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Using a Computer in High School Chemistry

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INTRODUCTION

The advent of the computer is having a great influence on our society and the educational system. Many public school systems have contracted with institutions and organizations for use of their computer facility in class scheduling, pupil accounting, fiscal accounting, preparation of student grades and the like. The computer has not, with the exception of some experimental situations, been widely used in the public schools as an instructional tool.

The advent of the time-sharing and multi-tasking computer provides the opportunity for public schools to avail themselves of an instructional computer at a reasonable cost without employing specialized computer scientists. It is this kind of facility that has been in use since August, 1969, at Ames Senior High.

FACILITIES

Ames High School is connected to the Iowa State University Computation Center. Incorporated in ISU's multi-tasking facility is the provision for using the Conversational Programming System (CPS). The ISU CPS system uses remote telephone connected external keyboard units.

At present, Ames High leases a Model 33 Automatic Send-Receive teletypewriter. The portable unit is easily moved to the classrooms that are equipped with standard telephone jacks. The teletype terminal is equipped to punch and read paper tape. Programs are usually punched off line and then fed into the computer at 100 words per minute.

PROGRAM LANGUAGES

The ISU CPS system allows the use of modified versions of both PL/1 and BASIC programming languages. PL/1 is primarily used in Ames High School science since it seems to provide for more flexibility in the narrative part of the computer program.

It has been a simple procedure to modify programs written in FORTRAN to fit the PL/1 language in the CPS system.

UTILIZATION

Our major attempt in this paper is to present some of the ways in which we have found the computer useful in the teaching of chemistry at the high school level.

Aid to Student Calculations

The ISU version of CPS has most of the standard mathematical functions available and hence can serve as a high speed calculator.

A use that we have found to be of value is the verification of student calculations. For example, the reaction of Mg with HCl solution to determine the equivalent weight of Mg requires several sequential calculations. As an aid to the student, a program has been written for the student to verify his calculations.

In the study of the emission spectrum of the visible lines of hydrogen it is often desired to decide which electron transitions are involved. The value of n_f and n_i corresponding to each line of the visible series must be determined. The student is instructed to use the Rydberg equation to decide the transition that accounts for the observed line. As an aid to the student, a series of

$$\nu = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

calculations of $\frac{1}{n_f^2}$, $\frac{1}{n_i^2}$ and $\frac{1}{n_f^2} - \frac{1}{n_i^2}$ are supplied for all possible sets of values for the first seven energy levels.

In an experiment (1) to determine the proper form of the Equilibrium Law expression and the equilibrium constant for

$$Fe^{+3} + SCN^{-1} \rightleftharpoons Fe(SCN)^{+2}$$

a series of cumbersome calculations are required. A FORTRAN program to perform all the calculations for this experiment is available in the teacher's guide to the laboratory manual. This program was modified to use the per cent transmittance values obtained with a Spectronic 20 or the measured height ratios as suggested by the procedures in the experiment. An alternate procedure suggested by Ramette (2) has also been used and a corresponding program to process the data has been prepared.

The modified program has been used to perform the calculations of the equilibrium constant for the less able student. More time is thus available for the student to analyze and understand the chemical principles of the experiment. It can serve as a check on the calculations for the more able chemistry student.

Curve Fitting of Data

In an experiment to determine the solubility curve of $K_2Cr_2O_7$, students were assigned the task of finding the saturation temperature and solubility of a given mass of the salt in 100g of water. The data from the students (solubility vs temperature) were analyzed by a method of least squares curve fitting program to determine a solubility curve equation. From the equation, values of the solubility (g/100g H_2O) of $K_2Cr_2O_7$ from 10°C to 90°C were determined.

The solubility of $K_2Cr_2O_7$ from student experimental data, the computer generated solubility data, data from the *Handbook of Chemistry* (3) were plotted and compared. The computer-generated solubility data agreed ± 2 g/100g H_2O with the handbook solubility values within the range of data gathered in the laboratory. The computer-generated solubility data did not match the handbook solubility values in the extrapolated range (50°C to 10°C). Although this was not anticipated, it served as an excellent illustration of the hazard of extrapolation beyond the limits of the data.

