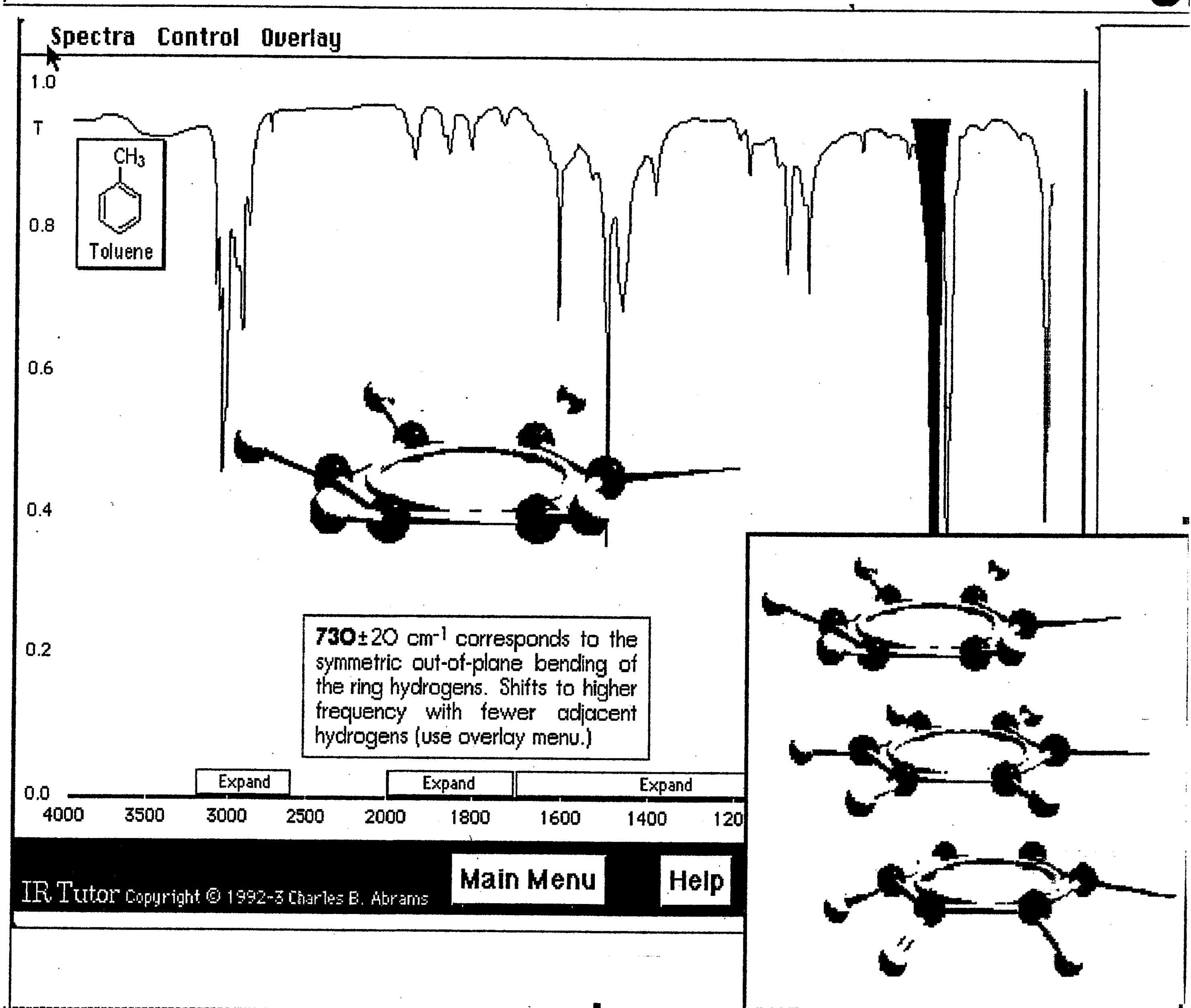
Computers in Chemical Education Newsletter

Spring 1994



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Don Rosenthal Chair

Contents

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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.

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

ALL NEW AND RENEWAL SUBSCRIPTIONS : PLEASE SEND REMITTANCE TO M. Lynn James, Dept. of Chemistry, University of Northern Colorado, Greely, CO 80639.

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Cover: Visualizing Infrared Spectroscopy with IR Tutor--see review by Bill Chipman in Fall 1993 edition

The newsletter is done using Aldus PageMaker.

FROM THE CHAIR

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In promoting and publicizing the use of computers in chemical education the ACS Division of Chemical Education's Committee on Computers in Chemical Education (CCCE) publishes this Newsletter, organizes symposia, workshops and on-line meetings. Let me describe some upcoming activities.

13TH BIENNIAL CONFERENCE ON CHEMICAL EDUCATION

July 31 - August 4, 1994 at Bucknell University A symposium entitled "Overview of Computer Use in Chemical Education: High School, General, Organic & Analytical Chemistry" will be held on Monday, August 1. Each of the four topics will be discussed by two speakers who will describe the courses which they teach. For each topic, an additional half hour will be devoted to informal questions, discussion and contributions from other participants. The preliminary Biennial announcement listed eight other computer and technology sessions and a number of computer workshops. On Tuesday, August 2 there will be an open meeting of the CCCE at which we will provide a little information, but mostly solicit comments and suggestions about present or possible activities. Topics which can be discussed include: A. Computers in Chemical Education Newsletter B. Future Symposia at National Meetings C. Online Conferencing D. National Computer Workshops E. Possible new Committee activities F. Other Matters: Those unable to attend this session may send suggestions or questions to me (Donald Rosenthal) or another member of the CCCE (see below)

208TH ACS NATIONAL MEETING, WASHINGTON DC

August 21 to 26, 1994 Symposium Sessions on Computers in Chemical Education

i. What Chemists Need to Know about Computers and Computing (Jointly sponsored by the Division of Computers in Chemistry and the Division of Chemical Education) Mary Swift (Howard University) and Raymond Dessy (VPI State University), Sessions organizers

ii. Use of Internet by Chemists Thomas O'Haver (University of Maryland), Session Organizer

iii. Integrating Computers into the Undergraduate Chemistry Curriculum Harry E. Pence (SUNY at Oneonta), Session Organizer

ON-LINE COMPUTER CONFERENCES

The CCCE sponsored the conference on "Applications of Technology in Teaching Chemistry" between June 14 and August 20, 1993. Fifteen papers were presented and discussed, and 450 registrants from 33 countries participated. Thomas O'Haver managed the conference using the LISTSERV facilities donated by the University of Maryland. Five topics which generated considerable discussion were extracted from the summer conference and served as the basis for extended post-conference discussion. The papers, graphics, discussion streams and related materials from the Conference and the post-conference discussions have been archived and are available on-line. Information on retrieving these documents can be obtained from the Usage Guidelines document which is obtained when the message SUBSCRIBE CHEMCONF <your name> is sent to LISTSERV@UMDD.BITNET or (LISTSERV@UMDD.UMD.EDU). As judged by participant responses (summarized in Fall 1993 C.C.E. Newsletter), this Conference was a success and on-line computer conferencing is a useful addition to the normal face-to-face conference. The Committee on Computers in Chemical Education has approached the Executive Committee of the Division of Chemical Education and the Program Committee of the Division of Chemical Education and encouraged them to schedule additional on-line programs.

Donald Jones (Western Maryland College and Past Chair of the Division of Chemical Education) organized an on-line open meeting of the Executive Committee of Division of Chemical Education which occurred in mid-April. This meeting informed participants of Division of Chemical Education activities and provided an opportunity for participants to ask questions and make suggestions. The documents and discussion can be retrieved by sending the message SUBSCRIBE EXECCOMM <your name> to LISTSERV@CLVM.CLARKSON.EDU or LISTSERV@CLVM.BITNET and following the instructions provided.

Arlene Russell from UCLA and a member of the Program Committee of the Division of Chemical Education will organize an on-line meeting during the summer of 1995.

The North American Chapter of the International Chemometrics Society is sponsoring its first on-line conference (InCINC'94) from September 26 to November 18, 1994. For further information contact Barry M. Wise (Chair, InCINC'94, Pacific Northwest Laboratory K2-12, P.O. Box 999, Richland, WA 99352; e-mail: bm_wise@PNL.GOV).

