APPLICATIONS OF MICROCOMPUTERS IN COLLEGE SCIENCE TEACHING LABS

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ABSTRACT: Two computer programs that automatically produce plots have been designed for use on microcomputers in college science teaching laboratories. LLSQPLOT determines the parameters and statistics of the best straight line through a set of input points, and GLC simulates a gas chromatograph with a selection of samples and operating conditions. Both programs contain special features beyond existing programs. Input, output and plots of sample data illustrate the use of both programs.

KEYWORDS: Science teaching laboratory, linear least-squares fit, gas chromatograph, plot routines, Apple II Plus microcomputer.

There are essentially four types of uses of computers in college laboratories for teaching science, namely data processing, process simulation, drill or tutorial, and management tasks such as maintaining records of grades or attendance. In this paper, we discuss instances of the first two of these functions that have resulted in microcomputer programs written in BASIC. Both these programs have applications in teaching beyond the confines of a single subject or department. The first program is statistical in nature; LLSQPLOT determines not only the slope and intercept of the best straight line through a given set of points but also some statistical measures of the goodness of fit. The other program simulates the operation of a gas chromatograph; GLC produces a chromatogram with various choices of samples and operating conditions. More detailed descriptions of the programs and their use follow.

LLSQPLOT

One of the most common tasks in college courses in chemistry (general, analytical or physical) and physics (general or advanced) is the determination of the slope and/or y-intercept of the best straight line through a set of points. These data may have been directly measured in the laboratory, or simply supplied by the instructor for an assigned problem. Of course, it is easy to write a program for a programmable calculator or a microcomputer to determine these quantities; indeed, to do this exercise is useful for students who are learning programming techniques. Only slightly more difficult is the computation of the standard errors of both the slope and the y-intercept, and the correlation coefficient of the fit, provided that the usual approximation is made that all the error is attributed to the dependent variable. In fact, some pocket calculators now available have such statistical functions internally programmed. When the results are displayed, however, the number of digits shown is almost inevitably the maximum number of which the machine is capable. Experience has demonstrated that students are prone either to transcribe all the displayed digits or to truncate them arbitrarily.

The program LLSQPLOT has therefore been designed with the following features. Correction of input data is possible. All the five calculated quantities — the slope, y-intercept, their estimated standard errors, and the correlation coefficient — are displayed as rounded values to show only the appropriate number of significant digits (the number of displayed digits is usually one greater than the formally significant number). The points and the fitted line are then plotted automatically, with no user intervention required for axis scaling etc; this plot enables the user to judge which points may need to be remeasured, if in the laboratory, or to be reentered, if input erroneously.

To use this program, the student specifies the number of pairs of coordinates to follow, then inputs these data according to prompts on the monitor. The user can then review those data pairs visible in the display in order to decide which cases may have been inaccurately entered. If the number of desired changes is not zero, then the appropriate case numbers are input followed by the corrected values (the values of both coordinates of any erroneously entered point must be input again). After this procedure for data correction, if necessary, the computer calculates the pertinent quantities, specified above, and displays their rounded values. The correlation coefficient, a measure of the goodness of fit of the linear model, takes values between the limits of plus and minus unity; these limits correspond to perfect fits with positive and negative slopes, respectively, whereas intervening values indicate a progressively less good fit the farther from the limits; in the physical sciences, correlation coefficients having magnitudes less than about 0.95 suggest either data of relatively poor quality, errors in handling them, or an inadequate linear model.

If the user then responds affirmatively (Y for yes) to the question of wanting to see the plot, the entire display becomes a graph with the input points shown as plus signs about the fitted line. The axes are always scaled such that the fitted line is close to a diagonal. The parameters of slope and y-intercept employed to construct the fitted line are those with the full calculated set of digits, not the rounded values. Although horizontal and vertical lines bound the bottom and left-hand edges of the display, these in general do not represent the positive x- and y-axes (the boundaries of the principal quadrant).

