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13 software packages

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Physical Sciences Educational Reviews

The journal of the LTSN Physical Sciences Subject Centre

LTSN Physical Sciences
...supporting learning and teaching in chemistry, physics and astronomy

Department of Chemistry
University of Hull
Hull
HU6 7RX

Phone: 01482 465418/465453
Fax: 01482 466410
Email: ltsn-psc@hull.ac.uk
Web: www.physsci.ltsn.ac.uk

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Physical Sciences Educational Reviews

ltsn Supporting Learning and Teaching

Physical Sciences

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Items for review and offers to contribute to the review process are welcomed. Please contact the Centre.

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Editor

Roger Gladwin
LTSN Physical Sciences
Chemistry Department
Liverpool University
Liverpool L69 7ZD
Tel: 0151 794 3576
Fax: 0151 794 3586
Email: rgladwin@liv.ac.uk

Editorial

Welcome to the first issue of Physical Sciences Educational Reviews. This is the new journal of the LTSN Physical Sciences Centre and we hope that you find it to be a useful publication. The ethos of the journal is to critically review all types of teaching and learning materials or resources which are potentially useful to teachers of the physical sciences in higher education. The journal builds on the highly successful *Software Reviews,* previously published by the former CTI centres.

We hope that the journal will provide academics with an invaluable source of information about what is available to them to use in their teaching. We intend to review books, software packages, websites, and any other resources generally available. If you come across anything which you think should be reviewed in the journal please contact the Editor, Roger Gladwin. We would also like to hear from you if you are interested in becoming a reviewer. I am sure that together we can provide a useful source of reviews which will help promote effective resources and go some way towards helping us all avoid 'reinventing wheels'.

Tina Overton
Director

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Electrochemical Impedance Spectroscopy

Subject area
Physical Chemistry.

Description
Revision notes for electrode kinetics/electrochemical techniques.

Authors
University of Bath.

Last updated
no data.

Level
Research.

Plugins required
None.

Other features used
None.

Reviewed using
PC running Windows 95 using Internet Explorer 5.

Web address
www.bath.ac.uk/~chsacf/solartron/electro/html/int.htm

Peter G Hall
School of Applied Sciences
University of Glamorgan
Pontypridd
Mid. Glamorgan CF37 1DL
August 2000

Summary Review

range: * very poor to ***** excellent

Ease of navigation	***
Speed of response	****
Ease of learning	**
Content	****
Relevance	***
Accuracy	****
Usefulness to student	*
Usefulness to teacher	***

I was asked to review this site for the teaching and learning of "Electrochemical Impedance Spectroscopy" but must stress first that this site is certainly not designed for that purpose. Nor in fact is it designed for use as a "teaching/learning package" for an audience beyond that for which it was designed. That original audience was participants attending a short course on electrochemical impedance spectroscopy at the University of Bath in April 2000. The site is intended as background lecture notes covering electrode kinetics, electrochemical techniques and associated mathematics and electrical circuit analysis. The level is advanced and, in the main, the chemistry is clear and concise with only a smattering of typographical errors. The material is probably not suitable for undergraduate students but may be of use to teachers of final year or postgraduate electrochemistry. They may wish to mention this site as an alternative to a chapter in a book. Other than cost, however, it offers no advantage over a textbook. The material is entirely text based with no interactions nor problems and questions for students to tackle.

"...If... you are a teacher looking for ideas or simply information about what others are doing, then this may well be useful..."

If my comments so far sound critical, this is not my intention. If you want "self-teaching" material in advanced electrochemistry then this is not where you would come. If, on the other hand, you are a teacher looking for ideas or simply information about what others are doing, then this may well be useful. I wish more teachers were prepared to allow free access to their web material and congratulate the Bath authors for their willingness to leave material on the web with no passwords or registrations required.

Rice Virtual Lab in Statistics

Subject area
General Science.

Description
A resource for the teaching and/or learning of statistics.

Authors
David M. Lane.

Last updated
A copyright of 2000 is mentioned.

Level
Undergraduate, research.

Plugins required
None apparent.

Other features used
Java, tables.

Reviewed using
PC with Intel Pentium II; 233 MHz processor with 640K System RAM and 512K Cache memory on a high-speed campus network, running Windows 95 using Netscape 4.7

Web address
www.ruf.rice.edu/~lane/rvls.html

Philip R. Dee
School of Physics and Astronomy
University of Birmingham
Edgbaston
Birmingham B15 2TT
July 2000

Overview
This site provides a set of resources in the teaching and learning of statistics appropriate to Undergraduate and through to Postgraduate level.

Summary Review

range: * very poor to ***** excellent	
Ease of navigation	****
Speed of response	****
Ease of learning	***
Content	*****
Relevance	no data
Accuracy	*****
Usefulness to student	****
Usefulness to teacher	****

Main Page
The welcome page is cluttered with references to awards and a permission statement (these could perhaps be relegated to simple links), but more importantly there is no clear description of the site's purpose. Indeed, within each of the four main strands from the welcome page ('HyperStat Online', 'Simulations/Demonstrations', 'Case Studies' & 'Analysis Lab'), there is an unfortunate absence of any discernible overview or introduction; the newcomer can quickly get the feeling of a random walk through the resource rather than being led in a logical and instructive way.

Navigation
As with any large resource there are the inevitable dead links (one of the awards, ironically, several of the java demonstrations and two of the 'Exercise' chapters), although I think their number could be reduced with simple management software. In spite of this and the previously mentioned lack of overall clarity and guidance, the structure of the resource is manageable, once familiarity is achieved.

Content
Overall there is a feeling of the four main areas essentially being stand-alone resources, although cross-referring does occur (particularly to the Glossary). For instance there is a search facility within each strand which only appears to return finds from that strand, rather than from the site as a whole. Even so, the content of these areas is of a high quality.

For me, the 'HyperStat Online' component is the most useful. It is an excellent self-referencing source with an extremely useful glossary, a set of 'Instructional Demos' and a series of 'Exercises'. These are very educational and I would consider using them as part of my own teaching. However, much of this area is simply a good book on statistics pasted onto the web (indeed a printed version can be ordered on-line). Admittedly the hyperlinks allow for more immediate cross-referring, but a glossary and index in a book could provide that. For me, it is in the departure from what can be achieved via a conventional book that carries more relevance in a multi-media resource. The 'Instructional Demos' already mentioned, and 'Analysis Tools' certainly provided the most useful examples in this respect. These are quick to load and manipulate and on the whole facilitate a greater understanding of the concepts being explained.

In addition, there is a useful range of statistics tools (although the difference between 'Analysis Lab' (from the main page) and 'Analysis Tools' (from within 'Hyperstat Online') was not made clear and had me wondering for some time if I was accessing the same set of resources (albeit differently ordered) but from different places (I was not). Liberally scattered throughout the resource are many useful links to external sites. These are often rich resources in their own right and certainly add to the value of this site as a starting point for study.

Overall, I was impressed by the sheer volume of material accessible from this resource and, with what would amount to only fine-tuning, feel it could be made easier to understand, navigate and use as part of a program of self-study or directed learning.

The Nine Planets website

Subject area
Astronomy.

Description
Information about the solar system.

Authors
Bill Arnett.

Last updated
no data.

Level
Foundation level and for general use.

Plugins required
None.

Other features used
None.

Reviewed using
UNIX workstation running Solaris 5.7 with Netscape 4.08.

Web address
seds.lpl.arizona.edu/nineplanets/nineplanets/nineplanets.html

Chris Done
Department of Physics
University of Durham
South Road
Durham DH1 3LE
July 2000

The Nine Planets website by Bill Arnett is a fantastic compilation of information about the Solar System. The non-technical text is generally well written and informative, the images are superb, and there are plenty of links for more details. It is aimed at a general audience, but there is material here which would provide useful backing for introductory undergraduate astronomy courses.

Summary Review

range: * very poor to ***** excellent	
Ease of navigation	*****
Speed of response	*****
Ease of learning	*****
Content	****
Relevance	***
Accuracy	****
Usefulness to student	*****
Usefulness to teacher	*****

The site is set out in a very intuitively obvious way, making navigating around it very easy. Information on all the planets and their moons is linked from the front page, together with pages on comets, asteroids, spacecraft, extrasolar planets and much much more. The sheer extent of it could be quite daunting, but there is a very nice 'Solar System Overview' page and then a 'Express Tour' which takes in only the major bodies. The text for each object is interspersed with many small pictures, but the pages load quickly. Each section ends with a list of links for more specialist information (though a small fraction of these do not work due to out of date addresses).

"...One aspect of the site which especially impressed me was the 'Open Issues'... While the text gives the extent of our knowledge, these 'Open Issues' show the extent of our ignorance..."

The information contained in the site is generally very accurate and fairly presented. The only quibble I have is with the assessment of the solar neutrino problem as 'probably a minor glitch in some esoteric calculations'. It is now widely accepted that this discrepancy between the observed and calculated neutrino fluxes is real and that it is extremely important in pointing to new physics beyond the 'standard model' of particle physics.

One aspect of the site which especially impressed me was the 'Open Issues' list of questions at the end of each section. While the text gives the extent of our knowledge, these 'Open Issues' show the extent of our ignorance. In a site aimed at a general audience it can be all too tempting to compile facts into a coherent story and miss out the current controversies as being too confusing. This is seen all too often in media coverage of science, where the story can be simplified to such an extent that the conclusions become much firmer than the data warrant! Instead, this site gives a short summary of some of the active research areas for each object, and so stresses the ongoing nature of scientific discovery, and conveys something of the excitement of Solar System study.

World Chemistry

Subject area
General Chemistry.

Description
A resource package for students and teachers.

Authors
W Bailey.

Last updated
26/08/00.

Level
AS and A-Level chemistry.

Plugins required
None.

Other features used
Java.

Reviewed using
PC Pentium 2, 350 MHz, 64MB RAM, 6MB hard drive with LAN plus dedicated fibre optic line, 512 band width running Windows 98 with Internet Explorer 5.0.

Web address
www.wbaileynet.com/wldchem/home/

Derek Denby
John Leggott College
West Common Lane
Scunthorpe
North Lincolnshire DN17 1DS
August 2000

World Chemistry is an extensive, free, resource package, which is suitable for students and teachers involved in Advanced Level Chemistry courses in the UK. It has received a number of awards including winning the education category of the 1998 Pirelli INTERNETional multimedia competition.

Summary Review

range: * very poor to ***** excellent	
Ease of navigation	*****
Speed of response	*****
Ease of learning	*****
Content	****
Relevance	*****
Accuracy	*****
Usefulness to student	****
Usefulness to teacher	****

The home page is clear and informative and provides easy and rapid access to a number of embedded features. The site also has extensive links to other sites providing information, tutorials, resources or materials that support advanced chemistry study.

The site contains a number of student tutorials. These are split into small sections, a few pages long, and are followed by interactive learning checks. Some tutorials and learning checks use virtual reality models, for example, a virtual periodic table, and/or Java applet programs, such as those which show movement of molecules in tutorials on reaction kinetics.

"...A particularly useful feature of the site is a collection of 3-dimensional interactive molecular models, which include most of the simple molecules met at this level..."

Students may choose to use the services of a website manager which recommends tutorials to be attempted and keeps a log file of associated self-assessment units.

A particularly useful feature of the site is a collection of 3-dimensional interactive molecular models, which include most of the simple molecules met at this level. The site also contains a quick reference guide that gives short definitions of over 200 chemical terms.

The website provides material which is relevant to advanced chemistry courses in schools and colleges in the UK. The range of topic is rather limited, covering some areas of physical and inorganic chemistry, but they are covered in an interactive and imaginative manner, which makes them suitable for guided independent study. The only minor error which I found was the intended link to the Royal Society of Chemistry which took me to the Royal Shakespeare Company!

A Question of Chemistry

Subject area
General Chemistry.

Description
A problem-solving text written to inspire students of chemistry to think both effectively and professionally.

Authors
John Garratt, Tina Overton, Terry Threlfall.

Publishers/Suppliers
Longman, available from
UK & International Trade, Customer Services, Pearson Education, Edinburgh Gate, Harlow, Essex CM20 2JE.
www.awl-he.com

Date/Edition
1999/ 1st Edition.

ISBN
0-582-29838-5

Level
Undergraduate.

Price
£12.99.

Mary Masson
Department of Chemistry
University of Aberdeen
Meston Walk
Aberdeen AB24 3UE
August 2000

Summary Review

range: * very poor to ***** excellent	
Academic content	*****
Usefulness to student	****
Usefulness to teacher	*****
Meets objectives	*****
Accuracy	*****

In recent years, it has come to be recognised that problem solving should be at the heart of any educational programme. For example, in the draft statement of benchmark standards for chemistry, the following is the second item in a list of eight transferable skills:

- Problem-solving skills, relating to qualitative and quantitative information, extending to situations where evaluations have to be made on the basis of limited information.

In chemistry, we have tended in the past to think smuggly that our "examples" were "problems", but gradually it has become apparent that training students to use known algorithms to find answers to questions is not teaching them about problem solving.

So what is problem solving? One definition is

- Problem solving is what you do when you don't know what to do; otherwise it's not a problem.

A more elaborate definition has been developed by the Scottish Qualifications Agency, in which the "core skill" of problem solving is considered to have three main components:

- Critical thinking
- Planning and Organising
- Reviewing and Evaluating

These are all important skills that we certainly should be attempting to develop in our students, but there is little help for us in standard chemistry textbooks, which provide many "examples", but few real problems. So how do we teach students to think? Or perhaps a better question is "How do we help students to learn *how* to think and not just *what* to think?"

The authors of *A Question of Chemistry* have recognised that there is a gap in the book market, and have attempted to provide a resource that will help students to recognise that learning to be a chemist involves more than chemical facts; that will encourage them to learn to question, to think critically and creatively, and to make judgements. They have devised several different types of exercise, some inspired by the MENO exercises of the Thinking Skills Service of the University of Cambridge.

The first section, *Understanding an Argument,* is concerned with learning to follow, and make a critical evaluation of, a chain of reasoning. Each of the 30 exercises consists of a short paragraph, together with a series of additional statements. Students are asked to identify the one statement which best strengthens the argument, identifies a flaw or weakness in the argument, most weakens the argument, or states an underlying assumption in the argument. The exercises cover a wide range of thought-provoking chemical questions; they seem well suited for use with small groups of students, and made me see that maybe it can be possible to stimulate, in our perennially non-interactive chemistry tutorials, the kind of discussion that would be expected from students of a social-science subject.

