceptable results, but a higher specification machine will increase the speed and smoothness of interactive structure manipulations. The package uses the Windows 16 colour system palette, which was chosen to increase the speed of redrawing during molecule manipulations.

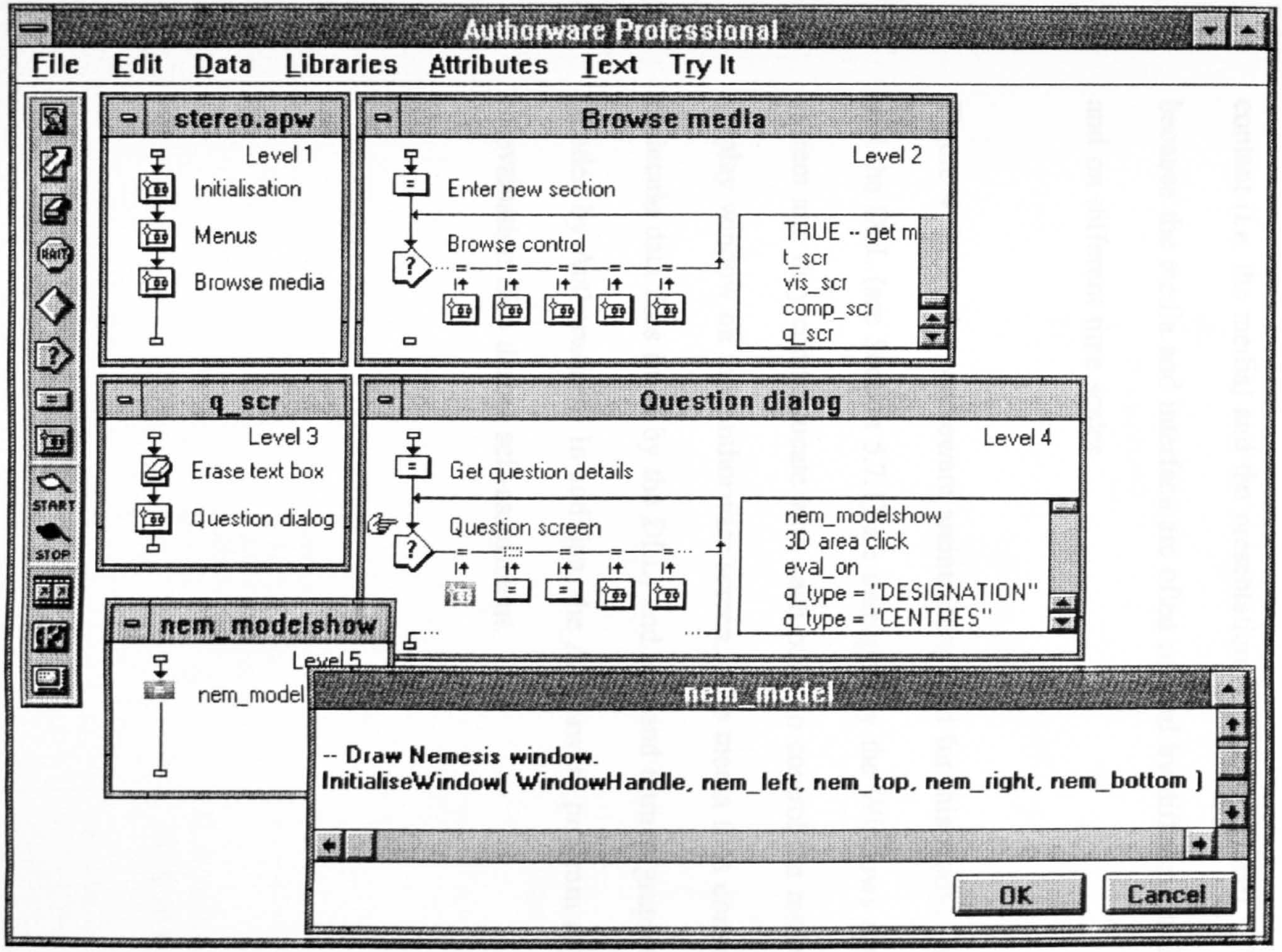
Authorware Professional for Windows (APW) v2.0 [181] was used to develop the courseware. It satisfied the following criteria, which were essential for different stages of the project:

- rapid production of prototype interface designs, allowing iterative revision of screens based on user feedback,
- communication with external programs and function libraries, enabling linkage with the molecular modelling algorithms, and

- widely adopted in the higher education environment, such that extensive distribution of the courseware for evaluation purposes would be possible.

APW is an object-based authoring system [49] that allows an author to create a series of flow diagrams using a set of eleven design icons. These icons control both the multimedia elements and the application logic. Figure 3 shows the APW design window and the flow of nested icons controlling the operation of the courseware. When the completed software is 'packaged', a read-only version is produced for distribution. The Authorware run-time software is either linked into the packaged program or resident on the host machine.

The C language source code for Nemesis v2.0 [177] for Windows was used to build a set of modelling tools that could be loaded by the APW courseware. Nemesis provides a series of tools for building, manipulating, analysing and displaying molecular structures. Structures may be displayed and manipulated in 3-D using the mouse as a 2-D control device. A full description of the program can be found in the manual [182]. Microsoft C/C++ v7.0 and the Microsoft Software Development Kit v3.1 were used to build the set of modelling tools from the Nemesis code.



```
-- Draw Nemesis window.
InitialiseWindow( WindowHandle, nem_left, nem_top, nem_right, nem_bottom )
```

Figure 3 The Authorware Professional design window.

5.4 Courseware Architecture

In Section 2.4, the advantages of a modular approach to courseware development are described, as is used for traditional software design. The most appropriate separation to make during CAL design is between the content (*i.e.* the media) and the presentation (*i.e.* the interface). This is because the media and interface are often revised by different individuals and on different time scales.

Figure 4 shows the courseware architecture used for this study. Authorware and the DLL (see Section 5.7.1) are managed by the Windows operating system and they communicate with each other to control the molecule display window on the Authorware screen. The media files consist of molecule data files (read by the DLL) and text and bitmap graphic files (loaded by Authorware). In addition, the Authorware program appends data to evaluation files during self-assessment.

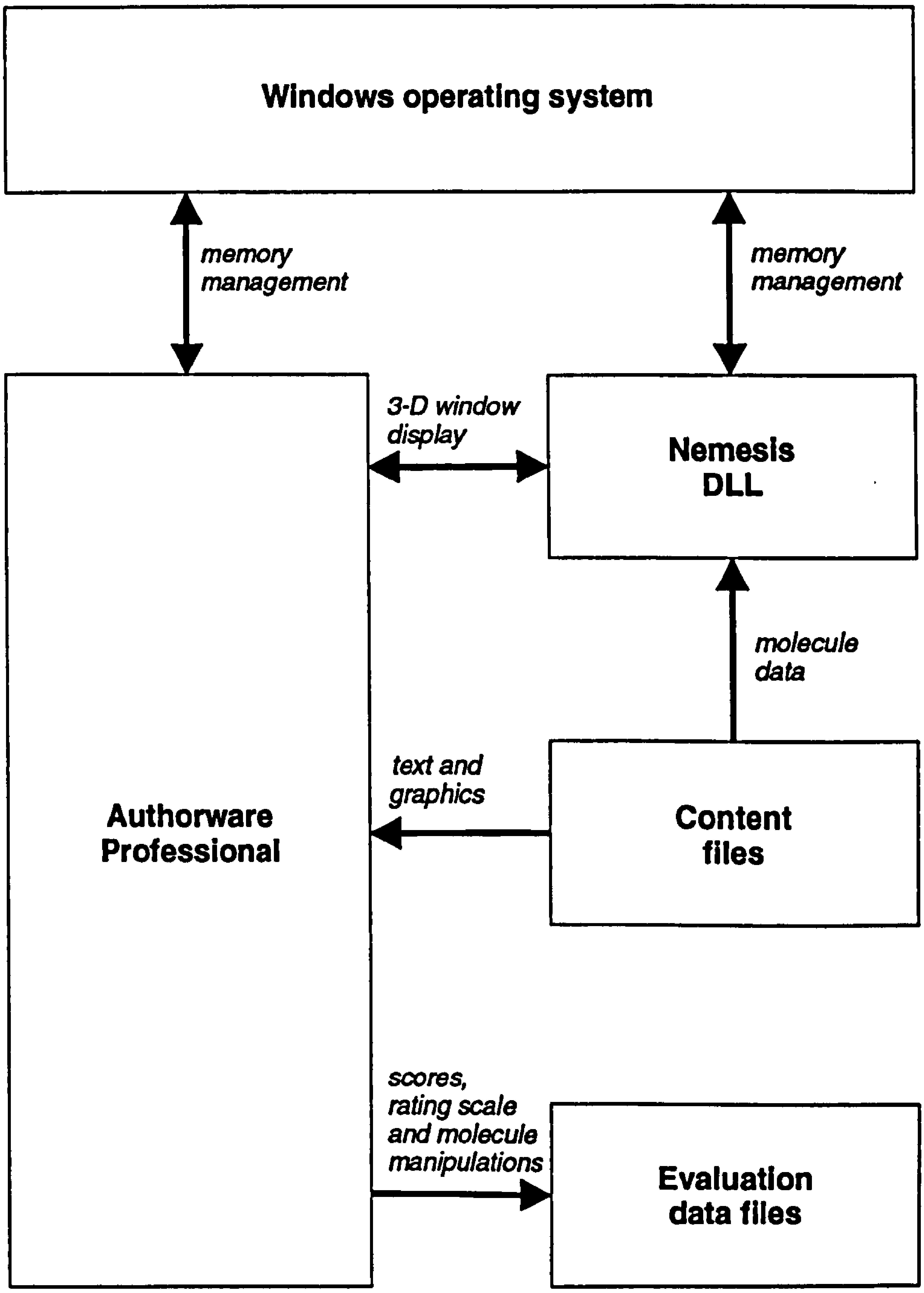


Figure 4 The architecture of the Authorware Professional and Nemesis DLL system.

5.5 Courseware Interface Design

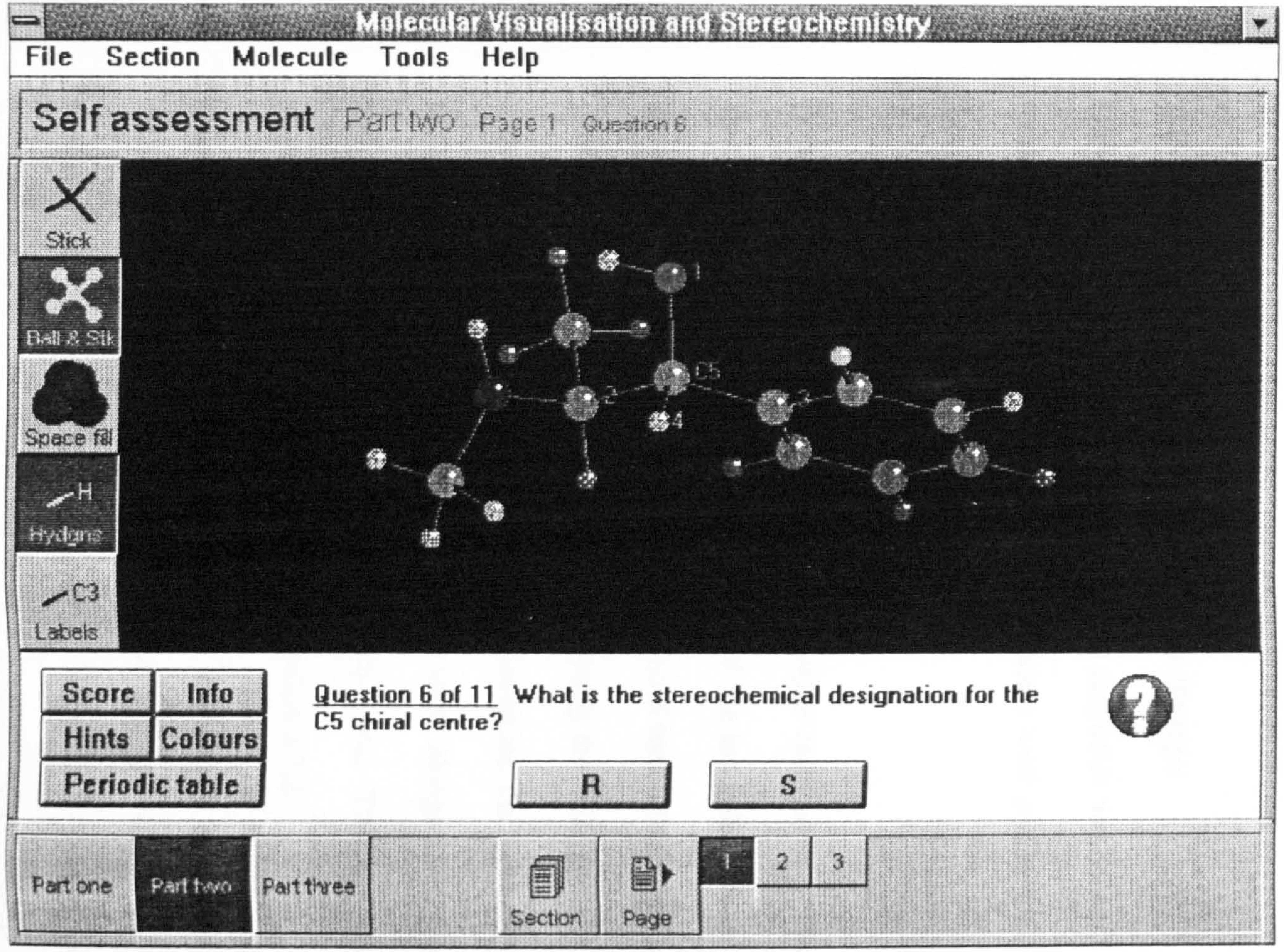
As discussed in Section 4.3.2, the user interface is often a neglected part of molecular modelling software design [163]. Conversely, it is usually taken as the starting point in CAL development. The production of an intuitive interface within which to embed the modelling tools was therefore the most important design element for this project.

A simple paging model was developed, using a set of standard screen layouts to incorporate the different media used. Figure 5 shows the functional areas used for the design and a screen shot from the self-assessment section of the package. A perpetual title is used to show the current section and sub-sections. The molecular modelling window is the largest functional area and is positioned in the centre of the screen, with the modelling tools grouped down its left side. The student tools and actions are presented directly below the modelling window. Navigational operations are grouped at the bottom of the screen. All navigational and molecular modelling operations are duplicated in the pull-down menus to help cater for different interaction styles.

A set of relevant tools are either presented on the screen or are accessible from the pull-down menus. These include a basic periodic table to help with the assignment of priorities during assessment. A glossary and a set of references are also included in the Windows 'cardfile' format.

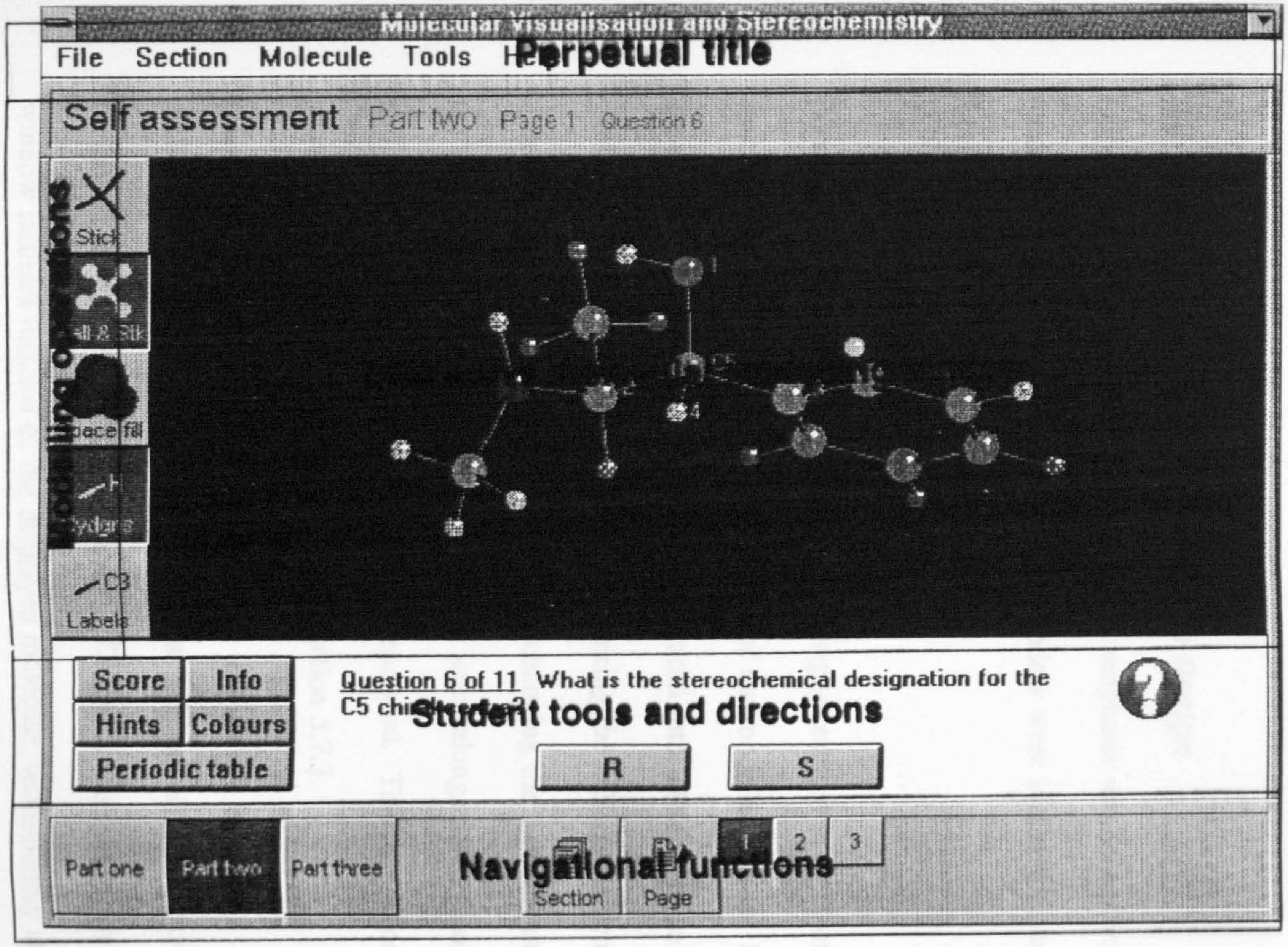
Supplementary information and help are presented using Windows dialogue boxes for consistency within the package. During self-assessment, for example, students can access information of pharmaceutical relevance about the currently presented molecule along with the atom colour scheme used in the package.

More fundamental screen design elements, such as colour, text and graphics are used consistently throughout the package. Colour coding of options is used to separate the different components of the interface. A few legible fonts are used for different classes of information. For example, Helvetica is used for screen titling, the Windows System font for the main text window and Microsoft sans-serif font for graphic captions.