In many applications, the raw chemical or physical data may need to be transformed or may not conform to a linear model. A further feature of the program LLSQPLOT is the provision for transformation of input data. For instance, in order to determine the molar heat of vaporization of a liquid according to the Clausius-Clapeyron equation, one must plot not the measured pressure against temperature (on the celsius scale) but logarithm of pressure against reciprocal of absolute temperature:

$$d(\ln P)/d(1/T) = -\Delta H^{o}/R$$

In order to facilitate such models of pseudo-linear regressions, the user must simply change the lines:

```
30 DEF FNX (X) = X

40 DEF FNY (Y) = Y
```

to read, in this particular case:

```
30 DEF FNX (X) = 1/(273.15 + X)

40 DEF FNY (Y) = LOG (Y)
```

In the derivative on the left-hand side of the Clausius-Clapeyron equation, there appear the quantities ln P in the numerator and 1/T in the denominator. The former is represented in Apple BASIC as LOG (Y), because we use the y-axis for the pressure axis, while the change of conventional temperature (in ^{o}C) to the absolute scale requires an addend of 273.15 before the reciprocal is formed to represent 1/T on the x-axis. Then the slope of the plot of log P against 1/T is the given derivative. These features of the program LLSQPLOT, whereby data transformation is automatically effected before data processing, make it possible for any desired conversion factors also to be incorporated; thus one can easily express the results in the most convenient units.

One characteristic of the programming techniques, related to the proper scaling of axes for a meaningful plot of data over any imaginable range of practical magnitudes of data values, causes problems if either perfect data (zero values of the standard error of either slope or y-intercept) or identically zero values of the slope or y-intercept occur. Experience with this program in several teaching laboratories has suggested that this situation is unlikely to happen if real data are gathered by students.

As a sample of input, output and plot, we present in Figure 1 the numerical data and

in Figure 2 a graph of the results. In Figure 1, the numbers between the question marks and the implied carriage returns are the input data, prompted by the messages as shown. The plot clearly shows how the best straight line through the five points lies close to a principal diagonal of the rectangular plot area, thus having good pedagogic value in illustrating proper graph construction.

```
RUN LLSQPLOT

NUMBER OF DATA POINTS = 25

X(1) = ?1
Y(1) = ?3.09
X(2) = ?2
Y(2) = ?4.95
X(3) = ?3
Y(3) = ?7.05
X(4) = ?4
Y(4) = ?8.95
X(5) = ?6
Y(5) = ?13

NUMBER OF DATA CHANGES = ?1
CASE NUMBER
CHANGE X(1) TO ?1
CHANGE Y(1) TO ?3.05

SLOPE = 1.9932 +- .014
Y-INTERCEPT = 1.022 +- .053
CORRELATION COEFFICIENTS = .999921
DO YOU WANT A PLOT? Y/N?
```

Figure 1. Typical input and results of the program LLSQPLOT.

GLC

Gas chromatography is an essential experimental method in chemistry, biochemistry and related fields in laboratory courses in all colleges and universities. In many countries, gas chromatographs of moderate cost are available (or may be assembled) that are quite suitable for instructional purposes. Because the operation of such instruments does not require a sophisticated technique, direct introduction of each student to the topic of gas chromatography by means of an actual instrument is clearly desirable. According to our experience, computer simulation can, however, usefully supplement use of an actual chromatograph. Where an appropriate instrument is not available, chromatograms simulated by a computer, in conjunction with appropriate diagrams, can greatly increase the instructional value of the diagrams alone. The current availability of microcomputers, especially valuable in association with the teaching laboratory, makes possible the effective coupling of an actual chromatograph with the speed and versatility of the simulated display to enhance the effectiveness of teaching this analytical method within a limited period of time. For these reasons, we have developed the program GLC that produces a realistic simulation of chromatograms, used interactively by means of selection of operating conditions appropriate to common existing instruments.