In the second section, *Constructing an Argument,* the reader is presented in each problem with a series of statements, and is asked to arrange them in a logical sequence, with addition of suitable linking words between the second and third statement. Here is a (short) example:

A Question of Chemistry

A. $SiCl_4$ is a tetrahedral molecule.
B. $SiCl_4$ is sp^3 hybridised.
C. sp^3 hybridisation gives rise to tetrahedral molecules.

The suggested answer to this is C, A, this suggests that B. [i.e. sp^3 hybridisation gives rise to tetrahedral molecules. $SiCl_4$ is a tetrahedral molecule. This suggests that $SiCl_4$ is sp^3 hybridised.]

These problems are not easy — sometimes they remind you of trying to decide whether the chicken or the egg came first — and again, they seem well suited for use in group discussions.

The *Critical Reading* section includes problems that consist of a short passage from, for example, a textbook, together with questions or statements about that passage. Sometimes, readers are asked to choose which statement best represents the message of the passage, or which they agree with most strongly; sometimes there is a series of comprehension questions. There may be an additional related assignment such as "Write a paragraph for a non-scientist which explains why you support the statement you have selected".

Section 4, *Making Judgements*, is designed to counter the "right answer" view of chemistry. In the authors' words "Chemistry is often seen as a subject in which all questions have a 'right answer', and that the student's job is to learn what the right answer is." Our best students do realise that science is not like this, but the majority need constant reminders that "Scientific knowledge is a body of knowledge of varying degrees of certainty—some most unsure, some nearly sure, but none *absolutely* certain … Now we scientists are used to this, and we take it for granted that it is perfectly consistent to be unsure, that it is possible to live and *not* know." [Richard Feynmann.].

"...the authors have written an admirable book that should be bought and read by everyone involved in HE chemistry teaching..."

The authors have made a collection of examples of situations where

- words do not have precise meanings
- there is no single correct method for making a particular measurement or testing a hypothesis
- there is more than one way to interpret experimental data
- there is not enough information to perform an exact calculation
- there is no right answer, but an estimate within a couple of orders of magnitude can be made.

The problems are divided into subsections, some of which relate to relatively specific areas of chemistry (e.g. solvents and solubility, atoms and molecules, analysis). Others are more general (equilibria, accuracy and precision, purity, yield, reactions, safety) and some (estimations) require "back of an envelope" calculations:

- "If all the molecules in a sugar cube were laid end-to-end, how far would they stretch?"
- "How much would a mole of peanuts weigh?".

Section 5, *Reference Trails*, designed to provide experience of finding information in the primary literature, is less novel as an idea, but nevertheless it is valuable in that the initial references and the set tasks have been carefully selected so that an answer can be located readily.

The final part, Section 6, *Commentaries,* provides discussion and sometimes answers for only the odd-numbered problems. As a teacher, I found this very valuable, because I often was not sure that I had thought about all aspects of a problem. Indeed, as a teacher, I would have welcomed commentaries for all the problems, but since the book is actually written for students themselves to use, I am prepared to accept the authors' compromise — it does allow half of the problems to be used for assessment (not desirable in an ideal world, but students rarely seem to put real effort into work that does not have marks attached.)

In an ideal world, students could be asked to buy this book, and an excellent course could be built around it, with use of regular small groups for discussion. Unfortunately, it is difficult to find time for new courses, and students are very reluctant to buy textbooks unless they are crammed with facts for learning. In a less than ideal situation, a possible approach is to make selections from the problems, and to embed these into an existing curriculum. For example, a "traditional" tutorial can be enriched by the inclusion of one or more of the problems from this book alongside the usual material. Our first attempts to try this last session were well received by our students.

In conclusion, I think that the authors have written an admirable book that should be bought and read by everyone involved in HE chemistry teaching, and that should be recommended to every chemistry student. I congratulate them on their efforts.

Chemistry Teaching Graphics for General Chemistry

Subject area
General Chemistry.

Description
A set of slides and animations to assist lecturers in undergraduate general chemistry.

Authors
Darrell J Woodman, Department of Chemistry, University of Washington.

Suppliers/Distributors
John Wiley and Sons, Inc.
www.wiley.co.uk

Date/Version
Oct 1997/Version 2.

ISBN
0-471-17584-6

Level
Undergraduate.

Type of Package
Simulation, teaching aid.

Price
$99.95 (single user, multi-user licence available on application).

Hardware required
PC: 8 MB RAM, 10 MB disk space, SVGA monitor with 256 colours, CD-ROM drive.
Mac: IIsi or better with 8 MB RAM, 10 MB disk space, 13" colour monitor, CD-ROM drive.

Software required
PC Windows 3.1 or later.
Mac: System 7.0.

John G Wright
Science Dept
MidKent College
Chatham
Kent ME5 9UQ
July 2000

Summary Review

range: * very poor to ***** excellent	
Ease of use	****
Ease of learning	***
Documentation quality	**
Academic content	****
Usefulness to student	***
Usefulness to teacher	****
Portability	****
Meets objectives	****
Accuracy	****

The package was tested on three PCs, a Pentium 120 MHz with 16MB RAM and 1 MB video RAM, a Pentium 200 MHz MMX, with 32 MB RAM and 2 MB video RAM, and a Pentium III 550 MHz with 64 MB RAM and 8 MB video RAM. Even the lowest specification machine ran the animations okay, if a little slowly, but its slow CD drive (an old 4 speed) occasionally caused horizontal interference lines or flickering to appear as the disk was read. There were no problems with the other CD drives (24 speed and 48 speed). The two lower specification PCs ran Windows 95, while the third one ran Windows 98.

The review package came as a single CD-ROM in a simple cardboard cover, illustrated with screen shots, and no paper manuals. The loading instructions cover the Macintosh and Windows versions, both of which are included on the CD. The Windows instructions didn't quite match the folders present on the CD, but any computer literate user would have little trouble in using the package from Windows Explorer by simply clicking on gctg95.exe for Windows 95 and above, or gctg31 (if anyone is still using Windows 3.1). This then presents the user with a scrolling menu screen, listing the main topic areas (Matter, Atomic Structure and Orbitals, Bonding and Molecular Orbitals, Intermolecular Forces and Properties, Gases, Solids and Crystals, Crystals II and Reactions) and their contents, which cover a total of 30 sub-topics.

Many sub-topics or units have an "about this topic" button on the opening slide which brings up short notes on what is covered, but these notes are just a bit too short sometimes. I felt that the on-disk documentation in general (a Word document and an ASCII text file) could also have been a bit more detailed.

The package can be run directly from the CD. However if the contents are copied to the hard disk, while maintaining the same sub-folder structure, it can be run from the hard disk, even if put in its own folder. There is no installation utility included, this would all have to be done manually.

The graphics are designed to assist lecturers in general chemistry where a slide show or animation could serve better than just a simple static OHP slide. The slides and animations are intended to be projected in a lecture hall or used in small group tutorials. The collection of units covers many of the topics likely to be taught in any first year general chemistry course, and some would also be suitable for parts of an A-level course. There are occasionally small differences between the way some units operate, but the documentation does state that two thirds of them have been updated and that work is continuing on improving and expanding the graphics available. These slight inconsistencies don't distract the user too much, except in the cases where animations unexpectedly don't start immediately and time is wasted waiting for something to happen.

In a typical unit, the user may be offered an auto-run feature to play the whole slide show or a section of it, a step forward and step back button, a re-start button, and a menu. The menu offers options to print the current screen, go forward, back, start, or end, or navigate to any named screen in the set, which would be handy for lecturers wishing to display only some of the screens, or to return to some for a lesson summary. Other options usually include a fast-medium-slow animation speed control, and information such as bond lengths and angles, or other structural details. Handouts of key or summary screens

Chemistry Teaching Graphics for General Chemistry

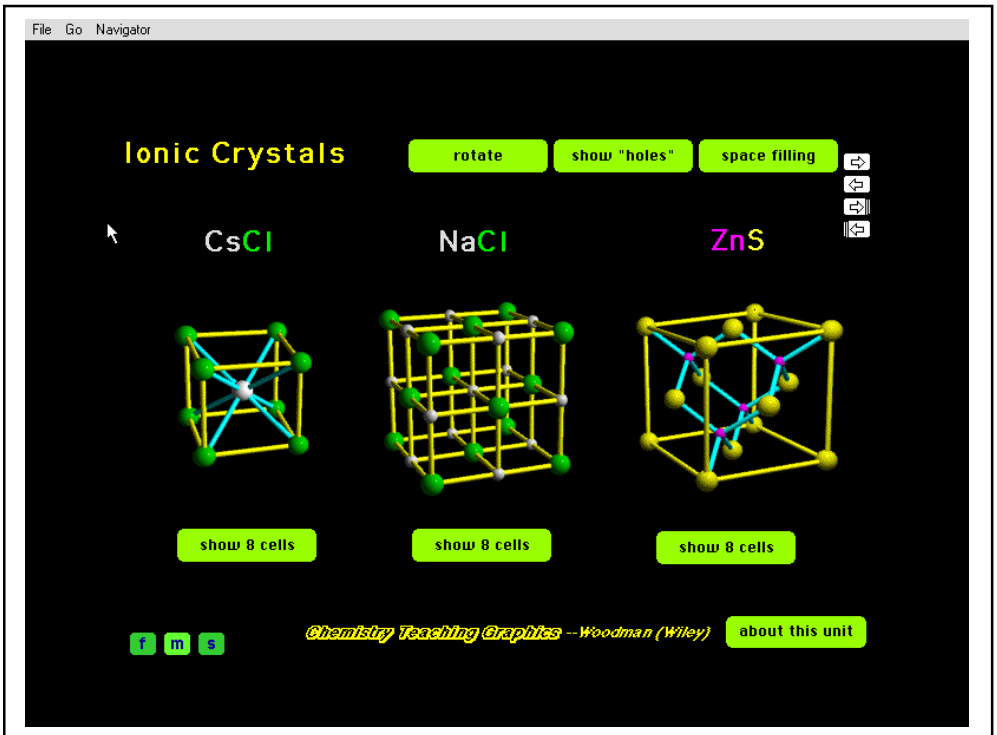

Figure 1: Example screen shot from Chemistry Teaching Graphics

While obviously tailored to the author's teaching, I didn't come across any chemistry that I was unhappy about, with the possible exception of part of the excited state animation and the 3-D perspective used in some molecular orbital diagrams, but it was soon easy to adapt to the latter.

Also included on the disk, in the Models folder, are a set of 68 structures produced using the well known RasMol package (Raswin.exe and Rasmacv2.5 are included), complete with an on-disk manual for RasMol (but not the Help files). These structures can't be accessed from the main menu, and the user has to resort to Windows Explorer again to activate RasMol. There is no documentation as to the actual molecules in the RasMol files, so some searching and note taking would be required before using them, although a reasonable selection is included and many small molecules simply have their formula as the filename. Structures included cover coordination compounds, crystal structures, elements, and some organic molecules. Again, no installation utility was available and Windows Explorer was used to copy files manually. The main documentation refers to an on-disk student exercise manual for this section, but none was found.

The author has produced as a separate CD-ROM a set of student exercises (currently available on special offer at $5 from Wiley's web site). Perhaps the missing section mentioned above has been expanded into this CD by the marketing department. There is also a separate Organic Graphics set at $99.95.

As for value for money, I don't think $99.95 is too much to pay for this set of high quality slides and animations. Some serious effort has gone into producing them and there is no way you could justify taking the time off teaching to produce even a limited set yourself given the price, although the reservations about some animation scenes being skipped over have to be kept in mind. Overall, a useful teaching aid.

can also be printed with gaps for students to add some details. Occasionally a model can be left rotating slowly on screen, perhaps while explaining the finer details to the class, then stopped with a mouse click. The display speed control system is planned to be improved for the next release, to give continuously variable speed, but usually it works satisfactorily as it stands.

More worrying than variations in the available options, some animations ran differently on the Windows 98 PC, with some steps completely missing, no matter which display speed was selected. It didn't seem as if this was a scene being displayed too rapidly to be detected, but just simply skipped past. In these cases much of the desired effect was totally lost. This may have been due to Windows 98, or just the faster clock speed (the files are dated 1997), but it could be rather annoying in a lecture, and something a user would have to check up on carefully. This must be one of the few packages where a slower machine might be beneficial.

The graphics are generally quite attractive, and of high quality, certainly far better than those that the average lecturer could possibly create. Students who viewed selected parts thought they were much better than any OHP they'd seen, although I did find it hard to keep a straight face while talking over the amusing animations of intermolecular forces pulling molecules together, when the student group burst out laughing. I'd have no hesitation in altering a lesson plan to include some of these units, and from the informal viewing's feedback, the students would appreciate it. They could be especially useful in small group tutorials to quickly illustrate some points.

Crocodile Chemistry

Subject area
General Chemistry.

Description
An on-screen chemistry laboratory.

Authors
Crocodile Clips.

Suppliers/Distributors
Crocodile Clips, 11 Randolph Place, Edinburgh, EH3 7TA, Scotland, UK.
www.crocodile-clips.com/education/

Date/Version
1999.

Level
GCSE, Basic A-Level.

Type of Package
Simulation, computer assisted learning, teaching aid.

Price
£175 for the first five users, £75 each for additional five users. Upgrades are available to all users for a 'nominal fee'.

Hardware required
486 processor or higher; 16MB RAM; CD-ROM drive; 16-bit soundcard (optional).

Software required
Windows 95, 98, NT 3.51 or later.

Wynne Evans
School of Applied Sciences
University of Glamorgan
Glamorgan CF37 1DL
July 2000

Introduction
Crocodile Chemistry is described as 'an on-screen chemistry lab.' allowing the user to choose chemicals and apparatus, then simulate experiments and see the results on-screen. The package is aimed primarily at students of basic chemistry (GCSE/very early A-Level) in secondary schools.

Summary Review

range: * very poor to ***** excellent

Ease of use	****
Ease of learning	***
Documentation quality	***
Academic content	**
Usefulness to student	***
Usefulness to teacher	****
Portability	****
Meets objectives	***
Accuracy	**

Content
The software includes a wide variety of sample experiments and activities. There is also a graphing facility which, together with a variety of probes/instrumentation to monitor properties such as temperature, pH and mass, allows you to plot data as an experiment proceeds. Equipment or chemicals are selected by dragging from the toolbars and Bunsen burners, burettes and gas cylinders are operated by a slider mechanism. In addition to suggested experiments and activities the user can design their own experiments with control over concentration, volume and experiment set-up. The chemicals are grouped together in ranges: for examples, metals, oxides, halides, sulphides gases and indicators. When a liquid is heated, the rate at which it boils is much faster than in reality. This increases the speed at which you are able to carry out your simulation.