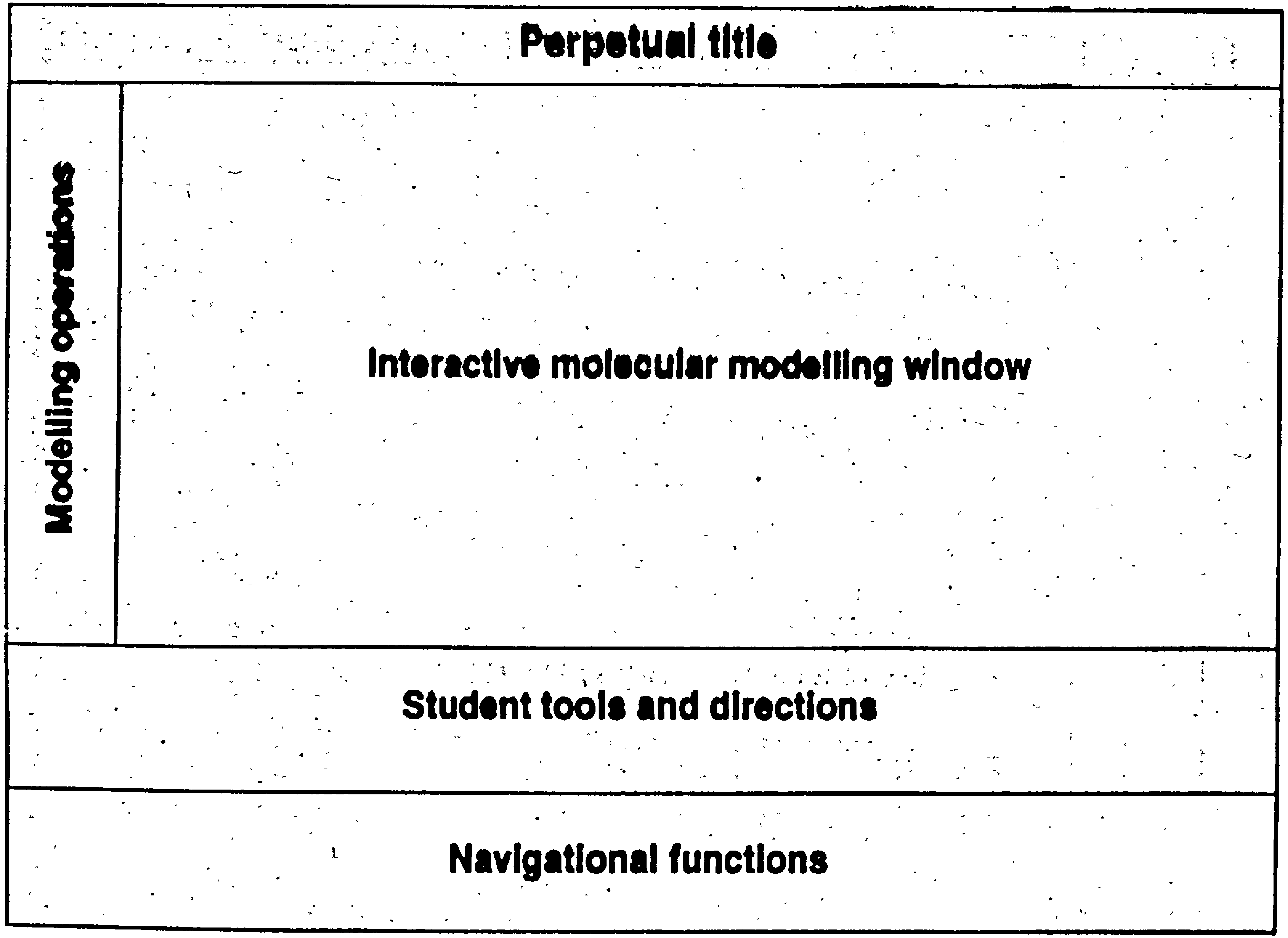
Question 6 of 11 What is the stereochemical designation for the C5 chiral centre?

Figure 5 The 'Self-assessment' section of the Authorware package showing the functional areas.



Question 6 of 11 What is the stereochemical designation for the C5 chiral centre?

Figure 5 The 'Self-assessment' section of the Authorware package showing the functional areas.


Perpetual title
Modelling operations
Interactive molecular modelling window
Student tools and directions
Navigational functions

Bitmap graphics are used throughout the courseware to accompany the tutorial material. All graphics are given an explanatory caption to link them to the text. When a piece of text has no relevant illustration, a default image is presented so that the same screen layout can be maintained.

5.6 Molecular Modelling Interface Design

During this stage of the design process, the emphasis was to ensure that the modelling tools and the interactive 3-D window were intuitive to use and integrated seamlessly with the courseware.

Formative evaluation of alternate screen designs resulted in a set of simple, spacious layouts for different applications of the modelling tools. Students are restricted to rotating molecules in the initial tutorial sections to gradually build their confidence. Upon entering the self-assessment section, a suite of extra tools is made available for changing the representation of the molecule. These tools are presented as icons alongside the molecule and the currently active functions appear depressed. The full set of tools provided in this section are described in Section 5.7.3.

Activation of a 'target' cursor shape over the 3-D modelling window is used to show a change of cursor functionality. Dragging the mouse over this window initiates rotation of the displayed molecule, immediately showing the nature of the interaction. The tension of holding down a mouse button and dragging to perform an action is an engaging operation [42], and this provides a direct feel to the interface. Figure 6 shows how the 3-D window is titled 'INTERACTIVE 3-D MOLECULAR MODEL' in the tutorial sections to further encourage the students to manipulate the molecule. This screen also illustrates the facility for presenting two interactive 3-D structures alongside for comparison.

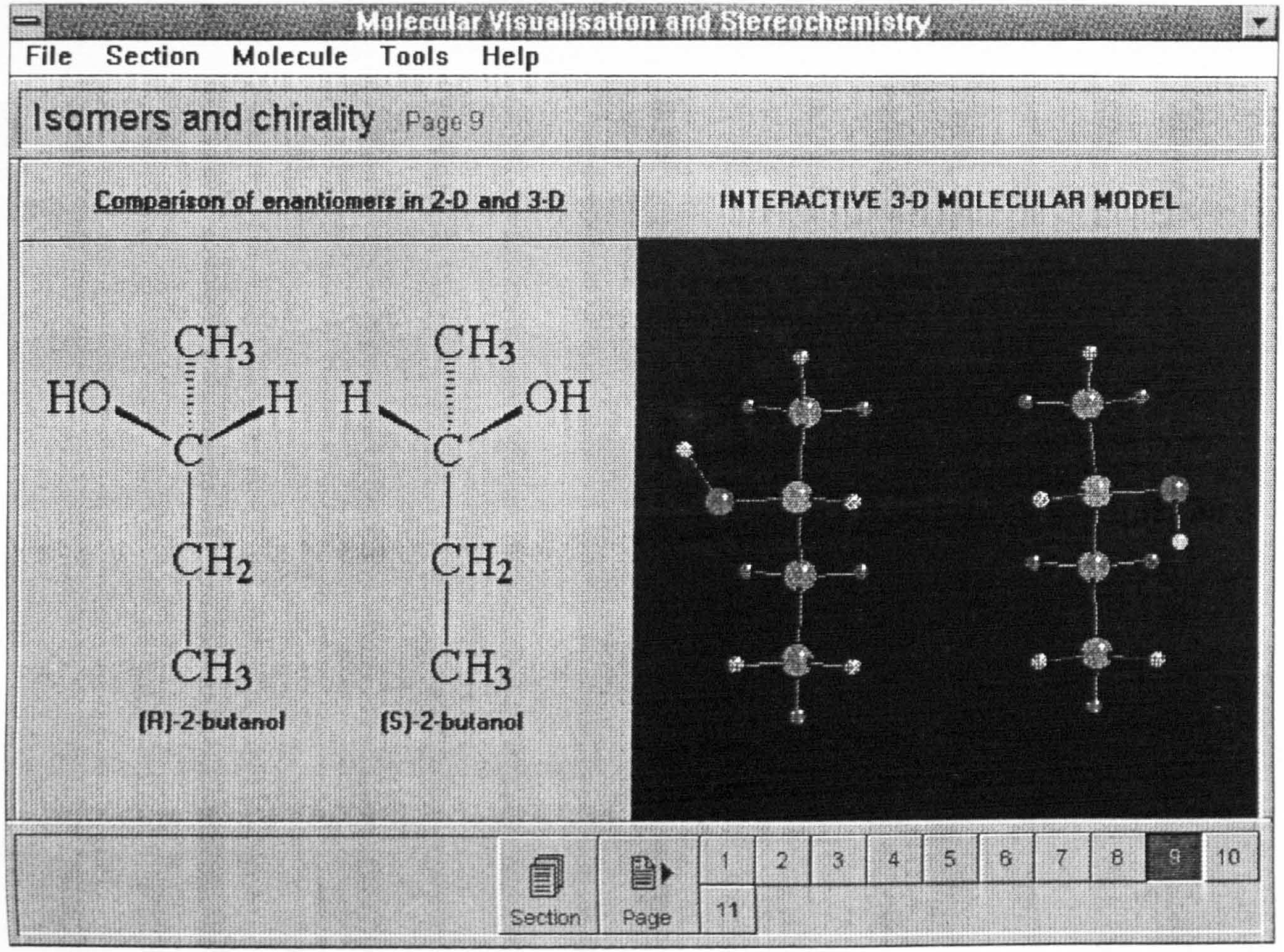


Figure 6 The integration of the molecular models with the Authorware interface in the tutorial section.

5.7 Molecular Modelling Programming

5.7.1 Dynamic Link Library Format

A dynamic link library (DLL) is a collection of one or more functions loaded dynamically during run time by another program. Such DLLs enable utilities (*e.g.* graphic or numerical operations) to be written independently, allowing other modules (programs or DLLs) to call the functions in the library. The benefits of using DLLs for customizing spreadsheet programs in teaching chemistry have already been demonstrated [183]. APW can use the functions contained in DLLs by linkage during the authoring process. Therefore, a DLL format was chosen for the development of a set of modelling functions.

5.7.2 Communication with Authorware Professional

Communication between APW and the DLL was enabled by including an object procedure in the amended Nemesis code to receive and send messages to the APW display manager. This procedure is shown in Appendix 2 (*APWMessageDispatch()*) along with the remaining code described below, that provides an interface between the Nemesis functions and APW. The use of an object procedure allows rectangular graphical objects to be posted onto the APW presentation window. APW then has control over the object and it can be moved or erased when required from within Authorware.

There are two basic types of messages used for communication between APW and a DLL object procedure: notification messages (prefixed *APWN_*) and control messages (prefixed *APWC_*). Notification messages are those received by the object procedure from APW, in response to some changing condition (*e.g.* display needs repainting). Control messages are sent to APW by a DLL, to instruct APW to perform an action (*e.g.* delete object) [184].

The DLL constructed from the Nemesis source code posts a window to the APW display that contains the molecular graphic. The image in this window is constructed using a double-buffering technique. Double buffering is an effective method for eliminating screen flicker during interactive manipulation of 3-D structures [185]. The molecule to be displayed is constructed in an off-screen (or secondary) buffer, which is then posted to the visible window whenever the display is invalidated. The DLL uses the 'WindowHandle' variable, which is passed to it from APW upon initialisation, to post the contents of the double-buffer to the APW visible window.

Figure 7 shows the life cycle of a graphical object posted from the Nemesis DLL onto the Authorware display. The DLL issues an *APWC_POST* message to request placing an object on the APW display. APW responds with an *APWN_INIT* message, prompting the DLL to draw into the double-buffer and send an *APWC_INVAL* message back to invalidate the APW display. APW returns with an *APWN_PAINT* message that instructs the DLL to copy the contents of the double-buffer to the APW display.

To remove the molecule window from the APW display it must be explicitly erased by an APW erase icon. Using the erase icon ensures that an *APWN_DESTROY* message is sent to the DLL. This causes the DLL to clear its allocated memory and it sends back an *APWC_UNPOST* message to APW when complete. This message removes the graphical object from the APW display manager list and therefore the display window.

Management of graphical objects in the above manner ensures that APW always displays the current contents of the double-buffer. This is essential for smooth molecule manipulation, which is achieved by *APWC_INVAL* and *APWN_PAINT* messages being passed between the DLL and APW in an iterative loop until the mouse is released.

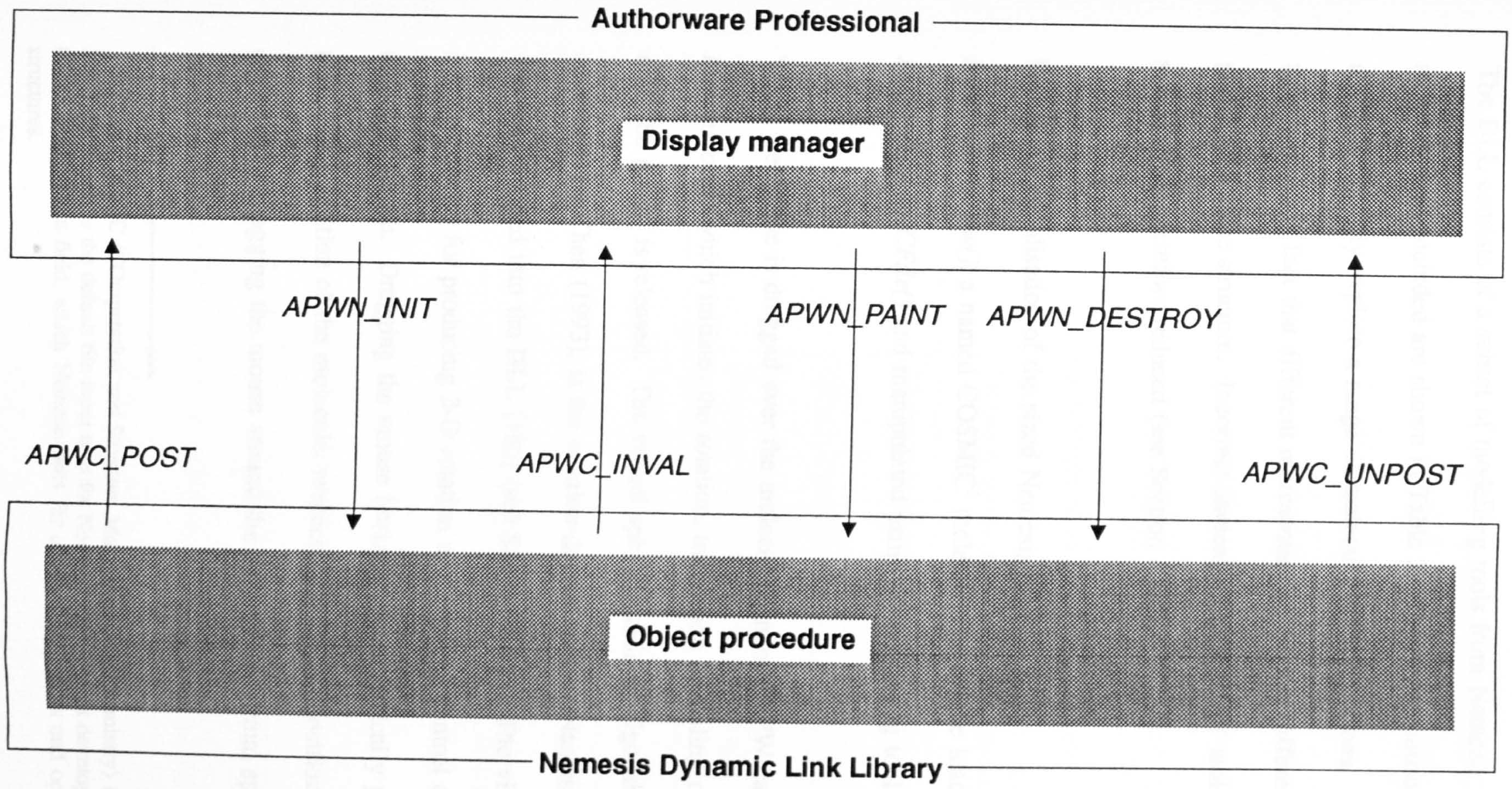


Figure 7 The life cycle of a graphical object posted from the Nemesis DLL onto the Authorware display.

5.7.3 Molecular Modelling Functionality

The DLL consists of a subset of modelling tools from Nemesis v2.0. The range of tools included are shown in Table 2. They were chosen to enable students to freely explore a range of molecular representations. This helps to reinforce the fact that different representations are just different ways to portray the same structure. Incorrect student perceptions of molecular structure are therefore reduced (see Section 4.3.2).

Following initialisation of the sized Nemesis window with *InitialiseWindow()*, a named COSMIC[2] molecule file can be loaded using *DisplayCOSMICFile()* and manipulated using the remaining tools.

When the mouse is dragged over the molecule window, APW calls *MouseMove()* which initiates the rotation, translation or scaling operation until the mouse is released. The virtual sphere rotational algorithm, as developed by Chen (1993), is the rotation device used by Nemesis and it was incorporated into the DLL [186] (see Section 4.3.2). The virtual sphere is a 2-D device for producing 3-D rotation under mouse control on a computer screen. Dragging the mouse horizontally or vertically produces pure *x* or *y* rotation of the molecule, respectively. Pure *z* rotation is achieved by dragging the mouse around the edge of the virtual sphere.

---

[2] The COSMIC (COmputation and Structure Manipulation In Chemistry) (Vinter *et al.*, 1987) file format is the default file input type for Nemesis v2.0. It was developed as part of the COSMIC force field, which Nemesis uses for energy calculations and optimisation of structures.

DLL function	Description
InitialiseWindow()	Sets up a sized Nemesis window on the APW display.
DisplayCOSMICFile()	Loads and displays a specified COSMIC molecule file.
MouseMove()	Initiates molecule manipulation. An atom label is returned if an atom was clicked.
Stick()	Displays molecule in stick representation.
BallandStick()	Displays molecule in ball & stick representation.
SpaceFill()	Displays molecule in space-fill representation.
Hydrogens()	Toggles hydrogen display on or off.
Labels()	Toggles label display on or off.
Active()	Toggles the active status of a molecule.
LabelAtom()	Labels an atom with a specified character string.
ResetLabels()	Resets atom labels to the default.
Highlight()	Turns atom highlighting ability on or off.

Table 2 The modelling tools accessible by APW from the Nemesis DLL.

If an atom is clicked in the manipulation process, its label is returned as a character string to APW. This feature, together with the functions *LabelAtom()*, *ResetLabels()* and *Highlight()* are used in the self-assessment section. Together, they enable the instruction to be designed so that students can click directly on atoms to answer questions.

The code to enable stick, ball & stick or space-fill representation of molecules is included in the DLL. These tools, together with those for hiding or displaying hydrogens and labels provide a flexible representational scheme to take account of different student learning styles.

The depth cueing facility of Nemesis is incorporated into the DLL for molecule display. This feature colours atoms and bonds that are further away along the *z* axis in darker colours than those that are closer.

Finally, the *Active()* function is included for use when two molecules are being displayed in the same window. This enables one structure to be manipulated while the other remains in a fixed orientation. For the study of stereochemical relationships this is an extremely useful facility.

5.8 Chapter Summary

This study has demonstrated the feasibility of integrating interactive molecular modelling tools with instructional courseware. This has been achieved by setting up a communication protocol between Authorware

Professional and an external library of functions (a DLL) extracted from a molecular modelling application. By placing the modelling tools in an external DLL, a generic system for the presentation of molecular structures in an instructional lesson has been created.

This chapter describes the programming and design of the integrated CAL package. Chapter 6 is concerned with the design and implementation of an evaluation scheme to assess the instructional effectiveness of the prototype courseware.

Chapter 6

Evaluation of an Integrated Stereochemistry CAL Package

"Years of quantitative studies of CBI have yielded an inadequate basis to guide our efforts to enhance education and training with interactive learning systems. Let us try some other ways."

(Thomas Reeves, 1993)

6.1 Introduction

CAL must be thoroughly evaluated to justify its incorporation into the curriculum (see Section 1.1). The aim of an evaluation is to investigate whether the program benefits the learning of the subject material and to discover what makes the courseware more effective than previous teaching methods. This will enable its quality to be finely tuned.

The traditional methodology for evaluating the effectiveness of CAL has been to compare the impact of new technology against the original teaching tools, in so-called media comparison studies (see Section 1.2). The lack of definitive results resulting from such work has lead to more integrated evaluation schemes being employed. Qualitative and quantitative data are often collected in such studies, to obtain the broadest representation of courseware use (see Section 1.7.3). By adopting this approach, more complex questions such as, "What features of CAL make it effective?" can be addressed by correlating the various data sets collected [1].

In addition, the evaluation of CAL in a natural environment has been recommended, as this will increase the ecological validity of the data obtained. To achieve this, the subject material must be of direct relevance to the students and the courseware evaluation should take place in a realistic setting (see Section 1.7.2).

Adoption of the integrated methodology described above is particularly important for innovative courseware, since unexpected learning gains and other positive features may be missed by a traditional comparative evaluation. This would prevent a designer from perfecting the design of the program by capitalising on its unique features.

The incorporation of interactive molecular modelling into CAL, as described in Chapter 5, is a novel approach for teaching molecular chemistry. This courseware must now be evaluated to discover whether an appropriate set of modelling tools have been provided and to determine how students use them during the learning process. In addition, by studying how the molecules are manipulated during the instructional sequence, it may be possible to judge how effective the 3-D tools are in improving spatial ability.

This study describes the summative evaluation of a CAL package that uses molecular modelling tools to teach basic stereochemistry, using the integrated design put forward in Chapter 5. The courseware was evaluated following its incorporation into the undergraduate pharmacy curriculum at several UK universities.

6.2 Aim

The aim of this study was to investigate whether the ability to interactively manipulate molecular structures in tutorial courseware helps with the 3-D visualisation of molecular chemistry concepts. An integrated evaluation scheme has been employed to demonstrate how multi-channelled data collection provides a comprehensive scenario of the effectiveness of the modelling tools.

