MICROCOMPUTER GRAPHICS IN CHEMICAL EDUCATION

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Microcomputer graphics are being used currently in several ways in chemical education software. Of course, microcomputer graphics can mean something as trivial as the display of the letter A on the axis of a graph or as complex as the display of a smoothly rotating molecular model. In this survey, the examples are taken from readily available software for the Apple II or IBM-PC series of microcomputers.

The simplest way that graphics are incorporated into software is as a static image used to illustrate some point. The image is prepared using a drawing utility such as Koala Painter and then stored for later use. This is by far the most common use of computer graphics and, although simple to produce, many more programs could benefit from this kind of graphic usage. It is easy to recognize because the images are commonly stored on disk so that the drive goes on and there is a short delay just before the image appears. Typically, such a program could show a Periodic Table on demand or a title page with an attractive image on it.

The better examples of the use of static images show up in the instrument simulations. These are intended for a tutorial or practice in the operation of a particular instrument. They can be useful when a student must practice the operation of a particular instrument before actually being allowed to operate it or when an instrument is not available but the skill to use it must be acquired anyway. These simulations can be relatively simple like the IR simulator of Krause for the MacIntosh (SERAPHIM MC1301). The user can control sample concentration and cell thickness before the simulation plots the spectrum of one of the available unknowns. A section of the program permits the user to make his own solution cell. The available parts have to be assembled in the right order and with some degree of precision.

More complex are the simulations of Paul Schatz (University of Wisconsin). The IR simulation mimics the Perkin-Elmer Model 1310 and the NMR models the Varian EH-360 instrument. The user must examine a mock-up of the main instrument panel and adjust the appropriate parameters just as in the actual machine. Then the spectrum is plotted.

HPLC by Rittenhouse and SPEC20 by Gable are under development through SERAPHIM. The former makes extensive use of very detailed, largely static images to simulate a High Pressure Liquid Chromatograph. The latter simulates the Spectronic - 20 visible-U.V. spectrophotometer. XENON by Whisnant (SERAPHIM AP606) simulates a vacuum line in which xenon and fluorine can react to form either or both of the xenon fluorides depending upon the temperature and concentration of the reactants initially chosen by the student user.

The most complex simulations use interactive animated graphics when the image on the screen responds to user input either directly, or indirectly, in that the image depends upon variables entered. The earliest examples were the Chem. Lab. simulations of Gelder. The one which illustrates the gas laws allows the student to vary P, V, N and T and to watch the simulated gas respond. Other modules available include acid-base titration, calorimetry and experiments involving equilibrium reactions. The simulations of Rittenhouse tend to favor re-enactments of famous historial experiments such as those of Rutherford. The user of this software can design and implement experiments on alpha particle scattering. The Rittenhouse simulations are excellent in that the graphics are very good and the user has to do the kind of thinking that the original experimenters did in order to reproduce the original results. The opportunity exists to accumulate extensive data from which the significant results must be culled.

The animated simulations of Bendall are not so difficult for the user. The objective is made obvious and the program is much more linear, reducing the possibility of being side-tracked. A typical example is Backtiter (SERAPHIM AP604) in which the object is to determine the concentration of carbonates in a mixture by adding it to standard acid and back-titrating the excess. The simulation requires the user to weigh samples on a top-loading balance and to titrate using a simulated buret. Along the way, the carbonate is shown bubbling as the acid is added, the buret flame flickers and the gas is shown escaping when the carbonate is heated.

Molecular modellers illustrate another use of microcomputer graphics. Typical of these are MOLEC by Owen and Curry and Molecular Graphics by Henkel and Clark. MOLEC was reviewed in J. Chem. Ed. in September 1984. Molecular Graphics can display and manipulate structures with more than a thousand atoms and bonds. The image can be translated along any coordinate, rotated about any axis or bond, enlarged or reduced. Standard molecules such as chymotrypsin are available, or one may enter a molecule by supplying atomic coordinates and bond connection tables. The image can be space filling in which case each atom is represented by a large sphere or made up of lines or lines with a small sphere at each intersection. The structural manipulations are slow. This is a common limitation of these packages. The calculation and drawing of a new view depends upon the number of atoms but can take up to eight seconds and is too slow for effective animation. Space filling representations take longer to draw than line drawings.