MEMBERS OF CCCE

Following is a list of current members of CCCE:

James W. Beatty - Ripon College, Ripon, WI Bruce N. Campbell, Jr. - SUNY College, Potsdam, NY Joseph Casanova - California State University, Los Angeles, CA Wilmon B. Chipman - Bridgewater State College, Bridgewater, MA Henry R. Derr - Laramie County Community College, Cheyenne, WY William Halpern - University of Western Florida, Pensacola, FL M. Lynn James - University of Northern Colorado, Greeley, CO Carolyn Sweeney Judd - Houston Community College System, Houston, TX Alfred Lata -

University of Kansas, Lawrence, KS Robert Megargle - Cleveland State University, Cleveland, OH Thomas C. O'Haver - University of Maryland, College Park, MD Brian Pankuch - Union County College, Cranford, NJ Harry E. Pence - SUNY College, Oneonta, NY Kenneth Ratzlaff - University of Kansas, Lawrence, KS Donald Rosenthal - Clarkson University, Potsdam, NY Barry Rowe - Champaign Centennial High School, Champaign, IL Gwen Sibert - Roanoke Valley Governor's School, Roanoke, VA Allan L. Smith - Drexel University, Philadelphia, PA Stanley Smith - University of Illinois, Urbana, IL Carl H. Snyder - University of Miami, Coral Gables, FL William J. Sondgerath - Harrison High School, West Lafayette, IN Theresa J. Zielinski - Niagara University, NY.

CONCLUSION: To be successful the CCCE must meet the needs of chemical educators. We rely on your contribution to and participation in our activities.

EDITOR

An interesting use of advanced graphics.

by Brian Pankuch,
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Princeton:

I arrived at the Art History class just at the start of the lecture. Kirk sat me down in front of the Silicon Graphics computer, toward the back of the room. The lighting was subdued, which made the 20" color screen quite bright. The main reason for the dark room was not for my screen but for the 20 foot projection screen at the front of the class. The projector itself was mounted out of the way from the ceiling.

He showed me some of the basics then hurried to the front to take his position with the powerful Silicon Graphics computer controlling the projection screen. Alice, a professor of Art History, explained we were to explore a database containing high quality reproductions of paintings, frescos, the buildings holding the art, artists who made it, people who commisioned it, or posed for it, etc.. She explained the overall tour and Kirk simultaneously showed demonstrations, on the projection screen, of methods we would use. Peter, the programmer of the database, moved around answering questions and making suggestions. My position toward the back of the room had the disadvantage of my not being able to read fine print on the projection screen, but had the advantage of being able to see what others were pursuing on their screens. Their were 7 students and 4 professors visiting from other universities and other departments at Princeton.

Some followed step by step with students generously helping visiting faculty find the correct material. Others flew into the system opening a wide variety of examples on their screens. We started by opening a few reproductions. The machines seemed quite slow to me, Peter confided to me that they were severely under strength for RAM- a mere 16 Meg. He feels they need at least 32 Meg each locally while being connected to a 12 processor server.

We proceeded to open architectural drawings of the building housing some frescoes. Alice confides this is the area that first caused her to request Kirk to help out with some computer simulation. Kirk uses his system to zoom into the building- very realistic on the large screen. It is a 40 ft high ceiling , a long building with frescoes on both long walls, stained glass windows at the end to provide some of the light.

Kirk changes the perspective and we turn to view the frescoes on the right wall. He pans up to the left corner sweeps the whole wall and Alice discovers some of the frescoes are in the wrong order-Kirk moves the frescoes, Alice discovers some more errors and Kirk expertly moves the frescoes again to the correct order. The frescoes are read starting at upper left to the right, then the next row below are read from left to right, then back at the left side we read the next row to the right. I didn't know that- but it makes sense, the building is long, it is easier to read this way. (Some ancient writings apparently were also written this way) . Alice had tried to do this with single photographs but felt it was not very clear.

Kirk adds that he can change the lighting for us - his system has the ability to make a light and realistically place and change resulting shadows, as we move. He shows us the affect as he speaks. The changes are quite effective, I want to try it on my machine. Peter laughs, it seems Kirk's machine has 128 Meg, compared to my poor 16 Meg. Kirk continues to add light sources and change our viewpoint. He reminds students not try the changes he is doing because they could affect the whole database. Maybe art students are different, but the computer science and engineering students I've worked with at Princeton would find this an irresistible challenge. I will have to check back and see if mysterious lights are appearing from unlikely places.

My system does allow me to continue doubling the size of the picture, and to scroll through at great magnification that allows me to see details that Alice is putting into context. Peter stays close to me because I keep exploring in all directions and crashing his neat interface. I find many relations I try to explore have no connection. Is this due to my lack of knowledge in the area or am I just pushing the system too far?

Alice and Kirk get into a discussion with some of us about how decisions were made to use the data in the relational database. It turns out that 700 or so pieces were put in, it could easily be 30-40,000. One reason at least why some connections were null.

The interactions with the system are interesting, the mouse we use has 3 buttons instead of the usual one. This allows some interesting abilities my Mac doesn't have, but it also leads to some problems if you get too many things going at the same time. Practice and learning more about the interface will help. Now its been 3 hours since the class started, this is the 3rd different system I've looked at today and I've got one more to go. Peter invites me back to play some more and discuss the interface. Sometimes I think programmers have a sadistic streak.

The students are left with the assignment to answer a number of questions by exporing the database on their own. Kirk shows where to leave messages if they come across possible errors such as the frescoes being out of order. It is interesting and challenging being only a few days ahead of the class.

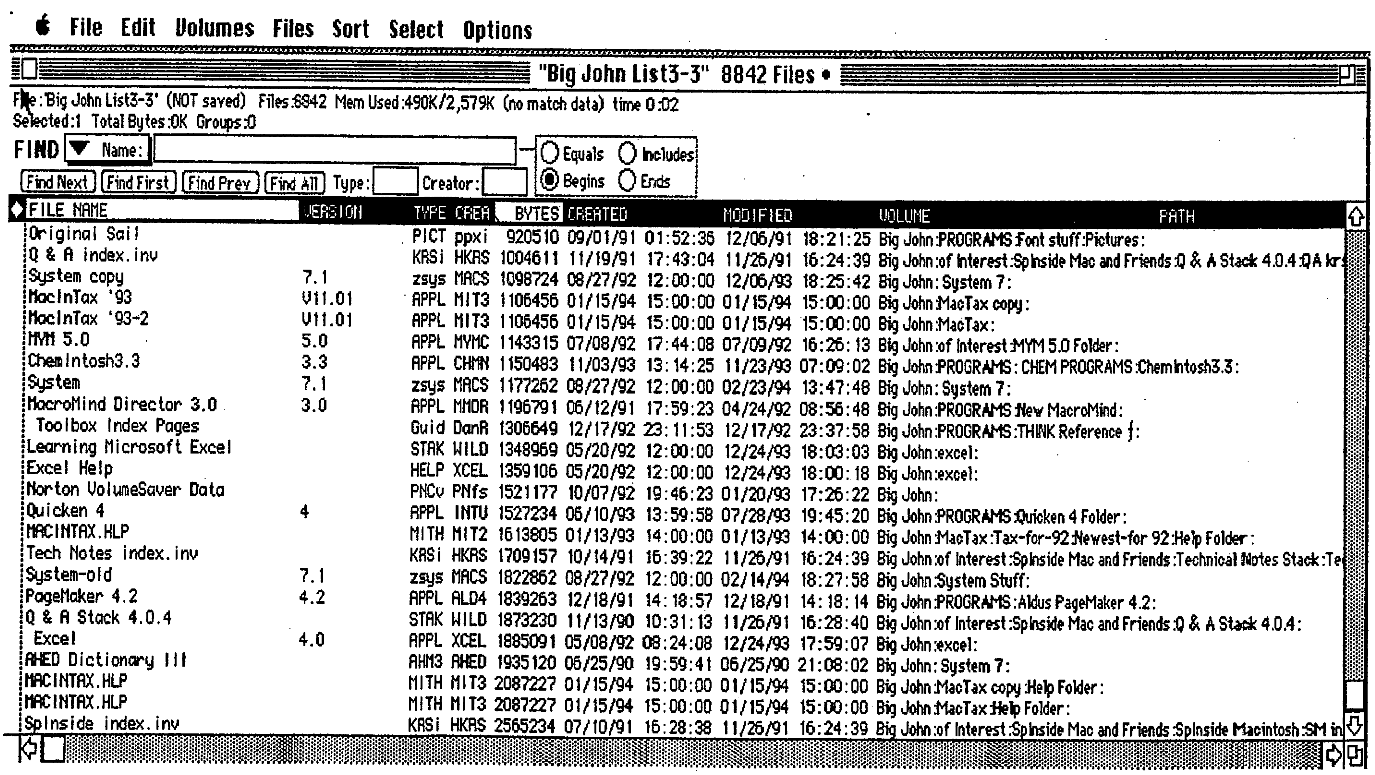
Why Art Histroy-because they are actually doing visualization with an undergraduate class. Imagine the building as a large molecule, we can enlarge our way to individual atoms, select an atom, a bond or a whole section of the molecule, and search an attached database for 'connections.' I have used databases about the periodic table - not particularly visual, but very interesting.