6.3 Instructional Design

Stereochemistry is a conceptually difficult subject for most chemistry students as it involves the visualisation of the 3-D arrangements of molecules (see Section 4.1). Therefore, this was a suitable subject around which to design a prototype package. The chosen subject was the assignment of stereochemical designations (*R* and *S*) to chiral molecules. The courseware is titled 'Molecular Visualisation and Stereochemistry' and consists of several prerequisite tutorial sections and a separate self-assessment section. The tutorial section titles are 'Molecular projections', 'Isomers and chirality', 'Assigning priorities', 'Orientating a molecule' and 'The final designation'.

The instructional sequence used for the assignment of an *R* or *S* designation is that taught for traditional 2-D media, as follows: Step 1. Identify the chiral carbon atom; Step 2. Assign priorities 1-4 to the four groups surrounding the chiral carbon atom; Step 3. Visualise group 4 (the lowest priority group) facing away from you; Step 4. Determine the direction of rotation going from group 1 to 2 to 3. If the direction of rotation is clockwise, an *R* designation is given to the molecule, otherwise an *S* designation is given.

The self-assessment section is divided into three parts. Parts one, two and three contain molecules with one, two and three chiral centres respectively. Part one comprises nine structures, part two has three structures and part three consists of a single structure. The molecules were carefully chosen by a member of academic staff, such that the students at Nottingham had encountered most of them in previous modules.

The structures are initially presented in one of two orientations, with respect to the spatial positioning of the lowest priority group. This group faces alternately out of and into the screen for successive question sequences, being slightly off-set from the *z* axis, so as not to be hidden by other atoms. Students are not prompted to manipulate the molecules before step 4 or at any other point in the instructional sequence.

The molecular modelling tools are used to create an exploratory environment within the self-assessment section, as described in Chapter 5. In addition, the atom coordinates and atom highlighting feature provide an interactive dialogue by allowing students to click the mouse directly on atoms to answer questions (see Section 5.7.3). This enables immediate feedback to be given, appearing as an atom type label[3] next to the selected atom. For every incorrect answer given a relevant hint is given as a guide towards the correct response. The students are allowed to make unlimited attempts to answer any of the questions. In addition, questions can be omitted and the courseware can be quit at any point in the instructional sequence.

6.4 Subjects and Implementation

The prototype package was distributed to UK universities by the Pharmacy Consortium for Computer-Aided Learning (PCCAL). The data presented here result from its integration into BPharmI modules covering basic stereochemistry at Nottingham and Manchester Universities. The students used the courseware while the module was being taught. A 'Computers & Pharmacy' module, covering basic personal computer skills, had been taken by all the students at Nottingham.

Since the rating scale was optional and the questions could be skipped, variable numbers of students are used in the data analysis described below. The number of participants are shown for each set of results.

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[3] Nemesis displays atom type labels as the atomic symbol of the atom followed by a unique number (*e.g.* C3 for a carbon atom).

6.5 Evaluation Methodology

To assess the mastery of *R* and *S* designation, cumulative scores obtained during self-assessment were recorded for individual students. A correct answer was recorded when the correct atom was identified in response to a question. Alternatively, for an *R* or *S* designation, a correct answer resulted from a click on the 'R' or 'S' labelled buttons that appear below the molecule window. An incorrect attempt was recorded following a click on the wrong atom or on the incorrect button for a designation. The percentage mastery, for each of the question types, was calculated as: (correct answers/questions answered) x 100.

An optional five point Likert rating scale (see Section 3.4.2) was presented in a Windows dialogue box, at the point when a student quit the program. The scale ranged from 'Strongly disagree' (1), through 'Neutral' (3), to 'Strongly agree' (5). Previous computer and subject experience were assessed before the rating scale was administered. Eight statements then assessed student attitudes towards the interface and the molecular modelling tools. Finally, two text entry questions allowed a student to enter text descriptions of particularly good or bad features about the program.

System monitoring of mouse drag operations during self-assessment was used to record the manipulation of molecules during the instructional sequence. The data obtained for chiral centre identification, priority assignment and designation questions were appended to separate data files.

Individual mouse drags were accumulated and as each correct answer was received, the total distance the molecule had been rotated was recorded. The drag distance was calculated in screen pixels as: $\sqrt{((\text{MouseUp}X - \text{MouseDown}X)^2 + (\text{MouseUp}Y - \text{MouseDown}Y)^2)}$.

6.6 Results

The average mastery scores and standard errors obtained during self-assessment are shown in Table 3. Students gave more correct first answers to questions the further through the instructional sequence they worked, from chiral centre identification (71%) to designation (88%). The total mastery of *R* and *S* designation was high (83%).

Question type	**Percentage mastery (SE)**
Chiral centre identification	71 (7.7)
Priority assignment	77 (6.9)
R and *S* designation	88 (4.6)
Overall	83 (3.9)

Table 3 Student mastery of self-assessment questions (*n* = 13).

The results from the rating scale are shown in Table 4. The percentage agreement with each of the statements has been calculated together with the standard error. Students had intermediate computer experience (53%) and were already familiar with *R* and *S* designation (79%). The screen displays were generally intuitive (77%) and the possibility of even more interactivity was attractive (78%). The students were occasionally disorientated in the courseware (43%), though they felt in control of their progress most of the time (78%). The facility to rotate molecules certainly made the instruction more interesting (88%) and manipulation of structures improved the learning experience (60%). The prospect of further programs incorporating interactive molecular modelling to teach chemistry was an attractive prospect (79%).

The results from the text entry questions that were appended to the rating scale are summarised in Tables 5 and 6. These results are categorised and each response is presented as a percentage of the total number of participants. Insignificant or inappropriate responses are grouped under 'Others' and the number of blank replies is also recorded.

Table 5 shows that 47% of the students picked out manipulation of molecular models as the most attractive feature of the courseware, with 31% not responding to the question. Conversely, Table 6 shows that the similarity of the questions was the least attractive feature (15%), with 71% not responding to this question.

Rating scale statements	Percentage agreement (SE)
I am a novice in the use of interactive computer systems.	53 (6.7)
I am familiar with the subject matter in the courseware.	79 (2.9)
The screen displays were uncluttered and easy to understand.	77 (4.4)
At times, I didn't know where I was in the courseware.	43 (5.1)
I felt in control of my progress while I was using the courseware.	78 (3.4)
I would have liked more interaction in the courseware.	78 (4.0)
The ability to rotate molecules in 3-D made the courseware more interesting.	88 (3.2)
Rotating the molecules didn't help me learn more.	40 (4.0)
3-D molecular modelling would help me understand other chemistry topics.	79 (3.9)

Table 4 Percentage responses to rating scale (n = 19).

The system monitoring of molecule manipulation during self-assessment has been categorised by question type in Figure 8. Clearly, molecules were dragged least during priority assignment (26 pixels) and most during *R* or *S* designation (93 pixels). During the identification of chiral centres, molecules were dragged by more variable distances, with the average lying between those for priority assignment and the final designation (73 pixels).

Figure 9 shows the molecule manipulation data categorised by initial molecule orientation. The mouse drag distances for a set of questions on a single molecule have been accumulated. Clearly, molecules were dragged more when the lowest priority group was initially presented as forward facing (111 pixels) as compared to backward facing (44 pixels). Welch's unpaired t test revealed that this difference was significant ($t = 2.03$, $p < 0.05$).

Response	**Percentage respondents**
"Manipulation of molecular models"	47
"Helps teach *R* & *S* stereochemistry"	4
"The screen displays"	4
Others	14
No response	31

Table 5 Categorised responses to the text entry question, "Is there one thing that stands out as being really good about the package?" ($n = 76$).

Response	**Percentage respondents**
"Questions too similar"	15
"Lack of atom colour key"	4
Others	10
No response	71

Table 6 Categorised responses to the text entry question, "Is there one thing that stands out as being really bad about the package?" ($n = 76$).

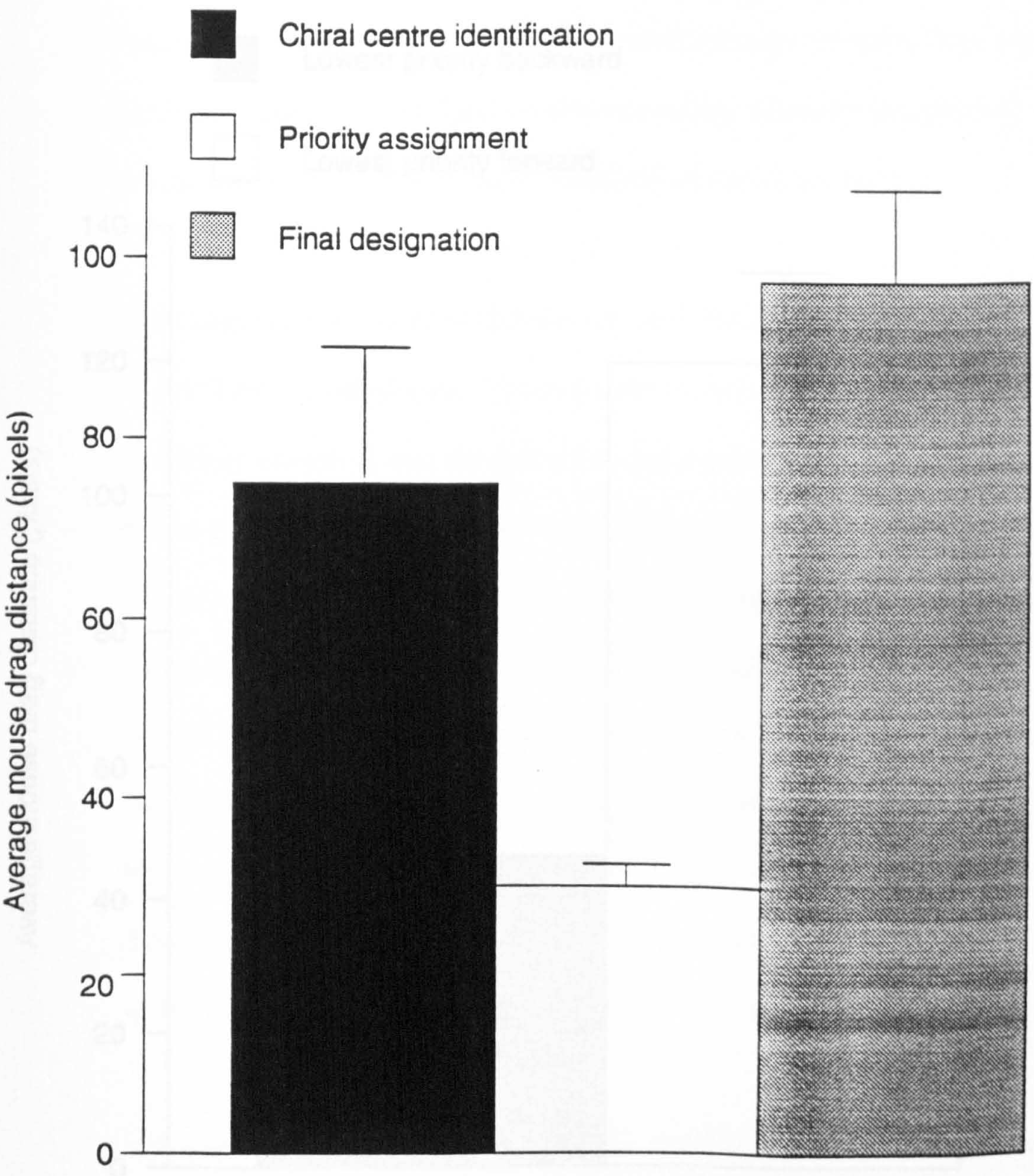

Figure 8 Mean mouse drag distances for chiral centre identification (n = 85), priority assignment (n = 571) and final designation (n = 144).

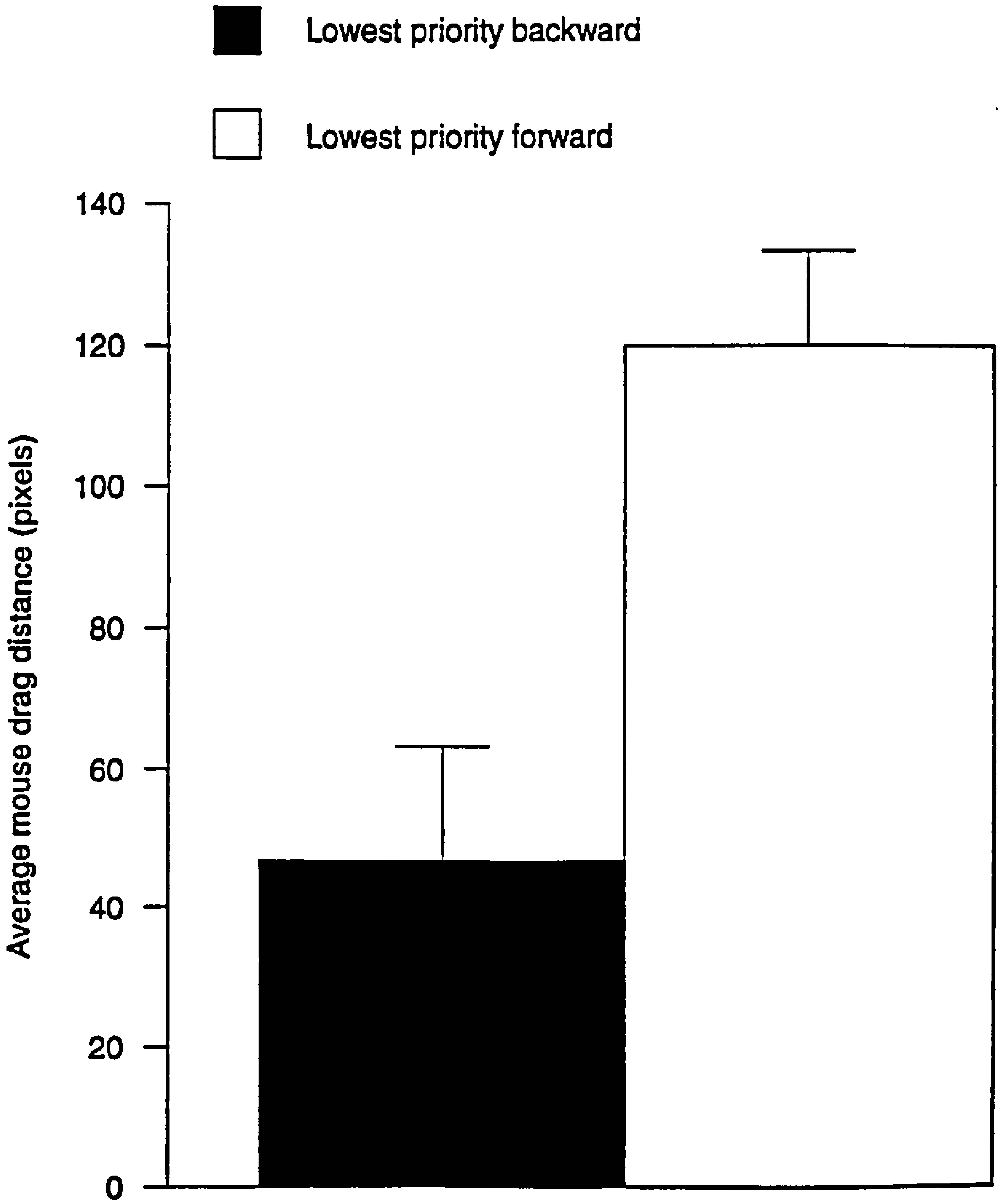

Figure 9 Mean mouse drag distances for initially forward facing ($n = 46$) and backward facing ($n = 30$) lowest priority groups.

6.7 Chapter Summary

The self-assessment scores obtained following the evaluation of the integrated courseware show that students achieved a high level of mastery of *R* and *S* designation. The weakest area was the identification of chiral centres. At this stage in the sequence the students were not focused on any particular region of the molecule and were possibly clicking randomly on several atoms before they correctly identified the chiral centre.

The rating scale results show that a usable and intuitive interface has been designed for the courseware. The molecular modelling tools have been seamlessly integrated with the instruction and most of the students found this an engaging and effective learning environment. The text entry questions gathered more casual observations about the package design. By far the most appealing feature was the ability to manipulate molecular models, which confirmed the finding from the rating scale. Conversely, the similarity of the questions was identified by the students as an unattractive feature. This latter result was predictable, since in the prototype courseware the questions are of the same type and in the same sequence by necessity, to enable a standard set of molecule manipulation data to be collected.

The molecule manipulation data show that students were intuitively rotating molecules to aid their visualisation of 3-D structure during the instructional sequence. In keeping with the traditionally taught method of assignment, molecules were rotated most during the final designation. At this stage the students had to visualise the lowest priority group facing away from them. They rotated the molecules to help them achieve this.

The manipulation data also reveal that molecules were rotated significantly more when the lowest priority group was initially presented as forward facing. This result highlights a possible weakness in the students' ability to form mental images of the 3-D structures of molecules in this orientation. They were either rotating the lowest priority group to face away from them, or they were rotating the molecule slightly in several directions and constructing a mental image of the 3-D structure.

The integrated evaluation scheme used in this study has provided substantial evidence concerning the effectiveness of the courseware. Both the qualitative and quantitative data show that 3-D molecular modelling can be integrated with tutorial instruction to help students understand spatial chemistry. An insight has also been gained into how the molecular modelling tools are used during the learning process. Weaknesses in the design of the program and the spatial abilities of the students have also been identified.

Chapter 7

Design and Evaluation of a Multimedia QSAR Training Package

"The development of a useful structure-activity relationship (SAR) from a body of physical, chemical and biological experimental work is an intellectual exercise."

(Michael Tute, 1994)

7.1 Introduction

The traditional method of searching for new medicinal drugs has often been described as chemical roulette [187]. In this manner, chemical intuition and isosteric considerations are used in an attempt to improve a chosen chemical structure with a known biological activity. The aim is to produce a highly active compound which possesses minimal side effects.

The quantitative structure-activity relationship (QSAR) approach is a structured and powerful technique for drug design which uses multiple properties in an analysis. A QSAR analysis begins with the selection of a series of related drug molecules and parameters are then assigned to the various functional groups in these molecules. These parameters provide an indication of the potential contribution of each group to a particular property of the parent molecule. The functional groups and their descriptive parameters are then compared with the biological activities of the drug compounds. The structures of the most active derivatives can then be identified using statistical techniques, such as multiple regression and principal components analysis. This in turn may enable new structures with higher activities to be predicted from the original set of drug molecules. QSAR analysis is therefore a highly intellectual exercise [188], involving the visualisation of complex data sets, with the aim of defining novel drug molecules.

Powerful computer programs are now available to assist the medicinal chemist in performing QSAR studies [189]. These packages provide a variety of analytical tools and enable complex data to be visualised in a form that the human brain can comprehend. To achieve this, QSAR applications often employ 3-D computer graphics and allow users to interact with multidimensional data in real-time [178]. Therefore, effective use of these programs requires high spatial ability and a wealth of experience. To reduce this learning curve, some form of training is a prerequisite before an analysis can be performed. Traditionally, worked examples in the accompanying manual have been the main teaching source available with QSAR applications [190]. Although effective, these methods are slow and lack the context and dynamic nature of actual QSAR studies.

The integration of multimedia into CAL has been shown to enhance learning (see Section 2.7.1). Consequently, the multimedia capabilities of modern computers provide a novel opportunity for producing effective on-line training materials. In particular, the dual-coding (see Section 2.7.1) of multimedia information in both visual and audio forms increases its retention, since the user then has two separate ways of finding the material in memory. A further quality of multimedia CAL is that it can create realistic contexts for the presentation of instruction. This technique is called situated learning (see Section 2.8.4) and the benefits of designing courseware in this way have been well documented. For example, Tennyson (1994) suggests that simulations, case studies or role-playing situations are created in multimedia instruction to ensure that users develop their cognitive skills in engaging and authentic environments. The contextual skills that they acquire will allow them to use the knowledge to undertake complex decision making, problem solving and/or trouble shooting in real life situations [30].

These developments in multimedia technology and computational chemistry tools have highlighted an opportunity for producing on-line courseware for training in QSAR techniques. Unfortunately, the pedagogical aspects of combining these two technologies have not kept pace with the capabilities of the hardware and software (see Section 4.3.2). Consequently, there is still no acceptable unifying theory describing the conditions under which these and other media influence learning [104]. It is possible that the integration of computational chemistry tools and multimedia into a CAL program will provide an engaging environment and produce novel learning benefits. However, it is also possible that the simultaneous presentation of two forms of dynamic media may exceed the cognitive capacity of the users, with detrimental effects on learning.

