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.

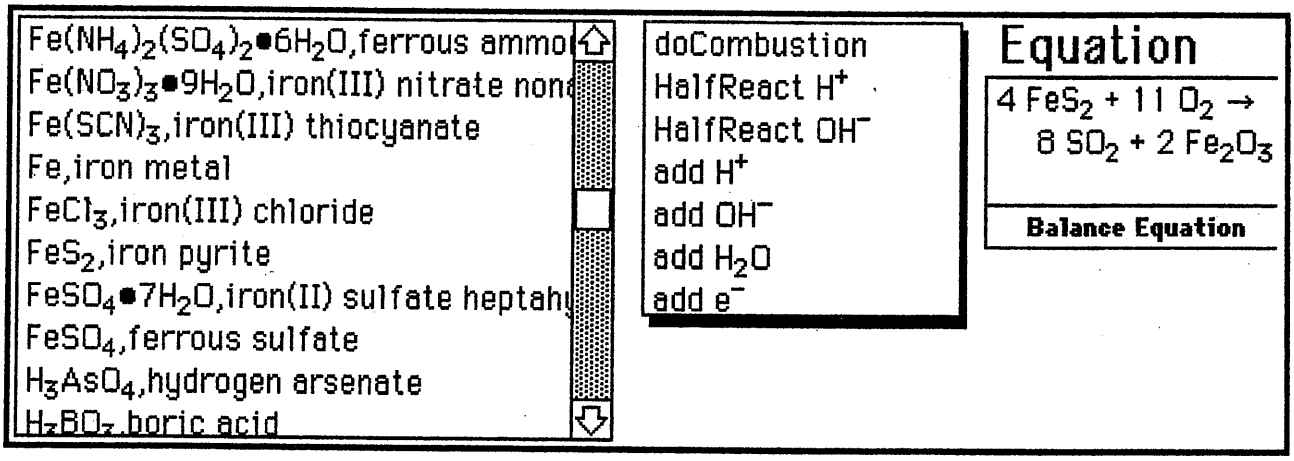

Figure 1. Balancing Equations. Substances may be selected by clicking in lists. Choosing FeS_2 and clicking in a reactants field identifies FeS_2 as a reactant. Most reactants and products must be selected individually. For some reactions, as here, selection from a palette (center) such as "doCombustion"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

