Nonlinear Parameter Estimation Using Spreadsheet Software

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ABSTRACT

Many fundamental processes in the natural and physical sciences exhibit substantial nonlinear relations among the component variables. Instructing students on how to identify parameters in models for such relations based on measured data, and providing a means to illustrate the impacts of specific components on the *behavior* of nonlinear relationships, is therefore a critical element of university science training. Commercially available spreadsheet software programs offer convenient and effective means for performing nonlinear parameter estimation. Among the advantages of the spreadsheet approach to nonlinear optimization and parameter estimation are its relative ease of use, general applicability, demonstration or reinforcement of least-squares principles, and the ability to interactively alter selected parameter values and immediately view the results via embedded graphics. In this paper we provide a brief discussion of nonlinear least-squares optimization, demonstrate its application within the context of some commercial spreadsheet software packages, and illustrate some of the capabilities of this approach using examples from our respective upper division Soil Physics lecture/laboratory courses. Our experiences indicate that students learn spreadsheet techniques more readily than often specialized mathematical or statistical programs, and that they provide a valuable tool in their future endeavors.

$\mathbf{M}$ANY fundamental processes in soil physics exhibit highly nonlinear relationships among the component states and/or rates. This is true of many other disciplines as well. The ability to determine or estimate the value of component parameters is a critical aspect in the practical application of these relationships, and thus is an important aspect of university instruction. Effective parameter estimation typically requires use of numerical optimization techniques or specialized software (e.g., SAS, MathCAD, Mathematica)[1]. However, recent versions of many commercial spreadsheet software programs offer powerful and flexible means of performing nonlinear optimization. This offers a functional alternative to the use of more specialized mathematical or statistical software, while providing skills and abilities having potentially much wider application to students' future endeavors. We have found through conversations with colleagues at other institutions that, although many of them use commercial spreadsheets extensively in teaching and research, the capacity to perform advanced

[1] Mention of company names or products is for the convenience of the reader and does not imply endorsement by the authors or their respective institutions.

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nonlinear optimization within this context is not well recognized. A contributing factor may be the fact that explicit instructions or potential applications are generally not emphasized in the spreadsheet software manuals.

We encourage our students to use spreadsheet software extensively. Specific applications include homework problem sets and a variety of laboratory exercises. Advantages of spreadsheets for these assignments include their general facility for data entry and/or transfer from other sources, data management, ease in performing simple or complex calculations, and often advanced graphics and reporting capabilities. These provide an effective tool for student use in many other venues, as well as for the immediate demands we place on them.

Our objectives in this paper are to outline the methods of performing nonlinear parameter optimization using the commercial spreadsheet software with which we are most familiar, to illustrate the approach using a few specific examples from our courses, and to discuss advantages of this approach relative to the use of more specialized mathematical/statistical software packages. Our treatment of nonlinear optimization itself is intended to serve only as a brief overview of the subject, and of the relevant options commonly available in the spreadsheet environment. More exhaustive treatments are available elsewhere (e.g., Press et al., 1986; Luenberger, 1984).

GENERAL APPROACH

Nonlinear Optimization by Least Squares Minimization of an Objective Function

In nonlinear parameter estimation we wish to fit N data points $\{(x_i, y_i); i = 1,\dots,N\}$ to a model having M adjustable parameters $\{a_j ; j = 1,\dots,M\}$. The functional relationship predicted by the measured independent and dependent model variables is then (Press et al., 1986)

$$y(x) = y(x;\mathbf{a}) \qquad [1]$$

A merit function is often defined to measure the agreement between the data and model (usually, small values in the merit function represent close agreement). The best fit parameters are obtained by adjusting the model parameters to achieve the minimal merit function value. The most common approach to the problem of parameter estimation is the Gaussian least-squares minimization, where the merit function to be minimized is the sum of squared error terms,

$$\chi 2\,(a) = \sum_{i=1}^{N} [y_i - y(x_i;a_1\dots a_M)]^2 \qquad [2]$$

with $\mathbf{a} = a_1,\dots a_M$, the vector of model parameters. With nonlinear model dependencies, the minimization must proceed