When a piece of apparatus is selected, a toolbar shows equations for reactions happening within or formulae of chemical contents if no reaction is taking place. For some demonstrations, a system can be selected so that a side panel reveals a molecular animation of the contents; the motion of particles during changes of state, for example, can be viewed. A 'record movie' command allows the user to capture their actions in the form of an animation, which can be played back at a later date.

The experiments and activities contain explanatory text; the theory behind the experiment, instructions as to how to perform the experiment and questions for students to answer. Answers to the questions are sometimes provided on-screen. Activities and experiments can be edited or written from scratch and saved.

Crocodile chemistry can handle chemistry of some complexity, but as further chemicals are added to a mixture, the simulation will slow down as the number of possible reactions increases. If more than 20 chemicals are placed in the same vessel, Crocodile Chemistry will warn you that the reactions are too complex and then undo your previous action.

Crocodile chemistry allows the simulation of experiments in the following subject areas:

Solutions and solubility
Dissolving solids, measuring solubility, solubility of gases, concentrations.

Acids and bases
Acids and alkalis, bases and neutralisation, titration experiments, making salts.

Metals
Metals and non-metals, alkali metals, alkaline earth metals, metals and the reactivity series, corrosion, transition metals.

Crocodile Chemistry

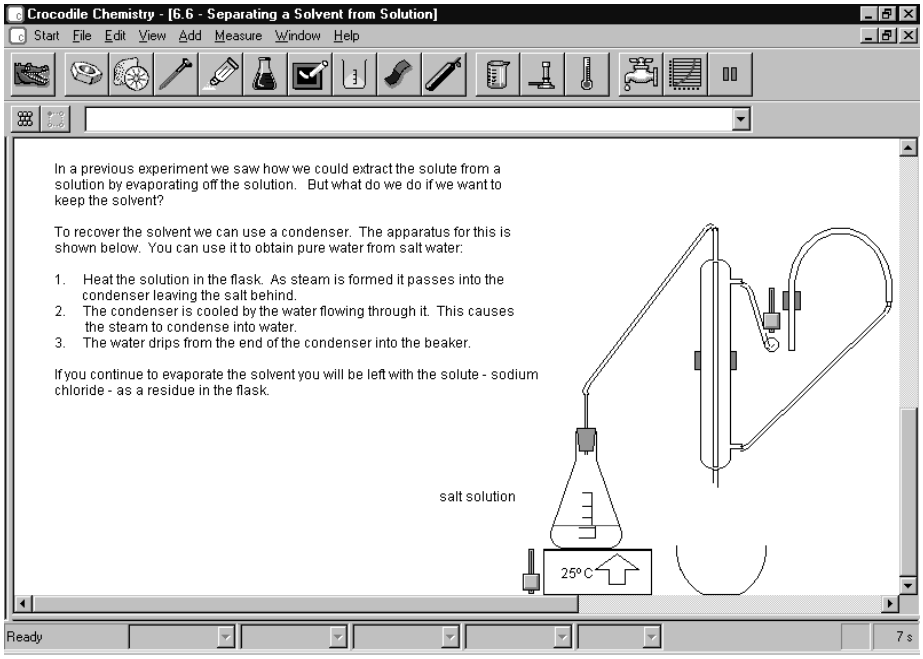

Figure 1: An example screen from Crocodile Chemistry

Reaction rates
Measuring reaction rates, changing reaction rates, reversible reactions, catalysts.

Physical chemistry
Physical changes in elements and compounds, properties of solids, liquids and gases, separating mixtures, heat capacity.

The periodic table
Introduction, different types of reaction, trends in the periodic table.

Non-metals and their compounds
Hydrogen, nitrogen and ammonia, fertilisers, oxygen and its properties, oxides: basic, neutral and acidic, sulphur and sulphur dioxide, sulphuric acid and sulphates, halogens, chlorine and its compounds, noble gases.

Evaluation
I tested Crocodile Chemistry using a 500 MHz processor, 64MB RAM and 6 GB hard disk, running Windows NT. The software is straightforward to install and run. Apparatus and chemicals are easily selected and dragged around the screen or transferred from one vessel to another. Instructions and apparatus are displayed on an area bigger than the computer screen – requiring the user to frequently scroll from left to right and back again, then down in order to read the instructions and perform the experiment - I found this a source of irritation. You can print out the instructions on-screen, but they are produced in a tiny font. Most set activities or experiments work well, but sometimes the arrangement of apparatus looks a little strange (for example as in distillation). If the user wishes to design an experiment, the permutations with respect to mixing chemicals are huge – I tried a variety of activities and most systems behave as they would in the laboratory. Clicking on vessels in which a chemical reaction is taking place reveals the equation for the reaction in the toolbar and at the end of the reaction, the chemical formulae of the products remain – I should imagine students would find this facility a valuable aid to revision. However, I did have some trouble with the graphing facility which inexplicably crashed the computer, in the middle of an experiment, quite a few times.
Although I appreciate that the package is aimed at an audience that does nor have a sophisticated knowledge of chemistry and making generalisations at this stage may aid memory and understanding; nevertheless, text accompanying the experiments contains information that is sometimes misleading:
“When equal amounts of acid and alkali are mixed they form a neutral solution”
or wrong:
“The strength of an acid is related to how concentrated it is”

Overall, this could be a useful addition to a chemistry department in a secondary school (I am sure that pupils would enjoy this package and the great variety of activities possible would ensure they would not get easily bored), but I do feel that the authors need to take a second look at the way that some of the theory is presented. Acceptance of statements, such as I have quoted, could lead the pupils into difficulties later on.

EasyPlot Version 4.0 for Windows

Subject area
General Science.

Description
A scientific plotting and data analysis package.

Authors
Stuart Karon.

Suppliers/Distributors
Spiral Software Europe, Garford, Abingdon, Oxon OX13 5PF.
http://www.spiralsoftware.com
(Formerly distributed by Cherwell Scientific Publishing Limited.)

Date/Version
1997/Version 4.0.

Level
A-Level, undergraduate.

Type of Package
Data analysis.

Price
A single user licence, for educational use, costs $384 for the software plus manual. Contact supplier for multiple user licences.

Hardware required
PC.

Software required
Windows 3.1, 95, NT.

Michael G.B.Drew
Department of Chemistry
University of Reading
Whiteknights
Reading RG6 6AD
July 2000

EasyPlot is a tool for viewing, analysing and plotting scientific data. According to the writers, it is designed for anyone who works with scientific data. The original EasyPlot was developed in the late 1980s at MIT Lincoln Laboratory and these academic origins are obvious in the current version. It is said to work under Windows 3.1, 95, NT but I only tried it under Windows95. It installed easily and ran immediately. I was provided with version 4.0 from 1997.

Summary Review

range: * very poor to ***** excellent	
Ease of use	****
Ease of learning	****
Documentation quality	****
Academic content	****
Usefulness to student	****
Usefulness to teacher	*****
Portability	*****
Meets objectives	*****
Accuracy	*****

I did not find the software easy to use to start with and needed to refer to the manual rather more often than I expected. Despite the claim in the manual that EasyPlot had an uncluttered appearance, I did not consider this statement to be valid. It was hard to find my way around the menus. Of course new users, particularly reviewers, often have initial problems which seem important at the time, but can persist less than a few days. Familiarity can take care of many an awkward menu system though that is not an argument for making software difficult to use.

I found that EasyPlot had a lot of well-designed features and that its scientific basis was sound. Data could be read in from ASCII, spreadsheet and binary files, or from the clipboard, or entered directly onto a spreadsheet facility within the program. It is a bonus that errors to the data values can be included within the input file if required and can be treated subsequently to produce error bars. However while data can be read into the spreadsheet, it is not designed to have many facilities as data manipulation is carried out on the plots. Plots can then be produced and the data transformed in a multitude of ways using a reasonably complete set of functions. There were many facilities to make plots look good, e.g. annotation, titles, grid lines, tic marks, labels, legends, a range of fonts which were easy to use and efficient. It was possible to drag curves and change axes and to resize and/or zoom or change the range of axes. Indeed it was hard to think of a facility for presentation that was not provided. The output from these plots printed out looked good and also could be pasted into other applications.

The scientific evaluation of data was less thorough. The curve fitting routines are easy to use with a range of polynomials and splines. However on looking at the statistics menu, there is only mean, standard deviation and histogram. No correlation coefficient was available and such routine statistical procedures such as ANOVA were not available. Even EXCEL has ANOVA!! Indeed in EXCEL it is also possible to carry out quite complicated mathematical operations involving iteration (e.g. solving equations via the Newton-Raphson method) which were not available here in EasyPlot. There is no multiple regression. There were however some welcome additional features provided. Thus EasyPlot uses the trapezoidal rule to sum the area or volume under a curve. It can also compute the derivative of a curve. There are data smoothing, range averaging and decimation facilities. There is also a procedure for Fourier Transform with an option of using Hamming or Kaiser windows.

It is also possible to plot 3-D Data though I found this complicated and far from intuitive to use. EasyPlot handles two types of 3-D data, surfaces and xyz triplets. However if you want to plot a surface with less than 20 columns, the manual says, you must put the command /td z in the file or plot the file, run Define Data and replace the xyyy... with z. I did this, rather reluctantly, and the data read in OK, but I never did manage to get the type of plot that I wanted. While the program comes with 3 test data files, none of them are for 3-D data which is a

EasyPlot Version 4.0 for Windows

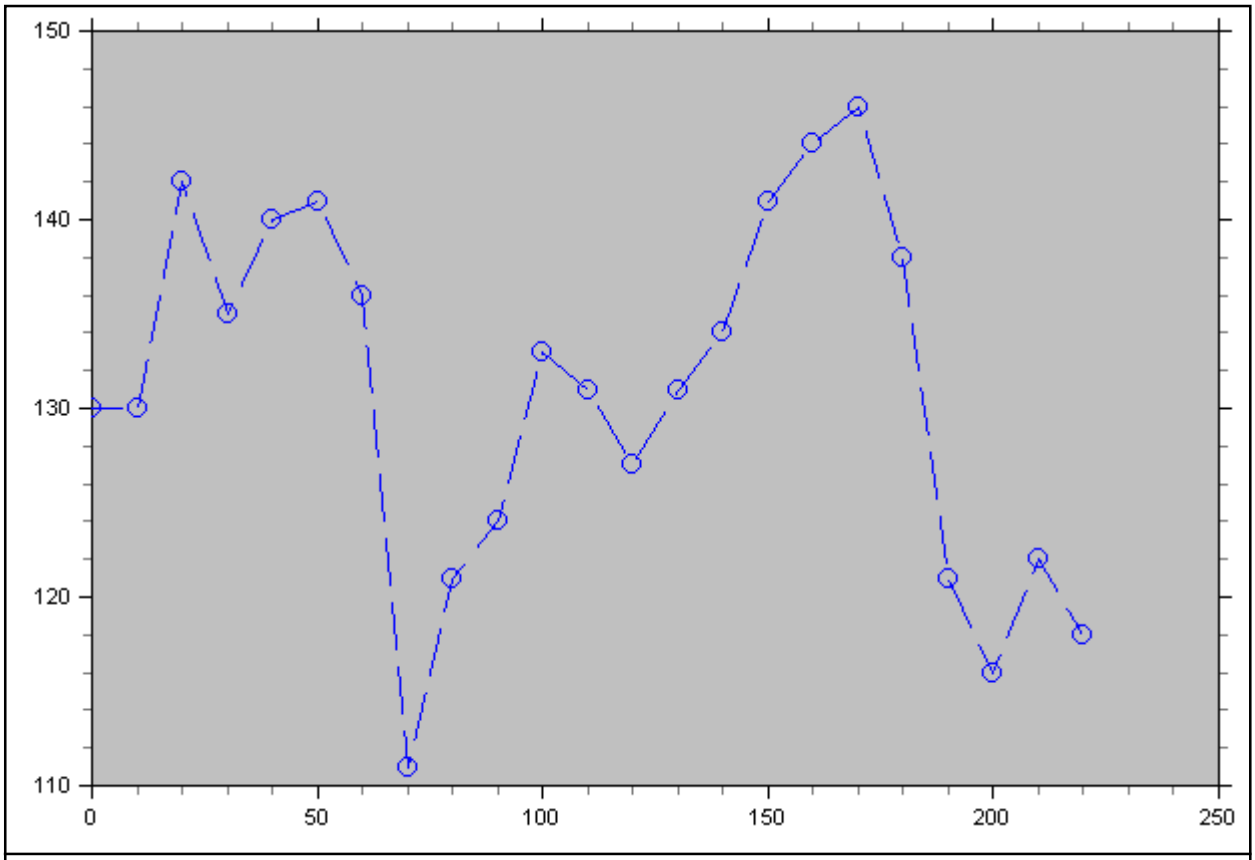

Figure1: Example output from EasyPlot

significant oversight. It would have been useful to find that the manual discussed the 3-D facility with the aid of a 3-D data set and that this could be followed through by users. I suspect if I had persevered, I would have got the plots I wanted but I would have expected the software to be more user friendly in this regard. The 3-D part of the package comes with a large number of presentation variations, thus the 3-D graphs can be rotated around axes, and there is a perspective option. It is also possible to use colour as a 3rd or 4th dimension associated with data values. The data can be shadowed onto axes planes to obtain contour plots. The manual states that arrays up to an order of 512*512 can be plotted in this way, but this was not tested.

EasyPlot also comes with a complete batch language that lets you speed repetitive tasks and automate graph production. It also has a programming language that lets you use EasyPlot as though it was a subroutine of your own Windows applications.

There are only three data files which are provided with the package and the manual starts off with a simple guide through the software using these files.

I thought that I would have welcomed several more test files for different applications in the program. The manual is well-written and the various descriptions are logically set out though it is in black and white; not even a limited number of colour pictures. There is a help facility which provides information about the facilities in the package. The program seemed reasonably robust; at least I did not manage to crash it. I did once obtain the message error *1 math error* which wasn't particularly informative.

In general then EasyPlot is a package with lots of nice features and it would certainly be among the packages to consider when buying a data analysis package. I think that undergraduates would find it far more difficult to use than EXCEL and except in a few cases would not find its extra facilities particularly useful. For postgraduates involved in large amounts of data collection that requires analysis using a method that is contained within EasyPlot, then it might prove to be a package worth acquiring.

electrochemLAB

Subject area
Physical chemistry.

Description
A package of six modules which simulate electrochemical systems illustrating basic principles of equilibrium electrochemistry.

Authors
J. Busby, D. Clow, A. Ruddick, A. Horn and J. Garratt.