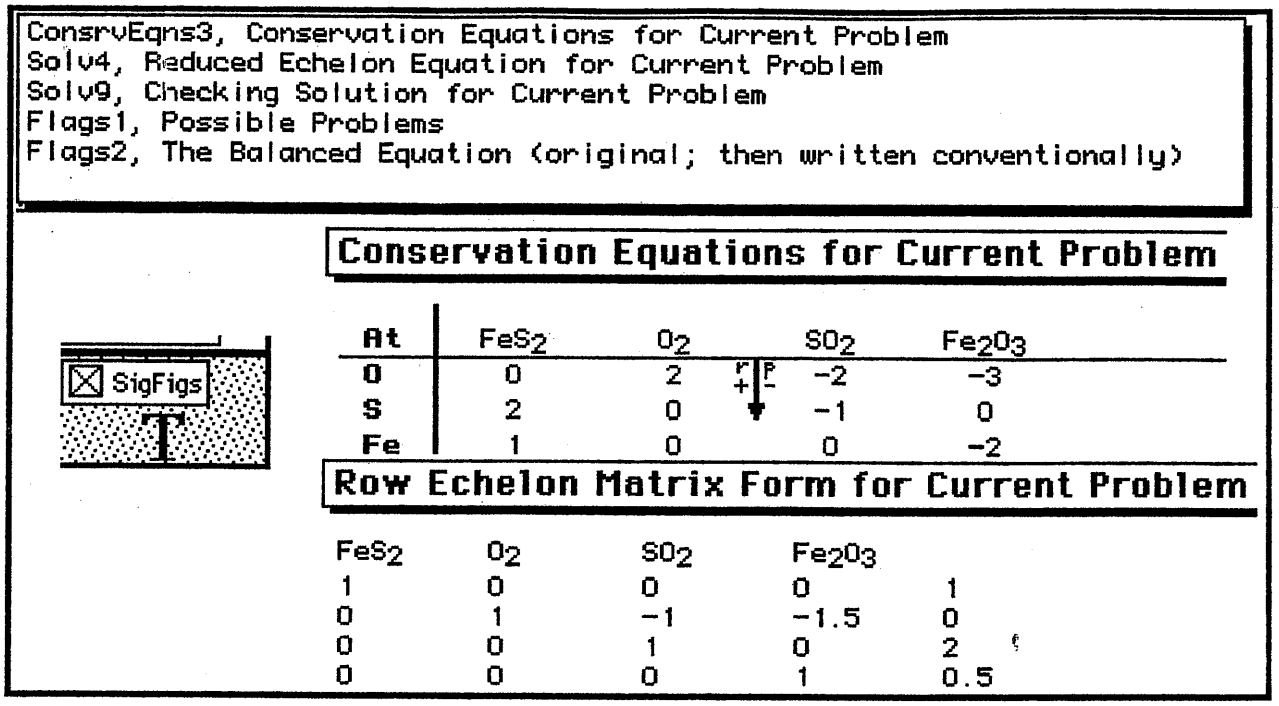

Figure 2. Context-Specific Tutoring for Balancing Equations. Clicking the "T" or tutoring button (center left) brings up a list of five choices for context specific tutoring (top of figure). Choosing the conservation equations brings up the middle list of equations. The row echelon form of the matrix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

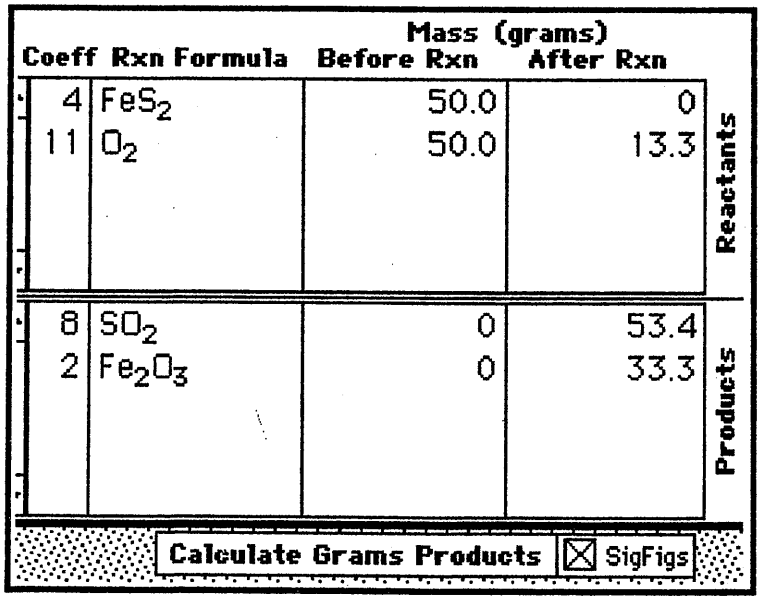

Figure 3. Mass Relationships. Entering the number 50.0 next to each reactant with the "Sig Figs" button hilited and clicking the "Calculate Grams Products" button leads to this result for final masses.