Abbreviations: SSE, sum of squared errors; CDE, convection–dispersion (model) equation.

iteratively (i.e., there is no closed-form solution) starting with a set of initial or trial parameter values denoted $\mathbf{a_0}$. At each iteration, the trial solution is improved until the $\chi^2(\mathbf{a})$ effectively stops decreasing. The challenge from a mathematical point of view is to devise efficient methods for minimization of the merit function $\chi^2(\mathbf{a})$. Most algorithms rely on approximation of the merit function χ^2 by its second order Taylor series about $\mathbf{a_0}$:

$$\chi^2(a) \approx \gamma - da + \frac{1}{2}\ \mathbf{aDa} \qquad [3]$$

where $\mathbf{d} = \nabla\chi^2|_a$ is an M vector (the gradient of χ^2), $\mathbf{D}$ is an $M \times M$ Hessian matrix with

$$[D]_{ij} = \frac{\partial^2 (\chi^2)}{\partial a_i \partial a_j}|_a,$$

and $\gamma = \chi^2(\mathbf{a_0})$ is a constant. The minimization schemes differ in the way information is used to drive the iterative process, or in finding *better* estimates of $\mathbf{a}$ than the current one in pursuit of a minimum $\chi^2(\mathbf{a})$. One of the most efficient schemes for minimization in the least squares context is the Levenberg-Marquardt algorithm (Press et al., 1986). Because the optimization routines in commercial spreadsheets are designed to efficiently handle a broader class of problems than solely least squares minimization, the algorithms used are somewhat less efficient in their minimization search and updating schemes for least-squares problems than the Levenberg-Marquardt. This has little effect on the solution to the minimization problem and the user may choose between *conjugate gradient* or *Newton* (*variable metric*) methods, both of which are considered equal alternatives for the multidimensional minimization problem (Press et al., 1986, p. 277).

Brief Description of the Optimizer

Recent versions of several commercial spreadsheet software programs include convenient and effective nonlinear optimization tools. We will focus on those in Quattro Pro and Excel, with which we are most familiar. The nonlinear optimizers in current versions of Quattro Pro, Excel, and Lotus 1-2-3 are nearly identical in terms of overall approach, options, and even menu structure. This facilitates a common instructional approach while providing students some flexibility in their choice of software based on previous experience, general preference, or availability/accessibility. The initial optimizer (*solver* in Excel) menu panel includes input locations to specify the solution or target cell location, and whether the goal is to maximize, minimize, or attain a specific value for this cell. The location of the variable cell(s) whose value(s) may be altered to achieve the desired target cell goal is specified, and constraints may be imposed on any cells involved in the problem (Fig. 1). Constraints take the form of a relationship among a variable, an arithmetic operator ($\leq$, $=$, $\geq$, integer), and a constant. An example might be (variable cell) D4 $\geq$ 1 (Fig. 1b); a given cell may be assigned up to two constraints, for example to bracket allowable values between lower and upper limits.

Several options are available to control or fine tune the optimizer. The maximum time, maximum iterations, preci-

sion, and tolerance of the iterative optimization process may be specified. For one-dimensional minimization (a subalgorithm), a user may use a tangent or quadratic approach to obtain the local minimum of basic variables in each iteration. Forward or central (finite) differencing options are available for estimates of partial derivatives (this is particularly important for an unspecified model structure). The search directions and updating schemes based on conjugate gradient or variable metric (Newton) methods may also be specified. We find that the default settings work well for most parameter estimation problems, but students or instructors may wish to explore conceptual or practical differences among these approaches. Once an optimization model has been developed using these menu options, it may be saved and subsequently reloaded from a user-specified location in the spreadsheet. The concepts described above will be illustrated in the following section using examples taken from our laboratory courses.

