

Computers in Chemical Education Newsletter Spring 1998

*Our thanks and best
wishes to retiring chair-
man Don Rosenthal for
his many contributions.
(but keep the articles
coming Don!!)*

Editor Brian Pankuch, Department of Chemistry, Union County College, Cranford, NJ 07016
pankuch@hawk.ucc.edu.

Submissions: General articles should be sent to editor Brian Pankuch at the above address. We would appreciate both 1) printed copy (hardcopy) and 2) a readable file on a Macintosh or IBM compatible 3 1/2" diskette. We have fewer problems with 3 1/2" diskettes. Email submissions are frequently lost, and formatting and special characters are changed. If attachments are used please send a description of what you're using such as Microsoft Word 6 with Netscape 4, separately. This gives me a chance to decode it.

Submission deadlines: Fall issue - Sept. 25; Spring issue - March 15.

ALL NEW AND RENEWAL SUBSCRIPTIONS: PLEASE SEND REMITTANCE TO:

Donald Rosenthal, CCE NEWSLETTER, Department of Chemistry, Clarkson University, Potsdam, NY 13699-5810.

ROSEN@CLVM.CLARKSON.EDU.

RATES: USA 1 year \$2.50, two years \$4.50; Other countries 1 yr \$5, two yr \$9. Please make a check or money order payable in US funds to Computers in Chemical Education Newsletter. Two issues are published per year.

Consulting Editor Donald Rosenthal, CCE NEWSLETTER Department of Chemistry, Clarkson University, Potsdam, NY 13699-5810. Send meeting notices, etc., to Don., ROSEN@CLVM.CLARKSON.EDU.

Managing Editor Henry R. Derr, Laramie County Community College, Cheyenne, WY 82007
HDERR@ eagles . lcc . whecn .EDU .

Contributing Editors:

Wilmon B. Chipman, Dept of Chemical Sciences, Bridgewater State College, Bridgewater, MA 02325,
chipman@topoat bsc.mass.edu

Thomas C. O'Haver - University of Maryland, College Park, MD 20742
Thomas O'Haver@UMAIL.UMD.EDU

CONTENTS

1. **CHAIRMAN'S COMMENTS**
Harry E. Pence
SUNY Oneonta
Oneonta, NY 13820
pencehe@oneonta.edu
1. **FROM THE EX-CHAIR**
Donald Rosenthal
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu
3. **FINISHING UP AT PRINCETON**
Brian Pankuch, Editor
Union County College
Cranford, NJ 07016
pankuch@hawk.ucc.edu
4. **MULTIMEDIA IN LECTURES AND
ON THE WORLD WIDE WEB, PART I**
Brian Pankuch, Editor
pankuch@hawk.ucc.edu
7. **AN INTRODUCTION TO CASCADING
STYLE SHEETS AND DYNAMIC HTML**
Susanne M. Dana
Roanoke Valley Governor's
School for Science and
Technology
Roanoke, VA 24015
sdana@rvgs.k12.va.us
Brian M. Tissue
Virginia Polytechnic Institute
and State University
Blacksburg, VA 24061-0212
tissue@vt.edu
9. **COLLABORATIVE INTERCOLLEGIATE
PHYSICAL CHEMISTRY PROJECTS**
David Whisnant
Wofford College
Spartanburg, SC 29303
whisnantdm@wofford.edu
Lisa Lever
University of South Carolina
at Spartanburg
Spartanburg, SC 29303
llever@gw.uscs.edu
Jerry Howe
Converse College
Spartanburg, SC 29303
jerry.howe@converse.edu
12. **SPARTAN IN ORGANIC CHEMISTRY**
Wilmon B. Chipman
Bridgewater State College
Bridgewater, MA 02325
wchipman@bridgew.edu
13. **CCCE NATIONAL WORKSHOPS**
Donald Rosenthal
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu
15. **PHARMACEUTICALS, THEIR DISCOVERY,
REGULATION AND MANUFACTURE OLCC-3**
James M. Beard
Catawba College
Salisbury, NC 28144
jbeard@catawba.edu
16. **SWITCHING STUDENTS ON TO SCIENCE**
An On-Line Conference in September
and October 1998
Hugh Cartwright
Oxford University
England
Hugh.Cartwright@chemistry.ox.ac.uk
17. **OTHER ON-LINE CONFERENCES**
Donald Rosenthal
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu
18. **COME JOIN US AT THE 1998 BCCE**
Donald Rosenthal
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu
18. **TO ERR IS HUMAN**
Donald Rosenthal
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu
19. **SOME USEFUL WWW SITES**
Donald Rosenthal
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu

Chairman's Comments

Harry E. Pence

SUNY Oneonta

Oneonta, NY 13820

pencehe@oneonta.edu

Paying homage to a retiring committee chair naturally produces mixed emotions, especially when the retiree has had such a productive period of service as Don Rosenthal. During Don's Chairmanship, there has been an incredible amount of progress in the application of computers to chemical education, and Don has ensured that the Committee has played a significant role in this development.

When Don became chair in 1992, the personal computer was just beginning to make an impact on chemical education. A few visionaries could see the promise of this new tool, but I'm not sure that anyone really appreciated the changes that were coming. Even the most far-sighted prophets couldn't anticipate applications that we now take for granted, such as the World Wide Web, desktop molecular modeling, symbolic mathematics programs, and many others.

The goal of the Committee is to encourage and support the use of computing technologies for chemical education. This sounds like a big order, since the Committee has relatively few resources, aside from some very dedicated members, and the community of chemical educators would seem to be too large and diverse for any small group to affect them. In fact, the various programs that the Committee has undertaken in the past few years have helped make many faculty aware of the potential of the new technologies and also have given many faculty members the skills that they needed to make significant changes in the ways that they teach.

Under Don's leadership, the Committee has sponsored symposia at many of the regional and national meetings of the American Chemical Society as well as the Biennial Conferences on Chemical Education. It has also developed and sponsored workshops to help college and high school teachers learn new techniques for teaching with computers. I don't have any solid data that show how effective this work has been, but I have heard a lot of anecdotal evidence to suggest that many of those who are currently active in the field got their start from these symposia and workshops.

Probably the most important contribution that the Committee made was not just talking about the new technologies, but actually using them in new ways to allow chemical educators to interact. Tom O'Haver, who is

retiring from the CCCE this year, proposed the development of the first on-line conference in chemical education, which was held in 1993. Based on the success of the first conference, there have been a succession of such on-line events. The most recent conference, held this spring, involves over 800 participants from 49 different countries. These are important, not only because they bring together an international roster of chemists to discuss common problems, but also because they give faculty a taste of the interconnected world in which our students will live and work.

More recently, the development of the On-Line Chemistry Courses has brought together chemistry students and faculty from all over North America, and enabled them to work with experts from industry to explore special topics in chemistry. The most recent course, which is being held this spring, involves approximately 130 students from 15 different colleges. The continued success of these on-line projects shows that the new technology can, indeed, turn the entire world into our classroom. The archives of the On-Line Courses and the On-Line Conferences represent a significant resource in chemical education, which is available to anyone with Web access.

Don has provided the inspiration, ideas, and hard work necessary to make sure that the Committee on Computers in Chemical Education has not simply encouraged faculty to use the new technologies, but has also demonstrated some of the new capabilities that these technologies make available. In doing so, he has served both the Committee and the community of chemical educators extremely well. We are all more aware of new educational possibilities because of his contributions. I am delighted to have this opportunity to express our appreciation to Don Rosenthal for his service as Chair of the Committee on Computers in Chemical Education. I am equally happy to report that Don will still be serving as a member of the Committee. We look forward to his continued contributions.

FROM THE EX-CHAIR

Donald Rosenthal

Department of Chemistry

Clarkson University

Potsdam NY 13699-5810

Phone: 315-268-2352

E-mail: ROSEN@CLVM.CLARKSON.EDU

NEW CHAIR

My term as Chair of the Committee on Computers in Chemical Education (CCCE) ended on January 1, 1998. The Committee recommended Harry Pence, SUNY Distinguished Teaching Professor, State University of New York at Oneonta for the Chairmanship of the CCCE. Harry was subsequently appointed to that position. Harry has been an active member of the Committee since 1987. For many years he wrote book reviews and served as book review editor for this publication. Harry has organized symposia at many of the ACS National Meetings as well as the BCCE meetings and presently serves as a member of the Division's Program Committee. He will serve as Co-Chair of the Division's program at the National Meeting in New Orleans in the Fall of 1999. I know that Harry will continue to promote and publicize the use of computers in chemical education. I wish him well.