This chapter describes the development of prototype courseware on the Unix platform designed to train users in the use of analytical tools for QSAR analysis. This is achieved through a series of case studies that integrate digital video and the interactive computational tools from a commercial QSAR application. A summative evaluation of the program is included which assesses the effectiveness of integrating these two forms of dynamic media.

7.2 Aim

The aim of this study was to demonstrate that tutorial courseware incorporating simultaneously presented computational chemistry tools and digital video provides an effective environment for learning complex analytical techniques.

7.3 Hardware and Software

A 100 MHz Silicon Graphics[4] Indy running IRIX 5.3 was used for the programming work. The machine had 96 MB of memory, a 1 GB hard disk and the graphics board supported 24-bit colour. The completed courseware occupies approximately 180 MB of the hard disk space.

The video material was recorded using a Sony camcorder mounted on a tripod. It was then digitised at 160 x 120 pixels and compressed in Apple Video (RPZA) QuickTime[5] format on a Macintosh Quadra 660AV, using FusionRecorder v1.0.2 (VideoFusion Inc.). Movie Converter v1.0[1] was used to make the movies playable on non-Apple computers.

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[4] Silicon Graphics (UK) Ltd., 1530 Arlington Business Park, Theale, Reading, Berks RG7 4SB.

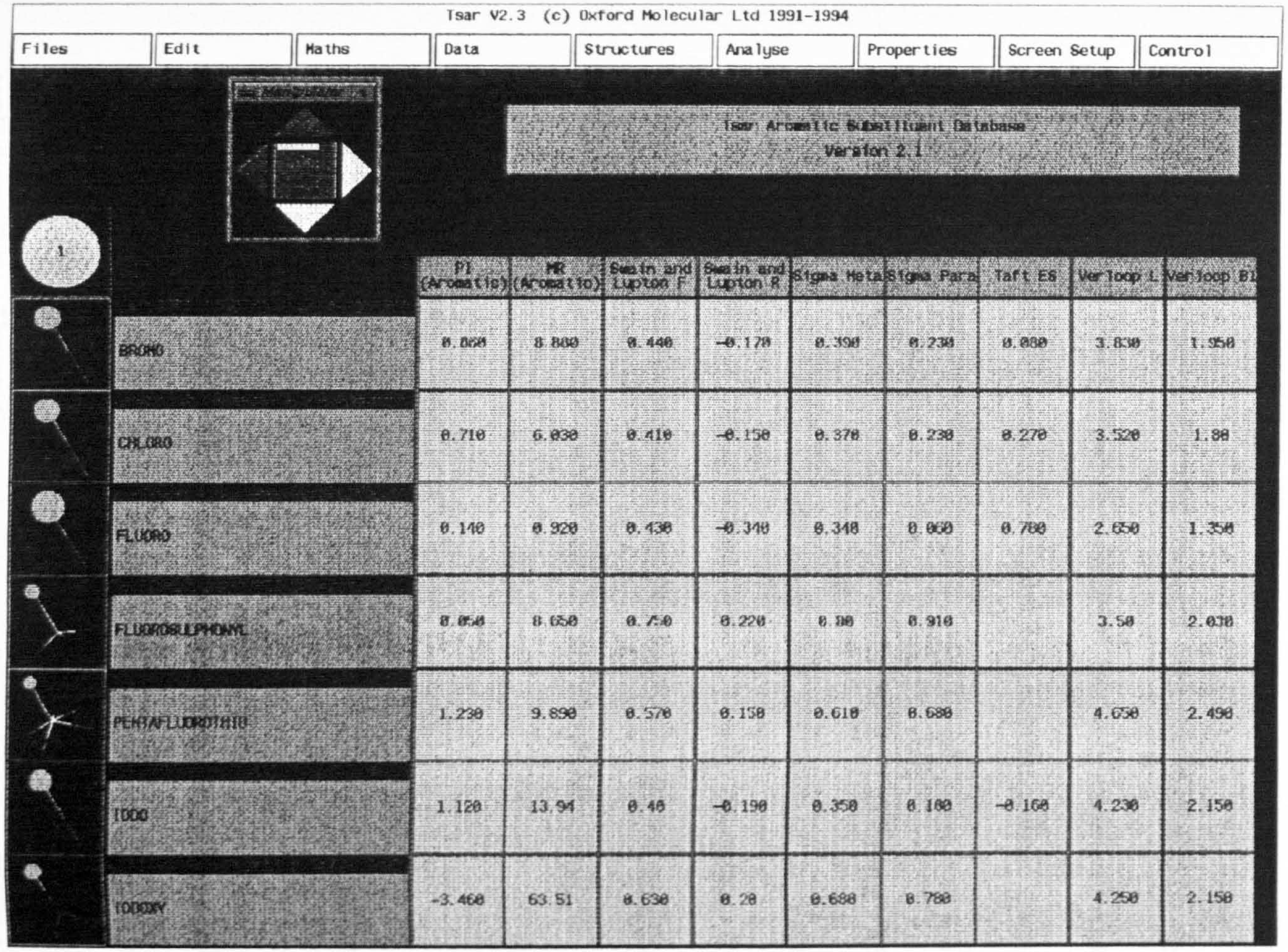
[5] Apple Computer, Inc. 20525 Nariani Avenue, Cupertino, CA 95014-6299.

The courseware was developed using Showcase v3.3[1]. Showcase satisfied comparable requirements to Authorware Professional (see Section 5.3), as follows:

- rapid prototyping of interface designs,
- the ability to run Unix shell scripts, enabling external programs to be executed at will, and
- freely distributed with all Silicon Graphics machines, allowing remote distribution of the courseware and subsequent evaluation.

Showcase is an object-oriented drawing and presentation program. It allows the construction of page-based courseware incorporating simple drawings and imported images. It also possesses audio and video tools for importing and displaying multimedia data. A hyperscript facility allows Unix shell scripts and external programs to be executed. This feature also allows a degree of interactivity to be incorporated into the authored material.

The source code for ***Tsar*** v2.3 [178] was used to build the set of computational tools for integration with the Showcase courseware. ***Tsar*** is a fully integrated program for the interactive investigation of QSARs. It allows all the data in a QSAR analysis to be stored as a data table. Figure 10 shows the ***Tsar*** table display with a data set loaded. The rows represent the substituents and the columns hold the different properties that will be



Tsar Aromatic Substituent Database
Version 2.1

	PI (Aromatic)	MR (Aromatic)	Swain and Lupton F	Swain and Lupton R	Sigma Meta	Sigma Para	Taft ES	Verloop L	Verloop B1
BROMO	0.860	8.880	0.440	-0.170	0.390	0.230	0.080	3.830	1.950
CHLORO	0.710	6.030	0.410	-0.150	0.370	0.230	0.270	3.520	1.80
FLUORO	0.140	0.920	0.430	-0.340	0.340	0.060	0.780	2.650	1.350
FLUOROSULPHONYL	0.050	8.650	0.750	0.220	0.80	0.910		3.50	2.030
PENTAFLUOROTHIO	1.230	9.890	0.570	0.150	0.610	0.680		4.650	2.490
IODO	1.120	13.94	0.40	-0.190	0.350	0.180	-0.160	4.230	2.150
IODOXY	-3.460	63.51	0.630	0.20	0.680	0.780		4.250	2.150

Figure 10 The *Tsar* user interface with a data table loaded.

used in the analysis. A full range of statistical functions for QSAR analysis are provided in the program, most of which provide fully interactive graphical output. Further details can be found in the manual [190].

7.4 Instructional Design

The courseware is titled '***Tsar*** Multimedia Training' and is split into three sections, each of which presents a different aspect of computer-based QSAR analysis. 'Background to QSAR' (Figure 11) provides a brief overview of the theoretical basis for QSAR analysis, from the early work of Corwin Hansch to the integration of computerised molecular modelling. 'Using ***Tsar***' (Figure 12) describes the analytical tools available in the ***Tsar*** program via a series of bitmap screen shots and audio narration. The computational tools are introduced in these sections with simultaneous audio narration which emphasises the interactive nature of the screens.

The '***Tsar*** case studies' section (Figure 13) consists of a set of five published QSAR analyses. The set of studies were chosen to enable a variety of tools from the ***Tsar*** program to be incorporated. A series of five studies were compiled with the assistance of users of the ***Tsar*** application. Contributors were asked to select a QSAR analysis based around a single data set that could be used to illustrate the use of one or more analytical tools from ***Tsar***. The studies and their contributors are listed in Table 7.

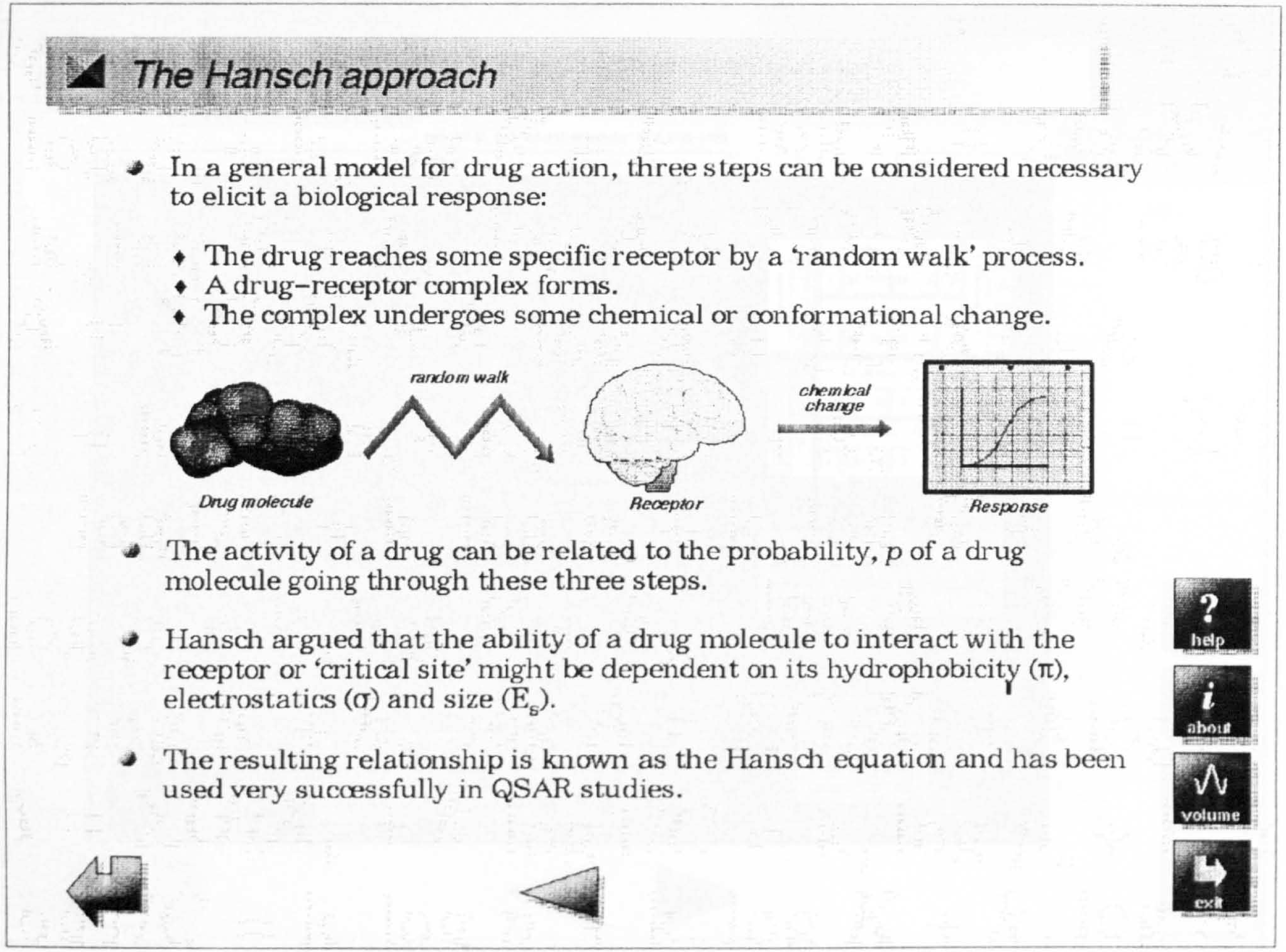
The case studies required the collection of sets of 'talking head' video clips. To provide consistency between the video material in the studies, a protocol was given to each contributor several weeks before the filming (Appendix 3). A set of key points were listed in this protocol around which the video script was constructed. The points were chosen such that a complete description of the analysis would be ensured. Therefore, each contributor was asked to explain their background, the aims of the analysis, the input data set, the QSAR analysis itself and their conclusions. The filming took place on site to provide authenticity and context to the footage. In all the case studies a head and shoulder's profile was used to shoot the video. The original data set was also obtained for inclusion in the courseware.

The video material was incorporated into the courseware by assigning one clip to each page of the case study section. The clips are played automatically as the user turns the pages within a case study. Clicking on the video window allows the clip to be replayed.

Predominantly, bitmap screen shots from the ***Tsar*** application accompany the presentation of each video clip in a case study. The images consist of screen shots from ***Tsar***, explanatory graphics or text summaries of the video clips. When the results of an analysis using a ***Tsar*** tool are described, the 'tsardemo' program is executed and the actual data set is used as a parameter (see Section 7.6.2). The appropriate video clip is then played on top of the ***Tsar*** window. In these cases, the contributors were told to encourage interaction with the presented data via their commentary in the video clip.

Contributor	**Study title**
Dr. R. Scoffin, Oxford Molecular Ltd., UK.	'Hansch analysis of steroid binding affinities' [190]
Dr. R. Scoffin, Oxford Molecular Ltd., UK.	'3-D QSAR analysis of steroid binding affinities' [190]
Dr A. Davis, Astra Charnwood Ltd., Loughborough, UK.	'Cluster analysis of calcium channel agonists' [191]
Mr M. Barratt, Unilever Research, UK.	'A predictive model for the corrosivity of acids' [192]
Dr. M. Tute and Dr. C. Montanari, University of Kent, UK.	'A similarity index for a set of bis-amidine derivatives' [193, 194]

Table 7 The *Tsar* case study contributors and the study titles.

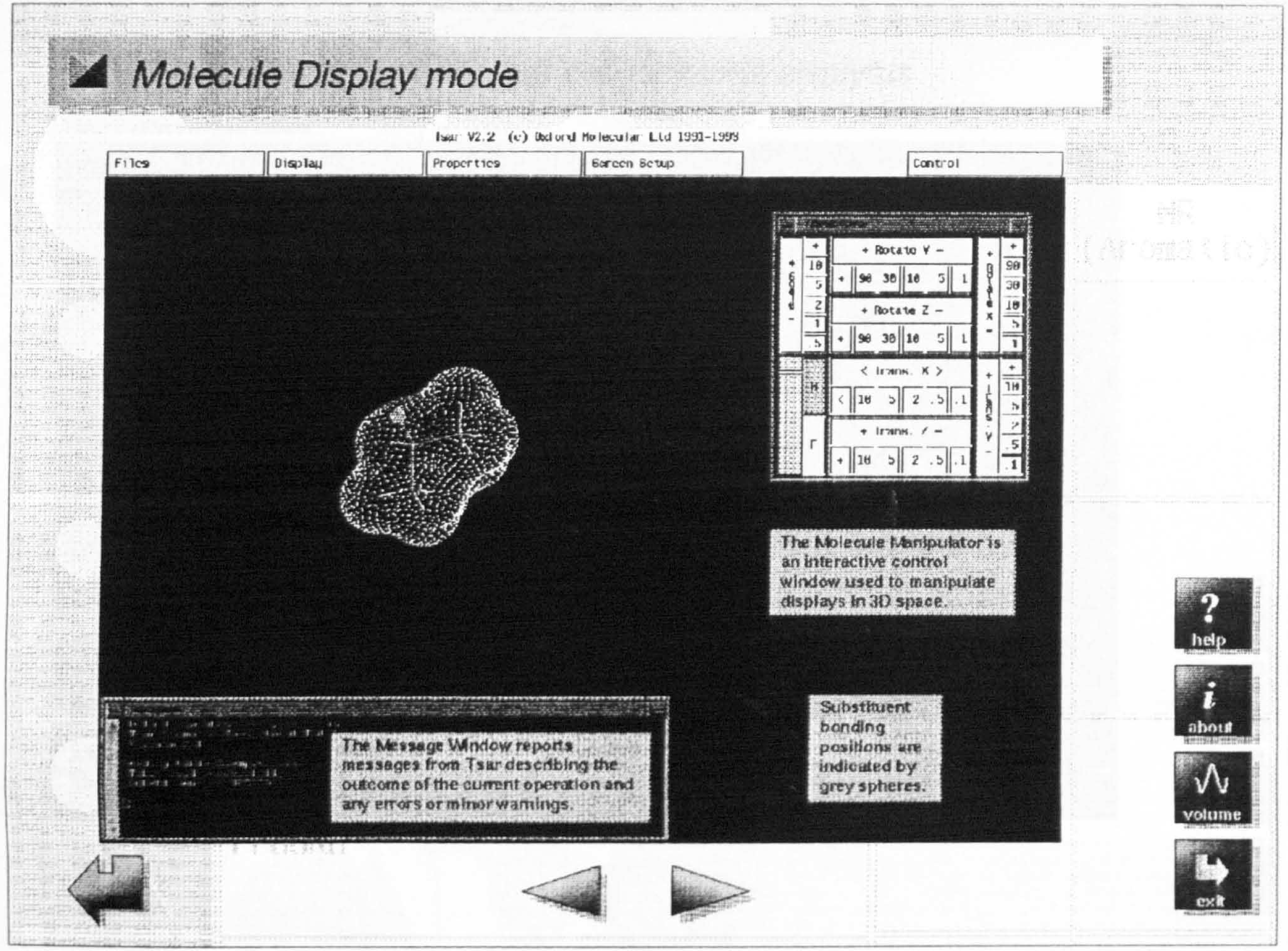


The Hansch approach

- In a general model for drug action, three steps can be considered necessary to elicit a biological response:
  - The drug reaches some specific receptor by a 'random walk' process.
  - A drug–receptor complex forms.
  - The complex undergoes some chemical or conformational change.

- The activity of a drug can be related to the probability, *p* of a drug molecule going through these three steps.
- Hansch argued that the ability of a drug molecule to interact with the receptor or 'critical site' might be dependent on its hydrophobicity (π), electrostatics (σ) and size (E_s).
- The resulting relationship is known as the Hansch equation and has been used very successfully in QSAR studies.

Figure 11 The 'Background to QSAR' section of the courseware.



The Molecule Manipulator is an interactive control window used to manipulate displays in 3D space.

Substituent bonding positions are indicated by grey spheres.

The Message Window reports messages from Tsar describing the outcome of the current operation and any errors or minor warnings.

Figure 12 The 'Using ***Tsar***' section of the courseware.