APPLICATIONS IN THE SPREADSHEET ENVIRONMENT

Stepwise Approach to Parameter Estimation of Soil Water Retention—Illustrative Example

A soil water retention curve describes the functional relationship between soil water content (θ) and matric potential (ψ) under equilibrium desorption conditions. It is an important soil property affected by soil structure and texture, and is critical for computer simulation modeling, estimating unsaturated hydraulic conductivity, and for related applications where inference of ψ based on θ or vice versa is required. A retention curve is a highly nonlinear function, and is relatively difficult to obtain accurately. Measured θ–ψ pairs are often fragmentary, and usually constitute relatively few measurements over the wetness range of interest. It is therefore beneficial to represent retention curves in a continuous and parametric form. An effective and commonly used retention model was proposed by van Genuchten (1980):

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)[1 + (\alpha|\psi|)^n]^{-m} \qquad [4]$$

where ψ is the matric potential, θ_r and θ_s are the residual and saturated water contents, respectively, and α, n, and m are fitting parameters directly dependent on the shape of the $\theta(\psi)$ curve. A considerable simplification is gained by assuming that $m = 1 - 1/n$. Thus, the basic model parameters are: θ_r, θ_s, α, and n. Because θ_s is often known and reliable values may be easily obtained experimentally, only three unknown parameters often need be estimated from the measured data.

Estimating retention curve parameters from experimental data requires: (i) sufficient data points (at least 5 to 8 θ–ψ pairs); and (ii) a program for performing nonlinear parameter estimation. The steps for fitting van Genuchten's retention equation to experimental data in Quattro Pro follow; these are nearly identical to those for Excel. The basic procedures will be the same for fitting other parametric models, or for any nonlinear least squares optimization of equation parameters to measured data.