RETIRING MEMBERS OF THE COMMITTEE The terms of William Halpern, Alfred Lata, Yuzhuo Li and Thomas C. O'Haver expired. I would like to thank them for their many contributions to the Committee. Tom O'Haver suggested the idea of CCE sponsored on-line conferences. He organized and chaired the first conference held during the summer of 1993. Tom has handled the Listserv and World Wide Web site for all of the subsequent conferences. Tom will retire from the University of Maryland in 1999. Alfred Lata is a former chair of the Committee. Al contributed to the work of the Committee by organizing symposia, a National Workshop, open and closed CCCE meetings at BCCE and writing articles for the Newsletter. Yuzhuo Li participated in a BCCE symposium and wrote a number of articles for this Newsletter. William Halpern manages the CHEMED-L discussion list.

CCCE MEMBERSHIP - 1998

Charles Abrams - Beloit College, Beloit WI

James Beard - Catawba College, Salisbury NC

James W. Beatty - Ripon College, Ripon, WI

Joseph Casanova - California State University, Los Angeles CA

Wilmon B. Chipman - Bridgewater State College, Bridgewater MA

Nancy S. Gettys - University of Wisconsin, Madison, WI

Carolyn Sweeney Judd - Houston Community

College, Houston TX

Paul Kelter * - University of Nebraska, Lincoln NE
George R. Long - Indiana University of Pennsylvania, Indiana PA

Steven K. Lower * - Simon Fraser University, Burnaby BC Canada

Marco Molinaro - University of California, Berkeley CA

Brian Pankuch - Union County College, Cranford NJ

Abby Parrill * - Michigan State University, East Lansing MI

Harry E. Pence - SUNY College, Oneonta NY

James H. Reeves * - University of North Carolina at Wilmington

Donald Rosenthal - Clarkson University, Potsdam NY

Gwen Sibert - Roanoke Valley Governor's School, Roanoke VA

Stanley Smith - University of Illinois, Urbana IL

Carl H. Snyder - University of Miami, Coral Gables FL

Brian Tissue - VPI and State University, Blacksburg VA

Scott Van Bramer * - Widener University, Chester PA

Gabriela C. Weaver * - University of Colorado at Denver

David M. Whisnant - Wofford College, Spartanburg SC

Theresa J. Zielinski - Niagara University, Niagara University NY

* identifies new committee members

ACTIVITIES

Many past, present and planned future activities are summarized in the Annual Report for 1997. This report is available at the URL:

<http://divched.chem.wisc.edu/divched/committees/ccce/report97.html>

Hot links are provided from the website to other pertinent information (#).

Some topics included in the annual report:
Symposia and Other Sessions at National Meetings
Computers in Chemical Education Newsletter
On-Line Computer Conferences # !

On-Line Courses # !
National Computer Workshops !
Committee Meeting at BCCE !
Div. of Chemical Education World Wide Web Site #
Publications #

Hot Links in 1997 Annual Report
! See article(s) elsewhere in this Newsletter

HOW YOU CAN HELP

The success of the Committee depends upon our interaction with you and other chemical educators. Please send us your ideas and suggestions. Your articles submitted to this Newsletter are published in a timely manner.

Finishing up at Princeton

Brian Pankuch, Editor
pankuch@hawk.ucc.edu

First sincere thanks to Don Rosenthal for all his help, advice and many contributions over the years, and a hearty welcome to Harry Pence the new Chair. Our thanks also to Tom O'Haver for the many pleasant and fruitful interactions we've had over the years.

We've finished up the course Chemistry of the Environment at Princeton. I outlined the details of how the course was using the World Wide Web to increase student discussions in lecture. We've had a symposium to show off the student web projects. You can view the projects at <http://pmi.princeton.edu/pathways/chm333/students/> and the course setup at <http://pmi.princeton.edu/pathways/chm333/welcome.html>.

Student evaluations showed that the students liked the text. They thought the Web projects were good, but a lot of work, and the daily Web questions were ok, but added too much busywork. We did have some very good discussions, generally on broad policy issues rather than the chemistry involved.

The students were asked to be innovative for the web projects, not to create the typical research project that could just be printed out. They were asked specifically to present their material in interesting ways, to use graphics and animations to make points clearer and more interesting.

It had originally been scheduled to have students hand in a detailed project outline, this was changed to putting the outline up as a webpage. This had the advantage of getting the students, most of whom had never created anything on the web before, a chance to assimilate the needed technology. I also put up a webpage to show some of the animations etc. they could use to make points clearer. You can see this at http://www.eclipse.net/~pankuch/use_animation.html

Having student projects upon the web proved to be valuable since we could track progress of the webpages at a click of the mouse. This provided a way of supplying reminders to those not showing significant progress. I should note that at Princeton as other Universities much of the work appeared the last week and a good deal the night before. Many students preferred to work off-line and put material up when it was pretty much finished.

At the symposium each project was presented by the entire group. Their webpage was up live on the large screen and each member of the group presented their part of the project. We had a few technical glitches, but it was informative and interesting. Each student was given a written form to evaluate other projects.

I was discussing their projects with some students after the symposium and a faculty member from the engineering department came up and complemented the students on the symposium and their webpages. He also offered to hire them during the summer to put up web pages for his research group. The students just glowed, and I felt pretty good myself!

As mentioned last time the text we used is excellent, Chemistry of the Environment by Tom Spiro and William Stigliani (Prentice Hall, NJ ISBN 0-02-415261-7). One can spend some pleasant worthwhile time with this book.

Multimedia in Lectures and on The World Wide Web. Part I

Brian Pankuch, Editor
pankuch@hawk.ucc.edu

Abstract:

How effective and efficient is the use of multimedia for learning in lecture and on the Internet? Most results are anecdotal and show positive outcomes, with students being enthusiastic about new methods of learning. It appears that most of this effect can be ascribed to using multimedia methods students are not familiar with (Hawthorne effect). No proof was found that multimedia learning is more efficient, i.e., that more is learned during the same time spent studying. Students did spend more time with the multimedia, so they learn more due to the increased time spent not because multimedia is inherently more efficient. This does not make the additional learning less meaningful.

It does suggest that a model for developing and using multimedia should include an awareness that the effect of 'new' multimedia may be short term. Development models should include the easiest ways possible of updating substantial parts of multimedia to include the newest and best material.

My intention is to explore the effectiveness and efficiency of multimedia in teaching chemistry, particularly its use on the World Wide Web (WWW). By multimedia I mean text accompanied by illustrations, graphs, simulations, animations, etc. Hypermedia, the ability to link a given page of material with other material is generally part of most multimedia packages. I'm principally addressing the effectiveness of this technology both in lecture and on the web not the advantages of new modes of 'distance learning'.

Most of us don't have the time (or perhaps the expertise) to develop teaching packages. We can, however, preview textbooks and their supporting materials. A number of publishers are beginning to include CD's filled with

material. Some include an outline of lecture notes with demonstrations and additional multimedia material. So as this is written in early 1998 we begin to have packages available so we don't have to be multimedia experts in design and general computer expert to use multimedia in lecture. We have a number of options for bringing multimedia material to our lectures. Such as using rooms set up for multimedia display, or carrying a laptop and portable projector into the lecture.

Full access to WWW plus ability to use material on a publisher's CD's in any order we wish and our own Powerpoint lecture notes would likely open a number of possibilities in learning most of us don't use now. Although there are many possibilities for how the equipment can be supplied, I'll just mention my personal preference based on 30 years of working with instruments and computers is to have my own laptop for my material. Sharing a computer for this type of work is possible but very difficult. I'd just as soon have a shared projector in my own department, again more control.

I'm basing this on recent experiences at Princeton University as well as my college where we had some problems keeping equipment working, and especially trying to get material live off the WWW.

I've tried to find well done research studies rather than anecdotal material to support or negate using multimedia and hypermedia for more effective learning. Generally I've come across of requests for massive research into how people learn. In other words we haven't proven that multimedia is more effective. Many users think it is and students appear to like it better, but do we know that it is more effective? Multimedia itself may be a means to more effective learning, by itself there is no assurance of increased learning.

Performance generally improves when the way material is presented is changed, and users feel something special is being done for them. This Hawthorne effect is known in psychology. For instance if a professors' lecture method is changed improved learning will probably occur. A 'reasonable' change causes an improvement in student learning. Students study harder when they perceive the professor is giving them attention that seems special. The increased learning falls off as the new methods become the norm. It's important to keep varying the course to keep it from getting stale. To keep experimenting to keep it a little bit new. So it is quite likely that many effects attributed to multimedia are going to be short term or ineffective as more students find it to be the norm. But are their multimedia aspects

which are more effective-learning the material long term?

Although much of what evolves below was done with K-12 in mind, most of the generalizations appear applicable at many colleges. Previous attempts to incorporate technology have been less than terrifically successful for a number of reasons:

From project 2061
Materials and Technology

...Previous technology reforms have almost always been hardware-driven and have largely ignored the content and structure of the curriculum they deliver. Therefore, the use of many technologies with potentially great educational value have followed a similar pattern: first, they are introduced with great fanfare and anticipation of the powerful impact they will have on student learning; then they are eagerly and hurriedly introduced into classrooms with little emphasis ever having been placed on examining their content or defining their role, and even less emphasis on training teachers to properly use them; and finally, their weaknesses are soon revealed to students, teachers and parents, and they are shelved permanently, their potential power forever wasted.