Plotting routines use graphics to plot graphs. The most general kind allows the user to enter data, process it, and present the plotted results. Data can be entered at the keyboard or directly from an instrument. ASYST is an elaborate example. It turns an IBM-PC into a data station where data can be collected, reduced and plotted. It has modules for graphical and statistical analyses. It uses the 8087 co-processor for computational speed. An interface board is required and about $1700 can purchase the complete system.

Many plotting routines are available. They can be almost trivial like LINGEN, which fits two variables to linear models, or they may be general like GRAFIT, which will draw 3-D data as contoured or gridded plots.

If you are reasonably certain of how you wish to process data and proficient in programming, then you are best off writing your own software. You are more likely to get fast code because you can optimize it for your particular application. If you want elegant displays including bar and pie charts, you should consider using one of the packages used by business in conjunction with a utility like Lotus 1-2-3.

A more specific kind of plotting software uses internal or external data to illustrate some principle. The graphics have to be calculated on the spot since the exact graph required cannot be predicted. The most common examples are the acid-base titration simulations which feature plots of pH versus Volume. KC Discoverer has a data base of the quantitative properties of the chemical elements and allows the user to plot any two variables. The software allows for some manipulation of the data. If you want a plot of Atomic Volume minus First Ionization Potential versus Atomic Number from twenty to sixty, then KC Discoverer can do that and give a hard copy of the result.

Graphic utilities are software intended to help others produce graphics for use in demonstrations or for inclusion in their own programs. To get an image on the monitor requires the author to specify the X, Y coordinates of each pixel that must be lit. While the coordinates can be individually entered at the keyboard, most authors use a utility such as a graphics tablet or a mouse. A tablet like Koala Pad and its accompanying software allows an image to be drawn freehand and manipulated. The software can help draw lines, boxes and circles and allows filling in areas with relative ease. The image can be manipulated by picking up pieces of it, moving them around, erasing or duplicating them.

Software which helps the programmer animate his graphics appears to have great potential. The latest software of this kind is Fantavision. If two different images are drawn using the Koala Pad, the software can transform one image into the other. Fantavision is easy to create a moving picture with up to eight colored objects moving smoothly around the screen. It is very impressive but the code is copy protected and the DOS is customized so that the disk you create must be specially formatted for that alone. To incorporate such a movie into CAI software would require the user to change disks for the animation and then return to the program disk when the animation concludes. The clumsy procedure effectively makes it impractical for incorporation into other packages.

CHANGE is a utility now available from SERAPHIM which is like Fantavision but is less sophisticated. It can animate only one unfilled object. If a triangle and a square are drawn, then CHANGE can smoothly change one into the other. The software automatically compensates for the different number of apexes in the two images. Since the points which define triangle and square are transformed on a one to one basis, then if the triangle is defined clockwise and the square defined anti-clockwise, the triangle will appear to turn over as it is transformed into the square.

I am pessimistic about the future of chemical educational software that uses animated graphics. There are two major problems. Graphically oriented software is very machine specific. Software that can only be used in locations which have identical hardware is not of great utility to the educational community at large. We need to standardize graphic software so that it will run on all common microcomputers or settle on the use of one or two microcomputers for CAI. Standardization of software means that the code will not be optimal for any one computer. There will be loss of animation speed. Standardization of hardware means that the introduction of new machines will be resisted. At the moment there is an unofficial unification in that the Apple II and IBM-PC are the two major microcomputers in education today. Unfortunately neither is particularly well suited for animation.

Two affordable microcomputers have appeared recently with superior graphic capability: the Amiga and the Atari ST. Sadly, both companies are viewed with suspicion by the buying public. Atari has teetered on the brink of insolvency for several years. Commodore has a reputation of being rather unfriendly to its buyers. Particularly irksome is the tendency to issue computers which cannot run the software of their predecessors. The company has also been having financial difficulties. The third machine to appear with a great deal of potential is the IBM PC-RT. However, it is expensive with an announced price of about $13,000.