Scientist

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Scientist[1] is a DOS based equation modeling program that was designed to provide solutions to problems involving ordinary differential equation solving and nonlinear curve fitting and parameter estimation. The package reviewed here consists of the software and a 225-page handbook. The program requires an IBM PS/2, PC, or AT compatible computer running with DOS 3.3 or above and 2MB of RAM and at least 2MB of hard disk space (4MB recommended). Most standard graphic options are supported. A mouse facilitates use of the program, and a math coprocessor is recommended. The installation of the program is straightforward.

The program interface is a tile window type environment with pull down menus for various operations such as plot, data, parameter choice, and model equation building. In the model window, dependent and independent variables are identified and the model equation with parameters is entered in standard ASCII text format. Compiling the model detects errors in model design. A data set for the model is defined through the data menu, which opens a spreadsheet type window. Data can be imported or typed. Supported file types include ASCII, Lotus123, dBase, Quattro Pro, SYLK, Excel, and DIF. Initial values of the fitting parameters are entered through a parameter window opened by a selection in the parameter menu. Fitting and simulation follow. Fitting finds the best values for the parameters within the constraints set by the investigator. The speed and success at curve fitting depends on the initial parameters provided by the user. Simulation uses the final fitted parameters to generate the fit curve. Selecting New Plot from the plot menu displays the data with the fitted curve superimposed. On screen plots are of high quality.

The program comes with 16 sample exercises that are fully described in the manual. Of particular interest to chemistry teachers are the following: A → B → C kinetics, Michaelis–Menten kinetics, polyprotic chemical equilibrium, pK from a titration curve, and chemical oscillator.

The description of the program caused me to think that it might be useful in a physical chemistry course and laboratory. With that in mind I proceeded to work with the program to try various learning activities that I would suggest to my students. The two primary applications of particular interest for students would be in preparing graphs and curve fitting data.

Experimental data are easily entered into the Scientist program by importing an ASCII file or typing the data into the spreadsheet window of the program. The sequence of steps required for normal operation are as follows: create a model, compile the model, select a data set, select a parameter set, plot results, and print graph and/or data. For simple plots only, the data set needs to be selected and incorporated into the Scientist's spreadsheet. The spreadsheet interface is straightforward but without the freedom of interaction found in more sophisticated commercial spreadsheet programs. Entering data by hand and changing cell position were somewhat clumsy in that the enter key and arrow keys had to be used for each datum. Loading ASCII files or spreadsheet data from other programs was straightforward. Once the data are entered, a plot is easily generated. Editing the plot to show titles, axis names, and different tic marks was relatively easy. However, this type of plot is more readily handled by one of the commercially available spreadsheet programs. The number of plotters supported was adequate. Support for a HP550C DeskJet was not available so that printing of color plots was not possible. Furthermore, the available choices in the print menu resulted in only half-page or quarter-page graphs with the HP550C. I expect that hard copies of graphs printed with laser printers would be excellent.

The curve fitting features of the program were a bit more difficult to implement in a straightforward manner because a model must be specified by the user. Here, experience in choosing equations for representative curves is essential. The sample exercises can serve as templates for constructing your own equation models and adjustable fitting parameters. Compiling helps in debugging the model and putting it into the form required for the program's fitting routines. Some experience with a higher order programming language is useful for interpreting error messages generated by the compile option. After a model is created, a simulation can be done to view the shape of the curve or data can be selected and the model fitted to the data using the least-squares (modified Powell algorithm) or simplex methods. Fitting proceeds smoothly if reasonable ranges for the fitting parameters are provided by the user. This is another place where experience is important. Once a fit is obtained, a wide variety of statistic measures are computed. These include parameter statistics, analysis of residuals, and goodness of fit statistics. Most students would not use these measures without extensive coaching from the instructor.

Simulations performed with successfully fitted models generate data corresponding to the model. These data are found in a new unnamed spreadsheet window. A plot generated at this point contains both the experimental data and the simulated curve. The optimized parameters for the fitting equation appear in a new parameter window. This creates a cluttered work surface on the screen and a potential for confusion for inexperienced users, especially students. For this reason the simple window environment in this program quickly become tedious.

The Scientist program can be used to simulate chemical kinetics studies. The sample model for two consecutive irreversible first-order reactions, A → B → C, could be used to explore the effects of changing the rate constants and initial concentrations. Both the integrated and differential forms of the equations could be used in the program. If the experimental data are available, then the integrated forms of the equation could be fitted to the data and the rate constants obtained directly as fitting parameters. Other kinetics expressions could be investigated with models generated by the user. It is not hard to imagine a set of models prepared and available for use in research or teaching. However, this type of simulation suffers from the need to switch back and forth between the

plot screen and the model/parameter screen. This minimizes the effectiveness of the program for experimentation with equations and parameters. Students in particular would be frustrated by this and loose sight of the chemical significance of the exercise.

Another example in the manual was the exploration of chemical equilibria in polyprotic acid systems. In this example concentrations of all species can be modeled for student interpretation. It seems that there would be some potential use for this program in analytical chemistry courses if the instructor developed the models for students to explore.

Overall the Scientist program is probably best suited for use by mature scientists who have the need to test model equations and do simulations. Routine use in the undergraduate physical chemistry classroom or laboratory is precluded by the relatively steep learning curve for inexperienced computer users. Effective use of the program requires some experience with a higher level programming language in order to quickly correct compilation errors. Undergraduate students would need to be provided with model equations, parameter ranges, and explicit instructions in order to successfully use the program for curve fitting. The type of simulations that students would do as undergraduate exercises would be better done with a program like Mathcad if integrated forms of the equations were used. Routine laboratory reports also would be better done using one of the commercially available spreadsheet programs such as Quattro Pro or Excel, where equations and data manipulation would be expedited by a more friendly and flexible user interface for the novice. For students with greater computer experience and a need for comprehensive numerical integration of differential equations or simulations of differential equations and modeling of data on a PC, the Scientist program would be a useful tool.

REFERENCES AND NOTES

(1) Scientist is produced by MicroMath Scientific Software, P.O. Box 21550, Salt Lake City, UT 84121, (801) 943-0290. The list price of the program is $295.