... Technology and media innovation in American schools has been characterized by cyclic fads and a failure to use the sound tools and processes of science to systematically and progressively improve the quality of instruction. As we enter the 21st century, technology has become a far too powerful and valuable learning tool to allow this pattern to repeat. (1)

Just transferring age old lecture notes to PowerPoint, Astound or some other presentation software will not likely increase learning. Nor does our average student necessarily need a great deal more information, they need to learn how to use information effectively. How to use it to solve problems.

... For decades, cutting edge technologies have been touted as groundbreaking boons to American education. But despite the optimism that frequently accompanies the introduction of new technologies into American classrooms, research on their use in schools has found a pervasive cycle of inappropriate use followed by disappointment and abandonment (Cuban, 1986). Perhaps the main reason for the repetition of this cycle is that when instructional "innovations" that use new technologies are introduced, the focus has centered on the lure of the new hardware and its ability to process or deliver information faster, in greater quantities, and from greater distances, rather than on the quality of instruction that the hardware carries or supports. These

are hardware-driven, rather than content- or instruction-driven, reforms.

Hardware-driven reforms are doomed for three major reasons. First, they assume that technology alone will improve student learning, ignoring how it might actually produce affective and cognitive results. Second, because the hardware is assumed to make the difference (as opposed to the teaching or the quality of its software), new hardware tends to be introduced into classrooms hurriedly on a wave of enthusiasm and public support, but with little time and few resources devoted to training teachers to integrate the hardware into their curriculum. Third, because technology is often hurriedly introduced, its role and purpose in instruction is usually left undefined. These severe problems cannot be solved without drastic changes in current practice by the producers and marketers of hardware, in the research on educational technology, and in the ways schools select and implement hardware.(1)

We are currently in a similar rush to keep up, to do the new because our competitors are doing it. With little regard to the effectiveness other than that it is new and other colleges may be more effective in attracting students (true). Of course sometimes just being new is enough to get a positive response from students even if they don't learn material any better.

... Although technology was important for providing access, these results were attributed in large part to the specific combination of pedagogy and curriculum organization in the program content.

... Teachers are, therefore, put in an extraordinarily difficult position. They are often charged with designing instructional materials to accompany technologies that they are not familiar with and whose educational purpose is often ill-defined. On the occasions when staff development does take place, methods for teaching with a new technology are often prescribed by individuals far removed from the classroom, and they have little relevance for the unique needs of each teacher's classroom. (1)

So if you don't have specific reasons to use new technologies tread carefully. If you don't have a need to show material not easily produced by cheaper means why are you changing? Keeping your job because the administration wants to try is a good reason, but may not be sufficient to increase student learning.

Many uses for the same technology may occur to each of us. We may very well be able to use instructional technology in innovative ways after tweaking it to our students needs.

... the machine alone makes no significant contributions to student performance.(1)

Well done research on the effectiveness of an entire package plus its implementation are difficult to come by. Even packages that are effective with some test groups may be less so with our students. Using a package and trying to separate out the material which works and changing what doesn't to be more effective is challenging, but rewarding.

... for decades researchers have studied whether one mechanical or electronic medium produced more student learning than another, with little reference to the educational context or pedagogical or curricular content of these media. Much of this research is confounded by uncontrolled variables, rendering it invalid and not replicable. A reasonable first step in future research would be to move away from comparing technologies or methods and begin to describe carefully the science teaching and learning situations in which technology has an impact on student performance and behavior. This research-based focus on observation, analysis, and synthesis of approaches that work would at the same time meet the need to tie technology to science content and provide science teachers with specific information about how to implement technology successfully.

... Effectively used technology would have three simple distinguishing characteristics. First and foremost, technologies should provide quality education to students. There are numerous examples of effective applications of technology that not only are better than traditional approaches, but also offer unique learning opportunities. Collaboration via the Internet, real-time data collection, computer modeling, and image analysis are all examples of science learning that is either impossible or cumbersome without technology. An important distinguishing characteristic of these applications is that they focus on the specific combination of teaching and curricular organization resident in the content of the program, and on the subsequent benefits to students, rather than on the hardware that carries the application. In these examples, technology can be integrated fully into the curriculum so that all students gain an understanding of its nature, power, and limitations. (1)

A good step would be to have well researched and designed packages from publishers of the text, a combination of CD and an accessible webpage for constantly updated material. Well designed, but editable by the professor teaching the course to take account of the needs of the particular group of students at a particular institution. Training in how and why to make effective changes for different student groups would be helpful.

... The first and most important way in which research on the use of technology must change to support science education reform is to make student outcomes the primary measure of a program's effectiveness. Observations of teacher behavior, costs, and physical and social infrastructure are important in assessing a technology's worth, but they are nonetheless secondary to that technology's ability to produce positive changes in cognitive and affective student performance.

Learning and teaching are going to be more deeply affected by the new availability of information than any other area of human life. There is a great need for a new approach in new methods, and new tools in teaching, man's oldest and most reactionary craft. There is a great need for a rapid increase in learning. There is above all, great need for methods that will make the teacher effective and multiply his or her efforts and competence. Teaching is, in fact, the only traditional craft in which we have not yet fashioned the tools that make an ordinary person capable of superior performance. (Heinrich, 1970, p. 56) 1 Along a similar line the "Report to the President on the Use of Technology to Strengthen K-12 Education in the United States" speaks to the need for definitive research to ascertain how people learn and how we can most effectively use technology to increase the ability to learn. Although the report doesn't deal directly with multimedia and hypermedia the call for meaningful research beyond anecdotal experience is clear.

Chaired by David E. Shaw, Ph.D.

Chairman, D. E. Shaw & Co., Inc. and Juno Online Services, L.P.

(David E. Shaw has a Ph.D. from Stanford in computer science and uses sophisticated computer modeling programs. He knows a lot about computers and what they can do.)

To some degree we need to know what we are trying to teach that goes beyond the important material of a discipline. Just facts and equations don't make the grade. Methods for learning new material has to be part of what we are teaching.

... It is widely believed that workers in the next century will require not just a larger set of facts or a larger repertoire of specific skills, but the capacity to readily acquire new knowledge, to solve new problems, and to employ creativity and critical thinking in the design of new approaches to existing problems.

... Initiate a major program of experimental research. The Panel believes that a large-scale program of rigorous, systematic research on education in general and educational technology in particular will ultimately prove

necessary to ensure both the efficacy and cost-effectiveness of technology use within our nation's schools.

... should encompass (a) basic research in various learning-related disciplines and on various educationally relevant technologies; (b) early-stage research aimed at developing new forms of educational software, content, and technology-enabled pedagogy; and (c) rigorous, well-controlled, peer-reviewed, large-scale empirical studies designed to determine which educational approaches are in fact most effective in practice. The Panel does not, however, recommend that the deployment of technology within America's schools be deferred pending the completion of such research.

...Section 8 focuses on the need for rigorous scientific research designed to evaluate the effectiveness and cost-effectiveness of alternative approaches to the use of technology in education, on the extent to which such research should be funded at the federal level, and on the manner in which it might best be organized and administered. (2)

So here are two national studies who conclude that technology might help, but call for substantial research to find out what will work efficiently. There are lots of anecdotal stories about successes, but not controlled well designed studies. We seem to be flying blind, as to what technology works long term to increase learning. So at this point we can't say definitively that technology will increase learning. We need to do more well designed research. We can't answer the question I started with.

We are, however, under a pressure to do something with this new technology. Areas such as multimedia and hypermedia and using the Web are popular with students and administrators. Funds are usually available. If nothing else the 'Hawthorne effect', using something new should increase learning and have the usual short term effect of increased learning. I'll go a little further and hope that combined with experience, an application of multimedia and hypermedia will have some longer term effect on learning. Perhaps tying the new methods to current learning theory would be beneficial. What do we mean by learning? The constructivist learning methods are close to what we do in some chemistry labs.

... (students) will thus need to be prepared not just with a larger set of facts or a larger repertoire of specific skills, but with the capacity to readily acquire new knowledge, to solve new problems, and to employ creativity and critical thinking in the design of new approaches to existing problems. In the words of Frank Withrow, the director of learning technologies at the Council of Chief State School Officers, "the US work

force does not need knowers,' it needs learners.'"