Suppliers/Distributors
The eLABorate Project, University of York, York, UK .
www.york.ac.uk/depts/chem/staff/elaborate/

Date/Version
August 2000.

Level
Undergraduate.

Type of Package
Simulation.

Price
Free to UK institutions of higher education.

Hardware required
PC with 486 processor.

Software required
Windows 3.1 (Asymetrix Toolbook 3.0 runtime files supplied).

Roger M. Nix
Department of Chemistry
Queen Mary, University of London
Mile End Road
London E1 4NS
August 2000

electrochemLAB is one of a series of simulation packages that were produced for the eLABorate Project, funded under the UK Teaching and Learning Technology Programme. As the name implies, this particular package aims to encourage students to investigate basic principles of equilibrium electrochemistry.

Summary Review

range: * very poor to ***** excellent	
Ease of use	****
Ease of learning	****
Documentation quality	****
Academic content	*****
Usefulness to student	****
Usefulness to teacher	****
Portability	***
Meets objectives	****
Accuracy	*****

In my experience, the subject of electrochemistry is perceived very negatively by most undergraduate students of chemistry, being widely regarded as both difficult and boring. Teaching aids which stimulate interest in the subject should therefore be welcomed, as few would question its importance, and I will say at the outset that I would regard the electrochemLAB package as a potentially useful addition to any course dealing with the basics of equilibrium electrochemistry (although it would need to be properly integrated for the students to really benefit educationally).

The package is composed of six modules, accessed from a straightforward menu page. The topics covered are summarized below.

Redox Equilibria
This module shows how the final concentrations of the two components of a redox couple vary as a solution of either the oxidised or reduced form of the metal (M) ion is added to a solution of Fe(II) and Fe(III) ions, and permits the student to investigate the effect of varying the redox potential.

Qualitative Electrochemistry
This module simulates a complete electric circuit based around a cell composed of a Fe(II)/Fe(III) redox half-cell connected to a redox half-cell of another metal. The cell voltage and circuit current are displayed qualitatively on analogue-style meters.

Quantitative Electrochemistry
This module displays the precise value of the potential across a cell constructed from half-cells selected by the user. The suggested exercises include an investigation of the use of such a cell for measuring pH and for estimating the potential across a cell membrane.

Activity
This module illustrates the effect of deviations from ideal behaviour, by calculating the potential for a cell composed of a standard hydrogen electrode connected to a Fe(II)/Fe(III) redox electrode. The user can vary the Fe(II)/Fe(III) concentrations and the type of counter ions, and select to perform the calculation using either unit activity coefficients or coefficients obtained from the standard or extended Debye-Hückel models. It is suggested that the student should investigate how the deviation from ideality varies with the concentration and type of ions in the Fe(II)/Fe(III) half-cell.

Temperature Dependence
This module illustrates how the potential of a cell varies with temperature, and it is suggested that the student should use values of the potentials obtained from the simulation to determine the ΔH and ΔS values for the reaction:
$Fe^{2+}_{(aq)} + Ag^{+}_{(aq)} = Fe^{3+}_{(aq)} + Ag_{(s)}$

electrochemLAB

Potentiometric Curves

This module can be used to simulate the results obtained in a potentiometric titration between a Fe(II)/Fe(III) solution and another pair of metal ions M(ox)/M(red). It is suggested that the student should first simulate results for a Fe(II)/Ce(IV) titration and then investigate what difference in redox potential is required in order to obtain a sharp end point.

All the simulations and associated exercises work well, and there are only a few minor issues regarding their use. For example, in the first module there is a problem in the suggested exercise with overlap of the Fe(III) and M(red) curves on the graph, whilst in the second module it is not immediately obvious that it is necessary to break the circuit ("disconnect cells") before it is possible to change either the E^o value for the metal half-cell or any of the ion concentrations. In general, however, I found the package very easy to use - the interface is always reasonably intuitive and not too cluttered. Context sensitive help is also available on the navigation bar at the bottom of the screen, whilst two additional buttons give access to useful Help and Introductory information (although it is a pity that the associated windows are not actually so-labelled).

"...UK HE institutes benefit from generous licensing terms which permit the software to be downloaded freely from the eLABorate website..."

Of all the modules my first impression was that the Qualitative Electrochemistry module seemed the least useful, and perhaps also a little gimmicky, but on reflection I feel that even this module will have served a useful purpose if it enables a student to better make the connection between the theoretical considerations, that tend to dominate in lectures, and real world applications such as batteries. It does, of course, assume that the student has a basic appreciation of the role and positioning of voltmeters and ammeters in electric circuits, which may not always be the case!

Regarding the scientific content and accuracy, I would first comment that there is nothing more annoying than teaching software which is sloppily prepared and contains scientific errors, but I am happy to say that I do not believe this package suffers from either of these problems. Those with access to an authoring copy of Asymmetrix ToolBook 3.0 can, furthermore, customize the program if they so wish.

Documentation

The package is supplied with various documents, including outlines of the principles and educational aims, installation instructions, tutors notes (useful for those of us who have done our best to forget the subject) and a set of student notes. These are reasonably comprehensive, but the student notes which are provided would not be sufficiently detailed or precise for your average student to simply work through on their own. In fairness the authors note that the package is most effectively used in a supervised session and unsupervised use would require adequate preparation and available tutorial support. Since this documentation is all provided as Word documents it would also be a simple matter to convert the existing notes to more structured instructions, if this were desired.

Installation Issues

The package is not demanding on hardware - it should run on any PC running Windows 3.1 or higher (say a 486 or better processor, with 4MB RAM) - and no additional supporting software is required as the essential Asymetrix Toolbook runtime files are supplied as a part of the installation. The latest version (August 2000) runs happily under Windows 95/98/NT4, although there may be minor issues of compatibility.

The main window is of a fixed size that will display satisfactorily for screen resolutions as low as 640x480, although higher resolutions (1024x768 upwards) offer the advantage that the Help and Introduction windows can be simultaneously displayed without overlapping with the main simulation window. One problem, certainly not unique to this package, is that the modules are not usable if the system display is set to "Large Fonts" since the windows are not resizable and the display overflows the window borders.

Licensing

UK HE institutes benefit from generous licensing terms which permit the software to be downloaded freely from the eLABorate website (http://www.york.ac.uk/depts/chem/staff/elaborate/) at York, and installed on multiple machines or local networks.

Conclusion

electrochemLAB is a stable, well-prepared simulation package and most introductory courses in electrochemistry would benefit from its inclusion.

enzymeLAB

Subject area
Biochemistry.

Description
A computer based exercise in the design and planning of experiments in enzyme kinetics.

Authors
Doug Clow, John Garratt, Anne Hodgson.

Suppliers/Distributors
The eLABorate Project, University of York, York, UK.
www.york.ac.uk/depts/chem/staff/elaborate/

Date/Version
Version1.2.

Level
Undergraduate.

Type of Package
Computer assisted learning.

Price
Free to UK institutions of higher education.

Hardware required
A 386PC.

Software required
Windows 3.1 or later (a spreadsheet is useful).

Alan Thomson
Department of Biological Sciences
Lancaster University
LANCASTER LA1 4YQ
August 2000

enzymeLAB is one of a number of packages produced by the eLABorate project to aid teaching of chemistry and biochemistry. Its aim is to provide students with experience of designing experiments to determine the steady-state Michaelis-Menten and inhibition constants of enzymes. It is not a simulation package, nor will it aid in the analysis of data from real experiments. Students would normally use this package just prior to conducting laboratory experiments in enzyme kinetics.

Summary Review

range: * very poor to ***** excellent	
Ease of use	****
Ease of learning	*****
Documentation quality	*****
Academic content	*****
Usefulness to student	*****
Usefulness to teacher	*****
Portability	***
Meets objectives	*****
Accuracy	*****

Users are told at the start that they have isolated a new bacterial enzyme and need to compare it to a mammalian one. They are asked to determine the K_m and k_{cat} values, the type of inhibition by azide and the pH-activity profile of the enzyme. Their total stock of enzyme is 6x0.5ml of frozen solution. They select a type of enzyme from a choice of 5 and are assigned an enzyme with known parameters summarised in a code number. The parameters are selected at random from a table within the program; there are 500 possible sets of kinetic parameters and 25 sets of pK_a values for each enzyme type so it is very unlikely that two students would get the same enzyme to analyse. The code number allows the tutor to determine the parameter set used.

The work is divided into simulated working days, with lunchtimes included. A kinetic run takes a simulated half-hour so a maximum of 14 or so runs can be carried out in a day, allowing for analysis time. In reality a run takes about 30sec including typing in the starting concentrations so the whole enzyme sample could be consumed in an hour. Each run generates an initial rate and the progress is simulated by drawing a straight line of appropriate slope on a graph. The analysis part of the program fits the data to a hyperbola for kinetic parameters, draws pH profiles and determines precision of a number of replicate runs. This part is intelligent at selecting the data points to use and no user input is required to select all those at a particular inhibitor concentration. The Michaelis-Menten data are graphed as a fitted hyperbola, the ability to show a linearised form might have been useful. The graphs can be printed but not copied. The data can be copied and then imported into a spreadsheet for further analysis though this is not strictly a necessary part of the learning experience.

All input from the student is numerical and it is not possible to enter anything other than numbers and decimal points into the input boxes. Out of range data is flagged. The screen outputs are clear and the graphs well-presented although colour is not used. The printed forms of the graphs are extended to fill a piece of A4 paper and look rather stretched when this is done. It is a pity that there is no way of saving the graphs by copying into a word-processor file; this would assist in report preparation and also avoid the queuing when a class using 50 computers simultaneously prints.

We have been investigating this software over the past few months as an introduction to an enzyme kinetics practical class for 80 students. We intend to start using it in October 2000. It has been trialled by some undergraduate project students who found it very helpful in making them think about selecting the right substrate and inhibitor concentrations at the start. The emphasis on 30min simulated time per kinetic run drove home to them that 30 minutes of thought could save hours in the laboratory. On their recommendation we will run it with pairs of students to promote discussion as to methodology.

enzymeLAB

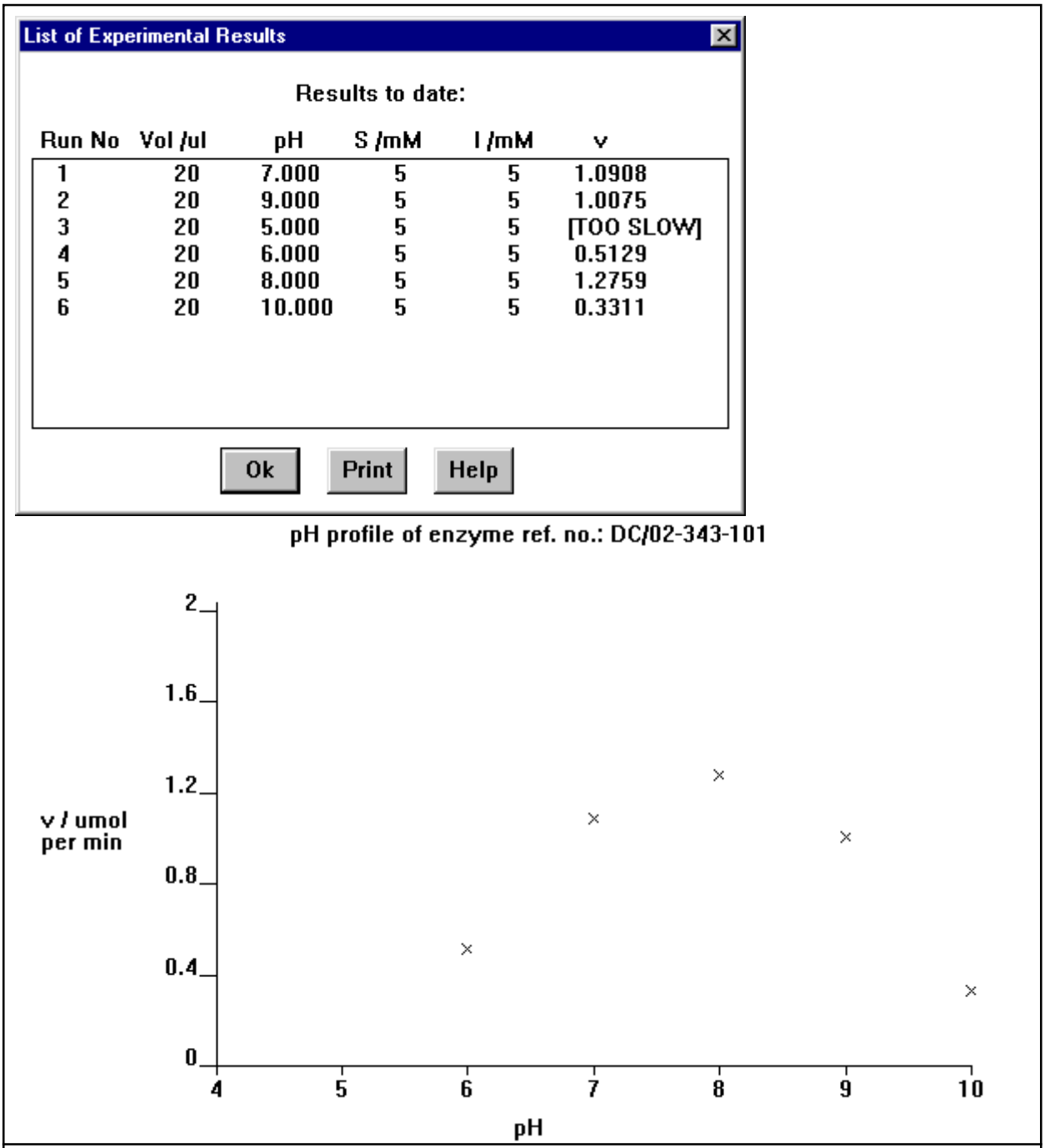

Figure 1: List of results and pH profile from enzymeLAB

The software was supplied as a web download from York and unpacked using a password. Most of the download is 3.5Mbytes of documentation as Word 6 files, the program and its helpfile take up a scant 200Kbytes. The documentation is very comprehensive with full tutor notes, full student handout and demonstration walk through. The program ran well on all the computers, the 25MHz 486 was not noticeably slower than the others.

In summary, an excellent teaching tool with clear aims well fulfilled. The only deficiency is the inability to copy the graphs and collect them in a word-processor file for later incorporation into a report.

Mathematica

Subject area
General science.

Description
A mathematics package combining interactive calculation, visualisation tools and a programming environment.

Authors
Wolfram Research.