USEFUL UTILITY:

FileList+ 1.0b21 is a utility I came across more or less the same time I realized that I had over10,000 files on my hard disk. FileList puts all your files with a great deal of information into an easy to use database. You can then easily see duplicates, strange files you were going to look at but never got to because they are now buried at the 8th level of the file system. You can rapidly set up search criteria and find special files. I was able to get rid of over 1200 files , about 70 Meg, in less than an hour.
Sorting by name can pick up duplicates, by size the files that can free up the most space. You can sort by several criteria at the same time.

The authors ordering information follows: "If you want me to send you the latest version of FileList+, send me an 800K or 400K floppy with an stamped mailer and I will be glad to send it to you. Please let me know if you want the last release or want to wait for the next one (if one is coming). If you donate $5 or more, I'll spring for the floppy, mailer, and postage and send you the latest, providing you request it." Mail to: Bill Patterson 805 Division St. Greenville, TX 75401

Below are some screen shots of the utility in use.



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MYM 5.0	5.0	APPL	MYMC	1143315	07/08/92 17:44:08	07/09/92 16:26:13	Big John:of Interest:MYM 5.0 Folder:
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System	7.1	zsys	MACS	1177262	08/27/92 12:00:00	02/23/94 13:47:48	Big John: System 7:
MacroMind Director 3.0	3.0	APPL	MMDR	1196791	06/12/91 17:59:23	04/24/92 08:56:48	Big John:PROGRAMS:New MacroMind:
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Excel	4.0	APPL	XCEL	1885091	05/08/92 08:24:08	12/24/93 17:59:07	Big John:excel:
AHED Dictionary III		AHM3	AHED	1935120	06/25/90 19:59:41	06/25/90 21:08:02	Big John: System 7:
MACINTAX.HLP		MITH	MIT3	2087227	01/15/94 15:00:00	01/15/94 15:00:00	Big John:MacTax copy:Help Folder:
MACINTAX.HLP		MITH	MIT3	2087227	01/15/94 15:00:00	01/15/94 15:00:00	Big John:MacTax:Help Folder:
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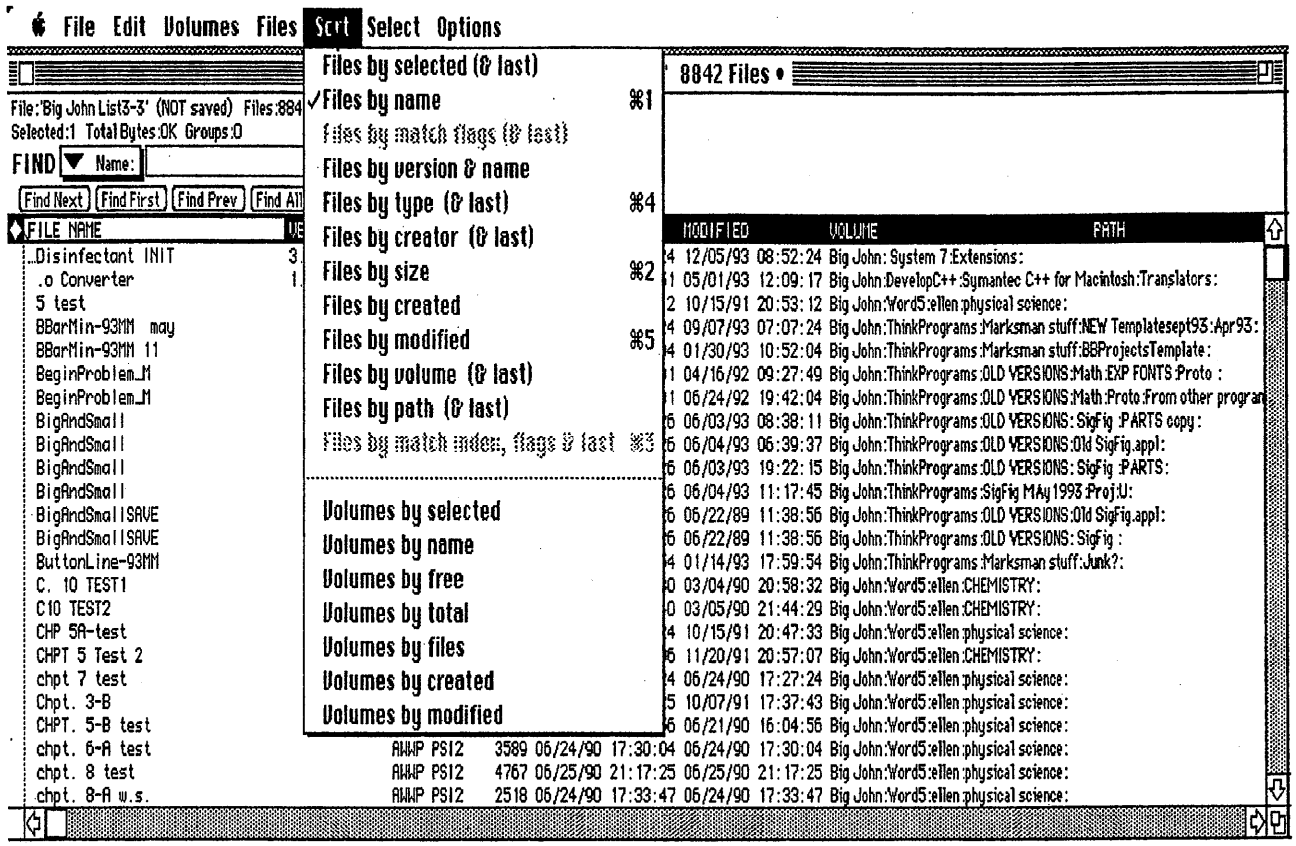
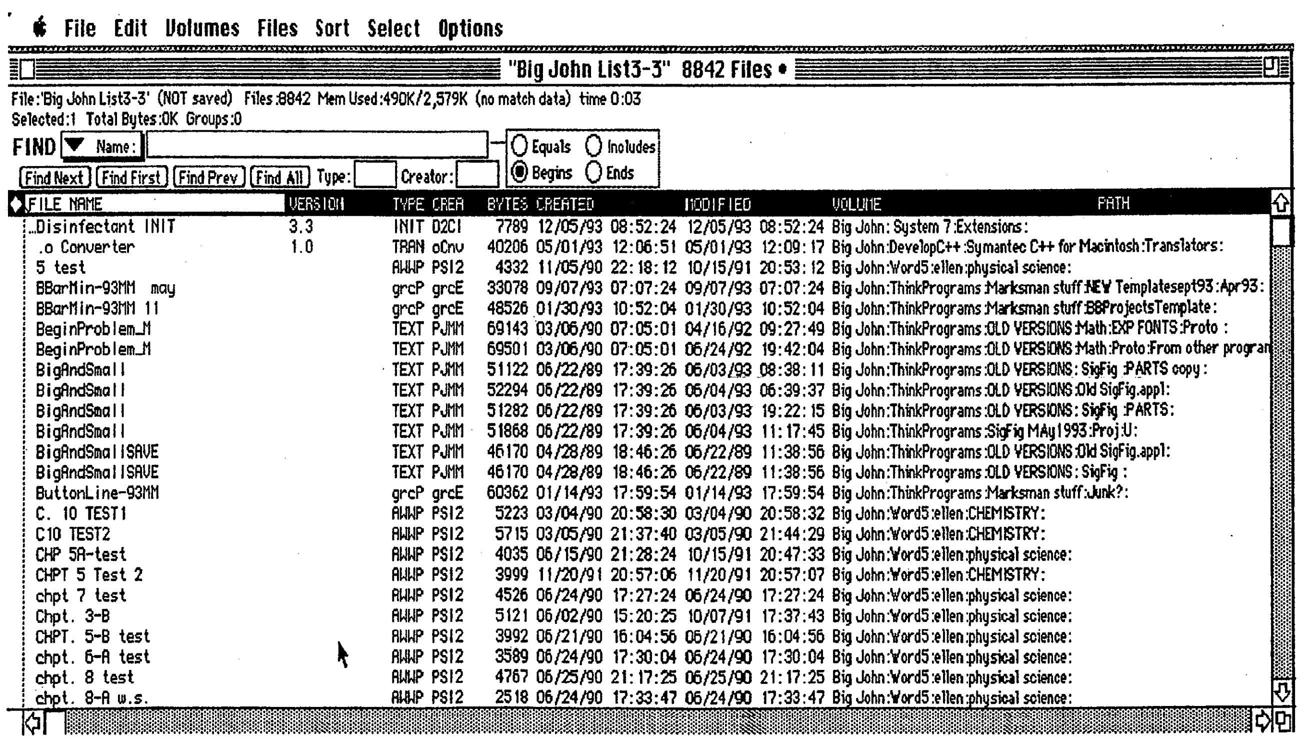
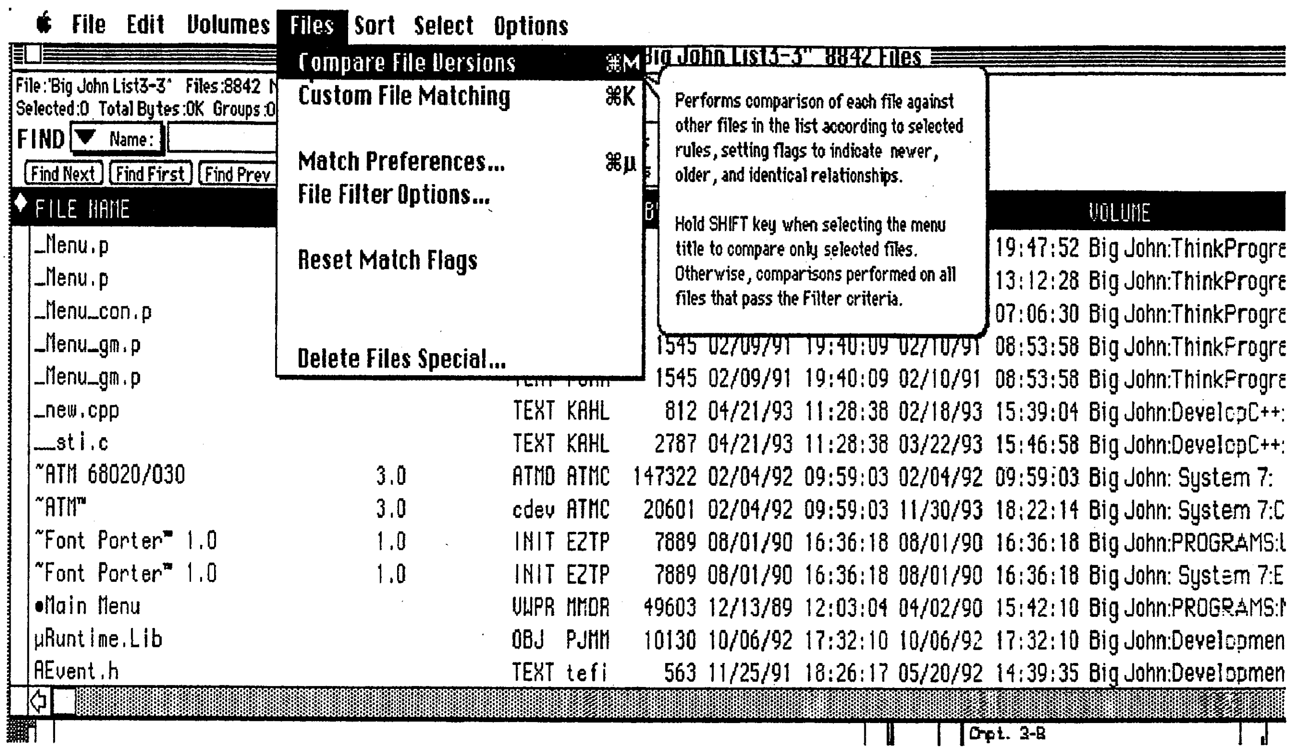