... constructivists believe that learning occurs through a process in which the student plays an active role in constructing the set of conceptual structures that constitute his or her own knowledge base. (2)

Bibliography

1. Project 2061 Blueprints On-Line
American Association for the Advancement of Science, Washington, DC 1997
URL = <http://project2061.aaas.org/products/bluepol/blpframe.html>
2. Report to the President on the Use of Technology to Strengthen K-12 Education in the United States
URL = www.whitehouse.gov/WH/EOP/OSTP/NSTC/PCAST/k-12ed.html

AN INTRODUCTION TO CASCADING STYLE SHEETS AND DYNAMIC HTML

Susanne M. Dana
Roanoke Valley Governor's School for Science and Technology
2104 Grandin Road, SW
Roanoke, Virginia 24015
sdana@rvgs.k12.va.us
and
Brian M. Tissue
Department of Chemistry
Virginia Polytechnic Institute and State University
Blacksburg, VA 24061-0212
tissue@vt.edu

INTRODUCTION

Cascading style sheets (CSS) and dynamic hypertext markup language (DHTML) provide new methods to control page layout and provide interactivity on Web pages. The benefits of CSS and DHTML include the ability to control the formatting and layout of the page content, and the ability to add animation, interactivity, and multimedia effects. These techniques, and some of the newer development tools, can simplify the development of interactive tutorials and

exercises for chemical education. DHTML pages do not require the loading of Java applets or ActiveX controls, the presence of browser plug-ins, or repetitive transfers from a Web server. Unfortunately, the current browsers that support DHTML, Netscape Navigator (ver. 4.0 and higher) and Microsoft Internet Explorer (ver. 3.0 and higher), implement many DHTML features differently. In the future, CSS and DHTML will be an integral part of HTML standards as part of the Document Object Model being developed by the World Wide Web Consortium (W3C) [Document Object Model (DOM): <http://www.w3.org/DOM/>].

Like other client-side programming methods such as JavaScript, DHTML is best suited for developing and delivering presentations, tutorials, or practice exercises [B. M. Tissue, "Overview of interactive programming methods for the World-Wide Web," *Trends Anal. Chem.* 16 (1997), 490-495; <http://www.elsevier.nl:80/inca/homepage/saa/trac/progmeth.htm>.] Applications that require an interface to a database for quiz generation, student tracking, or grading are still best programmed using server-based methods with the common-gateway interface (CGI) or server-side scripting. DHTML can animate graphics to replace animated GIF images, which lack user interactivity. Many multimedia development tools are more sophisticated and stable than DHTML to create presentations, but do require that users have the appropriate plug-in.

Our original intent in this article was to provide a simple tutorial of DHTML. Unfortunately, even defining DHTML is difficult since different authors and organizations use the term quite differently. DHTML might refer to any of a variety of Web-based programming methods or to a very specific set of HTML extensions or procedures supported by either Netscape Navigator or Internet Explorer. The best definition we have found for DHTML is from the W3C DOM Working Group [op. cit.: <http://www.w3.org/DOM/>]:

"Dynamic HTML" is a term used by some vendors to describe the combination of HTML, style sheets and scripts that allows documents to be animated.

To avoid adding to the confusion about DHTML, this article will concentrate on describing the underlying notion of cascading style sheets, and then qualitatively discuss some of the options for using and developing DHTML.

CASCADING STYLE SHEETS

Style sheets provide the means to control all attributes of a Web page [Web Style Sheets: <http://www.w3.org/Style/>]. They provide layout control to augment the document structure that HTML tags specify. Style sheets replace many HTML extensions such as , ,

and <I>, and layout work-arounds such as complicated tables or image spacers. For example, style sheets can specify the font type, color, line spacing, margins, and positioning of document components such as headings, <H1>, or paragraphs, <P>. Arbitrary styles can also be applied to any part of a document (see below). The following HTML code is an example of a cascading style sheet, which is placed in the header section of an HTML file or in a separate file.

```
<STYLE TYPE="text/css">
BODY {
  background: white;
  color: black;
  margin-left: 5%;
  margin-right: 5%;
}
H1 {
  margin-left: -5%;
  text-align: left;
  color: blue;
}
H2 {
  text-align: center;
  color: red;
}
#userdefined1 {
  font: italic bold 16pt Arial;
  color: green;
}
</STYLE>
```

In this example, the body text will be black on a white background. Any H1 headers will be flush to the left edge of the page, and everything else on the page will appear indented by 5% of the page width on both the left and right margins. The userdefined1 style can be applied to any text on the Web page by placing the and tags around the text to be highlighted. The ID attribute can also be used in <P> or <DIV> tags to format whole paragraphs or sections of a document. This simple example uses percentages for positioning. Style sheets allow absolute or relative positioning in percentage, pixels, points, and other units, for complete control of a Web page.

HTML files can be linked to external style sheets by placing a line of code such as the following in the header section:

```
<LINK REL=StyleSheet HREF="mystyle.css"
TYPE="text/css">
```

The mystyle.css is a text file that contains the <STYLE>...</STYLE> content, such as shown above, but not <HTML>, <HEAD>, or any other HTML tags. An external style sheet can control the formatting of mul-

multiple documents, allowing an author to create and maintain a consistent interface throughout a set of Web pages by editing only one file. More tools and information about cascading style sheets are available on the following Web sites:

CSS draft specifications: <http://www.w3.org/Style/css/>
HTML Help by The Web Design Group: <http://www.htmlhelp.com/>

DYNAMIC HTML

The cascading style sheets provide the tools to control style and layout on a Web page. Combining style sheets and scripting languages allows delivery of dynamic and interactive elements on a Web page. A useful feature for interactive tutorials is the ability for a text block or image to change based on the position of the pointer or on a mouse click in a certain area. Other examples include drop down menu boxes, text boxes, and animated text or image overlays.

Unfortunately, these dynamic features are where Netscape Navigator and Microsoft Explorer diverge in their implementation of DHTML. DHTML pages on the Web currently, are either browser-specific, or they incorporate browser testing and two sets of DHTML code. The more sophisticated DHTML development tools have the capability to produce browser-independent code. The following development tools support CSS and DHTML to varying extents.

HomeSite 3.0, Allaire Corp., <http://www.allaire.com/>
HoTMetaL PRO 4.0, SoftQuad Inc., <http://www.softquad.com/products/hotmetal/>
Interactor 1.1, mBED Software, <http://www.mbed.com/>
NetObjects Fusion 3.0, NetObjects Inc., <http://www.netobjects.com/>
Dreamweaver 1.0, Macromedia Inc., <http://www.macromedia.com/software/dreamweaver/>

More tools and information on DHTML are available on the following Web sites.

WebReference.com (sm) - The Webmaster's Reference Library: <http://www.webreference.com/>
ZDNet InternetUser / Garage / Dynamic HTML: <http://www.zdnet.com/products/garage/dhtml.html>

Collaborative Intercollegiate Physical Chemistry Projects

David Whisnant
Wofford College
Spartanburg, SC 29303
whisnantdm@wofford.edu

Lisa Lever
University of South
Carolina at Spartanburg
Spartanburg, SC 29303
llever@gw.uscs.edu

Jerry Howe
Converse College
Spartanburg, SC
jerry.howe@converse.edu

In Spartanburg, South Carolina, there are three relatively small colleges - Wofford College (1100 students), Converse College (1000 students), and the University of South Carolina - Spartanburg (3300 students). Our departments all are faced with the problem of small enrollments in our physical chemistry classes, which makes it difficult to justify the purchase of expensive equipment to update laboratories or to regularly use research-style collaborative projects. For the last four years, with support from two NSF ILI grants and Oxford Molecular Modeling (1) the three physical chemists from these colleges have cooperated by sharing equipment and collaborating on experiments in which all our students participate. The collaborative experiments have been particularly valuable because they have converted our sometimes small classes, in which there are only a limited number of students with whom to interact, into effectively larger classes.

Our first venture into collaborative experiments was during the 1996-97 academic year. Conversations with Theresa Zielinski of Niagara University had introduced one of us (Whisnant) to the potential of the Internet for promoting the interaction of students from different schools (2). For the two previous years we had struggled with problems involving a laser system designed to measure heat capacities by thermal lens calorimetry (3). Last year we decided to involve our students in a research-like project intended to narrow down the sources of error in the experiment. Groups from two of the colleges studied the effect of variable changes (e.g., cell positions, concentrations, or solvents) on the results of the experiment. They statistically analyzed their data and submitted the results to one of us who posted the results on the project Web page (4). When the students wrote their reports on the project, they were responsible not only for discussing

their own results, but also for drawing conclusions from the entire set. All three colleges continued this project this year, although experimental difficulties led to fewer results than we were able to obtain the year before. A recent communication from Ben DeGraff (5) has suggested changes in the experiment that may help us extend this project in the future.

