## SCIENTIST®

Experimental Data-Fitting Software. Salt Lake City, UT: MicroMath Scientific Software; 1995; $395.00 complete, $149.00 upgrade.

*Scientist* is a software package from MicroMath Scientific Software intended mainly for fitting curves to experimental data. The software is readily adapted to various mathematical modeling processes in the physical/biological/chemical sciences. *Scientist* runs under Microsoft Windows on MS-DOS-based computers and appears to be a much-improved version of an earlier software package, RSTRIP, that was developed for pharmacokinetic curve fitting. *Scientist* installs quickly and easily under Windows from three floppy disks, even when the user selects to install the optional equation editor word processing software. Much of the higher level mathematical power in *Scientist* is beyond the needs of a typical, practicing nuclear medicine technologist, but the software does handle some commonly encountered, simpler mathematical problems in nuclear medicine technology. The software is useful for determining half-lives, fitting least squares straight lines, creating presentation-quality hardcopy of graphs, and scientific word processing via the *Scientist* equation editor.

One of the main purposes of this software package is to fit a mathematical model curve to a set of experimental data. For example, we have a set of experimental data representing the counts from a radioactive source as a function of time such as shown in Table 1. Before running *Scientist*, the right-most column in Table 1 is blank. We want to determine the half-life of these data points using a least squares fit curve that includes all the data points. We enter the experimental data from the first two columns of Table 1 into the *Scientist* spreadsheet. We know the model, since we know that counts versus time for these data should follow the equation of radioactive decay:

$$COUNTS = C_0 * e^{-(0.693*TIME/THALF)}$$

We then enter this mathematical knowledge as the model equations on a *Scientist* text screen as follows:

IndVars: TIME
DepVars: COUNTS
Params: C0, THALF
COUNTS = C0 * EXP(-0.693
 * TIME/THALF)

These model equations simply define the independent and dependent variables, the parameters of the model ($C_0$ and THALF, the values *Scientist* will solve for), and the equation of the model, which is the equation of radioactive decay here. The next step is to provide guess estimates for the parameters. In this case, inspection of the data produces a quick, initial guess of $C_0$ = 20,000 (the initial guess for the fitted counts at zero time), and THALF = 30 (the initial guess for the half-life based on visual inspection of the data, which appears to decrease by one half about every 30 min). Then we simply click on Least Squares Fit which causes *Scientist* to fit the model curve to the data, calculate and display the best-fit values of the parameters $C_0$ and THALF, and produce an additional data column on the spreadsheet that contains the fitted data values as shown in the right-most column of Table 1. A final mouse click on Plot will produce a presentation-quality graph that can be printed by the laser printer, such as shown in Figure 1 for data in this example. Operation is summarized as: (a) enter experimental data values into the spreadsheet, (b) specify the model equations, (c) specify initial guess for parameters, (d) perform least squares fit and (e) plot results.

There are other mathematical nuances in the fitting procedures for more complex models since the techniques used by *Scientist* are those of nonlinear least squares fitting. This means that, for complicated mathematical models, the goodness of the initial guess parameters of the model can be crucial to the fitting results. These mathematical nuances in nonlinear curve fitting are often immaterial for our needs since the typical nuclear medicine technology problem is mathematically robust, using any reasonable techniques for determining the initial guess parameters. For the sample data in Figure 1, as long as we specify that $C_0$ and THALF are positive numbers, without regard to knowing any more detail of the magnitude of $C_0$ and THALF, *Scientist* will produce the same fitted results. For users for whom this type of nonlinear model analysis seems too complicated, *Scientist* provides a single mouse option for several commonly used linear curve-fitting methods including a straight-line curve fit, polynomial curve fit, spline fit, etc. In other words, for a straight line fit, instead of going through the above manipulations for the model:

$$Y = a + b * X,$$

we can just enter data in the spreadsheet and click on Linear Fitting without having to be concerned about model equations or initial parameter values.

An alternative way, to analyze the data of Figure 1 to find the half-life, is to use *Scientist* to transform the data column from Counts to natural log (Counts). This linearizes the exponential decay, changing the model from an exponential curve to a straight line fit. *Scientist* provides an easily used transform function to calculate the natural log. Then click on a Linear Straight Line Fit to get the slope (which is equal to the decay constant in the radioactive decay equation), from which THALF follows as 0.693/slope.

An even simpler data set, such as a straight line fit or correlation between X and Y data, would be handled by just entering the X and Y data in the *Scientist* spreadsheet and clicking on linear Straight Line Fit to produce the plot of the data points with the straight line fit. Many other types of spreadsheet software packages offer least squares linear curve fitting or regression analysis, but I have not found other packages as user-friendly for this application as is *Scientist*. This is probably because curve fitting is the main purpose of *Scientist*, whereas other software packages typically have many other uses.

Another use for this software is to

**TABLE 1**
**Counts versus Time from a Radioactive Sample**

| Time (min) | Counts (cpm) | Scientist fitted (cpm) |
|---|---|---|
| 0 | 20,893 | 20,447 |
| 10 | 14,765 | 15,974 |
| 20 | 13,198 | 12,480 |
| 30 | 10,112 | 9,749 |
| 40 | 7,042 | 7,617 |
| 50 | 6,668 | 5,951 |
| 60 | 4,183 | 4,649 |

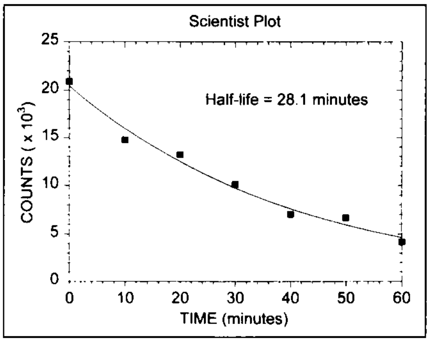


**FIGURE 1.** Presentation quality graph of counts versus time from a radioactive sample for the data in Table 1.

produce presentation-quality graphs of the type shown in Figure 1. Bar and other graphs can be plotted and the curves easily annotated with text, axes labels, etc. The plotting software may be some of the most graphically-crisp and user-friendly that I have encountered, although it may not have the power of a dedicated, but probably harder to use, software plotting package.