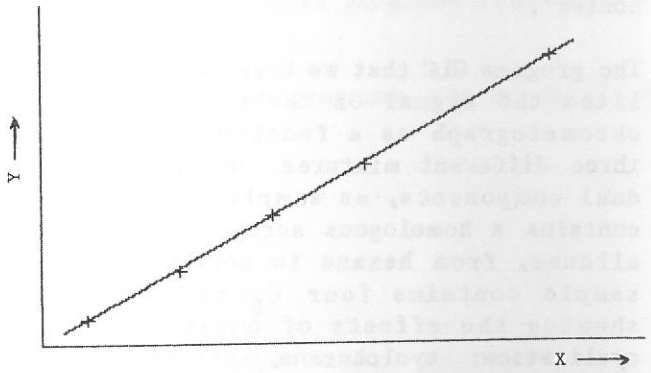

Figure 2. Plot generated by program LLSQPLOT from the data in Figure 1.

By way of a brief summary, gas chromatography not only is a method of separating a mixture of volatile chemical substances into its pure components, but also permits qualitative identification and quantitative estimation of such substances. In operation, a sample is injected into a stream of inert gas (mobile phase) that carries the components over a liquid (stationary phase) on a solid support within a tubular column; during its passage through the system to the detector, the sample is partitioned many

times between the mobile and stationary phases, such that a local quasi-equilibrium is attained. The time taken (relative to air (inevitably) admitted simultaneously with the sample) by any component to pass the column is called the retention time, generally taking a value characteristic of a given component in relation to a particular stationary phase (and length of column) at a particular temperature. The effect on the retention time of change of the column temperature is attributed to a thermodynamic quantity, the enthalpy change of solution of the sample component as solute in the liquid of the stationary phase. In accordance with the usual thermodynamic behavior, the retention time is observed to vary exponentially with the temperature. Thus a plot of logarithm of retention time against reciprocal temperature has a slope proportional to this heat of solution. The form of this relationship resembles that of the Clausius-Clapeyron equation quoted above, but the details are not essential in the present context.

The program GLC that we have developed simulates the signal of the detector in the chromatograph as a function of time for three different mixtures, or their individual components, as samples. One sample contains a homologous series of unbranched alkanes, from hexane to nonane. Another sample contains four C_6-hydrocarbons, showing the effects of unsaturation and cyclisation: cyclohexane, cyclohexene, benzene and hexane. The other sample contains members of four different families on the basis of organic functional groups: tetrahydrofuran (cyclic ether), 1-propanol (alkanol), butanone (carbonyl), and heptane (alkane). In addition to selection of one of these sample mixtures, one can however select any single component for a separate trial, for identification purposes for instance. Each of these mixtures or their components can be run on either of two stationary phases, a silicone oil (DC 200^{TM}) or a poly(hydroxyethene) (Carbowax 20M^{TM}), that may be considered to constitute nonpolar and polar solvents respectively. The other variables to be set are the temperature of the column and the attenuator. The realistic range of column temperature offered is 30–200°C, whereas the attenuator (accepting values in the range 1–10) is necessary for applications of quantitative analysis in order to keep the peaks within the ordinate range. All input is prompted by explanatory text. The values of input parameters are tested to lie within the acceptable range; erroneous responses cause repetition of the input prompt.

The chromatogram appears on the video monitor according to the standard program. The detector of the simulated instrument is supposed to be ideal — i.e. to have equal response to each substance on a molar basis. To facilitate identification, each of the three mixtures contains its components in the specified molar proportions 1:2:4:8, but confirmation of any peak can be made by a separate run of any component. A small peak due to air is found at the beginning of each chromatogram. The peak halfwidths are set to increase with retention time, thus mimicking experiment.

There are several advantages to use of the program GLC, best to complement use of an actual chromatograph. The effect of change of temperature is rapidly produced, in consecutive runs (each takes about two minutes); in fact, the derived heats of solution fairly accurately reflect the experimental data used as the basis of the program. The homologous series of alkanes elutes in the expected order on both polar and non-polar columns. The group of C_6-hydrocarbons, three of which have standard boiling points within a small range of 3K, demonstrates the efficiency of the chromatographic process of separation, without the student having to handle the toxic or noxious substances benzene and cyclohexene. The other group of compounds incorporating various organic functional groups elutes in opposite orders on the two columns, illustrating the effect of specific solvent-solute interactions within the column on the relative retention times. A particular advantage of GLC is the possibility to simulate the run of any single compound by itself on any column, just as in the laboratory calibration procedure.