This shows some of the many ways in which you may sort your files. Below are the files resorted by name taking only





The utility includes balloon help shown above explaining one of the listings below the menu heading files.

NOTE: Henry R. Derr, Laramie County Community College, Cheyenne, WY 82007 HDERR@eagles.lcc.whecn..EDU, WOULD APPRECIATE EVERYONE WHO HAS EMAIL TO SEND YOUR EMAIL ADDRESS TO HIM. THANKS

MOLECULAR DYNAMICS SIMULATION ON A MICROCOMPUTER

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Molecular dynamics simulations are important tools for under standing the behavior of large biomolecules. I have adapted a molecular dynamics simulation of the denaturing of a protein alpha helix (1) for use in a senior biochemistry course for chemistry and biology majors. The exercise consists of five parts:

1. Construction of a polyalanine alpha helix by template forcing.
2. Energy minimization of the alpha helix.
3. molecular dynamics simulation of denaturation.
4. examination of hydrogen bond lengths before, during and after the simulation.
5. viewing a "movie" of the denaturation.

A polymer of 15 alanine units was constructed by duplicating and connecting a minimized alanine structure found in a library of structures. Then a 15 amino acid alpha helix was "clipped" from cytochrome C for use as a template. By assigning constraints between corresponding atoms in the two polymers, the polyalanine polymer was forced to assume the conformation of the template alpha helix.

Then the template was removed, and an energy minimization was done on the polyalanine alpha helix. This adjusted the structure to a local energy minima for the actual methyl side chains. The use of an idealized alpha helix, with identical non-polar side chains, focuses the exercise on what happens to the hydrogen bonds between amides as the helix starts to denature.

Then the molecular dynamics simulation was run, using the Verlet algorithm. Since the actual simulation takes more than eight hours on a 386 PC with a floating point processor, the simulation was pre-run, and beginning, intermediate, and final structures were stored in a file library. The alpha helix was first heated to 100° C, and then allowed to denature. Structures from the simulation were saved at 2.5 picosecond intervals for a period of 305 picoseconds. During the simulation, hydrogen bonds lengthened, and broke, and sometimes reformed. (A total of 122 structures).

Selected files (wire frame models) were viewed to determine what happened to the length of the hydrogen bonds that hold the helix together as the simulation progressed. The hydrogen bond lengths can be color-coded (1.8-1.9~ is red, 1.9-2.0~ is green, etc.) so that the changes in bond length are obvious.

Finally, a "movie" was constructed from all of the 122 structures that were saved from the simulation. (2) This "movie" may be stepped thru rapidly to provide an animated picture of the simulation. All of the individual structures may be examined. The animated version of the simulation destroys the student's picture of proteins as the rigid immobile structures that they see in text books.

REFERENCES 1. HHoweler, U., MOBY 1.5: Molecular Modelling on the PC. Springer- Verlag, New York, 1993.

2. The construction of a movie cannot be done with version 1.5 of MOBY. It requires version 1.6 which is currently in beta testing.

Stoichiometer

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Background

When you view yourself as a teacher, you focus your efforts on student learning. In chemistry teaching we expect students to acquire an array of skills. When confronted with a powerful tool like a desktop computer, the first thing a chemistry teacher would do is figure out ways to have that tool enhance student learning or improve the process of teaching. This is the history of computers in chemistry education over the last two decades.

When you view yourself as a chemist, you focus your efforts on chemistry. You seek computer tools that make old tasks simpler, better, easier, etc., and you seek to accomplish new tasks heretofore too difficult or tedious or otherwise prohibitive.