*Scientist* also offers a powerful and user-friendly equation editor that is the MathType equation editor from Design Science (Long Beach, CA). This is the same equation editor that is used with Microsoft Word and will be familiar to MSWord users. The equation editor is basically a scientific word processor, intended for creating complex mathematical equations to be inserted into user's word processing document or onto the *Scientist* plot. The equations can contain mathematically specific symbols such as the summation symbol, integrals, derivatives and complicated algebraic expressions. This is of interest to users engaged in scientific/mathematical word processing who may not have access to an equation editor in their own word processing software.

*Scientist* accommodates users with a greater mathematical appetite. Any mathematical function can be typed into a model and Scientist readily produces a plot of the specified model, called a simulation. For example, entering the mathematical equations for the activity of $^{99m}Tc$ in a $^{99}Mo/^{99m}Tc$ generator can be used to produce a graph and spreadsheet values of the activity of $^{99m}Tc$ to be expected in the generator on an hourly basis throughout the week. Calculus functions make *Scientist* able to solve differential equations and produce simulation plots of the results. *Scientist* fits the solution of a differential equation to a set of experimental data. Laplace transform analysis is offered in some detail to aid in problems involving differential equations. These more complicated mathematical abilities and simulations are a boon to the student who wishes to analyze a mathematical model of a physical/biological/chemical process to concentrate on the results of the model, without being concerned with the mathematical drudgery of how the solution was obtained. *Scientist* offers several other mathematically complex capabilities, such as fast Fourier transform (FFT) analysis. Successful use of these higher mathematical capabilities depends upon the user's ability to comprehend this level of mathematical analysis. The operator's manual cannot be used as a tutorial for functions such as Fourier Transforms.

As with most software packages, there are drawbacks with *Scientist*. Some level of mathematical sophistication is needed to use this software for curve fitting or model simulation. The *Scientist* operator's manual states that this is a software package for researchers who "know what's going on" with their data. Many of us don't know what is going on with our data and wish that the computer would tell us what's going on. The uses for simple plotting or equation editing require less sophistication. Familiarity with Windows is a necessity and experience with spreadsheet or plotting software is a plus. I was up and running with the radioactive decay curve data shown here in just about 30 min by following the installation instructions and the examples in the manual. There are aggravating shortcomings in the operator's manual, such as a poor index. For example, the index indicates that the Equation Editor can be found only on page 163, whereas it actually occupies all of Chapter 8, pages 247-330. Although the software is intended for curve fitting, there are few curve graph illustrations in the manual.

I cannot recommend this package for its general statistical capabilities as it is inadequate for most analysis needed in nuclear medicine. Most of the statistics relate to the goodness of the fitting process and to producing statistics such as mean, standard deviation and the linear correlation coefficient. Unfortunately, although functions such as the linear correlation coefficient are produced by the software, the probability of the correlation is not produced. The user is left dangling or to look up the P-value in a statistical table. Other commonly used statistical functions, such as t-tests and chi-squared analysis and their probability values, are completely absent.

One strength of the *Scientist* package lies in curve fitting or simulation for mathematically complex problems, which are most likely to be useful to scientists or mathematically sophisticated users. Another strength is its curve fitting for simpler mathematical problems, such as straight line fits which is useful for many nuclear medicine technology problems. The package also provides user-friendly graph production and an equation editor in scientific word processing. Other software packages that are similarly useful for nuclear medicine technologists are Microsoft Excel, for spreadsheets, statistics and limited plotting, and Jandel Scientific Sigmaplot, for powerful but less easily used plotting.

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## RADIATION SCIENCE AND SOCIETAL DECISION-MAKING

Proceedings of the Twenty-Ninth Annual Meeting of the National Council on Radiation Protection and Measurement, No. 15. Leonard A. Sagan, ed. Bethesda, MD: NCRP; 1994, 329 pp, $40.00.

This latest edition of the excellent series of annual meeting proceedings of the National Council on Radiation Protection and Measurement (NCRP) reflects the departure from the previous meetings' format. Rather than a single lecturer discussing a pertinent topic at length, the NCRP Program Committee organized a series of presentations on the subject of radiation science and societal decision-making by a number of leading psychologists, radiation scientists, decision makers and regulators. These presentations were followed by four case studies that were reviewed in a panel discussion. The papers and the panel discussions form the content of the proceedings.

Each of the presenters does a credible job of framing the complex issue of risk management in radiation science. The background materials and the bibliographies provided by the guest lecturers are extensive. Several of the speakers recognize that there are "no win" issues and the bottom line is that better education and improved communication will help everyone. This book may provide useful preparation to those in the radiation medicine community who need to respond to our critics.

This publication also includes the Seventeenth Taylor Lecture, "Science, Radiation Protection and the NCRP," delivered by Dr. Warren K. Sinclair. The Taylor Lecture, which honors Dr. Lauriston S. Taylor, the first president of the NCRP, is an annual part of the NCRP meeting.

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