1. Enter the measured data in two columns corresponding to θ and $|\psi|$.
2. Establish a cell for each parameter in the model (θ_s, θ_r, α, n, m), and assign an initial value (estimate) to each. Note that reasonable initial estimates for all variables are often critical for proper convergence of nonlinear models. That is to say, if initial estimates are not reasonably near their true values, the fitting algorithm may converge on a local rather than the true global minimum, or even fail to converge on a solution at all. Consulting the literature for reasonable initial estimates may be appropriate in some cases.
3. Write the desired prediction model (i.e., equation) in a third column. Refer to the preassigned cells containing
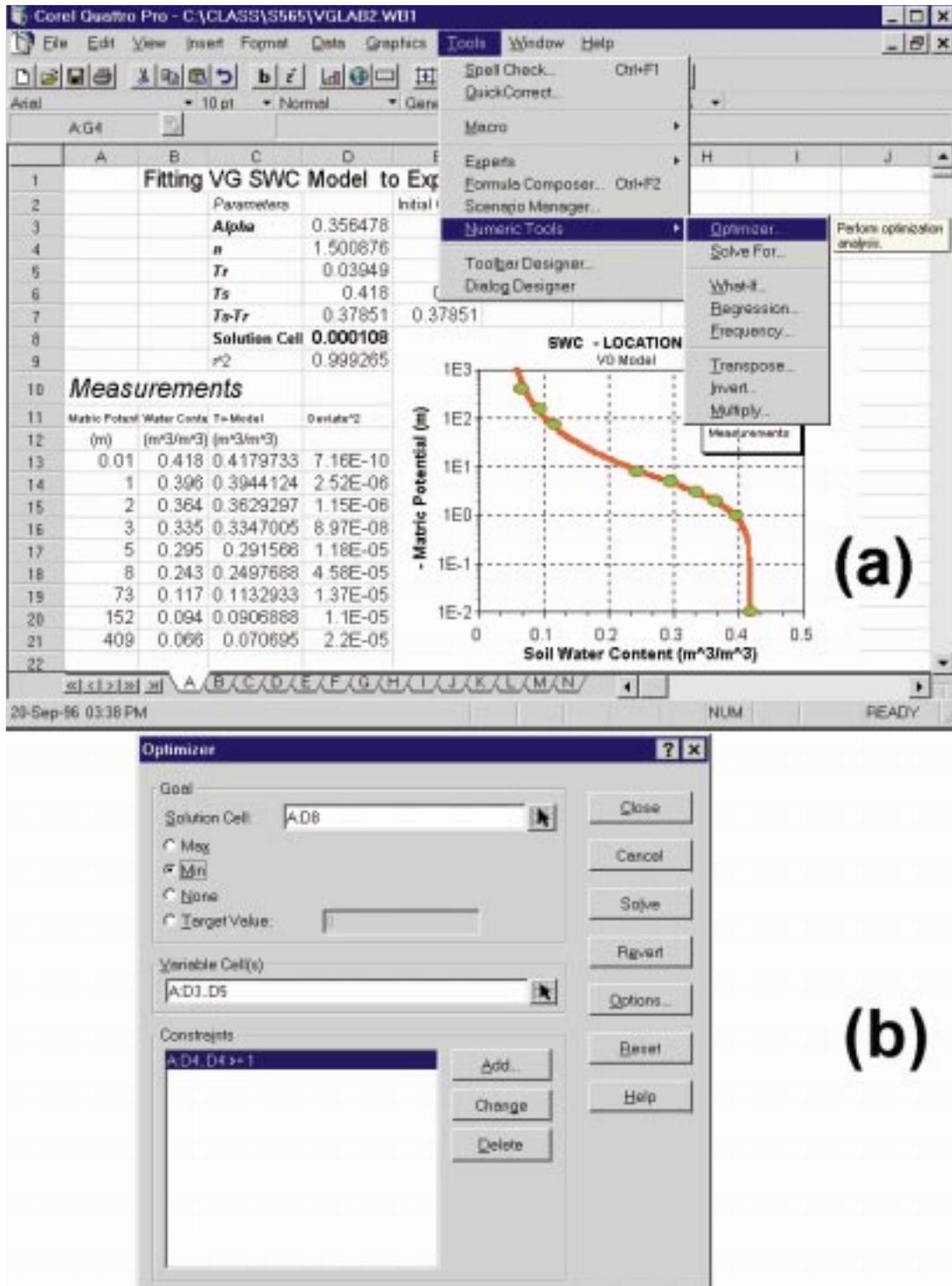

Fig. 1. (*a*) menu structure for the optimizer in Corel Quattro Pro (v. 7); and (*b*) the optimizer menu for defining the solution cell, variable range, and constraints.

your initial guesses for the fitting parameters, and to measured θ or ψ cells where appropriate in the equation. Note that Eq. [4] may be stated in terms of ψ(θ) as:

$$|\psi(\theta)| = \frac{1}{\alpha}\left[\left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{-1/m} - 1\right]^{1/n} \qquad [5]$$

We will assume for the current exercise that we are using Eq. [4]. The third column will thus contain predicted θ values (θ_{model}) for each measured value of |ψ|.

4. Form in a fourth column a deviate (or error) squared between θ and θ_{model}, i.e., $(\theta_{measured} - \theta_{model})^2$, for each data point.

5. Establish a cell containing the sum of squared deviations (errors) between measured and predicted values (sum the entire column of error-squared values using the @SUM() function). This is the merit function to be minimized.

6. Apply the nonlinear solver (Optimizer) to the problem by minimizing the sum of squared errors (SSE) cell using variable cells as defined in Step 2. You should include the following constraints: $0 \le m \le 1$, $\theta_r \ge 0$. The spreadsheet

menu structures for performing these steps are illustrated in Fig. 1.