As an example of the input, output and plot provided by the program GLC, we present in Figure 3 the information to prompt the user in the choice of samples and conditions, and in Figure 4 the resulting simulated chromatogram. The final two lines in Figure 3 are in fact displayed below the chromatogram for a period of about thirty seconds after the plot is completed; this period can be modified according to the value of the number in line 1999 of the program.

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RUN GLC

COLUMN CHOICES, POSSIBLE SAMPLES,
AND COLUMN TEMPERATURES ARE TO BE
SELECTED, ONE OF EACH, BY NUMBER.

COLUMN CHOICES ARE:  CARBOWAX 20M - 1,
    OR SILICONE DC200 = 2.

CHOICE OF SAMPLE MIXTURES FOLLOWS
    (COMPOUNDS AND PARTS BY MOLE).
SAMPLE 1:  CYCLOHEXENE, 8; CYCLOHEXANE, 4;
           BENZENE, 2; HEXANE, 1.
SAMPLE 2:  OCTANE, 8; HEPTANE, 4;
           NONANE, 2;  HEXANE, 1.
SAMPLE 3:  BUTANONE, 8; TETRAHYDROFURAN, 4;
           1-PROPANOL, 2;  HEXANE, 1.

COLUMN NO. = (1 OR 2) ?1
SAMPLE NO. = (1, 2, OR 3) ?2
SELECT MIXTURE = 1 OR SINGLE COMPONENT = 2;
    (1 OR 2) ?1
COLUMN TEMPERATURE/DEG C (30<T<200) = ?50
ATTENUATOR SETTING ( >0.99, <10.01 ) = ?1

COLUMN IS CARBOWAX 20M;
TEMPERATURE = 50 DEG C.
COMPOUNDS (PARTS) ARE OCTANE (8);  HEPTANE
(4); NONANE (2); HEXANE (1).
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Figure 3. Typical input and prompting material of the program GLC, plus the text displayed below the plot in Figure 4.

CONCLUSION

Both programs LLSQPLOT and GLC have been designed to operate on the popular Apple II Plus™ microcomputers (or compatible alternatives) with at least 32 kilobytes of core memory, one disk drive, the disk operating system 3.3, Applesoft™ and a video monitor for input prompts and display. If a printer is available, then hard copies of the text and the plots may be obtained. The BASIC statements are practically machine-independent, but the graphics sections of both programs require modification to be adapted to other computers. Of the ninety statements in the program LLSQPLOT, the last quarter is used to prepare the plot. The program GLC consists of about one hundred statements, of which a quarter is data statements containing the name and parameters of each compound for each column simulated; the various sections of the program are appropriately commented to explain their function. Experience in the use of these programs, even by students lacking previous contact with computers, has demonstrated that they are easy to use and that they fulfill a pedagogically valid purpose. Both programs incorporate features not included in the other available programs with similar functions.

Listings of these programs may be obtained from the author.

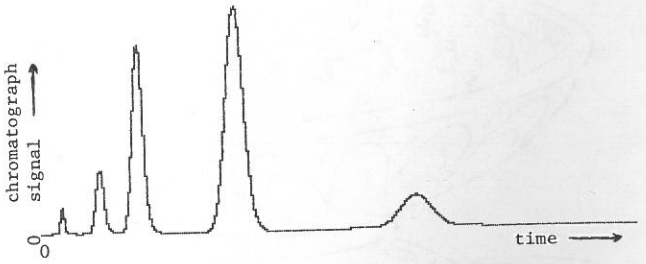

Figure 4. Plot generated by program GLC from the input shown in Figure 3.

BIOGRAPHICAL SKETCH

Born in Ottawa, Ontario, John Ogilvie was educated in the University of British Columbia and Cambridge University (England). He has held academic staff appointments in the universities of Cambridge, Newfoundland,

Kuwait and Bahrain, and has on several occasions been a Visiting Fellow in the Research School of Chemistry, Institute of Advanced Studies, at the Australian National University. Professor Ogilvie was first involved in computer-assisted learning in connection with teaching laboratories in physical chemistry in 1959; in recent years he has been keen to explore the applications of computer algebra for both scientific research and science education.

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