Suppliers/Distributors
Wolfram Research Europe Ltd, 10 Blenheim Office Park, Lower Rd, Long Hanborough, Oxon OX8 8LN.
www.wolfram.co.uk

Date/Version
2000/Version 4.0.

Level
Undergraduate, research.

Type of Package
Calculation, simulation, programming.

Price
Student version £75. Full professional version £1190.

Hardware required
A PC, Mac, Unix or Linux computer. For more details see supplier's web site.

Software required
For PC: Windows 95/98/NT/2000.
For PowerPC: Mac OS 7.5.3 or later.
For 680x0: Mac OS 7.1 or later.
For more details see supplier's web site.

Steve Walker
Department of Chemistry
Liverpool University
Liverpool L69 7ZD
September 2000

This is a difficult review for a variety of reasons. Mathematica has been around for a long time (1988) and has gathered such a well-deserved reputation for excellence that it is hard to say anything new. On the other hand, the program is so vast and versatile that even an expert will not have explored all of its potential. It is impossible, in this short review, to encompass the whole scope of this package, which has grown beyond the physical sciences and now pervades any modelling environment whether it is in financial analysis or computer art.

Summary Review

range: * very poor to ***** excellent

Ease of use	****
Ease of learning	**
Documentation quality	*****
Academic content	*****
Usefulness to student	*
Usefulness to teacher	****
Portability	*****
Meets objectives	*****
Accuracy	*****

Let me start at the beginning. Mathematica arrived in the usual enormous box that seems to be obligatory packaging these days. However, in this case it was necessary since the CD is accompanied by an enormous 1500 page hardback manual plus a 500-page description of add-on packages and a substantial 'Getting Started' brief. The installation presented me with the only negative aspect of this review in that none of the custom fonts appeared to be present. Since these are supremely important in what is basically a mathematical program, it was difficult to proceed. The on-line help uses these fonts (as does every aspect of this program) so it was impossible to understand the instructions for solving the problem and it was (shock, horror) necessary to read the manual. Unfortunately, none of the remedies were effective and neither was any number of re-installations so I E-mailed the UK agents for support. Sad to say, despite a half dozen attempts I received nothing, not even an acknowledgement, and I had to try support in the US. I received a holding response within a couple of days followed by detailed advice about a week later. None of their suggestions solved the problem and I was beginning to suspect a corrupt CD when I decided to look in detail at the custom fonts. The US support desk had provided me with a full list of these and I suspected that for some reason they had gone astray. In fact, they were all present as expected in the Fonts directory but a close examination revealed that their author was me! The mathematical, Greek etc. symbols were all present but the copyright and sundry information were identical to those written by me for a custom font of my own design. Removal of this font instantly restored all the Mathematica fonts. I have no explanation for this as others (e.g. c-cubed.ttf) do not cause a problem.

The program has five main strengths, all interlinked:-

Numerical Computation
Including matrix operations of any size, ordinary and partial differential equations, Fourier transforms, data manipulation and fitting, statistics etc., all with unlimited numerical precision.

Symbolic Computation
Including simplification, polynomial factoring, integration, and equation solving for both algebraic and differential equations.

A Programming Language
This is a fully featured symbolic language, which is easy to understand with even a smattering of knowledge of other languages.

Mathematica

Notebook

This is essentially a word processor incorporating text, equations, graphics and sound plus all the features you would expect such as spell checking with a scientific dictionary. The text can be exported to many other formats including HTML and LaTeX and is fully platform-independent in its own native format.

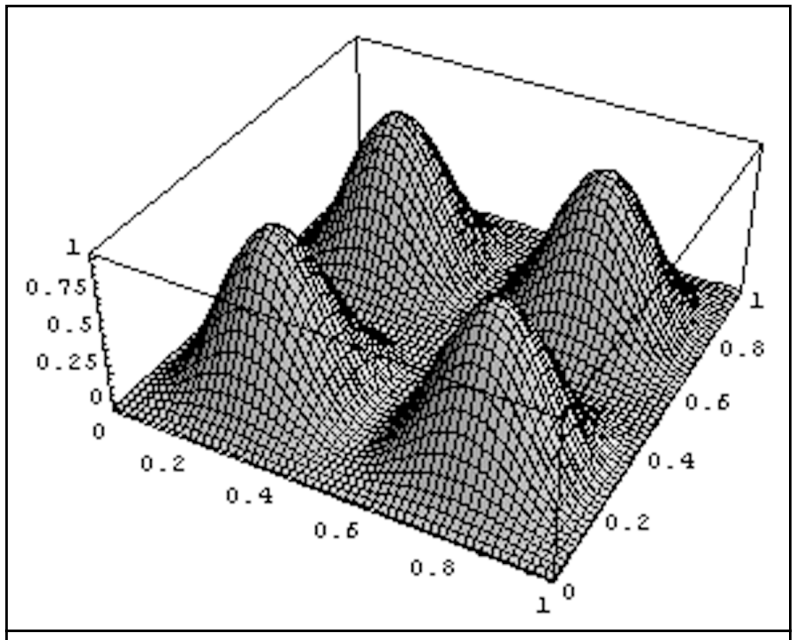

Figure 1: Equation 1 mapped in Mathematica

Graphics and Sound

This comprises a very full specification for 2D, 3D, contour and density plots with animation and sampled sound and export to all formats. To my mind, this is one of the most unexpected aspects of the program. I did expect to see beautiful images of the usual suspects – fractals and complex mathematical topologies, I did not expect to see circuit diagrams, geological maps, diagrams of apparatus or even recognisable portraits.

I have used Mathematica a great deal for numerical computations, particularly for solving numbers of large polynomials but never seem to have needed the graphics capabilities. For this review I decided to give it a go and chose something very simple to see how easy it was. I used Equation 1 to look at the probability density in the particle in a square box problem:

Equation 1: `Plot3D[(Sin[2 Pi * x] Sin[2 Pi * y])^2, {x, 0, 1}, {y, 0, 1}, PlotPoints → 55];`

At the outset it must be realised that Mathematica is extremely fussy about syntax and you must type in exactly what it expects to see. In this formula, the instruction Plot3D has a self-evident meaning but plot3D and Plot3d won't work (neither will sin, cos, pi, Plotpoints and so on). You must read the instructions thoroughly and be very careful about case, use of spaces, use of brackets (crucial – there are three very different ones above with specific meanings) etc. In this example we are plotting an un-normalised function, with unit box lengths (*x* and *y* go from 0 to 1), for quantum numbers of 2 in both directions using 55 points per variable. Figure 1 shows the result.

There are commands for producing some stunning results. The program allows full 16 bit colour to achieve the shading and you have total control of viewpoint, lighting position, colour table, axis appearance, hidden surface removal and so on.

Once a function has been defined and drawn, subsequent manipulations are simple using the % reference. It is not necessary to re-enter the function. For example:

```
Show[ContourGraphics[%]]
```

produces a contour map of equation 1. I find myself in two minds when it comes to the educational uses of Mathematica especially within a typical UK chemistry department. When I first encountered this program over 10 years ago, I was enthusiastic about its potential and this was reinforced by the introduction of the student edition. I was disappointed that students were not similarly excited and even the more mathematically able, despite recognising its power, strongly resisted it on the grounds that it was mathematics and not chemistry. I am aware of several chemistry departments using this program as part of their 'remedial' mathematics courses and I admire them for it but I cannot see it working for most of us. In an era when an A-level mathematics qualification is a rarity and maths is viewed with suspicion and fear (and as a punishment), I can see very little scope for using this program. I am afraid that the majority of us are unlikely to encounter students who can make the effort required to learn even the simplest applications and psychological barriers will prevent them from trying. The manual states …"Mathematica is heavily used in education and hundreds of courses from high school to graduate school are based on it". The collapse of maths teaching in the US and the concomitant decline in the physical sciences has led to chemistry courses featuring much less in this scenario. Teachers in the US are disappointed that we have followed their trend so quickly and so well.

In conclusion, a brilliant program, which I find myself using constantly, and which would both entertain and help any teacher and researcher but will only find limited application in UK university chemistry undergraduate courses.

ModelMaker 4

Subject area
General Science.

Description
Simulation modelling for physical sciences.

Authors
ModelKinetix.com.

Suppliers/Distributors
ModelKinetix.com, The Magdalen Centre, Oxford Science Park, Oxford OX4 4GA. (Formerly distributed by Cherwell Scientific Publishing Limited.)
www.modelkinetix.com/

Date/Version
2000/Version 4.

Level
Undergraduate, research.

Type of Package
Simulation, dynamical modelling.

Price
£145 (educational price). Manuals and CDs are extra at £30 plus postage.

Hardware required
PC; 16MB RAM; CD-ROM drive.

Software required
Windows 95, 98, NT.

Alan Hinchliffe
Chemistry Dept
UMIST
Manchester M60 1QD
July 2000

Summary Review

range: * very poor to ***** excellent

Ease of use	****
Ease of learning	****
Documentation quality	*****
Academic content	****
Usefulness to student	****
Usefulness to teacher	****
Portability	****
Meets objectives	****
Accuracy	****

I can't give a better start to this Review than by quoting the opening Paragraph from the User Manual. "A model is a quantitative description of a real-life process or system, and is typically composed of mathematical equations which give numerical answers. These answers can be substantiated against factual data to test the accuracy of a model. If a model is accurate, it can be used to make predictions."

Modelling is a hot topic in many branches of science, engineering and economics, and ModelMaker 4 is the latest version of a well-known package formerly from Cherwell Scientific. Earlier versions attracted good Reviews, and the package is well known amongst the modelling fraternity.

There are two manuals, the User Manual and the Reference Manual. Both are well written and informative. The User Manual has an excellent Tutorial concerned with the discharge of a pollutant into a water system comprising two lakes and a sea. A screen grab is shown below

The interface is divided into two panels, the Model Explorer on the left and the Model View on the right. The Model View is intuitively easy to use.

In this example, a pollutant P discharges into $Lake_1$, whose waters flow into $Lake_2$ via a River and hence into the Sea via an Estuary. The Lakes and the Sea are called "Compartments" and they are denoted by boxes in the screen grab. In order to find the concentration of pollutant in each Compartment as a function of time, we have to integrate the kinetic equations. If we focus on $Lake_2$, pollutant enters with a "Flow" F_1 and leaves with a "Flow" F_2, so that

$$\frac{dP}{dt} = F_1[Lake_1] - F_2[Lake_2]$$

and there are corresponding equations for the other two compartments. The three equations have to be integrated numerically, and this is done by one of Euler's method, the Mid-point method, Fourth Order Kunge-Kutta, Bulirsch-Stoer or Gear's method.

There is a good Graphical User Interface, the model above was made with very few mouse clicks. Visualization of the results is also good, with the possibility of graphs and tables. There is an extensive Help facility, and the input is quickly mastered.

Both the manual and the package demonstrate an amazingly cavalier treatment of quantity calculus. Inputs to the package are numbers (a discharge of 1000 units), which are magically transformed to kg and days for graphical and tabular purposes.

For a first try, one might make reasonable assumptions about F_1, F_2, $[Lake_1]$ and $[Lake_2]$ and then run the model for comparison with experiment. It is often useful to investigate the effect of changing one (or all) model parameters over a narrow range, and this *sensitivity analysis* can be done very easily with ModelMaker 4. If experimental data were available, one might also *optimize* some of the model parameters to give the best possible fit. The package caters for such optimizations with a choice of the Marquardt and Simplex methods.

ModelMaker 4

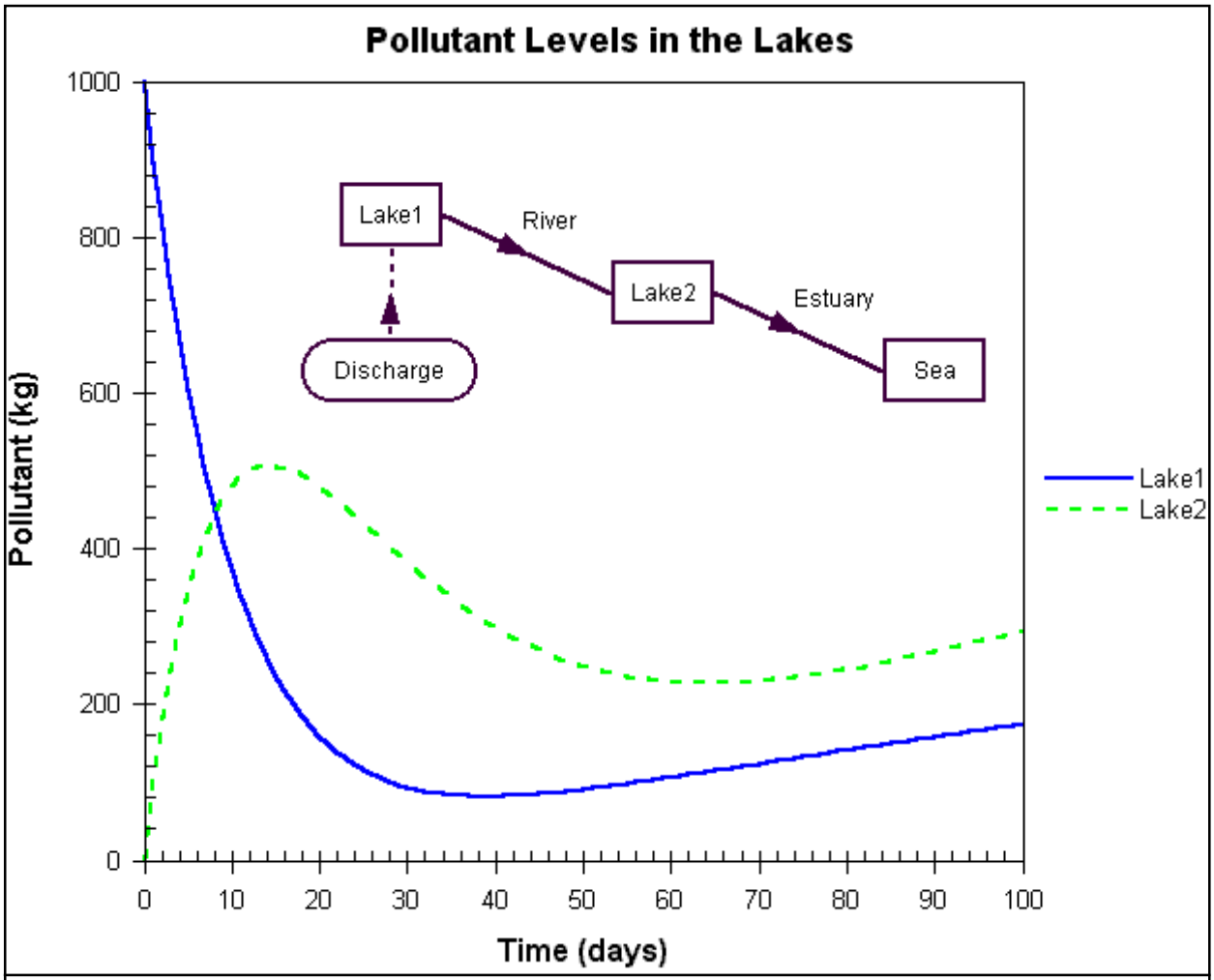

Figure 1: An example model and graph from Model Maker

Monte Carlo analysis is a new feature of ModelMaker 4. This enables model parameters to be specified as random distributions. For example, the discharge above might follow a normal distribution throughout a given time period.