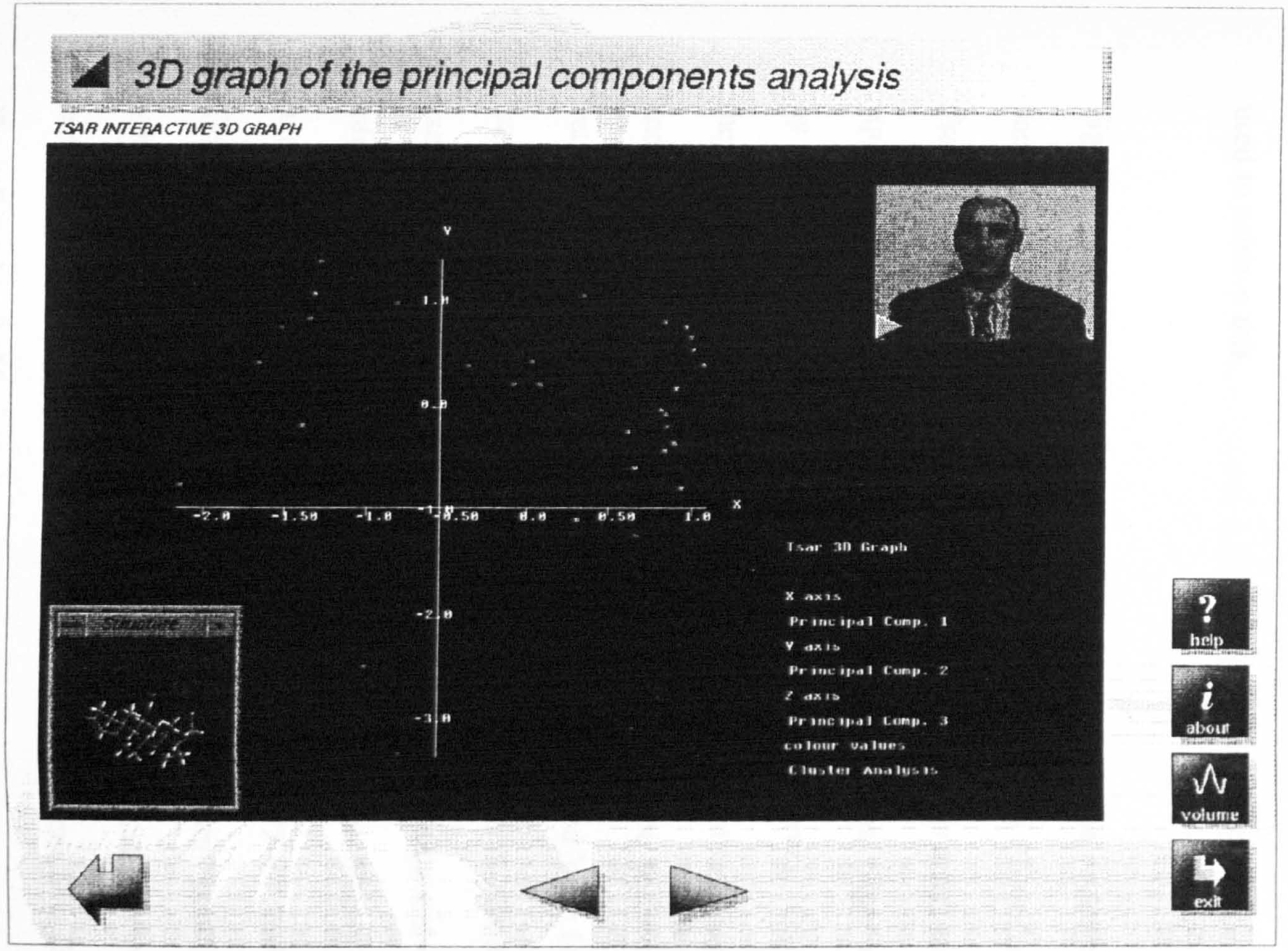


Figure 13 The '***Tsar*** case studies' section of the courseware.

7.5 Interface Design

The aim of the interface design process was to integrate the multimedia sequences and computational tools to create seamless and intuitive courseware. A graphical menu structure and simple paging model were used to achieve this.

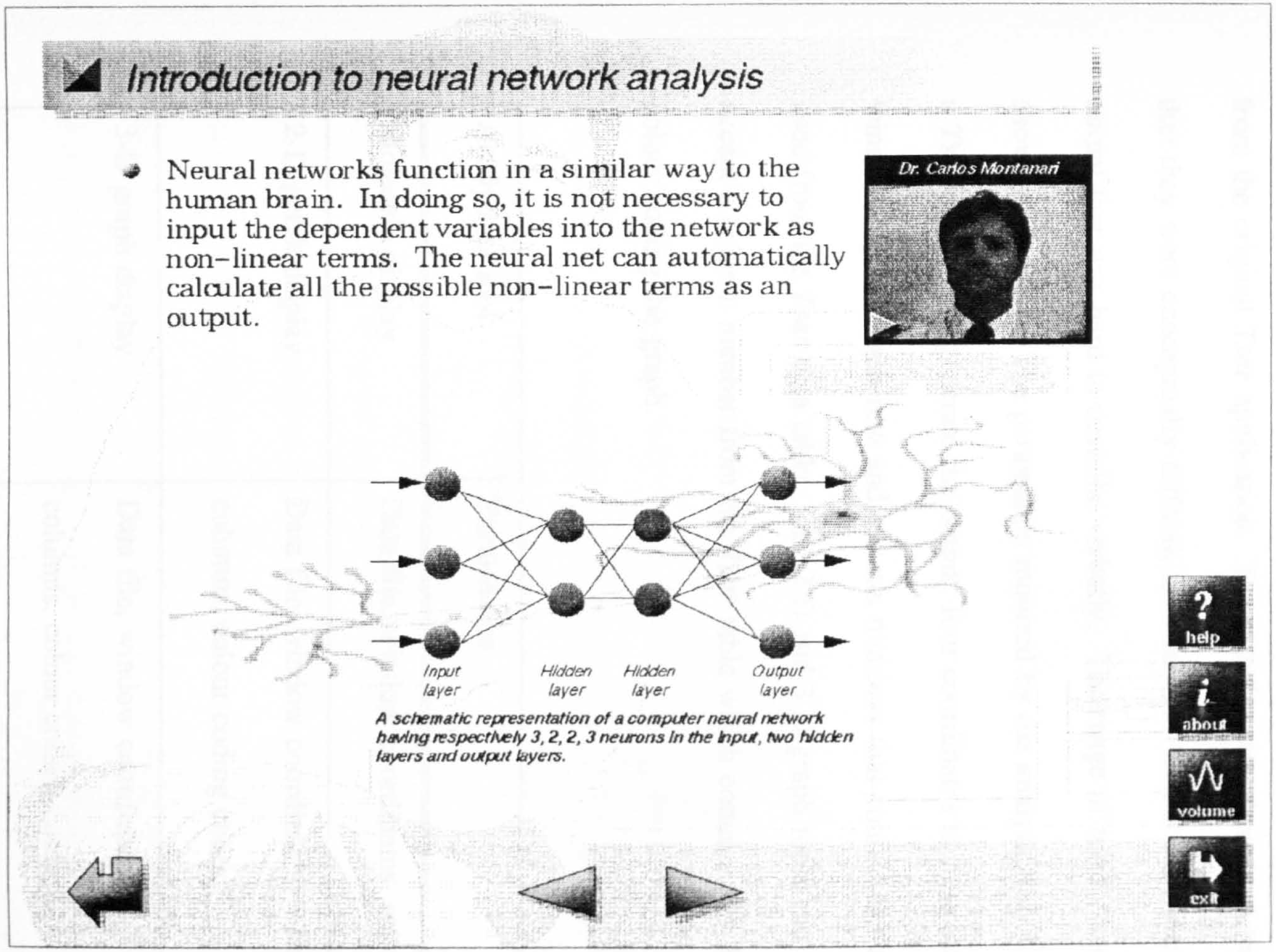
Figure 14 shows the functional areas used throughout the package. A background image is used to indicate the current section ('Introduction to ***Tsar***', 'Using ***Tsar*** 'or '***Tsar*** case studies'). This image is a full screen equivalent of the main menu image. Within each section, pages are chosen by clicking on reduced size images of the pages themselves. On each page, the perpetual features include a title that describes the current page contents and navigational icons that allow various operations to be performed. A 'return' icon enables the previous menu to be reached and 'page forward' and 'page backward' icons appear when appropriate. 'Help' and 'About' icons execute Showcase files that display navigational information and courseware information respectively. The 'Volume' icon executes the Silicon Graphics 'audiopanel', which allows the output volume to be set by the user. The 'Quit' icon allows a user to exit from the courseware at any point in a session. The media content area is a consistent size throughout the program and is used for the display of text, graphics and the interactive ***Tsar*** tools. The 'talking head' video window overlays the media area and appears in the top right corner.

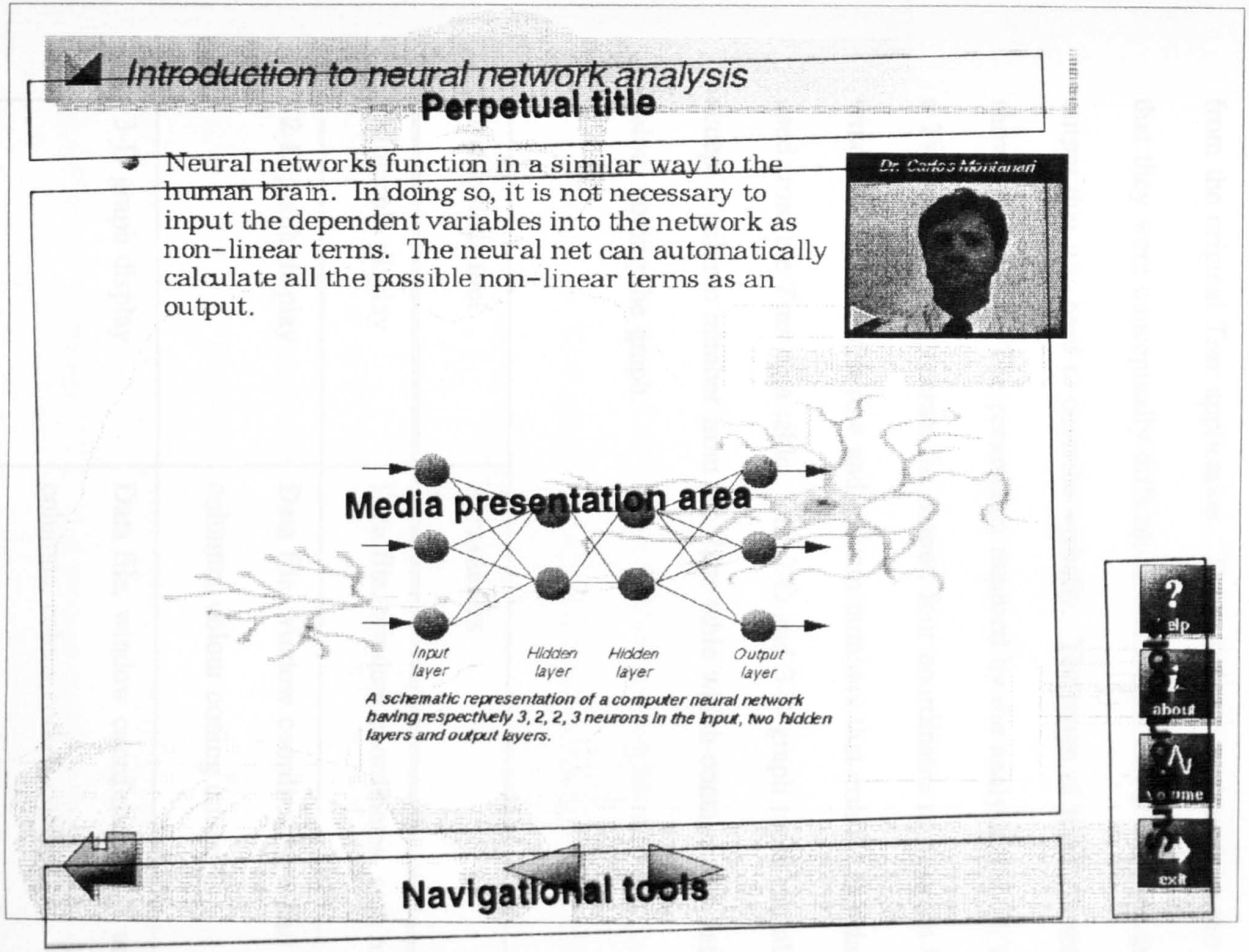
Colour and fonts are used discreetly throughout the courseware. Blue is a component of all navigational operations and information, which helps to separate these features from the media content (see Section 2.6.5). Helvetica font is used for screen titles and graphic labels and, to ensure readability, Times New Roman is used for all text passages.

7.6 Tsar Programming

7.6.1 Introduction

To integrate with the Showcase courseware, the ***Tsar*** application had to be modified so that the required analytical tools could be executed without displaying the data table and the rest of the user interface. Furthermore, the modified version had to accept several parameters passed to it from the courseware. This was to enable the results of an analysis to be displayed automatically, without the need for any user input. Re-compilation of the ***Tsar*** source code resulted in an executable program called 'tsardemo' that fulfilled these requirements. The design and implementation of this program are described in this section.



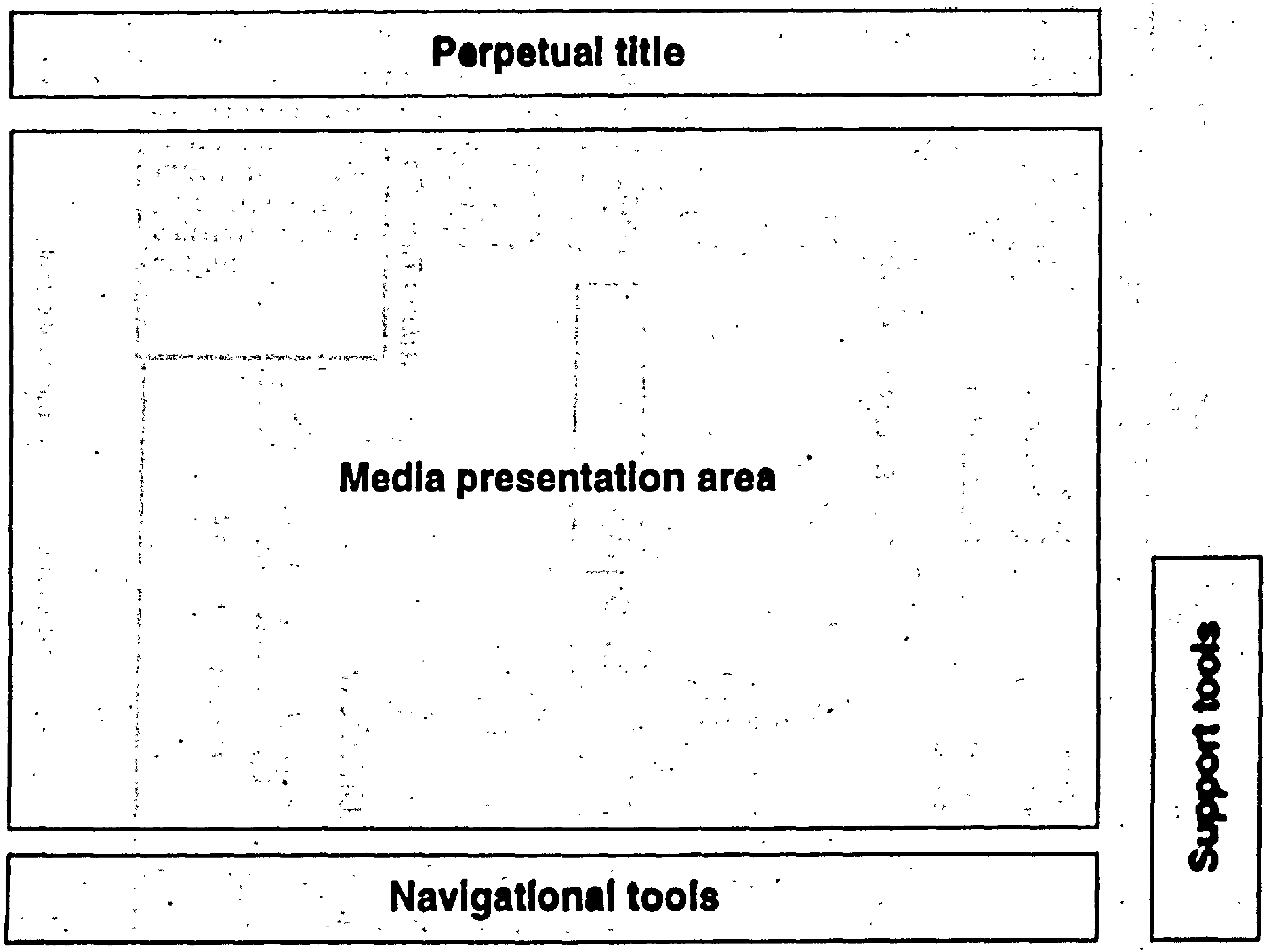


Introduction to neural network analysis

- Neural networks function in a similar way to the human brain. In doing so, it is not necessary to input the dependent variables into the network as non–linear terms. The neural net can automatically calculate all the possible non–linear terms as an output.

A schematic representation of a computer neural network having respectively 3, 2, 2, 3 neurons in the input, two hidden layers and output layers.

Figure 14 The functional areas used for the '*Tsar* Multimedia Training' courseware.


Perpetual title
Media presentation area
Navigational tools
Support tools

7.6.2 Tsar Functionality

The 'tsardemo' program was written to accept a parameter file as an input. These parameters included the data set to be displayed and the ***Tsar*** tool to be used. For this study, a reduced set of analytical tools were re-coded from the original ***Tsar*** application. These tools were chosen on the basis that they were conceptually difficult to understand and/or they produced an output that was hard to describe verbally. The range of tools chosen is shown in Table 8. The parameters required by the analytical tools include, a ***Tsar*** data file to generate the output, four coordinates to position the window, together with row and column numbers that contain the data to be used from the ***Tsar*** data table. The 2-D and 3-D graph tools can also accept a column number from the ***Tsar*** table which contains the data for colour coding the graph.

Analytical tool	**Parameters**
Molecule display	Data file, window coordinates, row number.
2-D graph display	Data file, window coordinates, x and y columns, colour coding column.
3-D graph display	Data file, window coordinates, x, y and z columns, colour coding column.

Table 8 The analytical tools in the 'tsardemo' program accessible from the Showcase courseware.

7.6.3 Integration with Showcase Courseware

To produce a dynamic and flexible courseware structure, a scheme was required that would allow external programs to be executed and 'killed' from within the Showcase document as pages were turned by the user.

The hyperscript facility of Showcase provides the necessary functionality by allowing Unix shell scripts to be attached to page turning events or to any object clicked on with the mouse. Upon turning to a page where an interactive tool is to be presented, a shell script can therefore be called from Showcase that executes the 'tsardemo' program and specifies a parameter file containing the display details (see Section 7.6.2). Simultaneously, the shell script can execute the 'movieplayer' program and pass to it the name of a video file to play. This scheme allows any combination of ***Tsar*** tool and video clip to be displayed on top of the Showcase courseware. Figure 15 shows this operation in diagrammatic form.

Upon initialisation of the 'tsardemo' executable, the unique process identification (pid) number of program instance is appended to the 'tsardemo.id' file. Turning a page in the Showcase courseware also executes the 'killTsar' program. This action 'kills' all processes with pid numbers stored in the 'tsardemo.id' file. This process management is also used to 'kill' movieplayer instances and it ensures that windows are efficiently removed as the user navigates through the courseware.

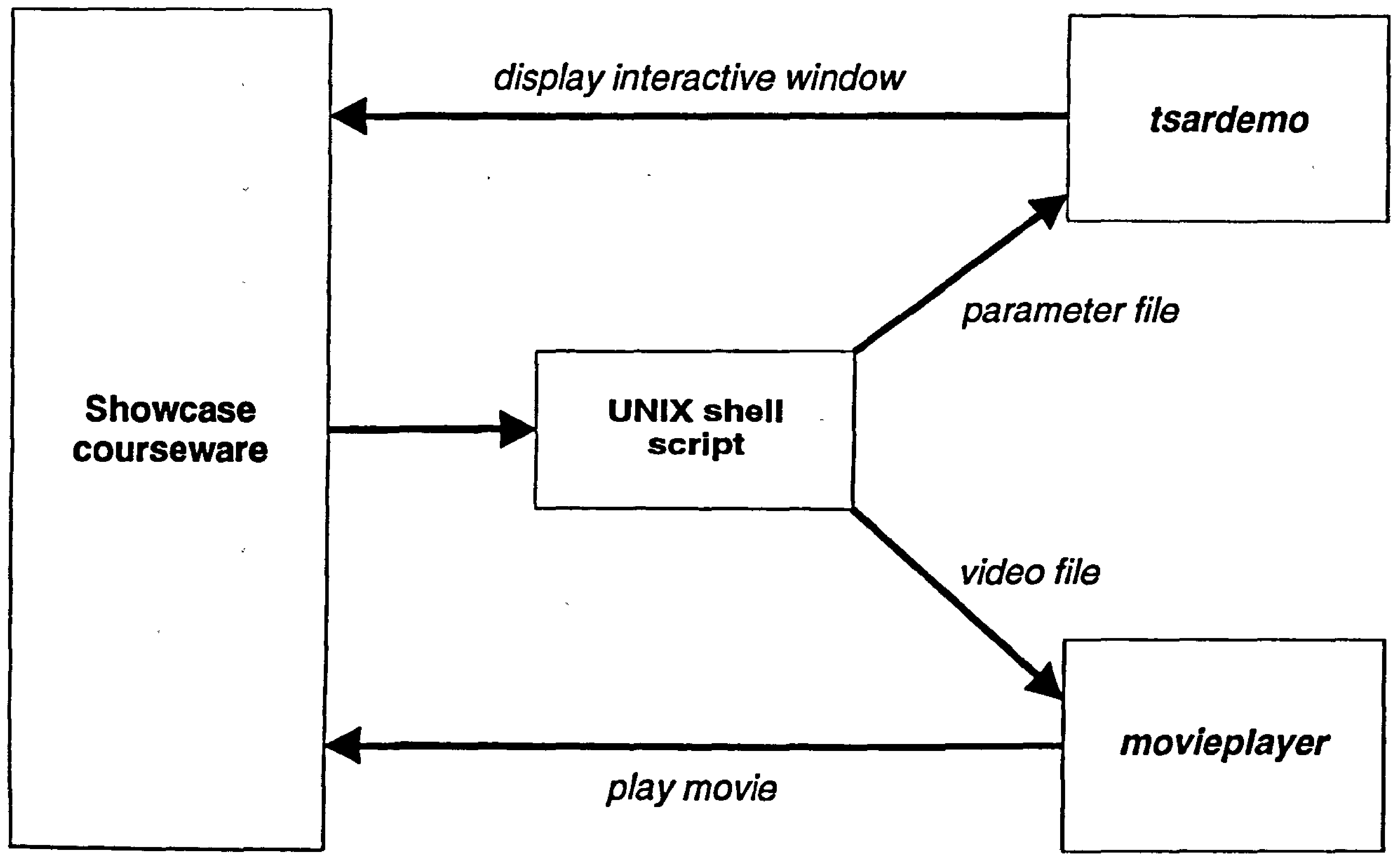


Figure 15 The execution of a *Tsar* tool and a video clip following a page turn event in the Showcase courseware.