This year, we have expanded our cooperation by adding two collaborative projects involving computational chemistry. In the first project, which was done during the first semester, the students played the role of R&D chemists working on hair dyes. They were told that the ready availability of benzene makes the project manager think that benzene derivatives might be a good place to start. Benzene compounds also are attractive because they are small and can penetrate hair fibers more readily than larger compounds such as azo dyes. The students were asked to do some preliminary work using semiempirical calculations to predict what types of benzene derivatives were more likely to give colored compounds.

The Hair Dye project lasted several weeks. The first student groups guessed a few derivatives to try, optimized geometries using Quantum CAChe MOPAC PM3 calculations (6), and predicted visible-UV spectra using ZINDO CI. After each group had completed their calculations, the structures and corresponding predicted spectra were added to the project Web page (7). We also encouraged an e-mail discussion of ideas about the experiment, with all messages being sent to one of the instructors, who forwarded the messages to a distribution list of all the students. Subsequent groups used the accumulated experience of the previous groups to make a more informed choice of derivatives. The compounds, such as 2,4-dinitroaniline, studied by some of the final groups were similar to compounds used as hair dyes (8).

The e-mail distribution list also gave the instructors the opportunity to ask questions of the group as a whole. For instance, toward the end of the first phase of the project when the students had homed in on likely compounds, we asked them how they could test the reliability of the spectra predictions. The students decided that they should record the spectra of some similar compounds and compare the experimental spectra with CAChe predictions (which do appear to be fairly reliable for these types of compounds). As part of this discussion, we were able to bring up solvent effects and the fact that the computational model was of gas-phase molecules. We also encouraged the students to make literature searches about compounds that are used in hair dyes and about potential health and environmental problems that might arise from use of these chemicals. Some of the students contributed information on these

topics from the World Wide Web and Chemical Abstracts Online.

At the end of the Hair Dye project we asked each of the students to decide on the compound they thought was most likely to be a good hair dye, and to use their knowledge of organic chemistry to devise a synthesis of the compound. We had reached the end of the semester by this time and were not able to have an online discussion of the proposed syntheses. This was unfortunate because many of the syntheses that students proposed in their final reports would have profited from such a discussion.

This semester we are in the middle of a third collaborative project, again involving computational chemistry. In 1989 scientists from the Kitt Peak National Observatory observed the absorption spectrum of the carbon star IRC+10216 and found a series of infrared absorption lines in the region of 2164 cm^{-1} (9). We have told the students that there is the possibility that these lines are due to a transition in a small carbon cluster molecule - probably C_3 , C_4 , or C_5 . We want to use computational chemistry to help identify the molecule that is being observed, and to infer some of its molecular properties from the spectra and computational results. We started the project by asking the students to list all the possible isomers of C_3 , C_4 , or C_5 . We then posted the combined lists to the project Web site (10) and assigned different isomers to groups of students from all the colleges for further work. During the next week the students optimized the geometries and predicted the heats of formation of their assigned isomers using CAChe PM3 semiempirical MO calculations. The PM3 calculations were not wholly successful, which did not come as a surprise to the instructors because the PM3 computational model is not always reliable for small carbon clusters (11). The calculated heats of formation did clearly favor linear isomers for all three carbon molecules, though.

We are in the third week of the project as this article is being written. As part of the e-mail discussion we have asked the students if the linear isomers make sense, given what they know about the bonding characteristics of carbon. We supplied the hint that they might check tables of covalent radii for carbon, which can be compared with the predicted bond lengths to help them draw Lewis structures for the molecules. The predicted bond lengths all turn out to be closest to double bonds, which does make sense. Double bonds give most of the carbon atoms four bonds and the 180° bond angles in the linear molecules correspond to those expected from VSEPR arguments. At the end of this week, we supply them the information that recent experiments (12) indicate the possible existence of a low energy cyclic C_4 isomer, and discuss what we can do to obtain more

reliable computational results. We also have asked them to recall the context of the project (identifying the source of IR lines in a carbon star), because conversations with some of the students had suggested that they were losing track of the project's purpose in the midst of all the calculations and e-mail discussion.

In the next phase of the experiment, the students will do ab initio calculations using Gaussian 94W (13). Different groups of students will optimize the geometries and calculate the vibrational frequencies for the linear isomers of C_3 , C_4 , and C_5 , and the cyclic isomer of C_4 at the HF/6-31G(d) and MP2/6-31G(d) levels (unrestricted for the triplet linear C_4 molecule). Again, the computational results will be communicated within the group by e-mail and posted to the project Web page. From our experience with these calculations, we expect the students to find that, at this theoretical level, the cyclic C_4 isomer is of slightly lower energy than the linear C_4 isomer. The most intense IR-active frequencies predicted for the C_3 and C_5 molecules are 2054 cm^{-1} and 2220 cm^{-1} respectively [MP2/6-31G(d) values scaled by 0.9434 (14)], which agree with literature values calculated using the same theoretical model (11). Both frequencies are within 5% of the 2164 cm^{-1} experimental value, with the C_5 value being slightly closer. The linear and cyclic C_4 frequencies are clearly different from the experimental value.

The final phase of the project will take place in two weeks, following the spring breaks at two of the colleges. The students first will be asked questions about the most stable C_4 isomer and the molecule most likely to be responsible for the 2164 cm^{-1} lines. As the discussion develops, we will give them the information that for linear C_n molecules the rotational lines in the vibrational-rotational spectrum should be separated by around $4B$, where B is the rotational constant, and ask how this can help us choose between C_3 and C_5 . Although the lines are not equally spaced, even a rough average gives an approximate rotational constant of 0.086 cm^{-1} , or 2.6 GHz , which is much closer to the value predicted by Gaussian for C_5 (2.6 GHz) than for C_3 (12.9 GHz), supplying additional evidence that the C_5 molecule is responsible for the series of experimental lines from the carbon star. During this phase we also will ask the students why some transitions are only IR active and some only Raman active, and whether we could observe linear C_3 or C_5 by pure rotational microwave spectroscopy.

Given the time we have left in the semester, this probably will conclude the on-line discussion phase of the project. In the student reports we can ask them to answer a few more questions. One set of questions will be about the reaction, cyclic $C_4 \rightarrow$ linear C_4 . From our project's calculations, why would we expect JH to be

small for the isomerization reaction? Thinking about the structures of the cyclic and linear isomers, what can we say about the sign of JH and the sign of JS , which form of C_4 might we expect to be more important at high temperatures? We also can ask the students to use point groups to classify all the isomers of C_3 , C_4 , and C_5 in the original list assembled by the group.

We are enthusiastic about collaborative projects such as these and plan to continue them in the future. They convert our small classes into a group large enough to use research-style projects that put some of our laboratory experiments into the context of a larger problem. The online nature of the projects also gives the students practical experience using the Internet as a routine tool in their work, both for communication and gathering information. The two computational projects have not been easy for the students, because the projects introduce methods of building computational models before we have reached this topic in lecture. A major advantage of having several students collaborate is the increased effectiveness of a group in solving problems, especially when the students are in new territory. Even if individual students may be mistaken on a particular point, the group discussion (sometimes with hints from the instructors) usually points the way to the correct answer.

Even though at times the students probably have felt deluged by e-mail (one student remarked that he had 10-12 new messages every time he opened his e-mail account), most of the students seem to be enjoying the experience. For one thing, other instructors have told us that they have heard students talking favorably about the projects in their classes, which has not been our usual experience. Of the nineteen students in our three classes this semester, fifteen are regular participants in the e-mail discussions and everyone has contributed at one time or the other. In fact, a certain amount of camaraderie appears to have developed among the students, few of whom know each other personally. Some of the students have asked us about having a "Carbon Clusters Convention" at the end of the semester so that they could meet the students from the other schools, which we are planning on.

We also are enjoying the collaboration as instructors, because it has effectively expanded our small departments to include three physical chemists. As was remarked one day when we were discussing a project, there is no way we could have done this alone. At various phases in our collaboration, each one of us has taken the lead on a particular project. This is good because these projects do take a lot of time. None of us were very experienced with the use of lasers when we began our cooperation, so developing the experi-

ments and finding "break-proof" ways of moving the equipment around was time-consuming. The multiweek collaborative projects also require a lot of time, both for planning and for managing the e-mail discussions and Web pages. We have been happy to have colleagues with whom to share the load.