The teachers' goals focus on fixed targets, and the chemists' goals focus on moving those same targets. This became very clear to this writer — a teacher — in 1990. Similar situations apply to all of the professions. Professionals are accustomed to cognition based upon intracranial changes involving carbon atoms. We live in a world where much cognition is based upon intradevice changes involving silicon atoms, however.

Over a decade ago my physicist colleague Robert Fuller suggested to me that spreadsheets would change our approach to science. In 1987 I taught a workshop for high school teachers in which spreadsheets performed calculations typically covered in introductory chemistry. Teachers created the necessary spreadsheet cell formulas. I never really thought about having them give their students templates such that computations would be more automated. I came to the problem from the perspective of the traditional chemistry teacher.

Two kinds of very powerful software have changed my perspective. The symbolic mathematics programs that *do* calculus and algebra for me are quite remarkable. Really, the amount of time I spent learning that stuff — the tedium — contrasts markedly with a newly found ability to *play* with mathematics. Molecular structure programs subsume vast amounts of chemical knowledge and know how. Three cheers for the silicon atoms. How are teachers able to prepare students to understand chemistry, to use chemistry, and, for a few, to do chemistry in a world of silicon cognition?

Stoichiometry is at the heart of a modern, mainline course in general chemistry. We expect our students to be able to apply the mole concept in a wide variety of contexts, on paper and in the laboratory. Ever since 1988 I have fooled around with stoichiometry problems on HyperCard. Late in 1993, a new idea finally gelled for me — why not provide after-the-fact tutoring, retrospective tutoring, in a chemists' tool? Stoichiometer is a chemists' tool that does most of the stoichiometric tasks that we ask students to do. It includes essentially all of the tasks chemists actually do, the latter being more of a subset than a superset of the former. Stoichiometer removes much of the tedium of stoichiometry. It remembers — storing substances and reactions in clickable lists. It can import whole catalogs from vendors. It handles significant figures. But, unlike other tutorial materials, the user can enter *any* problem. Stoichiometer will try to solve that problem and provide feedback when it detects difficulties (like an unbalanceable equation, or diluting 0.6 M NaCl to get 6.0 M NaCl, or getting the gaseous volume of $CuSO_4(H_2O)_5$). Most important, in the absence of getting stuck trying to solve the problem, Stoichiometer will give context-specific feedback about how it solved its most recent problem.

A conventional path that a teacher might follow when using software would be to pose a problem that the student would attempt to solve using that software. Creators of molecular structure programs have started offering materials using this instructional strategy. Another approach that might be valuable is to include tutoring within the mainstream program. There are cases when this might be especially effective, and those cases that are entirely rule based would seem optimal for this approach. Stoichiometry is entirely rule based, and it is a relatively easy matter to generate after-the-fact tutoring.

Stoichiometer was developed in HyperCard. A spreadsheet would have been preferred were it possible to adjust the user's interface. Disadvantages center on slowness and on limitations when performing calculations — spreadsheets handle numbers better. The best feature of HyperCard is the clickable lists that save significant amounts of user time.

Stoichiometer will be available from Synaps (334 South Cotner Blvd., Lincoln, NE 68510-2107, 402-489-0667). Pricing will not exceed $50.

Special Strategies

Three special strategies are used within Stoichiometer. Substances are entered using formulas that require a special font for subscripts and superscripts. Two such fonts, ChemSyn and ChemBook, have been in the public domain for three years. ChemSyn is a standard Geneva font with subscripted and superscripted numbers entered by typing numbers with the option key or shift and option keys depressed. When formulas are parsed into separate characters, each subscript and superscript gets a unique ACSII character number and this facilitates algorithmic interpretation.

After a substance is entered (from the keyboard or by 'clicking' on characters), Stoichiometer calls for a substance name. An algorithm determines the molar mass, and creates a vector of the number and kind of atoms in the substance. The resulting information may be stored for each substance either according to the elements present or by any of one or several special lists created by the user. Once stored, the substance always can be accessed by clicking and need never be entered again. Chemical suppliers have the opportunity to provide lists such that all of the substances they sell can be imported for use within Stoichiometer.

The next strategy relates to balancing equations. A matrix of conservation equations based upon conservation of atoms and charge can be written. Gaussian elimination converts this matrix into a so-called row echelon form from which solutions are readily obtained. There are a couple of issues here. First, there is no such thing as *the* balanced equation. An infinite number of solutions is always possible. In order to make the matrix solvable, the first coefficient is forced to have the value of unity. Any fractional coefficients are then removed in such a way as to get the set of smallest possible whole numbers. The row echelon matrix has the feature of discarding redundant information. There are times when conservation of atoms/charge is not sufficient. For these cases, additional equations can be entered. The permanganate oxidation of peroxide is such a case — where oxygen ends up present in three oxidation states. Several authors have suggested matrix procedures (see Blakeley, G. R. "Chemical equation balancing: A general method which is quick, simple, and has unexpected applications" *J. Chem. Educ.* 1982, ***59***, 728.) but chemists don't use them to balance equations. Once we automate the process of entering data, creating, and solving the resulting matrices, it is a wonder that we ever used any other method!

The final strategy involves mass relationships. Whenever the coefficient of a substance in a balanced equation is multiplied by the molar mass, a "magic" number results. Dorf, who published this procedure, called this number the reaction equivalent mass (Dorf, H. "The 'reaction equivalent' in stoichiometric problems." *J. Chem. Educ.* 1962, ***39***, 298). Stoichiometer uses this method to solve all mass relationships related to chemical equations.

Aside from these strategic variations, all of the other approaches within Stoichiometer are those chemistry teachers have come to know and love.

Retrospective Tutoring

Whenever an operation is performed, all aspects of the operation are saved in one global variable. The context-specific feedback is delivered from HyperCard cards. When a card opens, it tests the name in the tutoring global. If the name matches that in the card's script, it unbundles the data in the global to create the tutoring information. If it does not match, it indicates that some operation will need to be accomplished before that card can function as a tutor.

Each tutoring card has three strips. One strip provides access to just the context-specific portions of the most recently performed calculation. Another strip provides this information integrated within conventional text that helps either to set a foundation for or explain the meaning of the context-specific material. A third strip provides access to any of the tutoring cards.

Traditional tutoring is found in the stack. That is, there is written discourse on the law of conservation of atoms and the law of conservation of mass. It's all there, perhaps a bit toward the chatty side. Somewhere in Stoichiometer you are likely to find the same words that you would find in a book. There is also some practice. For example, one card presents learners with substances to use for practice calculations of molar masses. Another affords practice in balancing chemical equations by inspection.

Stoichiometer comes with detailed manuals. These include conventional chemistry textbook stuff—what we do, and how and why we do it. Using the software is used to accomplish chemistry is illustrated. Also, there is a computer reference manual.

Screen Samples

Stoichiometer has several special features. When a formula list pops up, typing the first few letters of a formula causes the list to scroll to the first appearance of those letters in the list. Many frequently accessed "transportation" features pop up when the cursor moves into a calling button; the amount of clicking required is reduced. Several standard equations illustrating different aspects of equation balancing are built in; all reactants and products for these are made ready to use with a single click. A reactants palette adds selected reactants automatically (e.g., H^+, H_2O, e^-) or adds oxygen and predicts oxidation products (based on a list). The following figures are created from partial and slightly modified screens from within Stoichiometer.

