USING COMPUTERS IN CHEMISTRY
by Brian Pankuch*

After being asked to comment on computer programs which I use, it was easy to choose my favorite two programs; not so easy to analyze why they are my favorites. Both do have several attributes in common. They:

1) Simulate moving particles that we can't see,
2) Give a more accurate model by showing movement and interaction at the same time,
3) Are interactive and give a wide choice of how information appears on the screen,
4) Allow the user to follow virtually any path desired through the program.

The first program demonstrates gas laws. It is available from High Technology Software Products, Inc., P. O. Box 14665, 8001 N. Classen Blvd., Oklahoma City, OK 73313 (405) 840-9900 for $100. You need an Apple with game paddles. The program draws a cylinder with a movable piston. You input the number of moles of gas using numbers 1-9. Other parameters such as temperature and pressure of the gas can be constantly changed using the game paddles. The gas molecules are shown bouncing around in the cylinder. If you increase the temperature or number of moles the volume is shown to increase by piston movement. At the same time, on the lower part of the screen, the current pressure, volume, number of moles, and absolute temperature are shown. The gas molecules move faster at higher temperature and slower at lower temperatures.

Before using the simulation in class, I discuss pressure, temperature, and volume measurements and units. The next period I wheel the computer and color monitor into lecture early enough to set it up and have a few students start using the program. Students choose the color of the cylinder, piston, and background on the screen, and the amount of noise molecules make when they collide with each other or the container. Enough time is

provided to play with the game paddles to *see* what happens. In some classes students cluster around making suggestions, and agitating for their turn. In other classes you are lucky to convince one or two students to try the program.

Once class starts I begin to lecture on Boyle's law deriving the formula and emphasizing what's happening physically. I use the simulation to show an example of increasing the pressure emphasizing physically what is happening. We set up the problem on the board, not just solving the equation but using the computer simulation. For instance "What happens when we increase the pressure - see the volume gets smaller." The students can see the volume get smaller. We check the numbers on the screen. Pressure is bigger since we increased it and the volume is smaller.

How do you set the problem up mathematically? If you know the pressure is increasing in the problem and you understand physically that this has to decrease the volume, then you already know the final volume has to be smaller. We multiply the original volume by a pressure correction factor. Since we already know the final volume has to be smaller, we put the smaller pressure on top and the larger pressure on the bottom. We get the answer from the monitor, then solve Boyle's law mathematically and get the same answer. We check to be sure that the final volume is amller than the initial volume.

We go over a similar sequence with Charles' law. Combining these relationships, the ideal gas taw is obtained. This is particularly useful since then we take the pressure and volume directly from the screen, multiply them (I usually set up numbers that are easily done in your head), then the number of moles and the absolute temperature from the screen and multiply these together with the ideal gas constant and show that the ideal gas law works for all examples we try. The simulation is part of the lecture.

I keep the equipment available for the next *week* or so during my conference hours to allow interested students to use it. Written evaluations and exams from students over seven semesters indicates that the program is very useful.

The second program is a molecular bonding simulation. I wrote this myself
to bridge the gap between my concretely-thinking students and a rather abstract area.
was especially interested in showing the geometry of the molecules, that moving electrons
are restricted to a probability space, and that two elements may form more than one compound.

This programs shows an abbreviated periodic table of about 70 elements. These are the elements included in the program. The program will only handle compounds containing two elements. The student is asked to choose the two elements, and is shown the three most likely oxidation states for each element. The student can then choose to see as many as three different molecules (appropriate messages are displayed if molecules are not formed). For linear, triangular planar, and tetrahedral molecules, bonding electrons are shown and the electrons may be animated in four different modes. With the trigonal bipyramid and the octahedron, stick models are presented on the screen.

My methodology is different with this program. I have previously covered VSEPR bonding thoroughly and have had students struggle with homework problems. As in the gas law case, I bring the computer in early before the lecture and get the students involved. In this case the students usually try a few simple molecules. Then someone gets the idea that the program may be used to solve problem 23h in the homework.

After a few students practice, I take over and use the animation in the HF to HI series to emphasize several points. The Lewis diagrams are useful but incomplete in visualizing what the electrons are doing. The electronegativity affects where the electrons
spend most of their time. One of the animation modes allows you to leave a mark where the s electron has been so that you get an approximate probability space or rough orbital pattern.

Students always want to do homework problems finding the molecule

that is most likely formed between two elements. A number seem surprised that you can get many molecules from the same two elements.

The program works not by having structures stored in memory, but by storing basic facts such as the number of valence electrons, oxidation numbers, electronegativity, etc. It then "calculates" the number of ligand positions, lone pairs, etc. It is a primitive "expert system" in which I programmed my expertise as a step by step procedure to find the most probable molecular structure. In this case, I did not use anything which isn't present in popular freshman texts.

I wrote this algorithm in English, or perhaps "chemicalese" is more appropriate, and hand it out to the students. We then take a homework problem and step our way through as indicated in the algorithm. Then we have the computer work the problem. I keep emphasizing the movement of the electrons - both the actual change in position and the higher electron density near the more electronegative element. We discuss and show how we can get more than one molecule from two elements.

Students are encouraged to come in, use the programs, and make suggestions or improvements, which they do. Feedback and testing show that interest is increased and ability improved as a result of using this program.

As the author of this program, I found that creating a realistic moving model brought up many questions which required considerable thought and research. In building this "expert knowledge-based system" I gained considerable insight into the subject matter and why and where students frequently go wrong.

Many areas may benefit from teaching with an "expert system". Areas that appear particularly appropriate are those in which you can combine the computer's vast memory and speed with your intelligence and experience. To enumerate the 6000 or so possibilities in this program from my memory would be difficult, but by connecting my expertise via an algorithm to the computer's stored facts, a more useful tool is created.

Areas of application would be (a) helping students solve problems by setting them up specifically for the problem the student inputs, (b) helping analyze lab data. The step-by-step procedure to interpret results such as an IR spectra could be improved. Instead of using a general approach the program could consider the specific spectrum a student is solving and go through each step using that spectrum as an example: This type of program is difficult to write *since* the path is variable and determined by the user.

We have experimented letting students customize an existing program. As more students have programming skills we should get them involved in programming worthwhile chemistry problems - not problems done more easily with a calculator. Programs are particularly useful which simulate (a) something you can't see otherwise (electrons, atoms, molecules), or (b) something which is dangerous or very time consuming, or (c) instruments which are expensive or dangerous.

The programming itself is an excellent learning experience and may make the effort of including it in an already crowded course and curriculum worthwhile.

For further information on "expert systems" you will find Expert Systems - Myth or Reality? by Bruce D'Ambrosio, pp. 275-282 Byte, Jan. 1985, and The Fifth Generation Artificial Intelligence and Japan's Compnter Challenge to the World by Feigenbaum and McCorduck, interesting.

This last program will only run in Pascal on a Terak computer. It will not run on an Apple or ISM. *See* J. Chem. Ed. Sept. '84 for availability.

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