References

1. Partial support for this work was provided by the National Science Foundation's Division of Undergraduate Education through grants DUE-9452453 and DUE-9751605 and a CAChe Scientific Higher Education program grant.
2. a) G. Long, R. Howald, C.A. Miderski, and T. J. Zielinski, "Physical chemistry online: a small-scale intercollegiate interactive learning experience," *The Chemical Educator* **1996**, *1* (3), <http://journals.springer-ny.com/chedr/zielinski.htm>.
b) G. R. Long and T. J. Zielinski, "Teaching Chemistry on-line: why it should be done," in a WWW article found at the URL, <http://www.elsevier.nl/freeinfo/trac/lc.htm>, August, 1996.
3. a) J. E. Salcido, J. S. Pilgrim, and M. A. Duncan, "Time-resolved thermal lens calorimetry with a helium-neon laser": in Moore, R.; Schwenz, R., Eds. *Physical Chemistry: Developing a Dynamic Curriculum*; American Chemical Society: Washington, D.C.; 1993, p.232.
b) J. M. Harris, N. J. Dovichi, "Thermal lens calorimetry," *Analytical Chemistry* **1980**, *52*, 695A.
4. <http://www.wofford.edu/~whisnantdm/thermal.htm>
5. B. A. DeGraff, "Suggestions Regarding Thermal Lens Calorimetry" and "Thermal Lens Calorimetry: The Heat Capacity of Fluids," Personal communications, October, 1997.
6. Quantum CAChe, Oxford Molecular Modeling Group, 2105 South Bascom Ave, Suite 200, Campbell, CA 95008
7. <http://www.wofford.edu/~whisnantdm/hair.htm>
8. K. Nassau, *The Physics and Chemistry of Color*, Wiley, 1983, p. 128.
9. P. F. Bernath, K. H. Hinkle, and John J. Keady,

Science, **1989**, *244*, 562.

10. <http://www.wofford.edu/~whisnantdm/cluster.htm>

11. J. M. L. Martin, J. P. Francois, and R. Gijbels, *J. Molec. Struct.*, **1993**, *294*, 21.

12. D. Zajfman, D. Kella, O. Heber, D. Majer, H. Feldman, Z. Vager, and R. Naaman, *Z. Phys. D*, **1993**, *26*, 343.

13. Gaussian, Inc., Carnegie Office Park, Building 6, Pittsburgh, PA, 15106

14. J. B. Foresman and J.E. Frisch, *Exploring Chemistry with Electronic Structure Methods*, 2nd Ed., Gaussian, Inc., Pittsburgh, PA, 1995-96, p.64.

Spartan in Organic Chemistry

Wilmon B. Chipman
Department of Chemical Sciences
Bridgewater State College
Bridgewater, Massachusetts 02325
wchipman@bridgew.edu

During the second semester of the last academic year, I used MacSpartan with students who had completed about two thirds of the usual first year organic course (chemistry and biology majors). I also used it in a first year graduate course in Organic Chemistry for chemistry master's degree students. Using the program at two different levels at the same time started me thinking about the best place(s) in the curriculum to teach molecular modeling and computational chemistry.

I was impressed with the way that Spartan helped students visualize molecules in three dimensions. A certain number of students seem to be able to get through the first semester of organic chemistry without making a good connection between three dimensional physical models and two dimensional formulas. Years ago, students were often exposed to mechanical drawing and solid geometry before they took organic chemistry. This suggested that, if you consider the percentage of chemistry majors in introductory and organic chemistry, it might be important to teach three dimensional visualization to students in freshman chemistry, particularly if the growing importance of this concept in biology and biochemistry is factored in. The molecular modeling capabilities of a program like Spartan are very useful in teaching students to visualize molecules in three dimensions. The ability to rotate the representation of a molecule under mouse or keyboard control helps students build a mental model of a molecule. It also helps students to move between models and three dimensional structures. These skills are useful to any student who will go on into biochemistry.

Chemistry majors need to learn to think like organic chemists. An important part of a chemist's mental picture of a molecule is an idea of the distribution of charge over the molecule. A **calculated** distribution of charge, clearly identified as such, can become an important part of a student's mental picture of a molecule. Both a mental picture of charge distribution and a calculated distribution of charge can be used to predict reactivity. The idea that computational chemistry is most valuable when it is used to predict an observable result is important. It gives students some idea of the validity, or lack thereof, of their computations. Spartan is a very fast computational package on current microcomputers; this suggests that the program can be very useful in the introductory organic course. The idea of making Spartan available to laboratory students who are waiting for one reason or another is an attractive one. Computations can be set up, submitted, and the results examined at separate times. Since computations run in the background, other students can use the program while computations are running.

I found the tutorials in the MacSpartan manual to be superb. After a brief demonstration of the capabilities of Spartan, organic students at either level quickly learned how to use Spartan as a computational package, with very little effort on my part. They were able to make the jump to applying the package to molecules that they were interested in with little or no hesitation. The ability to compute geometry, electron distribution, and even transition state geometry, allows students to ask all kinds of questions relevant to the understanding of organic chemistry. In fact, Spartan proved to be a very useful tool to get students to think like organic chemists.

Due to an institutional decision to phase out Macintosh computers, we are using PCSpartan this year. Wavefunction allowed us to upgrade our copies of MacSpartan to PCSpartan at a very reasonable fee (after return of the Macintosh hardware lock). We are running PCSpartan under Windows 95, on a TCP-IP network with a Windows NT server. So far, we have had no problems with the PC hardware lock.

CCCE National Workshops

Donald Rosenthal

<ROSEN@CLVM.CLARKSON.EDU>

Clarkson University

CCCE NATIONAL COMPUTER WORKSHOPS

Sponsored by the ACS Division of Chemical Education's Committee on Computers in Chemical Education (CCCE)

August 7 to August 9, 1998 (Just Prior to BCCE) at the University of Waterloo Waterloo, ON, Canada

The following workshops will be offered: (the title is followed by the name of workshop organizer)

A. INSTRUCTIONAL SOFTWARE FOR GENERAL AND ORGANIC CHEMISTRY What's Out There and How Are People Using It? Marco Molinaro (University of California, Berkeley)

B. USING THE WORLD WIDE WEB IN CHEMISTRY COURSES Brian Tissue (V.P.I. and State University)

C. DEVELOPING MULTIMEDIA MATERIALS FOR CHEMISTRY INSTRUCTION Charles Abrams (Beloit College)

D. PREDICTION OF PHYSICAL AND CHEMICAL

PROPERTIES BY COMPUTATIONAL CHEMISTRY

Paul M. Lahti (University of Massachusetts, Amherst)

Descriptions of the workshops are presented below.

Each participant will register for one workshop which will schedule morning, afternoon and evening sessions on Friday, August 7 and Saturday, August 8 and morning and afternoon sessions on Sunday, August 9. The workshops will include both lectures and hands-on sessions. The registration fee is \$ 120 Canadian (about \$ 85 U.S.) before June 1, 1998 and \$ 160 Canadian (about \$ 115 U.S.) after June 1, 1998. The number of participants in each workshop is limited. Registrants will be accepted in the order received.

Information about the CCCE National Computer Workshops is available:

* by sending the message: SUBSCRIBE WORKSHOP your-name to: listserv@clvm.clarkson.edu

* on the World Wide Web under "Pre-Conference Workshops" (<http://sciborg.uwaterloo.ca/bcce>)

* by contacting the CCCE National Computer Workshops Director:

Donald Rosenthal Department of Chemistry
Clarkson University
Potsdam, NY 13699-5810
rosen@clvm.clarkson.edu
Telephone: (315) 265-9242

WORKSHOP DESCRIPTIONS

A. INSTRUCTIONAL SOFTWARE FOR GENERAL AND ORGANIC CHEMISTRY - What's Out There and How Are People Using It?

Marco Molinaro, MultiCHEM - Director of Multimedia Development, Department of Chemistry, University of California, Berkeley CA 94720
molinaro@cchem.berkeley.edu - <http://mc2.cchem.berkeley.edu>

The amount of chemistry instructional software is increasing exponentially. The purpose of this workshop is to:

- 1) expose you to what is out there,
- 2) give you hands-on experience with the software, and
- 3) learn how others are using the software in the classroom, in the laboratory, and as take home work for the students.

We will take time to explore, critique, and discuss some material in depth from both the CD-ROM and the World Wide Web realms with the goal that everyone interested will leave with a clear plan for implementing appropriate technology in their classroom.

The software we will focus on will be both Macintosh and Windows compatible. Some Macintosh- or Windows-only software will be mentioned for completeness.

B. USING THE WORLD WIDE WEB IN CHEMISTRY COURSES

Brian Tissue, Department of Chemistry, V.P.I. and State University, Blacksburg VA 24061 - tissue@vt.edu

<http://www.chem.vt.edu/chem-ed/workshop/>

In this course participants will learn how to find, create, and use Web resources for their courses. We will begin by demonstrating and discussing what is available on the Internet. Participants will create basic HTML pages and FTP them to a server, and then progress to incorporating images, image maps, forms, JavaScripts, or other interactive elements into their pages. Discussions will focus on which Internet-based methods are best for different educational tasks. Participants should bring ideas and materials from which to develop Web pages. Either Macintosh or PC platforms may be used.