7.7 Evaluation of Courseware Effectiveness

7.7.1 Introduction

The integration of digital video and interactive computational tools into a CAL program is a novel approach for the teaching of QSAR analysis. As such, the effects on learning from this combination of media have been little studied and it has yet to be established how students learn from such an environment and what learning benefits will result. The preliminary evaluation of this courseware was therefore designed to demonstrate the effectiveness of this concept, recommend improvements to the design and provide pointers to more detailed evaluation studies.

The benefits of evaluating CAL in an authentic setting have been demonstrated in Chapter 6. The results from this study had high ecological validity and provided a thorough insight into the effectiveness of the courseware. The present study was designed with the same realistic approach. Furthermore, the evaluation scheme was wide-ranging and open-ended, which allowed innovative features to reveal themselves.

This section describes the design and conclusions obtained from the initial evaluation of the '*Tsar* Multimedia Training' package.

7.7.2 Subjects and Implementation

The subjects chosen for the evaluation were all research chemists with computer and molecular modelling experience but with more variable knowledge of QSAR analysis. The courseware was distributed to several research groups for remote data collection and it was demonstrated at QSAR related conferences. The users were encouraged to evaluate the package immediately following its use.

7.7.3 Evaluation Methodology

A five-point Likert rating scale (see Section 3.4.2) was designed for distribution with the courseware and is shown in Appendix 5. The rating scale was administered as a two-sided A4 sheet and gave background information and instructions for using the courseware. The Likert scale ranged from 'Very poor' (1), through 'Neutral' (3), to 'Excellent' (5) apart from specific statements that required a set of five more detailed responses. Two initial statements assessed previous computer experience and knowledge of QSAR analysis. A series of nine statements then determined the quality of the interface and the effectiveness of the courseware. Finally, two text entry questions allowed a user to enter descriptions of particularly good or bad features about the program.

7.8 Results

The results from the rating scale are shown in Table 9. The percentage agreement with each statement has been calculated as well as the standard error. Users had good computer skills (59%) and were familiar with QSAR analysis (49%). The user interface was generally acceptable (67%) and navigation through the courseware was intuitive (74%). When asked about the usability and quality of the digital video and ***Tsar*** tools, comparable results were obtained (65% and 62% respectively). The users were then asked how the video material affected their attention to the ***Tsar*** tools. The average response was equivalent to 'Enhanced' on the rating scale (64%). A further question queried the subject correspondence between the video and the data presented using the ***Tsar*** tools. A good correspondence was perceived by most users (68%). When the degree of learning from the video and ***Tsar*** tools was assessed, users determined that they had learnt equally from both media types (50%). The two final questions show that the users had learnt more because of the media combination (58%) and they would use further multimedia training material that incorporated computational chemistry tools (80%).

Tables 10 and 11 show the results from the text entry questions concerning the good and bad features of the program. These results are categorised and each response is presented as a percentage of the total number of participants. Insignificant or inappropriate responses are grouped under 'Others' and the number of blank replies is also recorded.

Table 10 shows a summary of good features that users identified about the courseware. The ability to interactively manipulate graphs and molecules in 3-D was the most popular feature (32%). This is followed by a characteristic of the case studies, which recommended when a particular ***Tsar*** tool technique is appropriate to use in an analysis (16%). The courseware was also seen as simple to use and particularly suitable for occasional users of QSAR analysis. In addition, the ability to use the program with no prior knowledge was highlighted.

Table 11 shows a summary of bad features that users identified about the courseware. The greatest criticism was the lack of detail on QSAR techniques in the case studies (26%). The other major criticisms were focused on the digital video component of the program. The variable quality of the video material was highlighted by several users (16%) and the inability to control the audio and visual channels independently was not popular (11%). The distraction of movement in the video clips was a minor problem and additional tools for manipulating objects in 3-D on the screen were also called for.

Rating scale statements	**Percentage agreement (SE)**
How experienced are you with interactive computer systems?	59 (6.9)
How experienced are your with QSAR analysis?	49 (4.8)
How usable was the interface to the courseware?	67 (2.3)
How easy was navigation through the courseware?	74 (2.6)
Was the video material easy to use and understand?	65 (1.5)
Were the ***Tsar*** tools easy to use and understand?	62 (3.3)
Did the video distract or enhance your use of the ***Tsar*** tools?	64 (4.4)
How good was the correspondence between the video and the ***Tsar*** tools?	68 (1.5)
How much did you learn from the video and the ***Tsar*** tools?	50 (3.2)
Overall, did the combination of video material and ***Tsar*** tools help you learn more?	58 (6.1)
Would you want to use more training material that combined multimedia with interactive computational chemistry tools?	80 (2.0)

Table 9 Percentage responses to rating scale ($n = 19$).

Response	**Percentage respondents**
"Manipulation of 3-D displays"	32
"Explanation of when to use a technique"	16
"Simple to use"	11
"No prior knowledge required"	5
"An ideal tool for occasional users"	5
"Video makes it a personal experience"	5
Others	21
No response	11

Table 10 Categorised responses to the text entry question, "Is there anything that stands out as particularly good about the courseware?" (*n* = 19).

Response	**Percentage respondents**
"More detailed tutorials on QSAR techniques"	26
"Variations in volume, brightness and speed of video were distracting"	16
"Ability to turn off visual/audio component of video"	11
"Shoulder shaking and flicker on video distracting"	5
"Use a dialogue box for manipulation of molecules"	5
Others	21
No response	16

Table 11 Categorised responses to the text entry question, "Is there anything that stands out as particularly bad about the courseware?" (*n* = 19).

7.9 Chapter Summary

The results from the rating scale showed that a usable and navigable interface has been produced following the integration of computational chemistry tools and digital video. This finding is confirmed by the text entry question asking for good features about the program, where users highlighted the simplicity and lack of prior knowledge required to use the package.

The most positive result from the rating scale is the request for further training packages that integrate multimedia with computational chemistry tools. Since the manipulation of 3-D displays was the most popular feature of the courseware received from the text entry question, it is evident that users see the interactive ***Tsar*** tools as the most useful feature in their learning of QSAR analysis. In addition, the explanation of when to use particular ***Tsar*** tools was another notable feature. Therefore, it appears that the users responded well to the authentic contexts created in the case studies. This is supported by the greatest criticism of the package, which was the insufficient detail on QSAR techniques in the studies. It is clear that several users became engaged in the realistic implementations of ***Tsar***, but were frustrated by the limited detail on particular QSAR techniques.

An additional criticism highlighted by the text entry question was the quality of the 'talking head' video clips. Although the video material was easy to use and corresponded well with the ***Tsar*** tool data, some users still found it distracted their learning. The movement, brightness and variations in volume of the video were all criticised. However, this conceptual problem is not apparent from the rating scale results, which indicate that the combination of video and interactive ***Tsar*** tools generally helps the learning process. The variation in user learning styles probably accounts for the diversity of responses received. Several users suggest including an option that disables the audio or visual component of the video clips to counter this problem.

This study has demonstrated the feasibility of combining digital video with interactive computational chemistry tools to teach QSAR analysis. The video clips and re-coded ***Tsar*** application have been transparently integrated using the hyperscript feature of the Showcase application. This has created a highly engaging and context-based system for the teaching of complex analytical techniques.

Chapter 8

Discussion and Future Work

"...you ain't seen nothin' yet!"

(J. Philip Bays, 1992)

8.1 Introduction

The introductory chapters to this thesis (Chapters 1 to 4) summarise the design and evaluation of CAL, together with the incorporation of computational chemistry tools into undergraduate chemistry courses. A recurring theme throughout the literature is the implementation of novel computer technology before design guidelines have been formulated. This has restricted the number of useful guidelines that have emerged for the design of instructional courseware. For example, screen design (see Section 2.6), multimedia design (see Section 2.7.1) and instructional design (see Section 2.8.1) are still exploratory areas for the courseware designer. For the same reason, the development of reliable methodologies for the evaluation of CAL has lagged behind its introduction into the curriculum (see Section 1.1).

The software development described in Chapters 5, 6 and 7 closely followed existing guidelines for the design and evaluation of instructional courseware. This ensured that the effectiveness of the packages could be reliably reported and innovative features could be identified.

This section begins with a discussion of the two CAL programs developed during the course of this project. Emerging guidelines for the integration of computational chemistry tools into multimedia courseware are discussed. Finally, the prospects for computational chemistry in the curriculum are considered. This includes potential enhancements to the software developed in this project and how emerging computer technologies may be exploited to create innovative tools for the teaching of undergraduate chemistry.

8.2 Integration of Molecular Modelling and Tutorial Courseware

Chapters 5 and 6 describe the design and evaluation of a novel CAL package that combines interactive molecular modelling with tutorial courseware.

The conclusion from Chapter 5 is that a generic environment for authoring chemistry courseware has been created. This integrated system gives the courseware author precise control over the modelling tools and so allows students of all abilities to use the software. For example, for a student with no prior experience of molecular modelling, the modelling functions can be introduced sequentially, increasing in complexity as they progress through a package. This is an important observation, since different learning styles should be allowed in a CAL lesson, through flexibility in its design (see Section 2.8.5).

Through using established principles of courseware design (see Section 2.6) during the development cycle, an intuitive user interface was produced for the prototype courseware. For example, all molecular modelling functions and navigational operations perform consistently and the interface remains uncluttered by ensuring that only directly relevant functions are visible on the screen for a particular task.

The integration of the interactive molecular modelling tools with the courseware interface presented a novel design problem, since there are few reliable guidelines for molecular modelling screen design (see Section 4.3.2). Consequently, the modelling tools were integrated as transparently as possible with the rest of the system. Disguising the underlying modelling application in this way enables a user to concentrate on the subject material and not on a plethora of potentially confusing functions. The modelling tools themselves included several different molecular representations which were accessible in the self assessment section. This helped to ensure that students did not rely one a single molecular representation and were made aware that different models are merely alternate ways of showing the same structure (see Section 4.3.2).

The evaluation of the prototype package in Chapter 6 shows that this integrated approach allows engaging courseware to be authored that assists students in the visualisation and comprehension of molecular chemistry concepts. The most positive feature of the package reported by the students was the ability to manipulate 3-D molecular structures during the assignment of *R* and *S* designation (see Table 5). This is supported by the interaction monitoring data, which show that the students manipulated the molecules significantly more during spatially complex operations (*i.e.* the designation stage). Since interactivity is a key determinant in learning from CAL (see Section 2.8.3), this is an encouraging observation as it is clear that the students' curiosity about the interactive device was motivating them to learn.

The evaluation scheme itself combined qualitative and quantitative methodologies to demonstrate the effectiveness of 'triangulation' in courseware evaluation (see Section 1.7.3). A complete picture was obtained by analysing user attitudes, scores obtained and interactions with the courseware. In addition, the application of the study as part of an actual undergraduate course showed the importance of a realistic environment for CAL evaluation, since the results obtained have both external and ecological validity (see Section 1.7.2).

The authentic environment used for the evaluation brought many benefits, but there was an inherent lack of control over data collection. Consequently, insufficient data were obtained to enable 3-D manipulation of molecules to be correlated with scores obtained in the self-assessment section. A more quantitative, controlled study would provide insights into the relationship between the visualisation of 3-D molecules and the learning of spatial chemistry concepts.

The effect of student attributes on their ability to learn from computerised 3-D molecular modelling is another important issue. For example, it is widely reported that males have better spatial ability than females of an equivalent age and spatial ability is often highest in ambidextrous males (see Section 4.2.1). Results from a study relating student characteristics to performance would highlight any confusion in visualising 3-D structure. If necessary, modifications could then be made to the interface to ensure that students of all abilities can benefit from this learning environment.

8.3 Integration of Multimedia and Computational Chemistry Tools

Chapter 7 describes the design and evaluation of an innovative training package that combines interactive computational chemistry tools and 'talking head' digital video to introduce the concepts of QSAR analysis. This package allows a user to experience computational chemistry tools in a visual and qualitative way, without knowing the underlying theory. The assumption is that this will help them to form an accurate mental model (see Section 2.5) of the technique and later gain a better understanding of the theoretical basis for the method.

A simple graphical user interface was developed for the courseware that employs established principles of CAL and multimedia interface design (see Sections 2.6 and 2.7). In this way, the users focus on the subject material rather than the complexity of a badly conceived interface.

Emerging instructional theories for multimedia design were also incorporated into the prototype courseware to evaluate their application to this novel combination of media types. For example, the concept of situated learning (see Section 2.8.4) is successfully exploited by using a realistic and engaging case study format. This was achieved by using experienced users of the ***Tsar*** program, who described an analysis they had carried out using the actual data set. This multimedia presentation is coupled with the interactive ***Tsar*** tools, which gives further realism by allowing the users to manipulate the data and observe the results (see

Section 2.8.3). The evaluation highlighted the users' appreciation of this format, since it explained to them the exact situation when a particular technique was appropriate (see Table 10).

The dual-coding theory (see Section 2.7.1) was used as a justification for presenting digital video and interactive computational tools simultaneously. This theory predicts that better retention results from an audiovisual presentation since audio and visual information are stored separately in memory. However, in this study, the theory was extended to assess the benefits of combining an audiovisual channel with an interactive visual channel. The results from the evaluation suggest that the simultaneous presentation of these two dynamic media may exceed the cognitive load of many users. This can be deduced from the request for an option to disable the visual and/or audio component of the video channel (see Table 11). The broad band width of the video channel (see Section 2.7.3) appears to distract the users from studying and manipulating the data displayed using the computational tool in sufficient detail.

Following evaluation of the package by medicinal chemists wishing to learn QSAR analysis, the effectiveness of the courseware could be enhanced in a number of ways. The main recommendation is the availability of an audio-only narration with interactive computational tool presentations. This is supported by work on narrated animations by Mayer and Sims (1994), who found that this approach led to better retention of the information and more creative solutions on problem solving tasks (see also Section 2.7.1) [97].

This is worthy of further investigation, since if the audio channel exactly complemented the data presented by the ***Tsar*** tool (see Section 2.7.5), attention would be completely focused on the ***Tsar*** window. In addition, the sudden change in modality (*i.e.* video to audio and 3-D graphic) would also gain attention (see Section 2.7.5). This would ensure the users experienced the information in both verbal and visual forms, increasing the chance of its retention.

Several other recommendations have been made by users who requested the ability to choose their own data sets and analytical tools. This could be combined with critical assistance from an animated or video 'guide' to arrive at the optimum analytical approach. The concept of the expert guide has been successfully used in interactive multimedia courseware (see Section 2.6.3.3). This approach could be exploited here by allowing users to study the points of view of a series of experts. This would provide a complete understanding of when to apply each of the computational chemistry tools available in the ***Tsar*** application.

8.4 Guidelines

A number of useful guidelines have emerged following the development of the two courseware packages described in this thesis. These are concerned with the integration of computational chemistry tools, interactive molecular modelling and multimedia to ensure instructionally effective CAL and they are listed below:

- *Use established principles of interface design*

The studies carried out in this thesis have shown that the integration of computational chemistry tools into CAL should follow established interface design principles to maximise usability and instructional effectiveness (*e.g.* simplicity, consistency, colour use and quality of interaction).

- *Account for different learning styles and abilities*

Interactive molecular modelling tools should be adaptable in order to account for different user learning styles and spatial abilities. This can be achieved by incorporating several molecular representations (*e.g.* stick, ball and stick, space fill), different rotational mechanisms (*e.g.* virtual trackball, sliders or scroll bars) and by allowing the display of atom colours, hydrogens and atom labels to be manipulated.

When combining digital video and interactive computational tools, users should be allowed to disable the audio and/or visual components of the video channel. The broad band width of video causes it to dominate all other media types (see Section 2.7.3). Therefore, audio and visual channel control is essential to allow users to tailor the presentation and attend to all relevant information.

- *Restrict functionality to what is required*

The idea of 3-D molecular modelling on a computer is a demanding conceptual task for novice users. Therefore, modelling tools should be carefully used and only the necessary tools should be presented for a particular task.

- *Provide an indication of the interactive nature of 3-D tools*

Novice users need encouragement to manipulate 3-D displays. They may also need an explanation of how rotation is taking place. For example, a description such as, "The molecule is inside a glass sphere which is being spun around by the mouse", would encourage the formation of a usable mental model of 3-D rotation.

- *Ensure there is high correspondence between video material and a computational chemistry tool display*

In keeping with established multimedia design guidelines, all information that is presented to the user must convey the same message otherwise confusion will result.

- *Present computational chemistry tools in a relevant context*

A case study, simulation or role playing format is the most engaging environment for presenting complex analytical techniques. This concept could be extended to include animated or video guides in a presentation who provide opinions and advice on using an analytical tool.

8.5 Future Work

8.5.1 Molecular Modelling in the Chemistry Curriculum

The feasibility of integrating molecular modelling into instructional courseware to teach basic stereochemistry has been demonstrated in Chapters 5 and 6. This suggests that the teaching of other molecular chemistry topics would benefit from integrated structure visualisation. For example, the study of reaction mechanisms, receptor-ligand interaction and trends in molecular series would also benefit from interactive 3-D molecular modelling.

To provide the functionality required for further chemistry topics, the Nemesis DLL would be extended to include more utilities from the full application. Students could then experience dynamic and visual representations such as real-time energy minimisation, molecular dot surface generation, atom centred partial charges and conformational scans. Further prototyping and evaluation of alternate interface layouts would be necessary to guide the development of these tools. A general purpose 'molecular viewer' would be the most appropriate approach to this problem. This would ensure that the modelling tools were presented consistently between courseware modules and the viewer could easily be updated with more functionality as required. In addition, tools that were inappropriate for a particular CAL module could easily be disabled, which would ensure that the simplicity of the viewer was maintained.

The relentless development of faster computer hardware and sophisticated software tools ensures that molecular modelling will continue to be incorporated into more aspects of chemistry education. For example, the recent introduction of fast, low-end workstations from Hewlett-Packard, IBM and Silicon Graphics have created exciting opportunities for computational and molecular visualisation resources [165, 175]. Students may soon be able to compute and visualise molecular mechanics, coloured bonding of molecular orbitals and semi-empirical or *ab initio* calculations as part of their undergraduate courses. However, these facilities will inevitably bring more complexity to the user interface. Therefore, further research is required to determine exactly how to present these tools to the student to maximise the learning benefits.

8.5.2 The World Wide Web

The World Wide Web (WWW) was established by a consortium of computer users in 1989 with the aim of creating a standard syntax called HyperText Markup Language (HTML) for composing documents for distribution over the Internet [195]. The HTML syntax combines text and formatting commands which allows it to combine images, movies, audio and animation. An HTML document is based on the HyperText concept of non-linearly linked information. Linked information can reside on any computer on the Internet and can consist of audio, video, animation and images.