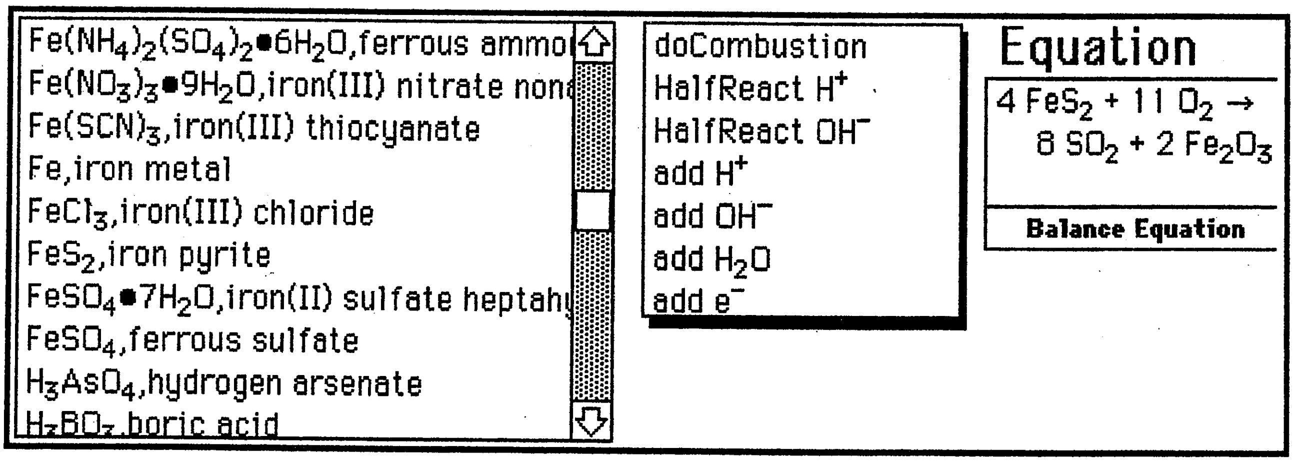

Figure 1. Balancing Equations. Substances may be selected by clicking in lists. Choosing FeS_2 and clicking in a reactants field identifies FeS_2 as a reactant. Most reactants and products must be selected individually. For some reactions, as here, selection from a palette (center) such as "doCombustion" simplifies the process. Clicking the "Balance Equation" button shown at the bottom right leads to the result shown at the right.

ConsrvEqns3, Conservation Equations for Current Problem
Solv4, Reduced Echelon Equation for Current Problem
Solv9, Checking Solution for Current Problem
Flags1, Possible Problems
Flags2, The Balanced Equation (original; then written conventionally)

☒ SigFigs

T

Conservation Equations for Current Problem

At	FeS_2	O_2	SO_2	Fe_2O_3
O	0	2	−2	−3
S	2	0	−1	0
Fe	1	0	0	−2

Row Echelon Matrix Form for Current Problem

FeS_2	O_2	SO_2	Fe_2O_3	
1	0	0	0	1
0	1	−1	−1.5	0
0	0	1	0	2
0	0	0	1	0.5

Figure 2. Context-Specific Tutoring for Balancing Equations. Clicking the "T" or tutoring button (center left) brings up a list of five choices for context specific tutoring (top of figure). Choosing the conservation equations brings up the middle list of equations. The row echelon form of the matrix produced in this case is shown at the bottom.

	Coeff	Rxn Formula	Mass (grams) Before Rxn	After Rxn
Reactants	4	FeS_2	50.0	0
	11	O_2	50.0	13.3
Products	8	SO_2	0	53.4
	2	Fe_2O_3	0	33.3

Calculate Grams Products ☒ SigFigs

Figure 3. Mass Relationships. Entering the number 50.0 next to each reactant with the "Sig Figs" button hilited and clicking the "Calculate Grams Products" button leads to this result for final masses.

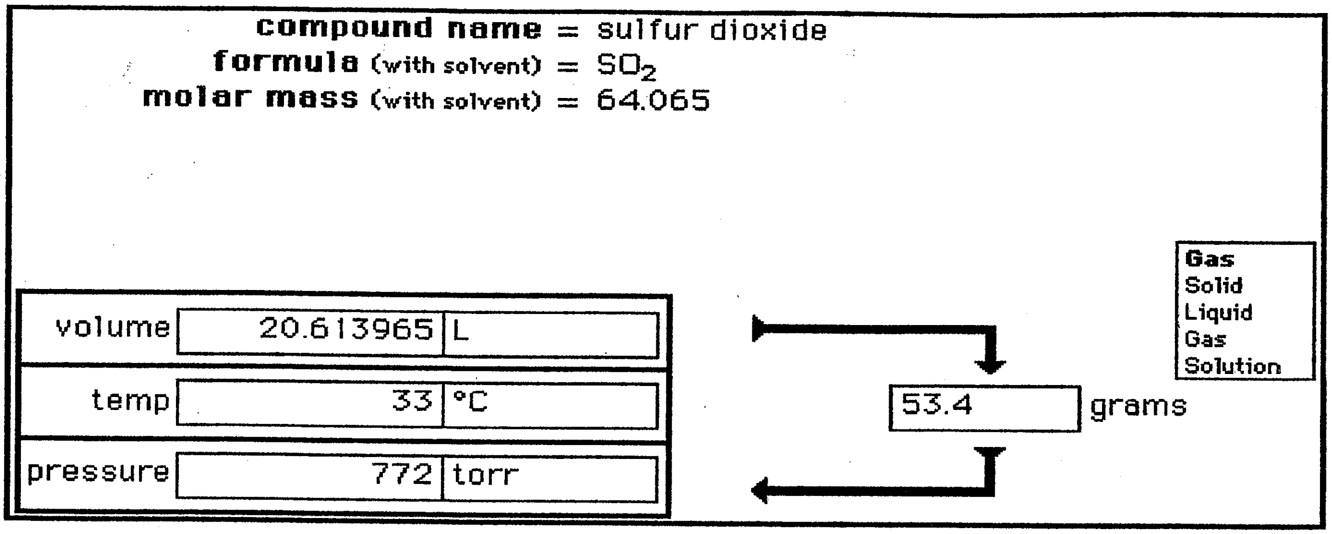

Figure 4. Converting Units. Clicking on the 53.4 grams next to sulfur dioxide (Figure 3, "After Rxn" side) brings up a card with pertinent information transferred. Clicking on "Gas" (upper right) brings up the boxes shown. Entering 33 for the temperature and 772 for the pressure and then clicking the bottom arrow with the "Sig Figs" button unhilited leads to the result shown (20.6..... L).

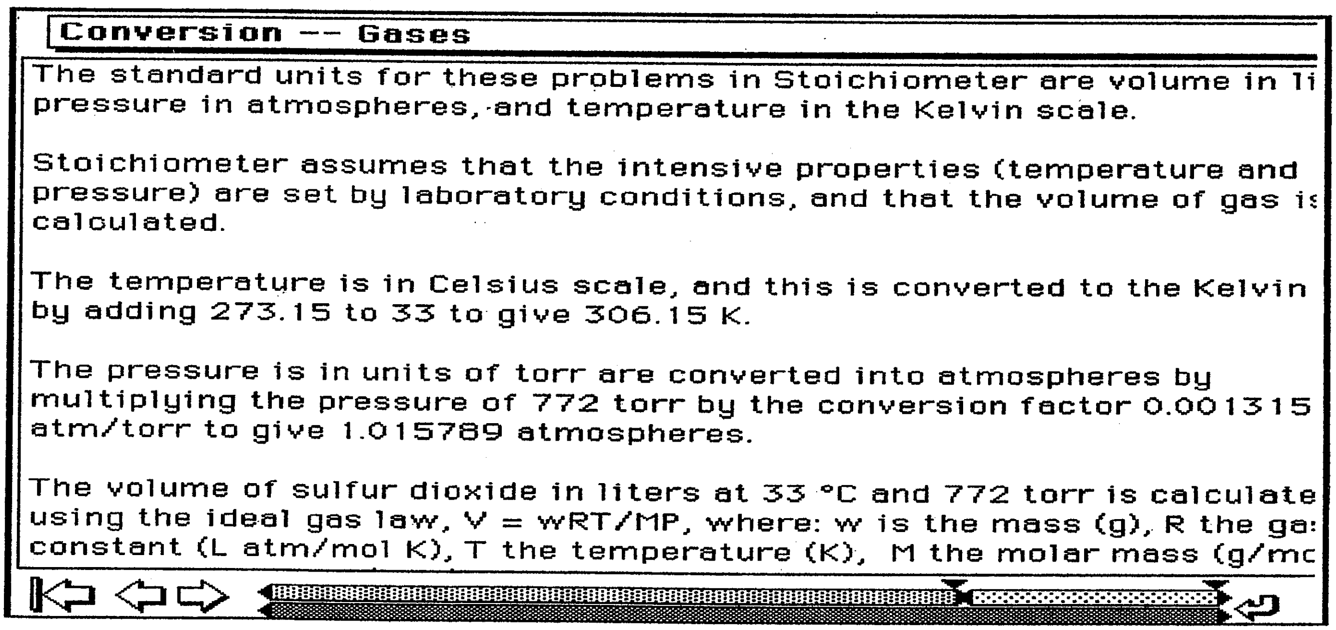

Figure 5. Context-Specific Tutoring for a Conversion. Clicking the "T" (tutoring button) at the bottom of the Conversion card brings up another card in the tutoring system with the information shown. The specifics of the problem are shown. The shaded strips at the bottom of the card permit access to any tutoring built into Stoichiometer. The lightly-shaded one accesses only context-specific tutoring (in this case, two cards). The strip to its left includes this card, but also includes a family of cards with background information especially germane to this topic (gas laws, conversions, dimensional analysis, etc.) The heavily-shaded strip permits access to any tutoring card. When the cursor is placed in any one of these strips, a window pops up and displays the name of the card that will be accessed if the mouse is clicked at that moment. The small inverted triangles indicate the relative position of the tutoring card in within the tutoring sequence.