The model discussed above has an ecology flavour, but it is just given as a simple example. The Website http://www.modelkinetix.com has the usual FAQs, news and Reviews but in addition it has a number of downloadable models from different branches of science, such as

- The flow of water into paddy fields
- Heat flow in soil
- Use of heroin and crime in the population
- Dosing regimes for drugs
- Simulation of AIDS in the population
- Effect of Pesticides on Insect Populations
- Predator/ Prey
- Autocatalysis

The Reference manual is comprehensive, and acts as a useful starting point for the literature. The package is shipped as a fully-functioning but time-limited product. Registration codes have to be obtained from ModelKinetix.com. Technical support is said to be available from the Web site. I always test such assertions when writing Reviews, and have to report a very positive experience.

Earlier versions of ModelMaker have featured in many scientific papers, and it is clear that the package is widely used by the modelling fraternity. Version 4 adds welcome and worthwhile options.

ModelMaker can be bought from ModelKinetix.com's online store for £199 (£145 Academic). Manuals and CDs are extra at £30 plus postage. The CD package comes with the two printed manuals. These are also on disk in Adobe Acrobat format, together with information about the ModelMaker Discussion Group.

Molecular Movies Version 1.0

Subject area
Organic Chemistry.

Description
Organic reaction mechanisms using 3D molecular movies.

Authors
ChemLibris.

Suppliers/Distributors
ChemLibris, Fatburs Brunnsgata11, 118 28 Stockholm, Sweden.
www.fatburen.org/chemlibris/chemlibris

Date/Version
1998/Version 1.0.

Level
A-Level, undergraduate.

Type of Package
Simulation, teaching aid.

Price
Single user licence, $30 until end 2000. Contact supplier for classroom licences.

Hardware required
PC: Pentium processor, 32MB RAM, colour monitor, 256 colours, sound, CD-ROM drive.
Mac: PowerPC processor, 32MB RAM, colour monitor, 256 colours, CD-ROM drive.

Software required
PC: Windows 95 or later or Windows NT.
Mac: OS 7 or 8.

Chris Wood
Rendcomb College
Cirencester
Gloucs GL7 7HA
May 2000

I reviewed this package using an IBM Aptiva AMD-K6 3D processor with 32MB RAM running Windows 98. There was no documentation available and no help within the program (however there is a readme file on the CD-ROM which gives a limited guide to troubleshooting as well as brief instructions for installation and use of the software).

Summary Review

range: * very poor to ***** excellent	
Ease of use	*****
Ease of learning	*****
Documentation quality	*
Academic content	***
Usefulness to student	***
Usefulness to teacher	***
Portability	no data
Meets objectives	no data
Accuracy	****

The software is extremely easy to install and may be run entirely from the CD-ROM. There is a choice of having screens with a dark background for PC monitors or a light background for multimedia projectors. The menu, which may be returned to at any point, is clear and accesses nine different reaction mechanisms. Each mechanism is in the form of an animated movie which may be controlled with forward, rewind, stop and play buttons like those encountered on tape/CD players. There is no facility to print the movies however it is possible to copy the active window (Alt Print Screen) into Word or other software (Ctrl V) if handouts are required. The transition from one sequence to another is fast even when running directly from the CD-ROM.

For each mechanism a reaction scheme is displayed followed by sequential electron movement. Stereochemistry is clear and reinforced by moving 3-D images of the species reacting. Such changes are accompanied by some entertaining sounds but these may be switched off if desired. Unfortunately $\delta+$ and $\delta-$ charges are represented mostly as small and feint pluses and minuses so this needs to be stated at the start of any session. After each mechanism movie has run, one can proceed to some useful notes, which in some cases take the student one or two steps further. For example, Markovnikoff's rule is discussed for electrophilic addition of hydrogen chloride and enantiomers are introduced for the electrophilic addition of bromine to cyclopentene.

Where appropriate rate equations are displayed and related to slow and fast steps and the Walden inversion is highlighted for SN2.

An additional feature for some mechanisms is an energy profile diagram, which is related to the movie although not explained, providing scope for the teacher but possibly meaning little for the student.

With the nomenclature adopted by current A-Level syllabuses there are a few niggles which would necessitate the production of a glossary for self study. These include R and S for enantiomers, acetate instead of ethanoate, Kekulé structures and ortho-, meta- and para- for aromatic compounds. The Scandinavian origins of this software are given away by the spelling of cyklopentene.

Overall this is a useful aid to teaching organic reaction mechanisms and the movies are visually effective. It is a pity that free radical mechanisms are not covered and the package would benefit from some sort of self-assessment section. Despite this I shall be using Molecular Movies to support classroom teaching, tutorials and self-study.

Motion in Electromagnetic Fields

Subject area
Electromagnetism.

Description
A tutorial covering the fundamental description of the motion of charged particles in electric and magnetic fields and related concepts.

Authors
WhistleSoft, Inc.
www.swcp.com/~silbar/software/

Suppliers/Distributors
Physics Academic Software, Box 8202, NCSU, Raleigh, NC 27695-8202.
wasnet03ws.physics.ncsu.edu/pasnew/

Date/Version
Windows Version 1.02.

ISBN
1-56396-870-X

Level
Undergraduate.

Type of Package
Computer assisted learning.

Price
Single user license $100, 10 user license $400.

Hardware required
A PC computer with 8 MB RAM or better, 256-color (8-bit) VGA graphics or better, 2X or better CD-ROM drive (MOTION can be run from the CD-ROM), (sound card recommended).

Software required
Windows 95/98/NT or later plus QuickTime for windows (installer included with package).

Nigel Glover
Dept. of Physics
South Road
Durham DH1 3LE
July 2000

Summary Review

range: * very poor to ***** excellent	
Ease of use	*****
Ease of learning	****
Documentation quality	*****
Academic content	*****
Usefulness to student	*****
Usefulness to teacher	*****
Portability	***
Meets objectives	*****
Accuracy	*****

This is a self-paced, interactive tutorial using hypertext in a way that allows the student to choose their own path through the material. The tutorial covers the fundamental description of the motion of charged particles in electric and magnetic fields in five sections. The basic material is quickly introduced in the first section and then illustrated through a series of applications, the spectrometer, the Wien filter (or velocity selector), the cyclotron and finally the magnetron. It is presented at a level that is accessible to a first year undergraduate physics student. Besides the hypertext links between the topics of the tutorial, there are other multimedia elements, such as animations, colored graphics, video clips and sound, which are well used to illustrate the historical aspects of the material as well as to develop an intuitive feeling for the subject. Backup material is available as sidebars and this allows access to slightly more advanced topics.

The package is extremely easy to install from the CD-ROM provided. The system requirements are quite modest, any PC computer running Windows 95/98/NT with at least 8 MB RAM, 256-color (8-bit) VGA graphics and a 2X or better CD-ROM drive. QuickTime is needed for the video clips and is also available on the CD-ROM. A sound card is recommended. I installed the package on the hard-disk – the executable occupies 4 MB and the video clips another 12 MB – although running the program directly from the CD-ROM is also possible. The program is also available to run on 16MHz 68030 CPU Macintosh systems with 8MB of RAM and 20 MB of hard disk. I had no problems running the program at all, however, there is a section on TroubleShooting in the manual provided with the software.

With a single user licence costing $100, the program can be installed on a single hard disk. Multiple-copy licences authorizing use of up to ten copies of the program are available for $400. The program may be loaded onto a networked computer system, but each computer operating the program simultaneously requires an authorized copy of the program. For up to date pricing, consult the publishers web-site. Information on other teaching and learning software packages written by WhistleSoft can be found at http://www.whistlesoft.com/~silbar.

Double clicking on the MOTION icon brings up the window giving access to the package which may be entered either by giving a Student ID or, if you don't want to customise or save the tutorial session by selecting No ID. All action takes place within this window which provides direct access to the 64 content pages, 17 question pages, 23 answer pages and 6 laboratory demonstrations that make up the tutorial.

There is an excellent built-in navigational help facility that explains how to use the tutorial – the navigation buttons, the multiple choice self-test questions and the interactive laboratory pages. There are also three main support pages, the table of contents, map and the scrollable index of hypertext links. Interaction with the package takes place via mouse clicks or keyboard shortcuts that are explained in the Help pages. Basically anything blue is a hypertext link which turns purple when accessed.

Motion in Electromagnetic Fields

Some pages have *progressive disclosures*, the speed of which are controlled by mouse clicks (or keystrokes). This is particularly useful for the derivation of equations and helps the student follow through the steps without being put off by a whole page of formulae at a time. It is also good for getting the student to think when reading through the page.

Another useful feature is the Report Card that can be accessed at any time by the pull down menu or on exiting the package. Here the number of content pages, question pages, answer pages and laboratory demonstrations accessed is recorded along with the percentage of correct answers to attempted questions. Reaccessing a saved session keeps track of which parts of the tutorial have been studied.

The content pages have colour coded borders – blue, orange and pink representing introductory, intermediate and advanced levels. In this tutorial, the intermediate material describes particle-cavity coupling in the magnetron, numerical solution of particle orbits in the magnetron and derivations of relativistic effects in the cyclotron. The Lorentz force, circular motion in a magnetic field, cyclotron frequency, the concept of magnetic rigidity, the magnetic spectrometer, the Wien filter (or crossed E and B field velocity selector), basic components of the cyclotron and how it works together with commercial examples and how relativity affects the cyclotron, the operating principles of the magnetron with device designs and applications such as the microwave oven form the introductory material. There is no advanced material in this tutorial.

One of the potential problems with point and click tutorials of this type is that students can go through it too quickly by just clicking on everything in sight to get to the end. For the most part, the material is presented in a sufficiently interesting and varied way that the user is likely to stop and think. The self test questions (and the answers) are well posed with solutions produced by the standard slip-ups as alternates.

For example, it is well known that relativistic effects limit the energy produced in a basic cyclotron. WhistleSoft have lost no opportunity in using this example to illustrate the general cycle in the progression of science: Design using known physics and technology ? build and test ? learn new physics or technology ? repeat. The interactive laboratories are also well used to bring out the physics and stimulate thought. To modify the basic cyclotron to attain higher particle energies we might consider adjusting the initial launch phase of the particle or the radio-frequency of the cyclotron itself. There are three laboratories that address these possibilities first separately and then together. In each case a mouse-controlled slider is used to control the variables and the acceleration voltage and phase are plotted as a function of the number of accelerating cycles. The final energy of the particle is given as a number in a box. For some values of the variables the particle doesn't make it from one side of the cyclotron to the other and the students are encouraged to think why small changes in the inputs can have such dramatic effects.

For the more mathematically minded, there are plenty of derivations hidden away – the relativistic phase lag of the cyclotron for example. I particularly appreciated the numerical methods that were introduced to solve particle orbits in the magnetron. In my experience this is something first year students find hard to understand but here it was done simply and made sure that we understood both what it was that we needed to know and why we were making the approximations to estimate it.

"...an average first year undergraduate student will accomplish all of the sections of the tutorial in about 4 hours and will end up with a very good idea of how particles move in electromagnetic fields..."

Another possible problem is that once material has disappeared from the screen, it disappears from the brain. It is necessary to advise the user to supplement the on-screen progress with notes made in a note-book or by getting a printout of the relevant pages.

Altogether, this is a very impressive package. It is very easy to use and the online help is very well organised, it covers the basic physics well and will engage the student through the applications and laboratories in a very hands-on way. In my view, an average first year undergraduate student will accomplish all of the sections of the tutorial in about 4 hours and will end up with a very good idea of how particles move in electromagnetic fields. I think that this would be four hours very well spent. It is hard to see how to incorporate this tutorial into an already packed first year course, however, I believe that it is well worth trying to do so.

Nightfall

Subject area
Astronomy.

Description
An interactive program which simulates properties of interacting binary stars.

Authors
Rainer Wichmann.

Suppliers/Distributors
Rainer Wichmann.
www.lsw.uni-heidelberg.de/~rwichman/Nightfall.html

Date/Version
1998/Version 0.18.

Level
GCSE, A-Level, undergraduate.

Type of Package
Simulation.

Price
Free.

Hardware required
PC running Linux, postscript printer.

Software required
Linux (tested on Redhat), C compiler, GTK library (for interactive use), GNUPLOT (version 3.5 (pre 3.6), patchlevel beta 347 or higher) or PGPLOT (plus Fortran compiler, e.g. g77) (for plots and graphs) [GNUPLOT version tested]. Gnome Desktop is supported. [Most Linux packages include all the above software].

Robert Connon Smith
School of Chemistry, Physics & Environmental Science
University of Sussex
Brighton BN1 9RH
July 2000

Summary Review

range: * very poor to ***** excellent	
Ease of use	*****
Ease of learning	*****
Documentation quality	****
Academic content	*****
Usefulness to student	****
Usefulness to teacher	***
Portability *(Linux only)*	*
Meets objectives	*****
Accuracy	*****

This interesting simulation program was written as a recreational activity in 1998 by Rainer Wichmann, a researcher on young stars and star formation at the Heidelberg Observatory (Landessternwarte Königstuhl). As a result, it is not aimed at any particular type of user. Rather, it attempts to introduce the user 'into the fascinating realm of eclipsing binary stars', to quote the extensive User Manual provided as part of the Nightfall package. This approach makes the package rather hard to classify: it does not fall into any obvious category. It could be used as illustrative material in an undergraduate or postgraduate course, it could be used for personal enjoyment by anyone interested in interacting binary stars, whether professional or amateur, and it could even be used as a serious research tool, although it is not fully tested for that purpose.