7. Compute the *variance* of the measured θ column (another *built-in* spreadsheet statistical function). The coefficient of determination (r^2) for the resulting curve fit may then be calculated using:

$$r^2 = 1 - \frac{SSE}{N\,\sigma_\theta^2} \qquad [6]$$

where σ_θ^2 denotes the variance of the measurements on the independent variable, θ. The @COUNT() function may be used to incorporate the number of data points, N, in Eq. [6]. Note that you may maximize the r^2 value as an alternative to minimizing the SSE in the Optimizer. An alternative to Eq. [6] is to use the @CORREL(array1, array2) function.

A modification that is sometimes useful is to assign a column of weights (e.g., ≠ 1) to the right of the squared errors (Step 4 above), and multiply the original squared errors by higher weights for data points you wish the fit-

Nonlinear Optimization of Water Retention Data to van Genuchten's Eq.

Fitting parameters

Step 2		
theta_r	0.029	
theta_s	0.403	
alpha	2.917	
n	1.576	
m=1-1/n	0.365	

	Step 5	Step 7	
	SSE	Var.	r²
	0.000587	0.014899	0.99821

Step 1		Step 3	Step 4
Matric Pot. [-m]	Measured Wtr. Cont.	Modeled Wtr. Cont.	Squared error
440.00	0.03	0.0346	2.11E-05
170.00	0.04	0.0390	9.36E-07
70.00	0.05	0.0460	1.56E-05
34.00	0.06	0.0551	2.42E-05
13.00	0.08	0.0747	2.84E-05
4.50	0.10	0.1131	0.000172
3.30	0.12	0.1292	8.54E-05
2.59	0.14	0.1438	1.43E-05
2.09	0.16	0.1582	3.32E-06
1.68	0.18	0.1744	3.18E-05
1.34	0.20	0.1927	5.31E-05
1.06	0.22	0.2133	4.45E-05
0.78	0.24	0.2422	4.83E-06
0.64	0.26	0.2614	2.08E-06
0.53	0.28	0.2798	5.97E-08
0.43	0.30	0.2995	2.91E-07
0.34	0.32	0.3201	8.18E-09
0.26	0.34	0.3408	6.44E-07
0.18	0.36	0.3632	1.03E-05
0.10	0.38	0.3853	2.83E-05
0.03	0.40	0.4003	1.13E-07
0.00	0.41	0.4032	4.57E-05

Water Release Curve linear-scaled potential
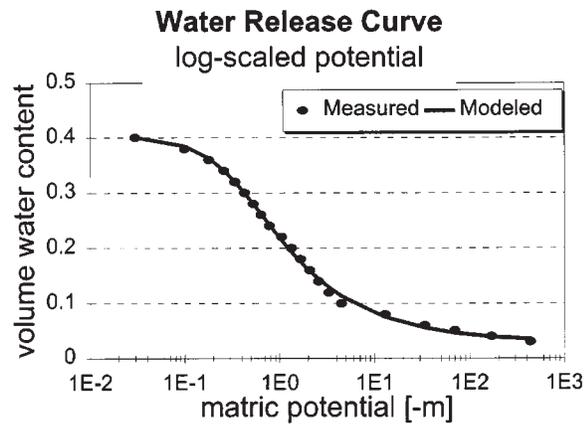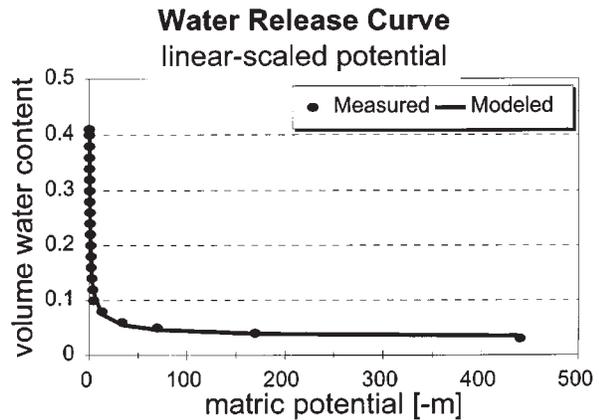