PRESENT AND FUTURES USES OF COMPUTERS IN EDUCATION: SOME QUOTES AND BRIEF COMMENTS

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A long time ago I learned that I was not a good predictor of future developments in technology. While a graduate student in the 1950's, I remember discussing manned space flights and landing on the moon. I did not believe a lunar mission was possible much before the beginning of the next century. In less than ten years manned space flight had occurred and within fifteen years a lunar landing had been made. Several decades later in the era of mainframes, I remember predictions that within a decade or so there would be portable hand-held computers as powerful as the computers we were then using. Again I was skeptical.

Recently, in flying across the country I was surprised to see several passengers working with lap tops during the flight. Announcements are made on planes these days asking those with lap tops to turn off their computers just prior to take off and landing. It is amazing to see how far we have come in such a short time.

A number of future developments are certain to have profound effects upon computing in general and educational computing in particular. For example, advances in interactive multimedia (hypermedia), artificial intelligence and expert systems, virtual reality, networking, information transfer, hardware and software will impact on how and what we teach and how students learn. Rather than making my own predictions, let me quote from some recent literature which indicates where we are and what is in the future. I have added some personal comments bracketed by asterisks (*).

WHERE WE ARE AND SOME PROBLEMS

"The national student:computer ratio is now 16:1. Over half the schools in the country use computers in almost every discipline. . . . Cable, satellite, and modems are in half to three-quarters of all *school* districts."

(1)

"The United States leads the world in the number of computers in its schools. Ninety-nine percent of all elementary and secondary schools in the U.S. have installed computers and 93 percent of the students use them during the school year.... Despite all that equipment, American students are less computer-knowledgeable than students in Austria, Germany, and the Netherlands. In addition, their teachers get less computer training than their counterparts in Europe and Japan. Those are just two of the findings of "Computers in American Schools, 1992: An Overview", a report sponsored by the International Association for the Evaluation of Education Achievement, and the Council of Chief State School Officers."

(2)

"In a world often over-enamored of change for change's sake - and thus technology for technology's sake - advocates of technology in our schools should have a compelling answer to the question: "Technology for what?" . . . "Educational technology will continue to advance whether we like it or not. As educators, it is our job to make sure that technology is planned for and implemented in ways that are best . . ."

(3)

". . . the body of knowledge will have doubled four times between 1988 and 2000, and college freshmen in 2000 will be exposed to more information in one year of study than their grandparents were in a lifetime. How can the existing instructional infrastructure in higher education handle this sheer volume of information without widespread utilization of CBT *Computer-Based Training*? More importantly, how can higher education provide students with the experiential basis for lifelong independent learning without the adoption of sophisticated intelligent simulations? In the final analysis, it is not a question of whether higher education will adopt CBT, but how effectively and efficiently it will do so."

(4)

" School districts are . . . exploring new ways to integrate technology into new ways of thinking about schools and instruction. As education moves into the 1990s, educators, parents and society in general appear to have made a longterm commitment to technology's role in education. What has contributed to this advancement of technology into the classroom? . . . four general reasons are proposed. First, there is a growing body of research on the positive effects of technology assisted instruction on student performance and attitudes. . . . science teachers have found that students can learn as much or more and with less risk from technology based simulations as from more costly lab experiments. Students who have been taught to use word processing systems write more and produce higher quality work than when using more traditional paper and pencil practices.... A second reason ... is that technology has expanded beyond the early capabilities of the microcomputer and the videotape.. . . Linking videodiscs and microcomputers can access data heretofore unavailable to most students. CD ROMS now make available entire reference libraries . . . Students and teachers alike are able to learn in an information rich environment.

A third reason . . . is teachers' acceptance of the technology as tools to help them perform multiple tasks more efficiently. Technology tools, such as word processing and graphic programs, allow teachers to create higher quality instructional materials more quickly than in the past. Electronic gradebooks help teachers manage student scores and grades. Sophisticated simulations permit teachers to use models that were once too difficult to manage with a group of students. . . . offer greater capacity to rationalize the notion of individualized instruction by monitoring student progress, diagnosing student competence, and assigning specific instructional tasks. . . . The fourth reason . . . is that more teachers are being prepared to use advanced technologies for instruction. While the commitment to better prepare teachers has been significant, the number of teachers who need training remains high. . . The lack of preparation of teachers to use technology effectively and to integrate it into instruction is a serious problem . . . To better meet the demands of improved technology education colleges and universities must make some significant changes. . . . faculty development must become a central issue."

((5)

LONG DISTANCE LEARNING

"Although computer science and technology have undergone tremendous changes in recent years, teaching methods in our colleges have hardly changed at all. Our colleges still operate under the assumption that a large group of students will sit in a lecture hall, take notes while the instructor drones on, and then regurgitate the facts at exam time. . . . established patterns of work and study are breaking down. Many people need continuing access to education throughout their lives. Our educational system needs to be more creative in how it conducts its business, while at the same time the consumer requires greater flexibility in managing the conflicting demands of family, work, and study. Our educational system has the opportunity to develop more efficient and cost-effective means to do business while filling a rapidly growing public need. . . . I believe it is time to offer a full range of college courses entirely by internet-working. Physically attending class is inefficient at best and impossible for many working people. The interpersonal benefits of class attendance have been overstated and, in any case, have their equivalent in Cyberspace."

(6)

"The technology explosion coupled with the information explosion has provided us with unimaginable possibilities. . . . Institutions of higher education have been integrating electronic capabilities for two or more decades. Some of the basic systems include electronic mail, telephone registration, and information storage and retrieval. Extensions of such systems allow for computer conferencing, access to library holdings and services, instructional management, and communications between students and faculty. Making use of such systems, colleges and universities have tapped into national and international networks which allow them new avenues for marketing, distance learning, and information sharing."

(7)

COMPUTERS IN THE LABORATORY

"Technology drives major changes in science. . . . Technology has not driven major changes in education. In "Intelligent Teaching Machines", Larry Cuban . . has documented the lack of impact of such heralded and truly wonderous technologies as the camera, the radio and TV in the classroom. Microcomputer-based labs (MBL) is an emerging technology that provides learners with new ways of seeing - and thinking about -scientific phenomena. In MBL, STUDENTS connect up all sorts of probes -temperature, pH, motion - to a personal computer through a d/a converter. The data from a probe is pumped straight into a spreadsheet and graphically displayed on the screen in real-time. MBL technology IS making a difference in education. . . . the students are engaged and thinking . . . students . . come to understand how to manipulate and interpret graphs, and come to develop deep understandings of the science underlying their experiments. . . . enable students to see scientific phenomena in new ways and ask new questions - questions that don't have answers at the end of the book. Why have TV and radio not impacted education? . . . TV has been used to deliver instruction . . Learning . . amounts to knowledge transfer: the expert knows something the student does not, and if the expert talks about the material well enough . . students come to know. This unfortunately, isn't necessarily true. On your job you learn all the time. How much of that learning takes place listening to a lecture? . . lectures are not a good way to learn; . . one learns through direct experience, through doing. . . lectures might well have a (small) place in the school day. . . as the dominant-instructional strategy (lectures) are overused and overrated. Just ask any student . . . what is the value in replicating experiments to which answers are already known? . . we learn through doing; we learn through constructing artifacts; we learn through engaging in genuine dialogue and conversation; we learn through the use of technological tools such as MBL. F. James Rutherford, former U.S. Secretary for Education (New York Times, October 25, 1993): ". . . existing curriculums try to cover too much (and) do not teach enough practical applications of science . . . curriculums should delve more deeply into scientific skills, and methods that have broader use, like devising and testing theories, or drawing conclusions from experimental data."