The software is designed for use with a Linux operating system, and is not guaranteed for any other form of Unix, although the author believes that it should run on other Unix systems. Like him, I have not tested this (through lack of time). My test was done on a Pentium Pro 200MHz PC, running Redhat Linux version 6.0 with a KDE window manager. The PC has 64 MB memory, a 2 GB hard disk and is networked to a server (a Sun workstation, running Solaris), along with 5 similar PCs, three other Sun workstations and several X-terminals (at the Sussex Starlink node). The networking caused some minor problems with the installation, because it was not possible to install the configuration, data and binary files in the default directories: the required new subdirectories in /usr/local could not be created without the root password. The installation, from a g-zipped file downloaded from the author's web site, was otherwise straightforward, and the instructions were clear and accurate. One other consequence of the non-standard installation was that it was necessary to issue the command './nightfall' instead of just 'nightfall' to start the program; this was not mentioned in the User Manual.

The User Manual is generally well written and helpfully structured. After a brief introduction to what the software does, and a suitable disclaimer, the technical requirements and installation instructions are given, together with solutions to some common compile/configure problems, and guidance on how to customise the configuration. Simple use from a command line is then described, followed by an introduction to the graphical user interface (GUI), which I found far more convenient and used almost exclusively for my test. After a brief introduction to binary stars, and in particular to the concept of Roche geometry, more advanced options are described, finishing with the use of the program to analyse real data and provide a best-fit binary model.

So what can the program do? It is remarkably versatile, and very easy to use from the menu-driven GUI, laid out in pages accessed by buttons. On the top page, there are boxes where the basic properties of the binary have to be inserted: the mass ratio, inclination, fill-out ratios (in units of the polar radius of the Roche lobe) and temperatures. It is possible to test the system straight away at this point, because there are default entries for these and the other binary properties (period, total mass, separation) defined on a later page [Advanced]. Above the pages there is a toolbar with buttons which allow a light curve to be computed [Compute] and an animation of the orbital motion to be run simultaneously [Animate]. The speed of computation is such that the binary components dance around one another in a leisurely way, allowing plenty of time to

Nightfall

take in what is happening. Alongside the animation, light and velocity curves are built up as they are computed, with the plotting scale automatically adjusting so that the full range of variation (and no more) is displayed. I tested the GNUPLOT version; the author admits that some of the plots (especially the radial velocity ones) are not perfect, but says that the animation is much less smooth with PGPLOT.

Once the computation is complete, it is possible to use another button on the toolbar to plot different light curves (UBVRIJHK and uvby) or the radial velocity curve in more detail. The filter or plot window can be selected on the [Plot Options] page; the same page also provides options for visualising the geometry (either the stars or the Roche surfaces). Non-spherical shapes for the stars are automatically included, according to the Roche approximation.

One of the best features of the interactive version is that, once the computation has been completed, it is possible to go to the [Output] button on the menu bar at the very top of the GUI and choose between various ways of visualizing the binary system. In some of these it is possible to alter interactively parameters such as the inclination and the phase angle. For example, it is possible by trial and error to discover the inclination for a grazing eclipse for a particular binary system. This facility is excellent for getting a feel for how changing parameters changes the appearance of a binary.

"...It is remarkably versatile, and very easy to use from the menu-driven GUI, laid out in pages accessed by buttons..."

To start the user off, there are eight binary systems available as configuration files: loading these in to the program provides a consistent set of data for some real examples of binaries, from the contact system TY Boo to the 51 Peg star plus planet system. Some of these illustrate some of the advanced options in the program: the possibility to include model atmosphere calculations instead of assuming black body spectra (for reasons of resources, the model atmosphere fluxes are taken from tables for a restricted range of temperature, and a single surface gravity and (solar) composition), to choose the limb-darkening law and to add dark or bright spots at various points on the stars' surfaces. Gravity brightening is automatically included, with a distinction between convective and radiative stars (divided arbitrarily at 7000K – but this can be changed). Irradiation and reflection can also be included.

It is even possible to construct an absorption line profile, at an arbitrary wavelength, and watch how the wavelength varies around the orbit. Because the line arises in both stars, with the strength depending on the brightness and the width on the temperature, there are some quite interesting line blending effects at conjunctions. Finally, there is the possibility of adding (non-eclipsing) third light to the system. This has no dynamical effect, and simply veils the eclipses. The author had not fully tested this when writing the Manual, and I did not explore the option thoroughly. All the details of how these options are implemented are given in a technical section at the end.

Once the user has mastered all the options – and the GUI and its on-line help facility makes this a fairly easy exercise – it is possible to explore other real systems, including one's own favourites. For example, I played with the parameters of a particular system to discover what total mass was necessary to produce the observed amplitudes of the radial velocity curves, given the known period and mass ratio. A more advanced option, which I did not have time to explore, is to take observed light and radial velocity curves for a system with a known period and to find the best-fit orbital parameters, using both a robust Simplex algorithm for local optimisation and a (very slow and not fully tested) stochastic search strategy for a global optimum. For research use, that could be extremely useful, if it proved reliable. The author issues a clear warning at the start of the Manual that for any serious use that might lead to a publication, the user should carefully test the program first! He is also suitably cautious in his specific claims for the optimisation codes. However, if you want such a facility, this easy-to-use program may be worth trying. But don't try the global optimising on a network if you value your friends; computing times of a day or more are predicted!

Some of the other options (for example, using a model atmosphere and proper reflection) take longer to compute than one would like, but that may have been partly a function of network traffic. There are some other negative points: if one gets bored with waiting for a slow computation, then the only recourse is to do something else: there appears to be no way of stopping it without closing down the whole program. Also, it is a pity that there is no option to add a simple accretion disk and stream to the simulation; this prevents any realistic simulations of cataclysmic and low-mass X-ray binaries.

In summary, however, I liked this program and I will probably use it to help me to visualise systems I am working on. However, use for undergraduate teaching is inhibited at my university by the fact that Linux machines are not generally available to undergraduates. A version that ran reliably on other Unix platforms would certainly help, although most of our machines are PCs, for which a complete rewrite would be needed. The program is probably also not suitable for use in schools, because it assumes a fair amount of background knowledge of astronomy in general and of interacting binary stars in particular, and also because most schools do not have any access to Linux or even Unix machines. Unfortunately, the same lack of access is true for most amateur astronomers, who normally use PCs; the package would otherwise be very well suited to them.

Papyrus for Macintosh

Subject area
General Science.

Description
Bibliographic software.

Authors
Dave Goldman.

Suppliers/Distributors
Research Software Design, 2718 SW Kelly Street, Suite 181, Portland OR 97201 (U.S.A.).
www.rsd.com
In UK from GeoMEM Consultants, 29 School Road, Kettins, Blairgowrie, Perthshire PH13 9JL.
www.geomem.co.uk/geomem

Date/Version
1999/Version 8.0.5.

Level
Undergraduate, research.

Type of Package
Information management, information retrieval.

Price
From $89 to $139 for single user licence. Contact supplier for details. CHEST deals also available for UK education.
www.chest.ac.uk

Hardware required
Macintosh (68K or PowerPC), at least 4 MB of spare RAM. Internet connection for online reference databases, online help, and updates.

Software required
MacOS System 7.x or later.

Nick Greeves
Chemistry Dept
University of Liverpool
Liverpool L69 7ZD
August 2000

Background/Introduction
Papyrus is described as a Bibliography System and Knowledge Manager designed to manage references and produce bibliographies for papers. It lives up to this title admirably. References may be typed in manually (not a method favoured by the author), imported from text files exported from other bibliographic software (e.g., EndNote, Reference Manager, Procite, Bookends, or BibTeX), or text files produced by on-line services such as ISI Web of Science. Papyrus is compatible with a range of word processors including Microsoft Word 5, 6, and 98, WordPerfect 3.x, and Nisus Writer 5.x and can also work with plain text, RTF or TeX/LaTeX documents. The references are stored in a database format which allows linking of references, notes, keywords, journal names, and graphic images to each other. Selected references may be collected into "groups," which can be independently sorted, formatted, spell-checked, exported, or edited without affecting the main database. Documentation is very well written with a sense of humour. There is a freely downloadable limited edition (=200 references) available http://www.rsd.com/Limited8.html. The software was tested on an iMac DV SE with 128 MB RAM running System 9.0.4 and Microsoft Office 98.

Summary Review

range: * very poor to ***** excellent	
Ease of use	****
Ease of learning	****
Documentation quality	*****
Academic content	***
Usefulness to student	****
Usefulness to teacher	*****
Portability	***
Meets objectives	****
Accuracy	****

Installation and Use
Installation was easy and operation with the extensive on-line help, including Balloon Help and HTML help files, which were both accessible from every window by a single click, was straightforward. Once the concepts of reference management software have been explained, undergraduate and postgraduate students should be capable of using the software with little further help. The detailed manuals, which comprise three volumes; Workbook (examples in a tutorial style), Concepts (underlying ideas), and Reference/Shortcuts (detailed), are also supplied as PDF files which is a useful touch as they exceed 1000 pages and this makes searching for a particular topic easier.

Analysis
In this review I will concentrate on the most important features for writing chemistry papers but Papyrus supports a much broader range of uses than that. I have used EndNote for many years (since version 2 now up to 4) and will make comparisons where appropriate.

Importing more than 100 references from ISI Web of Science proceeded smoothly via an intermediate text file. Unlike ISI supported products such as EndNote there is no direct export route to Papyrus, which is a shame and also unlike EndNote, Papyrus does not support the Z39.50 protocol for direct Internet connections to other databases. The strength of Papyrus was immediately apparent as it automatically compiled listings of the references by author, keyword, and journal. The individual windows are show in the screenshot, which highlights the automation of the process and the useful categorisation of information. I did not manipulate or add to these windows in any way except via the resize button and scroll bars prior to the screenshot. Each of these may be opened into a subset of the main database and formatted for output as desired. The generation and recognition of the standard abbreviations for journal titles for use in bibliographies was particularly impressive. In contrast these have to be individually entered and activated in EndNote.

Papyrus for Macintosh

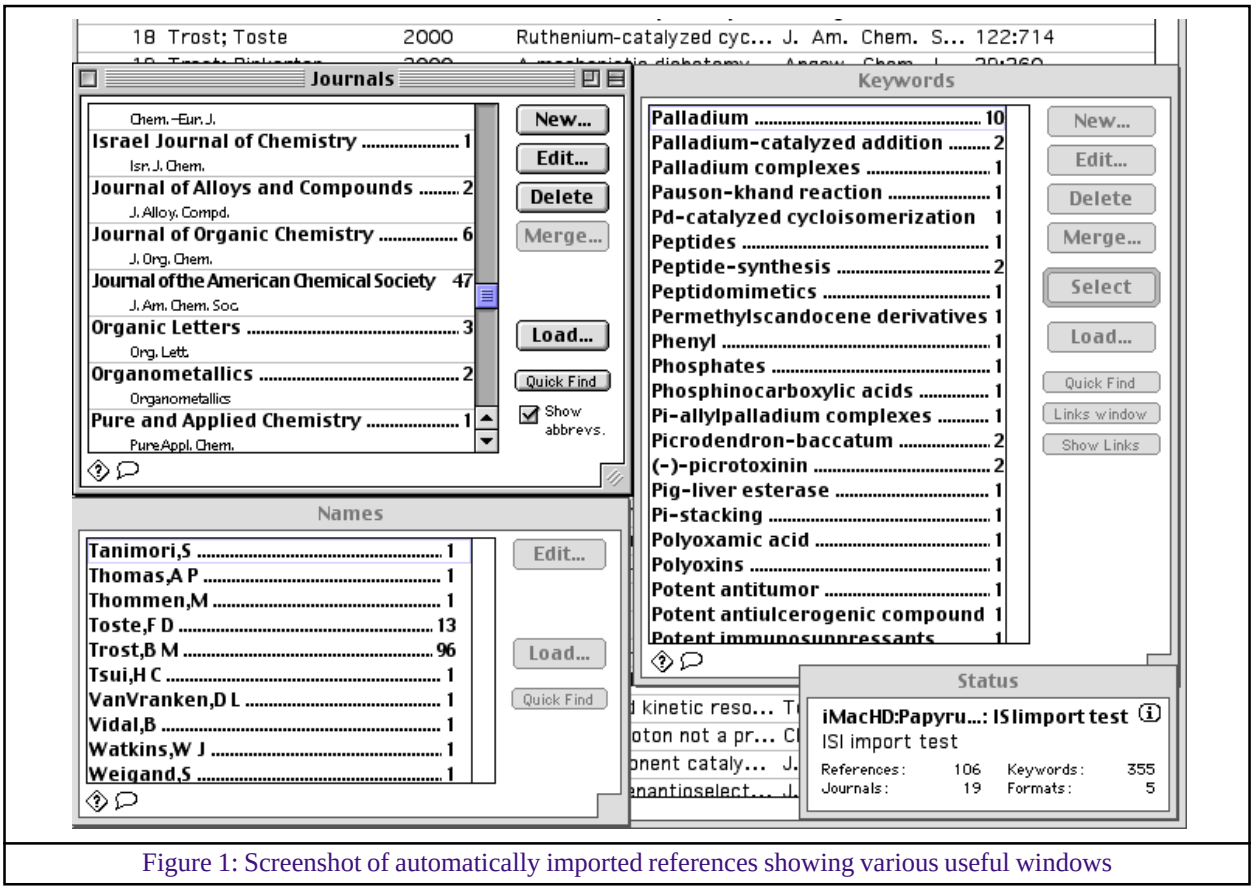

Figure 1: Screenshot of automatically imported references showing various useful windows

I tested the ability of Papyrus to produce a bibliography with MSWord 98. The process of citation insertion using either drag/drop or cut/paste and conversion to the final format in a wide range of different journal output formats was straightforward. One adverse comment is that it seemed significantly slower than EndNote at producing the final version. Following the Workbook instructions everything is customisable. Import and export formats, reference types, database fields, in-text citation styles, and bibliography styles can all be modified.

The quality of the data entered by hand is improved by clever use of the journal and keyword lists. Simply typing "jacs" in the journal field and pressing return twice is enough to produce "Journal of the American Chemical Society" and this works for all previously used titles eliminating mistakes which would cause problems later on. Similarly misspelling a keyword produces a dialog asking if this new keyword is really intended. These features will improve the accuracy of subsequent searches on the database.

The searching function is very powerful and simple to use once the slightly non-intuitive interface has been mastered. Simple or complex searches, using Boolean and relational operators with wildcards, may be performed. The results of each search may be kept separately or combined to produce a larger subset. This is far more flexible than the searching facility in EndNote.