Water Release Curve log-scaled potential

Fig. 2. Spreadsheet for optimization of van Genuchten (1980) equation parameters to measured soil water retention data. Step labels correspond with the description in the text.

ted relationship to be forced through, or to which greater emphasis should be placed (e.g., when data of varying degrees of reliability are being used). Then make the sum of these weighted deviates squared (or the r^2 based on these) the solution cell to be minimized (maximized). This approach may also be effective in cases where a range of substantially greater numeric values in the measured data dominate the error squared term, thus making it desirable to decrease their overall effects on the optimization process by assigning smaller weighting factors.

Figure 2 illustrates a spreadsheet page developed by a former student as part of a laboratory report covering measurement and characterization of soil water retention. Best-fit values for parameters of van Genuchten's (1980) equation were evaluated for a series of measured $\theta(\psi)$ data pairs. Embedded graphics provide immediate feedback for the student, and confirm the goodness-of-fit for student and instructor.

Additional Example Applications

Among the other applications of this technique in our laboratory courses are fitting nonlinear empirical or theoretical parametric expressions to measured data for one-dimensional infiltration and for miscible displacement of nonreactive solutes. We briefly explore each of these here to provide examples of the sort of disciplinary problem solving that may be easily presented to students having little previous experience or training in nonlinear optimization. Finally, we illustrate the important ability to interactively alter the value of selected equation parameters and view their effects using embedded graphics.

One-Dimensional Infiltration into Initially Dry Soil

An important class of flow events involves downward water movement through the soil surface in a process known as infiltration. The rate of this process relative to the rate of water supply determines how much water will enter the soil, and how much (if any) will pond and perhaps create overland flow (runoff). Based on field observations, the infiltration rate (denoted as i) is found to be dependent upon the initial soil water content, the hydraulic conductivity of the surface soil, and the elapsed time since the onset of water application. In most situations the infiltration rate is highest when water first enters the soil, and gradually decreases with time until a constant final rate is attained. This behavior is also reflected in the cumulative infiltration (I) showing a rapid increase in the volume of infiltration at short times, then decreasing gradually to a nearly linear time dependence at large times.

Based on a predictable and well-behaved shape of the infiltration rate vs. time relationship, several functions having shapes similar to the expected behavior have been proposed as predictive equations. Attempts were later made to attach physical significance to the various parameters of these empirical equations. Philip (1957, 1969) presented the first analytical solution to the Richards equation for vertical and horizontal infiltration. For vertical infiltration, Philip's solution describes the time dependence of cumulative infiltration as an infinite series in powers of $t^{1/2}$. In practice, the

series is truncated and only the first two terms are retained, resulting in the following equations:

$$\text{Cumulative: } I = St^{1/2} + At;$$

$$\text{Rate: } \frac{dI}{dt} = i = \frac{1}{2}St^{-1/2} + A \qquad [7]$$

where S is the sorptivity, t is time since water application, and A is a coefficient dependent upon the soil properties and on initial and boundary water contents. The first term in each describes the influence of the sorptive forces of (relatively) dry soil, and the second term the contribution of gravity. The influence of the first term diminishes with time and reflects the reduction in the hydraulic gradient as the surface soil becomes wetted.