Theoretical Calculations

This is one of the areas in which we think the computer has great potential. Many theoretical quantitative calculations are time consuming and difficult for the average beginning chemistry student; yet the results of these calculations can be very beneficial in learning the theories and concepts they support. For example, students can plot data as an aid to understanding the chemical concepts involved in titration. Computer programs have been designed to calculate and print out titration data in tabular form showing the volumes of both acid and base, the concentrations of both H+ and OH— ion and the pH for any chosen concentration of both acid and base (within normal laboratory limits). We have written such programs for various combinations of strong-weak acids and bases. The execution of weak acid-strong base titration is shown in Table 1.

Table 1

Titration of 0.15 N Acetic Acid With 0.10 N Sodium Hydroxide

Volume Acid	Volume Base	H+ Ion Concentration	OH— Ion Concentration	pH
25.00	5.00	.12E-03	.83E-10	3.92
25.00	10.00	.51E-04	.20E-09	4.29
25.00	15.00	.28E-04	.36E-09	4.56
25.00	20.00	.16E-04	.61E-09	4.79
25.00	25.00	.93E-05	.11E-08	5.03
25.00	30.00	.47E-05	.22E-08	5.33
25.00	35.00	.13E-05	.75E-08	5.88
25.00	36.00	.78E-06	.13E-07	6.11
25.00	37.00	.25E-06	.40E-07	6.60
25.00	37.30	.10E-06	.10E-06	7.00
25.00	37.40	.50E-07	.20E-06	7.30
25.00	37.50	.18E-08	.57E-05	8.75
25.00	37.60	.63E-10	.16E-03	10.20
25.00	37.70	.31E-10	.32E-03	10.50
25.00	37.80	.21E-10	.48E-03	10.68
25.00	38.46	.66E-11	.15E-02	11.17
25.00	39.86	.27E-11	.36E-02	11.56
25.00	40.86	.20E-11	.51E-02	11.70
25.00	42.46	.14E-11	.74E-02	11.86
25.00	47.46	.73E-12	.14E-01	12.13

Simulation of Data

One of the most exciting areas of future investigation appears to be using simulated laboratory data. Students may gain just as much understanding of the concepts in an experiment by processing computer produced data as those students who obtain the data through manipulation of laboratory equipment.

In a simulated Boyle's Law experiment, the student selects several values of pressures for input into the computer. The output will supply the input pressures along with corresponding volume values. A random error up to ± 5 per cent is built into the program. The student can plot the data in the usual ways to discover the mathematical relationship between volume and pressure.

The Charles Law experiment is similar except temperatures in degrees Celsius are provided by the student. The computer will generate temperatures and corresponding volumes with ± 5 per cent random error. Due to the built-in random values produced, each student is provided with different values of data each time the program is executed.

Two other experiments which have used simulated data are molar heat capacity of a metal and the heat of a chemical reaction.

Table 2 is a sample output for the heat capacity of lead (4). The data produced has a random error of ± 3 per cent. The instructor can have the computer generate as many sets of data as he desires.

Table 2
Sample Data for Molar Heat Capacity Experiment

Initial Water Temp.	Initial Temp. of Shot	Mass of Water	Mass of Shot	Maximum Temp. of Water	Calorimeter Constant
20.3 C	98.9 C	200 G	200 G	22.5 C	3.0 CAL/DEGREE C
22.4 C	93.6 C	200 G	200 G	24.5 C	3.0 CAL/DEGREE C
21.9 C	97.1 C	200 G	200 G	24.0 C	3.0 CAL/DEGREE C

The Heat of Reaction experiment in *Chemistry: Experiments and Principles* (1) is programmed to yield data for both the reaction of Mg with HCl and MgO with HCl. The student using the results of his calculations and applying Hess' Law of Heat Summation can then calculate the heat of reaction for magnesium with oxygen. An example of the data output is listed in Table 3. Again, as many sets of data as desired can be obtained by the instructor.