C. DEVELOPING MULTIMEDIA MATERIALS FOR CHEMISTRY INSTRUCTION

Charles Abrams, Department of Chemistry, Beloit College, Beloit WI 53511 - Abrams@Beloit.edu

Multimedia authoring is not as costly or difficult as it used to be. This workshop will introduce participants to several multimedia authoring tools and techniques, ultimately focussing on Macromedia Director. Instructors interested in creating their own multimedia presentations, or helping their students do so, are especially encouraged to attend. We will learn how to take advantage of unique capabilities of computerized instruction (interactivity, visualization, etc.) that cannot be duplicated by other instructional media. Incorporating multimedia elements into web pages (using Macromedia's Shockwave) will also be covered.

No prior programming or graphics experience is required. By the end of the workshop, participants will have developed a short multimedia tutorial on a topic from general or organic chemistry, with the help of graphics and templates provided.

Macintosh computers will be used. However, the skills learned and all the software used is available and readily transferable to the Windows platform.

D. PREDICTION OF PHYSICAL AND CHEMICAL PROPERTIES BY COMPUTATIONAL CHEMISTRY

Paul M. Lahti, University of Massachusetts,
Amherst MA 01003-4510 - lahti@chem.umass.edu

This workshop will be a hands-on session aimed at demonstrating and testing computational chemistry methods for the prediction of molecular properties. A survey of various force field, semiempirical molecular orbital, and ab initio molecular orbital methods will be made with consideration of their capabilities of predicting specific properties. Case studies will be carried out to evaluate properties such as: molecular geometry, conformational analysis, vibrational spectroscopy, UV-vis spectroscopy, dipole moments, and chemical reactivity. Time will be allotted for free-format labs when workshop attendees focus on problems of their own specific interest. Problems both of educational and research interest are encouraged. Extrapolation from molecular to macromolecular properties will be briefly considered, but generally will be outside the scope of this workshop.

Because of the applied nature of this workshop, some previous experience with computational modeling techniques will be expected. A brief overview of the methods used in the workshop will be given to orient workshop attendees sufficiently to proceed with the specific exercises given.

Pharmaceuticals, Their Discovery, Regulation and Manufacture OLCC-3

Jim Beard,
Catawba College
Salisbury, NC 28144
jbeard@catawba.edu

This is an invitation to register your school for the On-Line Chemistry Course for Upper Division Chemistry Students (Prerequisite - one year of organic chemistry) to be held during the Fall term of 1998. The on-line activities will be scheduled for September 14 to November 25, 1998. The title of the course will be "Pharmaceuticals, Their Discovery, Regulation and Manufacture." The course is sponsored by the American Chemical Society, Division of Chemical Education's Committee on Computers in Chemical Education (CCCE). In this course, the Internet will be used for discussions among students (student Listserv and WebBoard), faculty (faculty Listserv and WebBoard) and experts, all from around the world.

TOPICS MAY INCLUDE BUT ARE NOT NECESSARILY LIMITED TO:

1. Drug discovery including computer-aided design, combinatorial chemistry and other, earlier strategies
2. Development of clinically useable drugs including optimization of novel lead structures and assessment of pharmacodynamics, safety and efficacy of promising drug candidates
3. "Case studies" of the development and use of certain classes of widely used drugs including analgesics, antidepressants, anti-inflammatory drugs, antibiotics, AIDS and anti-cancer compounds
4. The FDA approval and FDA regulated testing process

PROCESS AND CONTENT RELATED GOALS OF THE PHARMACEUTICALS COURSE:

1. To provide an opportunity for students to investigate frequently used processes for discovery and manufacture of pharmaceuticals used as drugs for man and other animals
2. To provide the opportunity for students to gain an understanding of the general procedures for drug testing, its limitations, analysis, use and regulation
3. To provide an electronic forum which permits students to interact with professionals who are involved with the processes in 1 and 2
4. To provide an environment in which students will

interact locally and at a distance to do brain-storming, data-gathering, data analysis and problem-solving

tor, Dr. James Beard, e-mail: jbeard@catawba.edu to obtain the form.

5. To provide a forum for discovery of and discussion of industry's interaction with its regulatory, client and physical environment including such items as government inspections, user complaints and hazardous waste handling)

RESPONSIBILITIES OF PARTICIPANTS:

Students will participate in collaborative learning assignments where they can practice division of labor, teamwork, and individual responsibility. The Listservs and WebBoards will be used for the discussion of concepts and processes.

Instructors at local sites will guide "traditional" literature searches as well as on-line data-gathering. On-line, students will be guided by faculty and each other in their exploration of the content of this course. On-line questions from faculty will sometimes require critical thinking about industrial procedures in terms of a personal values framework.

It is the responsibility of each participating institution to register students and to provide college credit for the course. The role of the OLCC organizing committee and the CCCE is limited to assistance in organizing and administering electronic aspects of the course. The American Chemical Society will neither provide credit nor assess any fees. It is suggested that students receive three semester hours of credit for the course. It is the responsibility of each local faculty member to assign grades to their students. It is anticipated that a national evaluation will be administered.

For further information about previous on-line courses like this, see the Web Pages for OLCC-1 at <http://www.py.iup.edu/college/chemistry/chem-course/webpage.html> and additional information and evaluations of OLCC-1 at <http://www.clarkson.edu/~rosen2/olcc.html>.

Further information can also be obtained by contacting the course coordinator:

Dr. Lindy Harrison
Department of Chemistry
York College of Pennsylvania
York, PA 17405-7199
717-846-7788 X1210
aharriso@eagle.ycp.edu

Those interested in participating in this OLCC-3 course during the Fall of 1998 should complete a pre-registration form. Contact the OLCC-3 registration coordina-

SWITCHING STUDENTS ON TO SCIENCE **An On-Line Conference in September and October 1998**

In the fall of 1998 a CHEMCONF on-line conference will take place on the topic "Switching Students on to Science". The session has been organized and will be chaired by:

Dr. Hugh Cartwright
Physical and Theoretical Chemistry Laboratory
Oxford University, England
(Hugh.Cartwright@chemistry.oxford.ac.uk - <http://physchem.ox.ac.uk/~hmc>).

The focus of the conference will be: "How do we develop and maintain interest in science among students?"

It is a common observation that science is one of the most popular subjects with young school children.

Nearly every child finds simple science experiments fascinating. Yet, by the age of 15 or 16, many children have lost enthusiasm for science, or developed a positive dislike for the subject.

This session will deal with a number of issues related to "turning students on" to science, among them:

What are we doing wrong that turns teenagers off science?

What can we do to encourage students to pursue science careers and maintain their interest in the subject?

What can be learned from Science courses for non-scientists? There are many examples of such courses flourishing at Universities. What does the success of these courses tell us about how to maintain interest at the school level? How can a University-level course restore interest in science that may have been lost at school?

Is science inherently and unavoidably dull? If not, why don't our students appreciate its fascination?

Are alternative teaching schemes and syllabi, such as the Salter's scheme in the UK, more successful at retaining interest in science? Can we adjust the course content or teaching style to enhance interest without diminishing the academic worth of a course?

Is a science education essential for ALL students? If so, can we provide that with the current approaches? If not, how can the non-scientifically literate be meaningfully involved in scientific decision-making?

Would teaching science using the World Wide Web encourage more students to develop a scientific interest?

Papers will present research results, or be more personal reports of what does or (does not) work at school or university level. Papers are from those in school or college environments.

The final program is not presently available but the session will be broken into four sections. Each section will focus discussion on particular areas.

Section A "Catching them young - science at school"

Section B "Can we teach enthusiasm? Innovation in curriculum and learning"

Section C "Broadening the appeal - science for all"

Section D "Switching students on to science - let's do it"

Those who are interested in obtaining further information on the session should send the message: SUBSCRIBE CONFCHEM your-first-and-last-name To: LISTSERV@CLVM.CLARKSON.EDU This message must be sent from the e-mail address where you want conference messages to be sent and you must confirm your subscription by replying to the message sent by CONFCHEM. CONFCHEM is managed by Donald Rosenthal (ROSEN1@CLVM.CLARKSON.EDU).

Brian Tissue (tissue@vt.edu) is managing the CONFCHEM World Wide Web site: <http://www.chem.vt.edu/confchem/>

OTHER ON-LINE CONFERENCES

Donald Rosenthal
Clarkson University
E-mail: ROSEN@CLVM.CLARKSON.EDU

In addition to the fall 1998 conference session "Switching Students on to Science" described in the previous article, the following sessions are being planned:

"What Should Students Know When They Leave General Chemistry?" Fall 1999 - September and October Organizer:
Paul Kelter
Department of Chemistry
University of Nebraska

Lincoln NE 68588-0304
pkelter@unlinfo.unl.edu

"Teaching Spectroscopy" Fall 1999 - November and December

Organizer: Scott Van Brammer
Department of Chemistry
Widener University
Chester PA 19013
svanbram@science.widener.edu

your ideas and suggestions and the opportunity to talk about some of the Committee's plans for the future. The meeting is tentatively scheduled for Tuesday, August 11 beginning at 12:30 PM. Check the Conference schedule for the time and place of the meeting.