In the laboratory exercise, a permeameter is used to supply water to the top of a cylindrical column packed with air-dry soil. The elapsed time, wetting front position with respect to the soil surface (i.e., depth of wetting front), and the water level in the permeameter reservoir are monitored at predetermined time intervals during the experiment using a ruler and stopwatch. Changes in reservoir water level are subsequently converted to depth of water infiltrated across the soil surface area based on diameters of the water reservoir and soil column. From the measured data, cumulative infiltration, infiltration rate, and wetting front depth are calculated with respect to time. These relationships are then used to derive the relevant parameters in Eq. [7] (as well as for several empirical and quasi-analytical infiltration relationships), and plots of measured vs. predicted infiltration (cumulative, rate) and wetting front position are developed (e.g., Fig. 3).
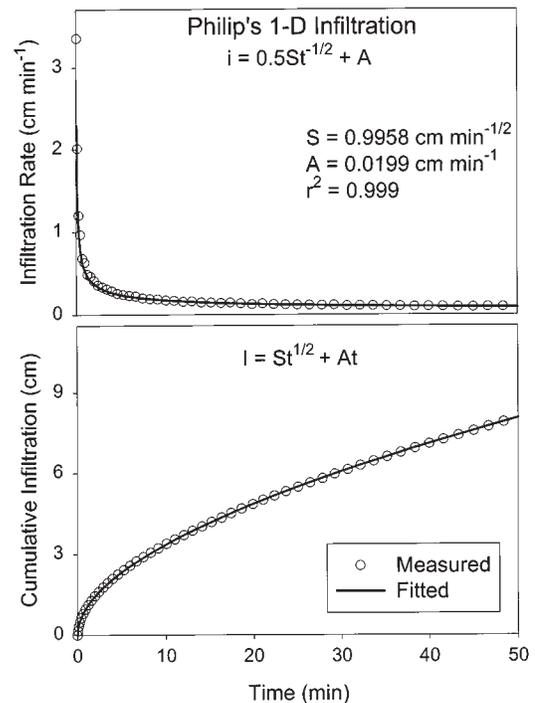
Fig. 3. (*top*) Measured and predicted one-dimensional infiltration rate and (*bottom*) cumulative infiltration into an initially dry soil column.

Estimation of Convection–Dispersion Model Parameters from Measured Breakthrough Curves

When a solution of different chemical concentration from the resident soil solution is passed through the soil, the chemical concentration in the composition of drainage water (effluent) will gradually change. The process of replacing the resident soil solution with a different solution is termed miscible displacement and is demonstrated by the leaching of salts, the distribution of fertilizer, pesticides, waste products, and other chemicals, and the use of tracers for following water movement through porous materials. By measuring the concentration change of the effluent of a soil column, information about the transport properties of the porous soil medium and the behavior of the solution moving through the soil can be obtained.

The convection–dispersion (model) equation (CDE) is often used to describe solute transport through soils. A common form of the CDE is:

$$R \, \frac{\partial c}{\partial t} = D \, \frac{\partial^2 c}{\partial x^2} - v \, \frac{\partial c}{\partial x} \qquad [8]$$

where c is solute concentration, t is time, D is the dispersion coefficient, v is pore water velocity, R is the retardation factor ($R = 1$ means no interaction of the solution with the solid matrix), and x represents a spatial coordinate (distance). Analytical solutions to Eq. [8] have been developed for a number of specific initial and boundary conditions, and many important soil science problems involve estimating solute transport parameters based on fitting analytical solu-

Miscible Displacement - Kidman Sand Using Step Solute Application

					Fitting Parameters		
Area of column		21.2	cm^2				
Flow rate		0.02	cm/s	P	30.98887		
Volume water content		0.42		R	1.308675		
Flow velocity (v)		2.88	cm/min	D	1.812263	cm^2/min	
Column length		19.5	cm				
				SSE	0.0017		
				r^2	0.999483		