Every HTML document and every computer on the Internet must be uniquely identifiable to prevent conflicts between machines using the same addresses. To cope with this requirement, the Uniform Resource Locator (URL) was developed. A URL consists of the address of the remote computer (*e.g.* www.nottingham.ac.uk) and the name of the HTML file (*e.g.* depts.html). Together, these two components allow a document to be uniquely accessed, for example, http://www.nottingham.ac.uk/depts.html.

Using the appropriate viewer software (*e.g.* Netscape[6] or Mosaic[7]), HTML documents are accessible across a variety of platforms including the Apple Macintosh, IBM-compatible computers and workstations running the Unix operating system. These document viewers provide a user-friendly, mouse-driven graphical interface for accessing interactive multimedia information.

The multimedia capabilities of the WWW offer a new and exciting opportunity for the distribution of teaching materials across the Internet. WWW information is accessible by any number of students throughout the world, the course material is readily revisable and students can add extra material to the information. Nevertheless, a number of workers have warned against over-exploiting this new technology before the pedagogical benefits have been properly assessed. For example, Woolston (1995) suggests that teaching material developed at one site may be inappropriate for users at another site because of different course requirements. In

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[6] Netscape Communications, Mountain View, CA.

[7] NCSA, Urbana-Champaign, IL.

addition, the current HTML viewers are restricted in the amount of interactivity that they allow and this is the most important feature of effective CAL (see Section 2.8.3). However, Woolston suggests that the collaborative development of teaching materials may be beneficial to course development, since specialist knowledge can be combined from many different sources [196].

Soloway (1995) adds that teaching practices will have to change dramatically to make effective use of the Internet. Students must be allowed to probe deeply into a topic over an extended period of time before the WWW is seen as a significant improvement over traditional teaching practices [197].

Despite the current limitations of the WWW, several academics have begun to experiment with the Internet as a medium for teaching chemistry. For example, Professor Peter Murray-Rust and Dr. Alan Mills have established an open-access WWW course called 'The Principles of Protein Structure' at Birkbeck College, London, UK (http://www.cryst.bbk.ac.uk/PPS/index.html). The course was run for the first time in January 1995 with over 250 undergraduate students and industrial scientists from around the world.

This innovative approach has introduced several new techniques to the teaching of molecular chemistry. Firstly, students are expected to contribute some of their own teaching materials, which produces a dynamically evolving teaching resource. The course also allows students to examine protein structures in 3-D as they study them. This is achieved by integrating the WWW document viewer with RasMol[8], which is an interactive molecular viewer. When a student clicks on a graphical 'hyperlink' to a molecular structure, the molecule data file is retrieved from the remote machine and loaded into RasMol, which is executed on the local machine. In this way, the mechanism for activating the molecules is embedded within the context of the discussion in the HTML document, creating an engaging learning environment.

Recently, work has begun on enhancing the distribution of chemical information over the Internet. Chemical Markup Language (CML) has been devised as an extension of HTML to standardise the way of 'marking-up' chemical structures and to cater for a wider range of datatypes than HTML (which deals primarily with hypertext) [198]. CML allows specific attributes of 3-D structures to be controlled. For example, instructions can be passed to RasMol to specify that individual residues in a molecule file are coloured differently from the rest and displayed in a different representation (*e.g.* space fill). In this way, attention can be focused on a particular structural attribute making an effective instructional tool. This technique has been extended to marking up structures associated with mass spectra, organic synthetic schemes and potential energy surfaces [199].

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[8] Obtainable by anonymous FTP from ftp.dcs.ed.ac.uk [129.215.160.5] in the directory /pub/rasmol. Written by Roger Sayle, BioMolecular Structures Group, Glaxo Research & Development, Greenford, Middlesex, UK.

An alternative approach for addressing the limited interactive capabilities of WWW material is to integrate Internet access into a multimedia authoring system. For example, the Formula Graphics System[9] allows multimedia courseware to be produced that has WWW connectivity. This enables HTML documents to be loaded and displayed as part of a multimedia presentation on a local machine. This technique is worthy of further investigation, particularly for enhancing the pedagogical quality of WWW material.

It has been said that by 2005 every person on the planet will have an Internet connection if the growth of the network continues at the present rate [196]. This fact alone suggests that the teaching potential of the WWW must be improved to facilitate the distribution of interactive multimedia instruction. Together with the further development of the concepts described in this section, this will undoubtedly lead to more important enhancements to the teaching of chemistry.

8.5.3 Virtual Reality

Virtual reality (VR) derives from aeronautics and space research and involves the integration of 3-D graphics and interactive devices. VR systems use peripheral vision to enhance the 3-D nature of an image, so when the user moves forward, parts of the image disappear behind the viewer, giving the feeling of motion. This allows the user to experience an artificial reality and simulates a feeling of 'being in the picture' [118]. VR

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[9] Harrow Software, Sydney 2001, Australia (http://www.magna.com.au/~formula/).

technology is still developing and the processing power it requires has limited its use on desktop personal computers to date [77].

Chemists have already recognised that molecular modelling and computational chemistry are ideal applications for VR technology [200]. DeKock *et al.* (1993) describe this as an exciting possibility, since it will allow students to study such things as reaction mechanisms and discover exactly how molecules orientate and fit together [160].

The integration of VR and the WWW (see Section 8.5.2) is another active research area that has implications for chemistry education. In particular, the recent development of Virtual Reality Modelling Language (VRML) is showing potential as a tool for teaching molecular chemistry on the Internet. VRML allows 3-D objects (*e.g.* spheres or cylinders) to be allocated a size, texture, colour and position and be represented in 3-D space using a visualisation program. Several commercial VRML viewers are under development (*e.g.* WebFX[10]) which can be combined with an HTML navigator such as Netscape, allowing VR objects to be viewed as an integral part of a multimedia WWW document.

Unfortunately, VRML is currently not sufficiently sophisticated to represent complex molecular structures. For example, tapered bonds, dot surfaces and ribbon representations are beyond the scope of VRML v1.0 [201]. The

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[10] Paper Software, Inc., 4 Deming St., Woodstock, NY 12498.

ability to annotate 3-D protein structures is another feature which would be valuable for educational purposes.

The WWW viewers that are emerging have also made real-time communication between remotely based chemists a possibility. For example, Casher and Rzepa (1995) have investigated the feasibility of so-called 'molecular video conferencing'. Their prototype system allows two or more remote collaborators to interact with a 3-D image of a molecule. Each participant can manipulate the image and these operations are viewed by the other participants in real-time. This information can also be accompanied by audio and/or video data. To achieve this functionality, the system integrates a WWW browser, a molecular visualiser and a browser implementing VRML scene descriptions. The molecular visualiser reads the chemical data files and exports them as 3-D VRML objects, which are then displayed by the VRML viewer. This technique has great potential for molecular chemistry education, but the limitations of desktop computer hardware and software have restricted its widespread acceptance by the chemical community. These workers also stress that the acceptance of this way of presenting information (*i.e.* navigating through a 3-D world) is another major consideration that needs further examination [202].

Using VRML in a collaborative environment is a top priority among the VRML community [200]. This fact alone ensures that WWW and VR technology will continue to be improved in the near future and consequently it will become more accessible to chemists and eventually students.

Therefore, further enhancements to VRML and viewer software are essential to enable chemistry educators to describe 3-D systems with the flexibility that they require. With these developments, an innovative and exciting medium for teaching molecular chemistry will emerge.

Another VR viewer and authoring tool, called QuickTime VR, is being developed by Apple Computer, Inc.[11] This system uses panoramic photographs to allow users to view a scene in 360 degrees, zoom in and out, change position within the 3-D space and pick up objects and look at them from any angle. The correct perspective is maintained during all operations, which creates a realistic environment for studying 3-D objects. This technology is at any early stage of development and only a few innovative applications have emerged. However, since QuickTime VR only requires QuickTime v2.0 for the Macintosh or Microsoft Windows to display VR objects, this technology will undoubtedly become integrated into desktop computer software in the near future.

The potential of QuickTime VR in undergraduate chemistry still needs to be assessed. Further development and evaluation of this software and its integration with instructional courseware may prove to be an invaluable tool for teaching molecular chemistry.

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[11] Apple Computer, Inc. 20525 Nariani Avenue, Cupertino, CA 95014-6299.

APPENDIX 1

Glossary

2-D Two-dimensional.

3-D Three-dimensional.

ab Initio In computational chemistry, this involves starting from first principles in a calculation.

APW (Authorware Professional for Windows) A commercial authoring system produced by Macromedia, Inc.

authoring system Computer software which allows the rapid development of courseware without the need for low level programming.

ATI (Aptitude-Treatment Interaction) A CAL research technique that assumes that learning involves interactions between the task the learner performs, the learner and the characteristics of the media.

band width The amount of information a medium can present to the user at any one time. High band width media (*e.g.* video) can easily overload human information processing capabilities.

bitmap A way of describing an image as a bit pattern or series of numbers that give the shade or colour of each pixel (*i.e.* each point that makes up the image).

CAI (Computer Aided Instruction) See CAL.

CAL (Computer Aided Learning) Computer software designed for education.

closed questions Questions in which the respondent selects from a predetermined set of replies (see also **open questions**).

CML (Chemical Markup Language) An extension to the HTML syntax which provides a standard method for 'marking up' chemical structures for distribution over the WWW.

cognitive load The load made on a person's cognitive resources, in particular memory.

continuing motivation The maintenance of user motivation (*i.e.* the will to learn) throughout an instructional lesson.

courseware Computer software designed for education. See also **CAL.**

depth cueing The display of objects on a computer screen in such a way that they appear to be three-dimensional.

digital video Video sequences stored on a computer as machine-readable binary numbers instead of analogue recording techniques.

DLL (Dynamic Link Library) A library of general purpose functions that can be called by other computer programs while they are running.

double buffer A copy of a visible graphical object that is stored in computer memory.

dual-coding The theory that information will be retained better if it is stored in both visual and verbal forms in memory.

ecological validity The degree to which the environment in which a study is carried out affects the results that are obtained.

external validity The degree to which the results from a study can be generalised to apply to other populations, settings, or levels of variables.

formative evaluation An evaluation which takes place before the actual implementation of a product and influences its development.

functional area An area of the computer screen reserved for related operations (*e.g.* navigational functions).

GB (Gigabyte) A unit of computer storage. One gigabyte is 1,073,741,824 bytes.

guide A virtual character creating by the computer that initiates action.

HCI (Human-Computer Interaction) The processes, dialogues and actions that a user employs to interact with a computer.

HTML (HyperText Markup Language) A standardised method for creating documents containing multimedia information for access across the Internet.

HyperCard A Macintosh-based product that uses hypertext to allow the organisation of information in a random manner.

hypermedia A collection of non-linearly linked information, that may include text, video, sound or animation.

hyperscript A feature of Showcase (Silicon Graphics presentation software) that allows dynamic courseware to be produced. A hyperscript consists of an event that causes the script to run and execute a list of actions.

HyperText A system that is designed on the notion of documents being non-linear, with pointers from words or points in the text to other words or points in the text.

icon A symbolic, pictorial representation of any function or task.

interface metaphor The use of a familiar object to represent the structure of a computer system (*e.g.* the desktop metaphor).

interaction The exchange that occurs between users and computers.

internal validity The degree to which an experimental design allows for uncontrolled results.

Internet An international network of computers that connects government agencies, universities and industry and uses standardised protocols for the exchange of information. It is estimated that there are now 6 to 7 million computers connected to the Internet.

Likert scale A multi-point rating scale that measures the strength of a subject's agreement with a clear statement.

MB (Megabyte) A unit of computer storage. One megabyte is 1,048,576 bytes.

media comparison A CAL research technique that compares new technology directly with the traditional method of instruction.

media replication A research technique that investigates the relative effectiveness of one or more dimensions of CAL (*e.g.* screen design).

mental model A model that evolves in the mind of the user as they learn and interact with a computer system. An ideal mental model is consistent with the conceptual model of the system developed by designers.

metaanalysis The combination of the effect sizes of individual studies (expressed as the average distance between experimental and control groups) into one common effect size.

multimedia The use of several different kinds of input and output media in combination (*e.g.* sound, text, video and animation).

object procedure In the Windows environment, a function that receives and sends messages to manage objects on the visual display.

observational evaluation A software evaluation technique that involves watching or recording user interaction with a system.

open questions Questions where the respondent is free to provide their own reply (see also **closed questions**).

palette The total number of colours available for pictorial representation on the computer screen.

PID number (Process Identification number) A unique number assigned to every active process on a Unix system.

prototyping The act of developing a computer system that is functionally incomplete for testing purposes.

QSAR analysis (Quantitative Structure-Activity Relationship analysis) A computational chemistry technique for drug design. Multiple properties of a set of related drug molecules are analysed statistically with the aim of predicting new structures with higher activities.

QuickTime An extension of the Macintosh system software which integrates time-based data types into mainstream macintosh applications. In QuickTime, the time-based data are referred to as movies.

QuickTime VR (QuickTime Virtual Reality) A 3-D virtual reality viewer and authoring tool that is an extension of QuickTime v2.0.

RAM (Random Access Memory) Readable and writable computer memory.

serif/sans serif font A serif font has embellishments to improve the readability of long passages of text (*e.g.* Times Roman). Sans serif fonts have no embellishments and are commonly used for titles (*e.g.* Helvetica).

shell A program that provides the primary interface to a Unix system by acting as a command processor and by interpreting scripts of commands.

shell script A list of commands that can be executed by a shell.

short term memory A small working space in which limited information can be held for a short period (also known as working memory).

situated learning Learning that occurs in a particular context.

spatial ability The ability to mentally visualise objects in three-dimensional space.

summative evaluation An evaluation which takes place after implementation of a product and has the aim of testing the proper functioning of the application.

survey evaluation A software evaluation technique that involves recording user attitudes about a system.

task analysis The investigation of a problem by breaking down tasks that a user does, or would do, into sequences of actions and objects.

trackball An input device consisting of a ball that a user can rotate in any direction within a fixed socket.

triangulation The use of multiple measures in an evaluation with the aim of converging more accurately on a variable associated with learning.

URL (Uniform Resource Locator) An unique identifier used to locate a WWW document on the Internet. It consists of the Internet computer's address and a file name (*e.g.* http://www.nottingham.ac.uk/depts.html).

unix Any operating system that meets generally accepted Unix-like standards with respect to providing user and programming services. This usually includes multi-tasking and multi-user capabilities.

usability A measure of the ease with which a system can be learned or used, its safety, effectiveness and efficiency and the attitude of users towards it.

user interface The complete surface features of a computer system, which includes its input and output devices and the information presented and received from the user.

virtual sphere An interface control device that uses the mouse to simulate the mechanics of a physical 3-D trackball (see also **trackball**).

VR (Virtual Reality) A computer-generated 'reality' which users may enter by virtue of bodily peripherals such as data gloves and head-mounted computer graphic displays. Now appearing in desktop multimedia.

VRML (Virtual Reality Modelling Language) A protocol that extends the HTML concept by allowing 3-D scenes to be described on the WWW. It is based on the Open Inventor file format (3-D modelling application).

window A bounded area of the computer screen, manipulated by a graphical user interface.

WWW (World Wide Web) An Internet service that allows a user to find multimedia information stored in a large number of hypertext-based databases by using a keyword search.