General Papers Summer 1999

Organizers:

Donald Rosenthal and Brian Tissue
Chemistry Department Chemistry Department
Clarkson University VPI & State University
Potsdam NY 13699 Blacksburg VA 24061
rosen@clvm.clarkson.edu tissue@vt.edu

TO ERR IS HUMAN

Donald Rosenthal
Clarkson University
E-mail: ROSEN@CLVM.CLARKSON.EDU

Other sessions are in the early planning stages. Anyone interested in organizing a future on-line session should contact Donald Rosenthal or Brian Tissue. The CONFCHEM Discussion List and WWW site are available for these sessions. (See the previous article for subscription information and the URL.)

The next time you read predictions about what will or will not happen in the future you might ponder some of these quotations taken from the Guffaws humor list edited by Peter Lytle (plytle@capital.edu).

Ever notice how some people just seem to have psychic abilities? (These folks don't!)

"Computers in the future may weigh no more than 1.5 tons." --Popular Mechanics, forecasting the relentless march of science, 1949

"I think there is a world market for maybe five computers." --Thomas Watson, chairman of IBM, 1943

"I have traveled the length and breadth of this country and talked with the best people, and I can assure you that data processing is a fad that won't last out the year." --The editor in charge of business books for Prentice Hall, 1957

"But what . . . is it good for?" --Engineer at the Advanced

COME JOIN US AT THE 1998 BCCE

Donald Rosenthal
Clarkson University
E-mail: ROSEN@CLVM.CLARKSON.EDU

The Committee on Computers in Chemical Education (CCCE) will hold an open meeting at the BCCE at the University of Waterloo. This meeting provides an opportunity for Committee members to meet you and for you to meet the members of the Committee. We welcome

Computing Systems Division of IBM, 1968, commenting on the microchip.

"There is no reason anyone would want a computer in their home." --Ken Olson, president, chairman and founder of Digital Equipment Corp., 1977

"So we went to Atari and said, 'Hey, we've got this amazing thing, even built with some of your parts, and what do you think about funding us? Or we'll give it to you. We just want to do it. Pay our salary, we'll come work for you.' And they said, 'No.' So then we went to Hewlett-Packard, and they said, 'Hey, we don't need you. You haven't got through college yet.'" --Apple Computer Inc. founder Steve Jobs on attempts to get Atari and HP interested in his and Steve Wozniak's personal computer.

"640K ought to be enough for anybody." --Bill Gates, 1981

"To go from Linux to NT is like going from the SST to the Wright brothers plane." --Joe Klemmer, 10 October, 1997

"Everything that can be invented has been invented." --Charles H. Duell, Commissioner, US Office of Patents, 1899.



SOME USEFUL WWW SITES

Donald Rosenthal
Clarkson University
E-mail: ROSEN@CLVM.CLARKSON.EDU

Here are some sites which contain hot links to a large number of sites.

B. J. Pinchbeck's Homework Helper

This site was described in the Fall 1997 issue of this Newsletter. Unfortunately, an incomplete URL was given. The correct URL is: <http://tristate.pgh.net/~pinch13/index.html>

ChemDex

<http://www.shef.ac.uk/chemistry/chemdex/welcome.html>

This is an index of Chemistry WWW sites compiled by Mark Winter, Department of Chemistry, University of Sheffield, England. Hot links are provided to all of the websites which are cited. The left portion of the screen contains the index. The major topics are listed below, usually followed by the number of hot links in parentheses.

Universities and Institutes all over the World
(e.g. 291 in Europe)

Government - Agencies (61) and Laboratories (52)

Companies - U.S.A. (237), Rest of the World (173)

Institutions - Societies and Organizations (145)

Chemistry - subdivided into categories such as Analytical (17), Biological (46), Computational (53), Education (86), Environmental (11), General (14), Inorganic (6), Organic (19), Physical (10), Theoretical (9) and others (19 categories in all)

Databases - Databases (47), Periodic Tables (102) and WebElements

Communication - Journals (77), Publishers, Discussion Groups (41), News Groups (32) and Conferences (35). For example under Conferences 9 links are provided to Electronic Conferences.

Software Packages - Archives, Multimedia and Software

WWW - Chemistry WWW Development

Other Links - Other Chemistry Lists (109 links),

Miscellaneous Links (25 Links), New Chemdex Links (31 links)

WEB-sters' Organic Chemistry

<http://ep.llnl.gov/msds/orgchem/>

Compiled by Professor Nick Turro (Columbia University) and Ron Rusay (Diablo Valley College)

Many hot links are provided in each of the following categories:

Organic Chemistry Instruction

Chemistry Web Sites with Links

Atomic and Molecular Orbitals

Molecular Modeling, Viewing and Drawing

Spectroscopy

Isomerism and Stereochemistry

Nomenclature

Synthesis and Reaction Mechanisms

Natural Products

Molecule of the Month

Chemical Toxicity and Safety

Data Bases

General Interest

Macromolecules

Biochemistry/Bio-Organic/Biotechnology

Laboratory Techniques

Graphics and Animations

- Discussion Lists
- Web-Texts
- Chemistry and Related Publications and Conferences
- Consortia and Projects in Chemical Education Software
- Chemical Industry: Commercial Sites
- Non-Organic and Uncategorized Topics
- Student Web Sites
- Student Interest
- Web Page Authoring Tools and Resources

**ChemCAI: Instructional Software and Other Resources
for Chemical Education**

<http://www.sfu.ca/chemcai/>

Compiled and maintained by Steve Lower,
Department of Chemistry, Simon Fraser University,
Canada.

Information is provided for teachers and course designers on what's available from both commercial and non-commercial sources. Many links are provided to other instructional resources. CAI demos, digital texts and other materials from Simon Fraser University are downloadable.

Some of the information which is available:

- Instructional Software Links
- Organizations and periodicals
- Development projects
- Visualization and graphics
- Textbooks and publishers
- Major web collections
- Selected home pages
- K to 12 resources

Homework, problem solving, quizzes and testing

Specific areas of chemistry

General Chemistry: starting points for students

COMPUTERS IN CHEMICAL EDUCATION

SUBSCRIPTION FORM

To subscribe fill out this form and return it with your remittance to:

Dr. Donald Rosenthal, CCCE Newsletter
Department of Chemistry
Clarkson University
Potsdam NY 13699-5810

Please check one: _____ 1 issue for \$ 1.25
USA: _____ 1 yr. for \$ 2.50 _____ 2 yrs. for \$ 4.50
Other Countries: _____ 1 yr. for \$ 5.00 _____ 2 yrs. for \$ 9.00

Payment MUST accompany this form. Please make your check or money
order payable in US funds to:
Computers in Chemical Education Newsletter

Your Name: _____

Address: _____

Telephone: Work _____ Home _____

BITNET, INTERNET, or other electronic mail address _____

Courses which you teach _____

Name of school or professional affiliation
(if not indicated in the above address) _____

Types of articles you would like to see in future issues:
Rate on the following scale: 1 - Very important, 2 - Important,
3 - Average importance 4 - Not important

1. General articles on how teachers are using computers _____
2. Reviews of 'useful' software _____
3. Reviews of hardware _____
4. Brief "Who Done It" _____
5. Queries and Answers _____
6. Book Reviews _____
7. Programming tips _____
8. Calendar of Events of interest to computer users _____
9. Networking and networks _____
10. Other - please describe _____

OVER PLEASE

11. Are you a member of the:

ACS?

_____ Yes _____ No

Division of Chemical Education?

_____ Yes _____ No

Division of Computers in Chemistry?

_____ Yes _____ No

12. Areas of Computer Activity and Interest:

Leave the space provided below blank, if you have no present interest or activity. Insert a number from 1 to 4 depending on the amount of activity.

1 means with a consuming passion, 2 means considerable

3 means moderate, and 4 means a little.

	Activity	Interest	Description of Use
Word Processing	_____	_____	_____
Spreadsheets	_____	_____	_____
Data Bases	_____	_____	_____
Other Languages	_____	_____	_____
Simulation	_____	_____	_____
Numerical and Statistical Methods	_____	_____	_____
Graphics	_____	_____	_____
Interfacing	_____	_____	_____
Laboratory Automation	_____	_____	_____
Drill and Practice	_____	_____	_____
Other (specify)	_____	_____	_____

13. Provide a brief description of the hardware you use.

14. Other Comments or Suggestions:

COMPUTERS IN CHEMICAL
EDUCATION NEWSLETTER
ISSN 8756-8829

Brian J. Pankuch, Editor
Department of Chemistry
Union County College
Cranford, New Jersey 07016

Donald Rosenthal, Consulting Editor
Department of Chemistry
Clarkson University
Potsdam, NY 13699-5810