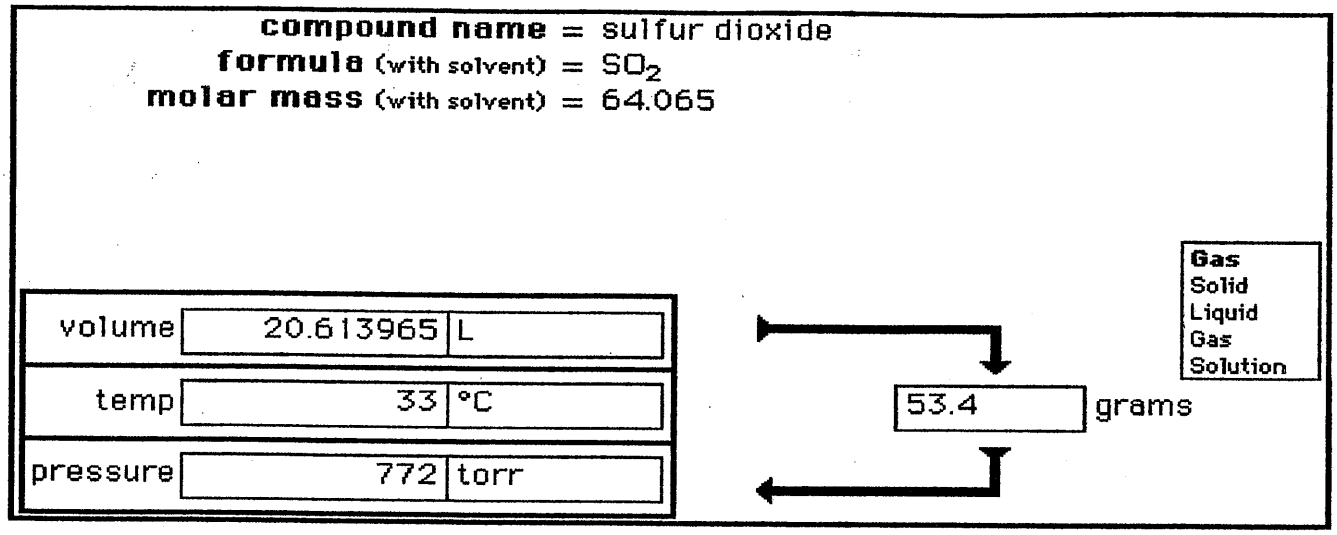

Figure 4. Converting Units. Clicking on the 53.4 grams next to sulfur dioxide (Figure 3, "After Rxn" side) brings up a card with pertinent information transferred. Clicking on "Gas" (upper right) brings up the boxes shown. Entering 33 for the temperature and 772 for the pressure and then clicking the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

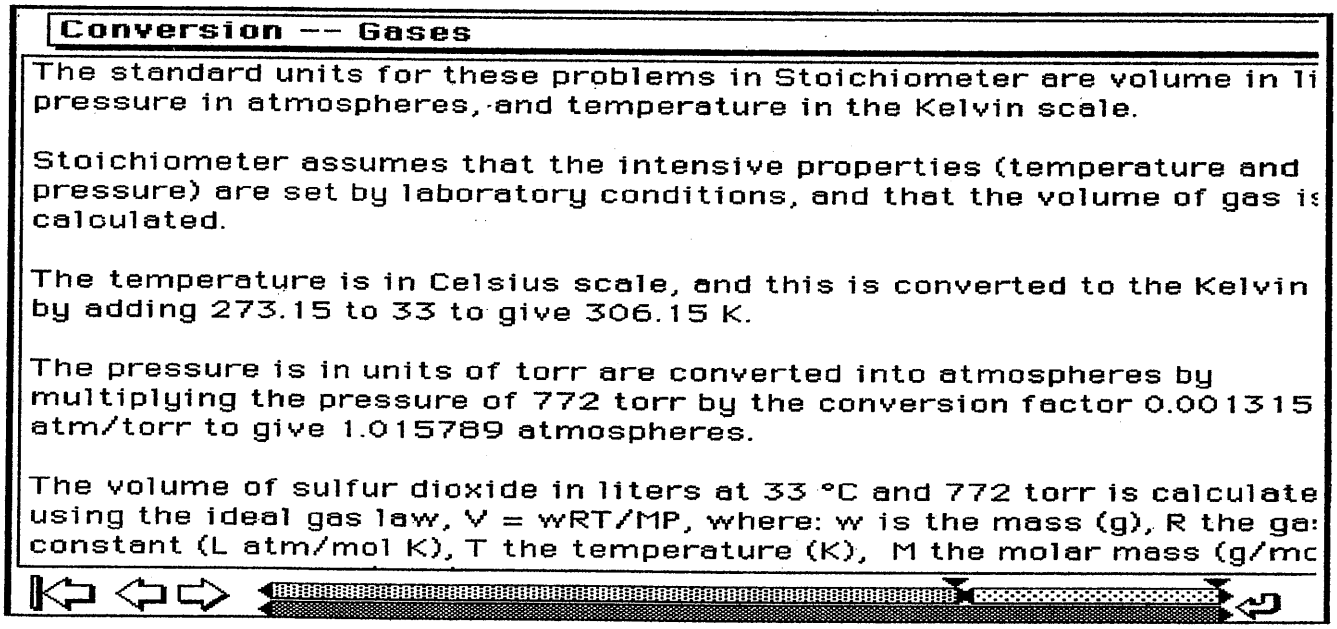

Figure 5. Context-Specific Tutoring for a Conversion. Clicking the "T" (tutoring button) at the bottom of the Conversion card brings up another card in the tutoring system with the information shown. The specifics of the problem are shown. The shaded strips at the bottom of the card permit access to 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.