(8)

***ARTIFICIAL INTELLIGENCE AND**

EXPERT SYSTEMS*

"'*Computers* will be capable of conversing with their users in their natural languages, preparing documents by voice-activated typewriter, and providing expert advisory services. . . . expert systems on chips embedded within equipment for diagnostic applications and enhanced user interfaces featuring voice dialog options."

(9)

". . . vision systems and speech recognition in order to create the "intelligent" talking, listening, thinking machines of the future. Tom Forester, "High-Tech Society", MIT Press, Cambridge MA 1987, p. 42.

(10)

* This book (9) contains a bibliography on Education, Instruction, Tutoring - p. 49 - 52; Modeling and Simulation - p. 67; Robotics - p. 69; Science - p. 70; and Hypertext - p. 78 - 89. *

" . . . development of strategic problem-solving capability is a critical educational goal that can be speeded and enhanced substantially through the application of artificial intelligence to the design of computer-assisted instruction. Specifically, we see the need for intelligent tutoring systems that not only design and present problem-solving tasks compatible with a student's prior knowledge, motivational history, and current instructional goals, but that also can analyze task performance online while the student is solving problems, providing maximally effective guidance, correction, and encouragements directed at improving the problem solving process. In order . . . to operate in this sophisticated manner, it must, in some sense, possess all of the following subsystems: 1. An intelligent problem-solving expert that recognizes all feasible plans and strategies possible for any given problem. 2. A sophisticated problem-generation system that can create whatever type of problem the system needs to tutor the student and that matches the student on characteristics such as age, world knowledge, gender, and interests. 3. A multipurpose interface that provides concept-enhancing problem-solving tools for the student to use in solving problems and that also helps make explicit the student's strategies, plans, and misunderstandings. 4. A coaching expert that can recognize and respond not only to correct moves, but also to errors and indicators of motivational breakdowns. 5. A lesson planner that selects problems and instructional routines and assembles them into lessons designed to accomplish instructional goals. 6. A sophisticated student record system for developing and storing student knowledge models and for establishing instructional goals for students. Machine-based intelligent tutoring systems might eventually achieve remarkable power through integration of these capabilities. . . . . . . vary the difficulty of its problem and tutoring routines to meet the instructional need of students ranging from grade 4 through remedial college level. . . . the intelligent machine-based tutor will be capable of many different instructional strategies and routines known to enhance learning."

(11)

HYPERMEDIA AND VIRTUAL REALITY

"Hypermedia -A hypertext consisting of different kinds of information (e.g. text, photographs, sound/ speech, video)."

(12)

"Hypertext is . . . the nonlinear viewing of information. "Nonlinear means that you can examine information in any order you wish by selecting the topic you want to see next."

(13)

"Hypermedia technology can revolutionize a student's view of learning. The educational environment will advance beyond lectures, taking notes, computer-assisted instruction, and other forms of teaching. Students will be able to access unlimited amounts of information from a universal library and enter computer-based worlds that imitate reality. . . . By integrating text, audio, graphics and video, hypermedia presentations both entertain and educate. . . . Hypermedia systems will become common in homes. Future home and school hypermedia systems will access information from databases located throughout the world. Students will have the world's data at their fingertips by having ready access to magazines, audio and video, journals, and other reports in electronic form. . . . One of the most talked about extensions of hypermedia is virtual reality. . . . Students . . . will choose from numerous virtual realities to match their educational needs. From the inside of an atom to the edge of the universe, students will be able to experience whatever environment they require. When microcomputers were first introduced in the schools, many teachers were concerned that they would be replaced by a machine. Instead of superseding the classroom teacher, computers illustrated the need for competent teachers who could design meaningful learning environments. Research demonstrated that incorporating technology into the classroom could both increase and decrease the amount of learning. Only when the classroom teacher evaluated the technology and rationally incorporated well-designed computer applications into the curriculum did learning increase. . . . Educators claim that one of their goals is to provide students with the best-possible learning environment. By continually assessing technology and its implications for learning, teachers will be able to design curricula today that will best prepare their students for the future. By incorporating hypermedia into the curriculum, teachers allow students to control access to information. This gives them a sense of ownership in the ideas and concepts that are represented, thus advancing the learning process."

(14)
TECHNOLOGY AND COLLEGES OF EDUCATION

Alan November: "We currently have enough technology to automate every menial task in the country, from making autos to wiping out middle management. . . . Whether we like it or not, technology has/will forever change the way we learn and work. It is not a question of applying technology to improve current reality. We have a new reality." David Thornburg: "Technology is the response, not the cause. Overall, technology has helped change and shape culture, but only because certain human beings applied technology in certain ways to bring about these changes. . . ." "How should we educate future teachers?" Alan: "This may be the first time in history that teachers do not have a clue about the kinds of jobs students will have. Eighty percent of the jobs that today's kindergarten kids will apply for do not exist today. If this is true, how do we know what content to teach? . . . We have to let go of curriculum and teacher training that are based on confined content and move toward helping students apply their knowledge to solve problems that have not yet been solved. And to do that, we have to see technology as more than a tool. It represents a new medium, a new culture, as sure as the Industrial Age represented a new culture." David: "Technology should play a role in redefining teacher preparation . . . As everything becomes digital, and as bandwidth explodes through the roof, universal access to information through homes, offices and (someday) schools will allow education to acquire a new face. Teachers need to see their roles differently in that technology allows much of the "content" to be acquired online . . . Also, educators need authoring skills in the new media so they can evaluate student work submitted in that form." Can undergraduate education schools provide what either of you are talking about? Alan: NO! David: YES! Alan: "This country has to commit itself to a massive overhaul of teacher preparation, and the last people I would put in charge are the current professors of education. We need the equivalent of the Manhattan Project." David: "If the schools of education are isolated from the needs of society, it is because we allowed that to happen." Alan: "David, do you think ed. schools as a group have the organizational incentive to change?" David: "Of course not, but we should provide it. They are not just arbitrary structures imposed by some alien force, they are part of society and should respond accordingly."

(15)
INFORMATION RETRIEVAL - NEW TOOLS VS. OLD METHODS

"The object you hold in your hands has three centuries of tradition behind it as a medium of communication in the sciences. . . . But printed periodicals will not remain the scientist's medium of choice for another three centuries, or even another three decades.. Their future beyond the next three years is somewhat cloudy. Already, much of the day-to-day discourse of science flows over computer networks, and dozens of electronically distributed journals have sprung up. Sooner or later, ink on paper will be superfluous. The new schemes of electronic publication have an irresistible appeal. Information is delivered in minutes instead of days or weeks. . . . Computer-based methods of searching and indexing make it easier to find what you want. . . . (documents) can be enriched with large data sets, sounds, video clips, animations or simulations. In the right computing environment they could become active documents, which invite the reader to participate as well as to peruse . . . Computers will be standardized, portable, lighter than an average book, with wireless links to a universal network. . . . The time will come when the printing press will be a computer peripheral device not much different from what the laser printer is today. . . . By the time the printed version of a paper appears - often years after it was written - workers have long since read it in preprint form."

(16)
SOME CONCLUSIONS

* The future as predicted by many of these individuals is both challenging an exciting. The prospect of an expert hypermedia system which could interact with students and individualize instruction for an ENTIRE course is mind boggling. Such a system needs to be carefully designed by a team with expertise in diverse disciplines. What a boon for distance learning and large general chemistry courses containing students with diverse backgrounds and abilities! I wonder how long it will be before a really successful chemical system of this kind will come along? Because chemistry is so dynamic, a chemistry system will be difficult to design and maintain. One point made by David Brooks in the recent Computer Conference (17) is that, if computers are able to guide students in solving general-type problems, then computers should be able to solve such problems by themselves. Perhaps it is no longer necessary to teach students how to solve such problems. Perhaps all that is needed is for students to be able to ask computers the appropriate questions. (Such asking will eventually be done by voice in our natural language!) This will affect what we teach students. That is, we need to consider what computers know, and what problems computers are capable of solving before deciding what we should be teaching our students! *

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