Computer Assisted Instruction

There is much written about the use of CAI in the classroom (5, 6). There is no question in our minds that this is a feasible and workable aspect of the CPS system. Cost is a factor that enters into CAI. For example, to execute a simple 10 question CAI program for one student costs approximately $0.50. This would prove to be a very expensive program if very many students were involved. Printed programmed instructional material seems to be more eco-

Table 3
Sample Data for Heat of Reaction Experiment

Initial HCl Temperature	Mass HCl	Mass MgO	Max-Temp HCl	Calorimeter Constant
21.0 C	91.4 G	.55 G	25.9 C	3.0 CAL/DEGREE
24.4 C	96.0 G	.51 G	28.5 C	3.0 CAL/DEGREE
27.9 C	99.8 G	.59 G	32.6 C	3.0 CAL/DEGREE
Initial HCl Temperature	**Mass HCl**	**Mass Mg**	**Max-Temp HCl**	**Calorimeter Constant**
22.2 C	91.5 G	.41 G	41.3 C	3.0 CAL/DEGREE
23.0 C	99.6 G	.57 G	48.0 C	3.0 CAL/DEGREE
29.7 C	97.5 G	.57 G	55.1 C	3.0 CAL/DEGREE

nomical than using CAI with the CPS system. CPS would be very useful for the development of branching programmed learning materials.

Problem Generation

A final area of computer use is the production of daily problem sets in chemistry. Textbooks always have some problems at the end of each chapter but often these are too few or of the wrong type. A teacher often spends a great deal of time making up additional problem sets for the student to work on to improve his competence in solving a certain kind of problem. In most cases this amounts to the same type of problem but with different numerical values to use in the solution. Some of this work can be alleviated by a computer program that randomly generates numerical values for a specific kind of problem format and also calculates the correct answer for grading. The teacher can have the computer generate as many problems of a specific kind as he desires. The authors have found these kinds of problems to be very useful as review problems in which the computer printout is duplicated and given to the students as supplemental practice problems.

FUTURE PLANS

The use of the computer as an instructional tool has proven to be a very exciting experience. As we gain skill in programming techniques, greater possibilities become apparent for using the computer as an instructional tool in chemistry. One of the areas that we are most interested in pursuing is that of simulation of laboratory experiences. We plan to conduct some controlled experiments comparing the performance of two groups of students, one using simulated data and the other gathering the data in the laboratory.

MATERIAL AVAILABLE

It is somewhat difficult to learn the programming language from the CPS terminal manual (7). We have spent some time gathering materials that will help students and teachers learn to write effective computer programs. For teachers of mathematics, the CAMP (8) materials are excellent. They make use of the BASIC language which is available on the CPS system and are designed to be used with a remote facility such as the one described. There are six books in the series ranging from seventh grade mathematics through introductory calculus and probability and statistics. As of this date the geometry and advanced mathematics books are not yet available but are scheduled for release in 1970. Also available for mathematics is a book entitled *Problem Solving With the Computer* (9). This book is designed as a supplement to secondary school mathematics programs uses of the BASIC language.

We have examined several other books on data processing and computer science. These references have been of help in learning to write computer programs and in suggesting applications of the computer to chemistry: *Computer Science: A First Course* (10), *Introduction to Data Processing* (11), *The Computer and Chemistry* (12), and *Numerical Methods and FORTRAN Programming* (13). The first book listed offers a great deal of material on basic programming and is designed for readers with only a good high school background in mathematics.

SUMMARY

The computer has not only made many aspects of our present chemistry courses easier but has indeed added a new dimension to our science curriculum. The computer has provided us with a new and exciting motivational device for students and staff members alike. The kinds of activities we can now offer to students is no longer limited by many hours of tedious calculation or, in some cases, mathematics they are unable to handle. The computer allows students to explore problems of their own creation with no limit but their own imagination. Simulation of laboratory experiences before students actually perform the experiment may add a new insight to the student's perspective on the objectives of his investigation.

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