MICROCOMPUTERS IN PHYSICAL CHEMISTRY ANIMATIONS

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For the past several years, I have been introducing students to the use of microcomputers by assigning projects to create interactive animated simulations of physical chemical phenomena. The following describes the evolution of this process.

The first projects were carried out as senior studies. They consisted of programs that could number crunch and were used to evaluate and simulate theoretical and laboratory data. The students used Apples and were successful at modelling kinetic and equilibrium systems. There were six to ten students over a two year time span that worked on this type of project.

The next significant step in the evolution of this work involved the introduction of students to three CROMEMCO microcomputers. These microcomputers had very good color and animation capabilities. However, there were some major disadvantages: the systems were expensive; we were using an outdated language (FORTRAN IV); and the CROMEMCO's were not widely available for others to use the software that was produced from this work.

This stage was important for two reasons. First, twenty to twenty-five students were involved as a part of special projects in the third quarter of the regular physical chemistry laboratory course, where they worked in groups of two or three. Second, we became convinced that interactive animated simulation in color contributed to the success of our efforts.

The third stage of development was the widespread appearance of IBM PC's on our campus. Although at that time they did not have the capabilities of the CROMEMCO systems, they were more available for student use. This permitted the inclusion of a required computer project as an integral part of the regular physical chemistry lecture course. That was done in the third quarter of the course, consisting of ninety-five students, and counted as twenty percent of each student's grade. They used primarily Pascal and Basic as the programming languages.

The preceding describes the development of the introduction of our students to microcomputers via creation of interactive animated simulations for physical chemistry. Now I will describe some of the characteristics of and observations garnered from these projects.

The students involved in these projects were split about 20/80 chemist/chemical engineer and the class sizes ranged from 100 to 140. The engineers had had a one quarter course in programming mostly for main frame computers. The chemists normally had not had that background. I did not observe any significant differences in performance between students in the two groups. I have noted that for the past two years more students have a working knowledge of Basic. I expect this trend to continue. In any case, the lack of prior programming skills did not prevent the completion of the projects.

Each project contained the following steps:

1. Create a visual model.
2. Create a mathematical model.
3. Connect the models so that the visual model interacts with the mathematical model.
4. Provide parameters in the program which the user can change.

The significance of these steps is that the students are required to visualize the chemical phenomena and make the mathematical connections. I believe that this enables them to understand ideas and concepts more readily.

At the end of the quarter, each group of students did a "show and tell" presentation of their work before the entire class. This is important as it provides a strong incentive to complete the project and is the first part of evaluation of the results. I, as the instructor, completed the evaluation and assigned the grades for the projects.

I acted as an advisor on the chemical concepts and ideas. I did not give advice on details of programming: I expected each student to develop the necessary skills on their own, as they did. Most of my time was spent consulting with them on effective visual and mathematical models.

I hope that this sharing of my experience will give you some ideas on how to incorporate microcomputers into your classes. I have found it to be very rewarding and look forward to future hardware and software developments that will allow us to better describe and teach chemistry. Walt Disney is at our fingertips. Let us take full advantage of this opportunity.

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