Spellchecking of the entire database is facilitated by the Word Services interface which allows third-party spellcheckers such as Spellswell Plus by Working Software http://www.webcom.com/~working/spellswell.html, and Excalibur (available free by download http://www.eg.bucknell.edu/~excalibr/excalibur.html). Technical words pose a problem for conventional dictionaries which restricts the value of this feature until they have been added to the dictionary.

Access codes allow the use of the database without modification or with the addition of new data or even changing the database settings. This is useful in a teaching situation where unauthorised changes would be likely.

Cross-platform compatibility

I did not test the Windows version.

Conclusions

Overall Papyrus is a well-featured application, which delivers its objectives in an efficient and friendly manner. In the UK a CHEST Agreement makes purchase in academic institutions even more attractive but ongoing negations for a similar arrangement for the more expensive EndNote may reduce this advantage.

Personally the lack of a direct interface with Web of Science and familiarity will not tempt me away from EndNote but should these shortcomings be addressed in a future version I would seriously consider switching.

Practical Laboratory Chemistry – Disk 3

Subject area
General Chemistry.

Description
A laboratory teaching resource covering gravity and suction filtration, recrystallisation, sublimation and refluxing.

Authors
Chemistry Video Consortium.
www.soton.ac.uk/~chemweb/cvc/

Suppliers/Distributors
Educational Media & Video Ltd, 235 Imperial Drive, Rayners Lane, Harrow, Middx HA2 7HE.

Date/Version
1999.

Level
A-Level, undergraduate.

Type of Package
Teaching aid.

Price
£35.00 (plus PP & VAT).

Hardware required
Pentium PC 100 MHz, 32MB RAM, 4 speed CD ROM Drive, Sound Card (Windows 3.x software systems require a hardware MPEG card for video playback).

Software required
Windows 3.x, 95, 98, NT.

David Allen Symon
University College Northampton
St George's Ave
Northampton NN2 6JD
August 2000

The software is supplied on CD-ROM with an eight page CD sized instruction booklet that covers the installation for Windows 3.x and Windows 95/98/NT4.0 and the operation of the software.

Summary Review

range: * very poor to ***** excellent	
Ease of use	****
Ease of learning	****
Documentation quality	**
Academic content	*****
Usefulness to student	*****
Usefulness to teacher	****
Portability	***
Meets objectives	*****
Accuracy	****

The review was carried out on a PC fitted with an AMD 350 MHz CPU, 128 MB RAM, 32X CD player, 10.2 GB hard disk and 17-inch display running in true colour at a resolution of 1280 by 1024 with a Matrox Millennium graphics card. Sound was provided by a C-Media on board sound chip and 80 watt stereo speakers. The operating system was Windows NT 4.0 service pack 6. Printing was via an Epson Stylus 900 inkjet printer.

The installation was straightforward and installed a movie player and then the support files on to the computer hard disk. Opportunity is given to select the destination folder for the program and the movie player. Warnings are given if the destinations on the hard disk are considered inappropriate. There did not appear to be any on line help provided by this package.

The installation process did not add the program to the programs on the task bar. A computer novice may have then experienced difficulty in starting the software. Once the software program PLC.TBK was located and double clicked the program started without problem. When installing the software on a second computer with a Pentium II 355 MHz processor running Windows NT 4.0 service pack 6 it was unable to correctly register the MSDXM.OCX file in the folder winnt\system32. This installation did however install the program to the programs on the task bar.

Although the installation is not without some shortcomings it is well worth the effort to sort out the problems as the academic content is of a very good standard and should prove useful in demonstrating and improving the understanding of the techniques covered.

The start-up screen is clean, easy to read and generally well presented. The full screen button does not expand the picture but places a grey background around the functional screen image. Pressing the CD-ROM symbol caused the CD-ROM to start and load the individual modules. Up to eight subsections titles of the module are displayed at once on the screen, any additional subsections can be viewed by on screen "previous and next buttons".

The audio-visual presentation can be reinforced using the on screen text display by toggling the text on / text off button on the screen. The text on / text off toggle button displays "text off" when text is being displayed and "text on" when no text is being displayed.

Although the manual provided suggested that the written summary could be printed this feature did not work properly on the reviewer's machine. A message suggesting the text was being sent to the printer and some printer activity was noted but no printed output was ever achieved from this feature.

The video controls consist of the normal symbols for forward, pause and stop; no fast forward or fast rewind facility is provided. Gross movement of the video can be achieved by sliding the progress bar at the bottom of the video image. The video can be displayed either in a small window or full screen by toggling

Practical Laboratory Chemistry – Disk 3

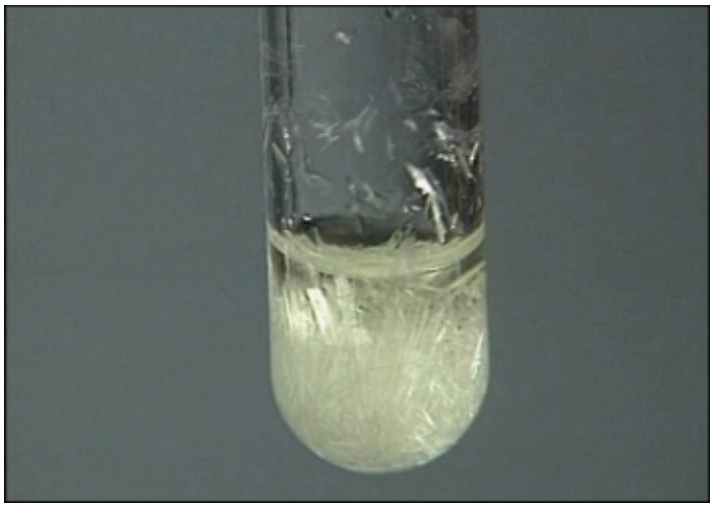

Figure 1: A still from recrystallisation

the screen icon on the display. The video is perfectly clear in both the small window and the full screen modes, although the reviewer tended to prefer the full screen mode. Return from the full screen mode to small window mode is achieved by use of the "Esc" key.

The topics covered are gravity filtration, folding filter papers, suction filtration, and recrystallisation. An appendix contains information on solubility testing, promoting crystallisation, handling oils and dealing with discoloured samples as well as the techniques of sublimation and refluxing.

The video display is of an excellent standard even when viewed full screen and the sound and images move smoothly. The content of the package is of a very high standard and clearly demonstrates all essential elements of the topics covered. Demonstrations of the techniques are clear, pay good attention to safety, clearly identify all the key equipment used and are free of distractions. The sound is of CD standard with clear diction of the words and is clearly of human origin rather than of a computer generated origin.

The viewer can choose to take a multi-choice quiz on the content covered in each of the modules and print out their identity and score. The number of questions for each module varies significantly. The questions answered incorrectly are identified on the hard copy but not on the screen. Printing out from this part of the program was without problem. Correct answers are not provided for those questions answered incorrectly either on screen or on the hardcopy. Again the presentation of this section is up to the usual high standard of the package.

There did not appear to be any readily available opportunity for printing out hard copy of screen shots from the video, which could be useful for students to illustrate a written report of related experimental work. The package appears to be excerpts of videos put onto CD-ROM with the addition of the quiz feature, and this tends to lack the sophistication of CAL packages where more feedback and help is provided when incorrect answers are entered.

Overall the package is presented to a very high standard and should encourage positive responses from the user. The package is suitable for use with people from a wide range of educational backgrounds and experience in the range of experimental techniques covered. The gravity filtration section, for example, could be used to introduce the topic in schools or to improve the techniques for more experienced practitioners in chemical laboratory techniques. The use of this package prior to carrying out practical work should result in much higher standards of laboratory techniques being achieved.

"...The video display is of an excellent standard even when viewed full screen and the sound and images move smoothly. The content of the package is of a very high standard..."

This is a very useful package that has wide applicability in an area where there is often insufficient attention paid to the basic practical technique. This package would make a useful addition to the resource base of any establishment using these techniques and should be included as "essential viewing" for all people studying chemistry or using these techniques.

Wizard Test Maker v2.04

Subject area
General Science.

Description
A database of geology, physics, biology and chemistry questions.

Authors
Eduware.

Suppliers/Distributors
Eduware Inc, 292 Main St, Huntingdon, NY 11743.
www.eduware.com/

Date/Version
1999/Version 2.04.

Level
A-Level, undergraduate.

Type of Package
Examination preparation, database.

Price
Prices start at $109.95. Contact supplier for more details.

Hardware required
PC.

Software required
Windows 95, 98, NT.

Margaret Greenhall
Department of Chemical and Biological Sciences
Huddersfield University
Huddersfield HD1 3DH
November 1999

Background & installation
Installation was easy - you just run setup off the CD. The only slight problem I had was locating the introductory tour after it had completed installation - as I used Explorer - but it was under the Windows Start menu.

Wizard test maker is a database of multiple choice questions. You can either use the ones in the database or use the program to write your own. There are four main topic areas - physics, chemistry, earth science and biology. Wizard will allow you to put together a test and then print it out. It does not allow on line testing.

Summary Review

range: * very poor to ***** excellent

Ease of use	**
Ease of learning	*
Documentation quality	*
Academic content	****
Usefulness to student	*
Usefulness to teacher	***
Portability	***
Meets objectives	***
Accuracy	***

Intended Audience
The level of questions appears to be A-Level or first year of a degree - in other words it seems to be aimed at the 'Freshman' market.

Program content and layout
In each topic area there are many questions which have been developed by teachers. In the chemistry section there are the following topics : Lab activities, Nuclear, Redox and Electrochemistry, Acids and Bases, Kinetics and Equilibria, Maths (which means chemical calculations not maths), Periodic table, Bonding, Atomic structure and Matter & Energy. Each of these topics has around 200-250 multiple choice questions, with four answers to choose from. These topics are sub-divided into more specific areas.

The questions I looked at seemed to be well written and correct and in SI units not imperial. You can get a print out of the whole of a topic as there are tests stored which are just all of the questions. All questions can be edited so if a question isn't quite right you can alter it. If you choose to design your own questions you can allocate them to either topics already available or to your own topic areas. There is a lot of scope for creating sub-categories to enable a tutor to select a random selection from a very specific area.

Ease of use
The interface looks very like many encyclopaedia CD-ROMS with a picture of books to chose your main topic and then an alchemist's studio for the chemistry section. At first this led me to believe that it was aimed at students but this is not the case, it is for teaching staff to create tests. When I started to use it I found it very difficult and had to resort to running the tour (which was on the Windows Start menu but not in the folder when I used Explorer) which was unexpected as usually I am able to just plunge in and use a program. The tour worked well on my home PC which is set up for sound but my work PC has no sound and there was no option to see a text version of the tour.

Even after a couple of hours I was still struggling a bit to do exactly what I wanted to and in some cases bugs appeared (such as two crashes and 2 cases of the menus not reverting to the correct ones as I went back up the levels of the program). Thus I would rate the interface high on looks and low on user friendliness. Help was not very good.

Wizard Test Maker v2.04

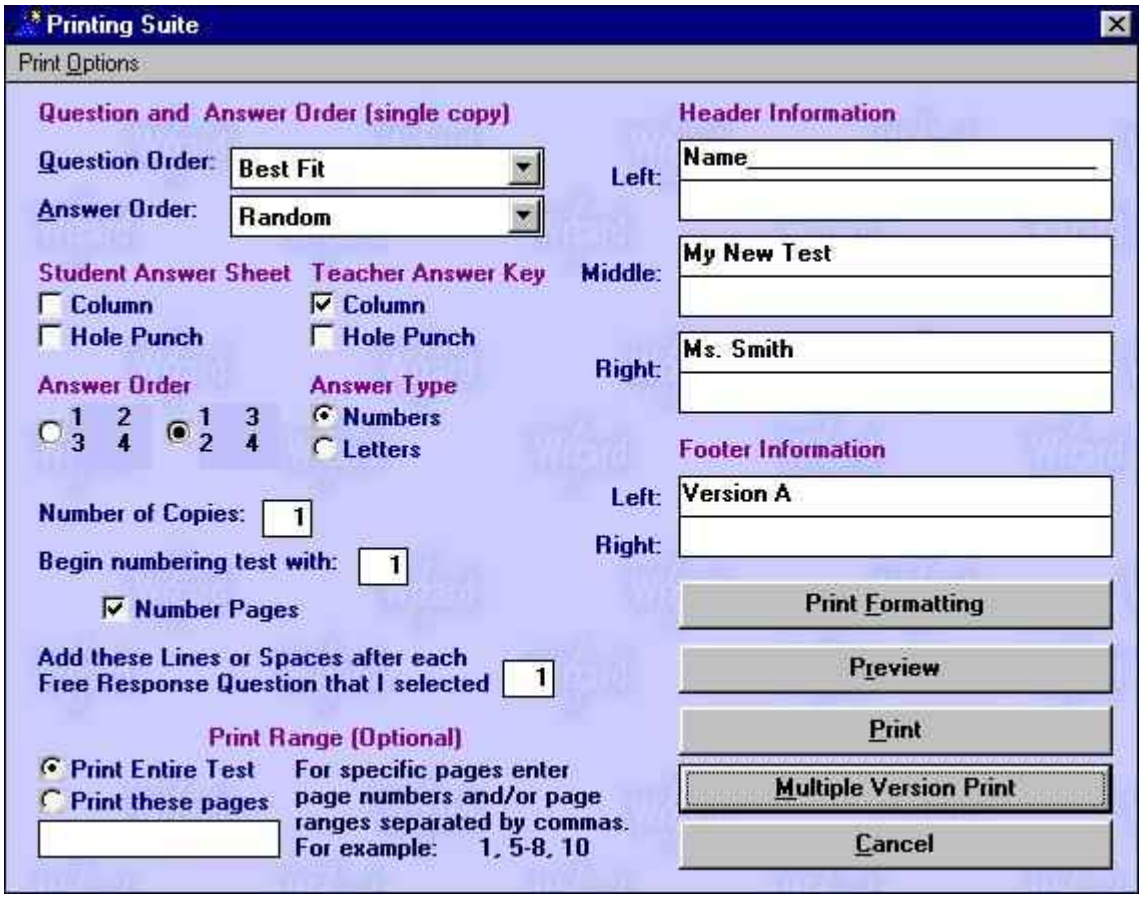

Figure 1: Printing features include randomizing questions and answers for multiple versions

Figure 2: The study for test creation

The questions come with some pictures such as measuring cylinders and graphs but I couldn't find an index of them so that when I started to write my own questions I could only use a picture if I first found a question with it on and then alter that question.

Recommendation

I think that too much design had gone into the looks and not enough into the ease of use. As a database of multiple choice questions it was excellent but as an interface to write your own questions you'd be better off with a more flexible program that can offer not only ease of use but also on line testing.

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