APPENDIX 2

DLL Source Code

```
/****************************************************************************
 *                                                                          *
 *  Name: Nemesis.c             - main message handler for the DLL.         *
 *  Functions: LibMain()        - entry point to the DLL.                   *
 *         WEP()                - exit routine.                             *
 *         ValidWindow()        - assigns APW HWND to a global.             *
 *         APWMessageDispatch() - message handler for the DLL.              *
 *         CopyObject()         - copy object to memory.                    *
 *         EraseObject()        - erase object from APW display manager.    *
 *         InvalidateDisplay()  - BitBlt the double buffer to APW.          *
 *         PaintMolecule()      - BitBlt invalid part of buffer to APW.     *
 *                                                                          *
 *         APW callable:                                                    *
 *         InitialiseWindow()   - draws the window on the APW screen.       *
 *         ReadCOSMICDataFile() - displays a COSMIC file.                   *
 *         MouseMove()          - initiates 3D operations.                  *
 *         Stick()              - draws the molecule in stick mode.         *
 *         BallandStick()       - draws in ball & stick mode.               *
 *         SpaceFill()          - draws in space fill mode.                 *
 *         Hydrogens()          - Hides/displays hydrogens.                 *
 *         Labels()             - Hides/displays labels.                    *
 *         ResetLabels()        - Resets labels to original.                *
 *         Active()             - Activates/deactivates a molecule.         *
 *         Highlight()          - Ability to highlight atoms (on/off).      *
 *         GetAtom()            - Was the atom clicked was correct ?        *
 *         WarningBox()         - Puts up a Windows warning box.            *
 *--------------------------------------------------------------------------*
 *    Author: Richard T Hyde                                                *
 *      Date: 1/10/93                                                       *
 *--------------------------------------------------------------------------*
 * Modification Record                                                      *
 * Date      Inits  Comments                                                *
 ****************************************************************************/

#ifdef NULL
    #undef NULL
#endif

#include <windows.h>
#include <apwpost.h>
#include <string.h>
#include <FileIO.h>
#include <Headers.h>
#include <Colour.h>
#include <DrwFcnTy.h>
#include <StrTab.h>
#define _INIT_GLOBALS_
#include <Globals.h>
#include <Nemesis.h>

#define _WANT_FATALS_
#include <Atoms.pro>
#include <Inits.pro>
#include <Main.pro>
#include <Menu.pro>
#include <APWdll.pro>
```

```
#include <Fortc2.pro>
#include <Controls.pro>
#include <Memory.pro>
#include <chmanip.pro>

/* Make NULL an invalid window */
#define VALID_WINDOW(w) ((w) && IsWindow(w))

static char *function_ptr = "APWMessageDispatch";  /* The object procedure */
static char dll[ 200 ];  /* Stores the name of the DLL */


/*******************
 * DLL entry point *
 *******************/
short FAR PASCAL LibMain( HANDLE hModule, WORD wDataSeg, WORD cbHeapSize,
                          LPSTR lpszCmdLine )
{
    gInst = hModule;
    if( cbHeapSize != 0 ) /* If data segment is MOVEABLE */
    UnlockData( 0 );
    return 1;
}


/***************************
 * Exit point for the DLL *
 ***************************/
short FAR PASCAL WEP( short bSystemExit )
{
    return 1;
}


/****************************************
 * The initial function called from APW *
 ****************************************/
void FAR PASCAL InitialiseWindow( HWND hWnd, short left, short top,
                                  short right, short bottom )
{
    extern APWC_POSTPB  gPost;
    extern HWND         gDisplayWindow;
    extern RECT         g3DRect;
    extern short        gId;

    /* Check to see if a valid window was passed */
    gDisplayWindow = ValidWindow( hWnd );

    GetModuleFileName( gInst, dll, sizeof( dll ));  /* Who am I ? */

    /* Fill in the structure to be passed back to APW */
    gPost.size =          sizeof( APWC_POSTPB );
    gPost.function_ptr =  function_ptr; /* The routine to receive messages */
    gPost.dll_ptr =       dll;
    gPost.port =          STATIC_PORT;  /* DLL will handle buffering */
    gPost.rect.left =     left;
    gPost.rect.top =      top;
    gPost.rect.right =    right;
    gPost.rect.bottom =   bottom;
    gPost.data_ptr =      &gdcDB;  /* The address of the double buffer */
    gPost.data_size =     sizeof( gdcDB );


    /* Setup off-screen RECT */
    g3DRect.left =    0;
    g3DRect.top =     0;
    g3DRect.right =  gPost.rect.right - gPost.rect.left;
    g3DRect.bottom = gPost.rect.bottom - gPost.rect.top;
```

```
    /* Initialise 3-D window, common blocks, colours, fonts, atoms */
    Initialize();

    /* Inform APW that an object is to be posted */
    gId = SendMessage( gDisplayWindow, APWC_POST, 0,
                       ( long )( APWC_POSTPB_PTR )&gPost );
}


/**********************************************************
 * Check to see if a valid window handle has been passed *
 **********************************************************/
HWND ValidWindow( HWND hWnd )
{
    if( !VALID_WINDOW( hWnd )) /* Test if a valid window has been passed */
    {
        return 0;
    }
    else
    {
        return( hWnd );
    }
}


/*********************************************
 * Receive a message from APW and act on it *
 *********************************************/
long FAR PASCAL APWMessageDispatch( APWN_AB_PTR args, unsigned msg )
{
    switch ( msg )
    {
        case APWN_INIT:
            return(0);

        case APWN_PAINT:
            PaintDisplay( args -> wparam );
            return(0);

        case APWN_DESTROY: /* Remove object and all handles used */
            EraseObject( args -> display, args -> id );
            CheckQuit();
            return( 0 );

        case APWN_SAVE:  /* Copy object to memory */
            if ( *(( WORD FAR * ) args -> data_ptr ))
                return CopyObject( *(( WORD FAR * ) args -> data_ptr ));

        case APWN_RESTORE: /* Recreate object from memory */
            *(( WORD FAR * ) args -> data_ptr ) = args -> wparam;
            break;

        case APWN_LBDOWN:
            return( 0 );

        default:
            break;
    }
}


/**********************************************************************
 * Copy the passed object to memory and returns a HANDLE to the copy *
 **********************************************************************/
static HANDLE NEAR PASCAL CopyObject( HANDLE hObject )
{
```

```
    HANDLE    rv;
    DWORD     size;
    char huge *s;
    char huge *d;

    size = GlobalSize( hObject );
    if (( rv = GlobalAlloc( GHND, size )) != NULL )
    {
        d = ( char huge * )GlobalLock( rv );
        s = ( char huge * )GlobalLock( hObject );
        for( ; size > 0; ++s, ++d, --size )
            *d = *s;

        GlobalUnlock( rv );
        GlobalUnlock( hObject );
    }
    return rv;
}


/***************************************************************
 * Unpost the posted object 'id' from the APW display manager *
 ***************************************************************/
void FAR PASCAL EraseObject( HWND hWnd, long id )
{
    if ( VALID_WINDOW( hWnd ))
        SendMessage( hWnd, APWC_UNPOST, 0, id );
}


/***********************************************************
 * Update the APW display - BitBlt from the double buffer *
 ***********************************************************/
void PaintDisplay( HDC hDC )
{
    extern APWC_POSTPB gPost;
    extern HDC         gdcAPW;
    extern HDC         gdcDB;

    short nWidth, nHeight;

    /* Bitblt the entire double buffer to APW */
    nWidth = gPost.rect.right - gPost.rect.left;
    nHeight = gPost.rect.bottom - gPost.rect.top;
    BitBlt( hDC, gPost.rect.left, gPost.rect.top, nWidth, nHeight,
            gdcDB, 0, 0, SRCCOPY );
}


/*******************************
 * Invalidate the APW display *
 *******************************/
void InvalidateDisplay( void )
{
    extern APWC_POSTPB gPost;
    extern HWND        gDisplayWindow;
    extern short       gId;

    APWC_INVALPB inval;

    inval.id = gId;
    inval.inval_type = INVAL_BACKWARD;
    CopyRect( &inval.rect, &gPost.rect );

    SendMessage( gDisplayWindow, APWC_INVAL, 0,
                 ( long )( APWC_INVALPB_PTR )&inval );
}
```

```
/*************************************************************************
 * Update the APW display - BitBlt the invalid part of the double buffer *
 *************************************************************************/
void PaintMolecule( void )
{
    extern APWC_POSTPB gPost;
    extern HDC         gdcDB;
    extern HDC         gdcAPW;
    extern RECT        gUpdateSize;

    short nWidth, nHeight;

    nWidth = gUpdateSize.right - gUpdateSize.left;
    nHeight = gUpdateSize.bottom - gUpdateSize.top;

    /* Copy the invalid part of the double buffer to APW */
    BitBlt( gdcAPW, gPost.rect.left + gUpdateSize.left,
            gPost.rect.top + gUpdateSize.top, nWidth, nHeight,
            gdcDB, gUpdateSize.left, gUpdateSize.top, SRCCOPY );
}


/****************************************
 * Fill the double buffer with black *
 ****************************************/
void ClearBuffer( void )
{
   extern RECT g3DRect;
   extern HDC  gdcDB;

   short nWidth, nHeight;

   /* Set the size of the off-screen bitmap */
   nWidth =  g3DRect.right - g3DRect.left;
   nHeight = g3DRect.bottom - g3DRect.top;

   /* Fill the off-screen device context with black */
   BitBlt( gdcDB, 0, 0, nWidth, nHeight, NULL, 0, 0, BLACKNESS );
}


/**********************************************************************
 * Called when the mouse is pressed.  Calculates the current cursor *
 * position and runs the trackball until the mouse is released     *
 **********************************************************************/
HANDLE FAR PASCAL MouseMove( void )
{
    extern DrawFunctions gCurrentDraw;
    extern HWND      gDisplayWindow;
    extern BOOL            gActiveUtility;
    extern HDC       gdcAPW;

    POINT  mouse;
    char   label[LABELLENGTH + 1];
    short  i, lmouseDown;

    GetCursorPos( &mouse );

    /* NULL return when no label is found */
    for (i = 0; i < LABELLENGTH + 1; i++)
        label[i] = NULLCHAR;

    /* Check that the left mouse button is still down */
    lmouseDown = GetKeyState( VK_LBUTTON );

    /* Do trackball if mouse is still down */
    if( lmouseDown )
```

```
    {
        SetCapture( gDisplayWindow );
        /* Activate the trackball until the mouse is released */
        DoTrackBall( gDisplayWindow, mouse );
    }

    /* Get the atom the user attemped to highlight - if active */
    if ( gActiveUtility )
    {
        Do3DClick( mouse, label );

        /* Use the current drawing function to draw the molecule */
        (*gCurrentDraw.windowFcn)();

        /* BitBlt the double buffer to APW */
        PaintDisplay( gdcAPW );
    }

    /* Invalidate the APW display */
    InvalidateDisplay();

    return( ReturnString( label ));
}


/*******************************************************
 * Label the passed atom number with the passed label *
 *******************************************************/
void FAR PASCAL LabelAtom( short atom, LPSTR newLabel )
{
    extern AtomLabelsCommonPtr gAtomLabels;
    extern DrawFunctions       gCurrentDraw;
    extern HDC                 gdcAPW;

    _fstrcpy( (char *)gAtomLabels -> AtomLabel[atom - 1], (char *)newLabel );

    /* Add newly labelled atom to the list of highlighted atoms */
    AddtoHighlightedAtoms( atom - 1 );

    /* Use the current drawing function to draw the molecule */
    ClearBuffer();
    ( *gCurrentDraw.windowFcn )();

    /* Update the whole APW display */
    PaintDisplay( gdcAPW );
}


/**************************************************************************
 * Load a COSMIC data file and display it in the current represenation *
 **************************************************************************/
short FAR PASCAL DisplayCOSMICFile( LPSTR FileName, short status )
{
    extern DrawFunctions gCurrentDraw;
    extern HWND          gDisplayWindow;
    extern short         gStatus;
    extern WDMap         g3DSpace;
    extern HDC           gdcAPW;

    POINT transstart, transend;
    short errorCode;

    transstart.x = transstart.y = 0;
    transend.y = 0;

    /* Determine whether 1 or 2 molecules are to be drawn */
    switch ( status )
    {
```

```
        case 1:
            gStatus = MOLECULE_ONE;
            break;
            case 2:
            gStatus = MOLECULE_TWO;
            break;
        default:
            gStatus = SINGLE;
    }

    /* Open a COSMIC file if valid filename */
    if( errorCode = ReadMolFile( FileName ))
    {
        WarningBox( gDisplayWindow,
        "File error",
        "The COSMIC data file was unreadable. The molecule will not show." );
        return( errorCode );
    }

    /* Determine whether 1 or 2 molecules are to be drawn */
    switch ( status )
    {
        case 1:
            transend.x = -( g3DSpace.iRight - g3DSpace.iLeft ) / 4;
            ( *gCurrentDraw.windowFcn )();  /* The current drawing function */
            TrnTrackball( transstart, transend, 0 ); /* Translate molecule 1 */
            break;
        case 2:
            transend.x = ( g3DSpace.iRight - g3DSpace.iLeft ) / 4;
            Active( 1 );                    /* Deactivate molecule 1 */
            TrnTrackball( transstart, transend, 0 ); /* Translate molecule 2 */
            Active( 1 );                    /* Reactivate molecule 1 */
            ClearBuffer();
            ( *gCurrentDraw.windowFcn )();  /* The current drawing function */
            break;
        default:    /* One molecule displayed */
            ( *gCurrentDraw.windowFcn )();  /* The current drawing function */
        break;
    }

    /* Update the whole APW display */
    InvalidateDisplay();

    return( errorCode );
}


/****************************************
 * Display the molecule in stick mode *
 ****************************************/
void FAR PASCAL Stick( void )
{
    extern DrawFunctions gCurrentDraw;
    extern DrawFunctions gPreviousDraw;
    extern BOOL          gSpaceFill;

    ClearBuffer();

    /* Draw a stick molecule into the double buffer */
    Draw3DWindow();

    /* Revert to stick display */
    gSpaceFill = FALSE;
    gCurrentDraw.windowFcn = Draw3DWindow;
    gCurrentDraw.drawFcn = Draw3DImage;
    gPreviousDraw = gCurrentDraw;
```

```
    /* Update the whole APW display */
    InvalidateDisplay();
}


/************************************************
 * Display the molecule in ball and stick mode *
 ************************************************/
void FAR PASCAL BallandStick( void )
{
    extern DrawFunctions gCurrentDraw;
    extern DrawFunctions gPreviousDraw;
    extern BOOL      gSpaceFill;

    ClearBuffer();

    /* Draw a ball and stick molecule into the double buffer */
    DrawBallandStickWindow();

    /* Switch to Ball & Stick display */
    gSpaceFill = FALSE;
    gCurrentDraw.windowFcn = DrawBallandStickWindow;
    gCurrentDraw.drawFcn = DrawBallandStickImage;
    gPreviousDraw = gCurrentDraw;

    /* Update the whole APW display */
    InvalidateDisplay();
}


/*******************************************************
 * Display the molecule in CPK mode - medium space fill *
 *******************************************************/
void FAR PASCAL SpaceFill( void )
{
    extern DrawFunctions gCurrentDraw;
    extern DrawFunctions gPreviousDraw;
    extern BOOL      gSpaceFill;

    ClearBuffer();

    /* Draw a space fill molecule into the double buffer */
    DrawSpaceFillWindow();

    /* Switch to space fill display */
    gSpaceFill = TRUE;
    gCurrentDraw.windowFcn = DrawSpaceFillWindow;
    gCurrentDraw.drawFcn = DrawSpaceFill;
    gPreviousDraw = gCurrentDraw;

    /* Update the whole APW display */
    InvalidateDisplay();
}


/***************************************************************
 * Toggle the hydrogens on and off on the displayed molecule *
 ***************************************************************/

void FAR PASCAL Hydrogens( BOOL hydrogens )
{
    extern DrawFunctions gCurrentDraw;

    /* Turn hydrogen display on or off */
    SetHydrogenDisplay( hydrogens );

    FortSETBDR();     /* create new bond draw list */
```

```
    ClearBuffer();

    /* Use the current drawing function to draw the molecule. */
    ( *gCurrentDraw.windowFcn )();

    /* Update the whole APW display */
    InvalidateDisplay();
}


/*****************************************************************
 * Resets labels to original values after priority assignments *
 *****************************************************************/
void FAR PASCAL ResetLabels( void )
{
    short imol;

    for ( imol = 0; imol < MAXMOL; imol++ )
    {
        AutoLabelMolecule( imol );
    }
}


/***********************************************************
 * Toggle the labels on and off on the displayed molecule *
 ***********************************************************/
void FAR PASCAL Labels( BOOL labels )
{
    extern DrawFunctions gCurrentDraw;

    /* Turn labels display on or off */
    SetLabelsDisplay( labels );

    FortSETBDR();     /* create new bond draw list */

    ClearBuffer();

    /* Use the current drawing function to draw the molecule. */
    ( *gCurrentDraw.windowFcn )();

    /* Update the whole APW display */
    InvalidateDisplay();
}


/***********************************************************
 * Toggle the active status of the passed molecule number *
 ***********************************************************/
void FAR PASCAL Active( short imol )
{
    /* Offset imol to the correct array value */
    imol--;

    /* Toggle the active status of the passed molecule number */
    ToggleActiveStatus( imol );
}


/*********************************************************
 * Toggle the ability to highlight atoms on the display *
 *********************************************************/
void FAR PASCAL Highlight( short highlight )
{
    extern BOOL gActiveUtility;
    extern HDC  gdcAPW;
```

```
    /* Clear all highligted atoms when finished */
    ClearHighlightedAtoms();

    if( highlight )
        gActiveUtility = TRUE;
    else
    {
        gActiveUtility = FALSE;
    }
}


/*******************************************************************
 * Takes the APW WindowHandle, caption and message.       *
 * Displays a Windows message box with exclamation an OK button. *
 ********************************************************************/
void FAR PASCAL WarningBox( HWND WindowHandle, LPSTR caption,
                LPSTR message )
{
    MessageBeep( -1 );
    MessageBox( WindowHandle,
                message,
                caption,
                MB_ICONEXCLAMATION | MB_OK );
}
```

APPENDIX 3

Case Study Video Collection Protocol

Tsar Multimedia Training case studies– contributor guidelines

The aim of a case study in the proposed ***Tsar*** training package will be to present a successful implementation of ***Tsar*** in a multimedia format. Talking head video clips, ***Tsar*** analytical tools, the original data set and relevant illustrations will be used to form a study. The material below should be put together to prepare for a case study:

Video script

A series of video clips will be used to provide an overview of the analysis at various stages in a case study. The individual clips should be 30 seconds or less in length. The script should answer the following questions as far as possible:

- Who are you and what is your research background?
- What was the problem you hoped to solve?
- Why did you choose ***Tsar*** for the analysis?
- What did you aim to achieve?
- How did you obtain the input data set?
- How did you use ***Tsar*** to make your analysis?
- Describe your data set as displayed by a ***Tsar*** analytical tool.
- What output data set did you obtain?
- What conclusions did you make from the analysis?

Tsar analytical tools

The ***Tsar*** analytical tools for use in the case studies. This will allow users to interactively manipulate a data set. The 3-D graph facility will be the first tool to undergo this treatment. Therefore, we shall require access to the data set to allow a user to interactively manipulate the data. If a ***Tsar*** tool has not been re-coded for the package, a series of screen shots of the data set being analysed will be required.

Illustrations/data/references

Relevant illustrations, data or references should be collated for inclusion in the package.

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APPENDIX 4

Rating Scale for Tsar Multimedia Training

Tsar Multimedia Training Evaluation

Tsar is a software package produced by Oxford Molecular Ltd. for QSAR analysis. "***Tsar*** Multimedia Training" is a prototype computer-aided learning package produced as part of a research project at the University of Nottingham. The courseware is divided into a "Background to QSAR", an "Introduction to ***Tsar***" and a series of "***Tsar*** case studies". Each case study focuses on a specific aspect of QSAR analysis and how ***Tsar*** was used to solve the problem.

Please follow the sequence below:

1. Click on the "***Tsar*** case studies" section.
2. Browse three or more case studies, viewing all pages.
4. Complete the questionnaire below, circling your responses.

Questionnaire

1. How experienced are you with interactive computer systems?

Very poor *Poor* *Neutral* *Good* *Excellent*

2. How experienced are your with QSAR analysis?

Very poor *Poor* *Neutral* *Good* *Excellent*

3. How usable was the interface to the courseware?

Very poor *Poor* *Neutral* *Good* *Excellent*

4. How easy was navigation through the courseware?

Very poor *Poor* *Neutral* *Good* *Excellent*

5. Was the video material easy to use and understand?

Very poor *Poor* *Neutral* *Good* *Excellent*

6. Were the ***Tsar*** tools easy to use and understand?

Very poor *Poor* *Neutral* *Good* *Excellent*

7. Did the video distract or enhance your use of the ***Tsar*** tools?

Greatly distracted *Distracted* *Neutral* *Enhanced* *Greatly enhanced*

8. How good was the correspondence between the video and the ***Tsar*** tools?

Very poor *Poor* *Neutral* *Good* *Excellent*

9. How much did you learn from the video and the ***Tsar*** tools?

Only video *Mainly video* *Equal* *Mainly* ***Tsar*** *tools* *Only* ***Tsar*** *tools*

10. Overall, did the combination of video material and ***Tsar*** tools help you learn more?

Learnt nothing *Learnt little* *Neutral* *Learnt something* *Learnt a lot*

11. Would you want to use more training material that combined multimedia with interactive computational chemistry tools?

Never *Not really* *Neutral* *Maybe* *Definitely*

12. Is there anything that stands out as particularly good about the courseware?

....

13. Is there anything that stands out as particularly bad about the courseware?

....

Thankyou for taking part in this evaluation.

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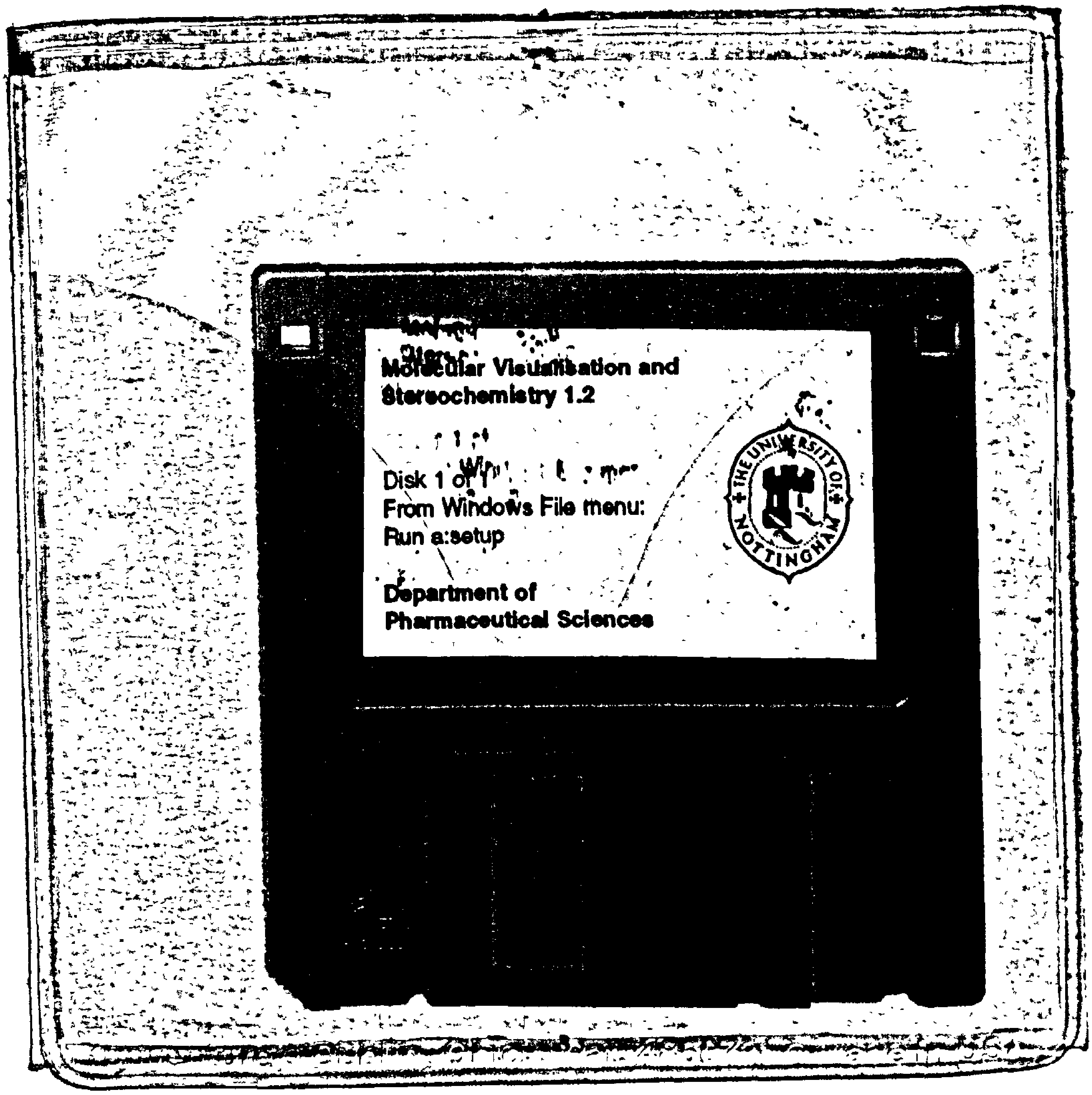
APPENDIX 5

Demonstration Courseware



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