| Time (min)	EC (dS/m)	Measured C/Co (rel. EC)	Cumulative outflow (cm^3)	T=vt/L	u	Predicted	Error^2
1	0.19	0.000	21.4	0.148	7.3503	0.0000	2.08E-43
2	0.285	0.002	44.6	0.295	4.5362	0.0000	6.09E-06
3	0.294	0.003	67.2	0.443	3.1640	0.0000	7.27E-06
4	0.294	0.003	90.3	0.591	2.2726	0.0007	4.19E-06
5	0.461	0.007	114.4	0.738	1.6145	0.0112	1.74E-05
6	2.32	0.055	135.9	0.886	1.0921	0.0612	3.52E-05
7	6.98	0.176	158.7	1.034	0.6576	0.1762	2.11E-08
8	13.4	0.343	181.5	1.182	0.2846	0.3437	4.18E-07
9	20.3	0.522	204.9	1.329	-0.0434	0.5245	5.09E-06
10	26.3	0.678	228.3	1.477	-0.3368	0.6831	2.59E-05
11	31.8	0.821	251.4	1.625	-0.6031	0.8031	0.000313
12	34.9	0.901	274.5	1.772	-0.8473	0.8846	0.00028
13	35.7	0.922	299.8	1.920	-1.0734	0.9355	0.00018
14	37.3	0.964	321.2	2.068	-1.2843	0.9653	2.86E-06
15	36.9	0.953	345.8	2.215	-1.4822	0.9820	0.000824
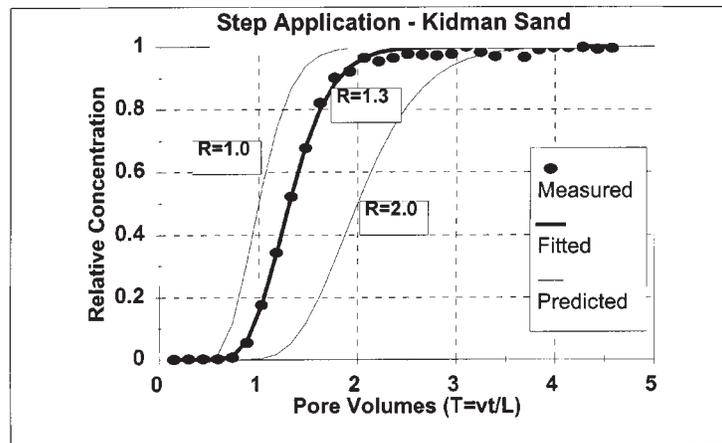
Fig. 4. Portion of nonlinear optimization spreadsheet for miscible displacement laboratory exercise with embedded graphic. The potential for visual feedback concerning the impacts of various parameters is illustrated by the predicted breakthrough curves for $R = 1.0$ and $R = 2.0$.

tions of the CDE or alternative models to measured breakthrough curves from miscible displacement experiments. Butters and Bandaranayake (1993) have provided an excellent discussion of this approach in the context of Soils laboratory instruction.

The solute concentration distribution in a soil column with uniform initial (resident) concentration c_i under steady state flow replaced at $t = 0$ with a solution of constant concentration c_0 is amenable to an analytical solution. The initial and boundary conditions are given by:

$$c(x,0) = c_i$$
$$c(0, t) = c_o \qquad [9]$$
$$\frac{\partial c}{\partial x}(\infty, t) = 0$$

The solution to Eq. [8] subject to these initial and boundary conditions is (Nielsen and Biggar, 1963; van Genuchten and Wierenga, 1986):

$$\frac{c(x,t) - c_i}{c_0 - c_i} = \frac{1}{2}\ erfc\left[\frac{Rx - vt}{\sqrt{4DRt}}\right] + \frac{1}{2}\ e^{vx/D}\ erfc\left[\frac{Rx + vt}{\sqrt{4DRt}}\right] \quad [10]$$

where $erfc(u)$ is the complementary error function and the remaining components were defined previously. Many spreadsheet software programs include a built-in $erfc(u)$ function. Note that when u assumes negative values, $erfc(u)$ will return an error message. To overcome this potential problem the relationship $erfc(-u) = 1 + erf(u)$, based on the identities $erfc(u) = 1 - erf(u)$ and $erf(-u) = -erf(u)$, may be used within an @IF() statement. Other transformations are also available.

A simpler solution commonly used in displacement experiments is obtained by retaining only the first term on the right-hand side of Eq. [10]:

$$\frac{c}{c_o} = \frac{1}{2}\ erfc\left[\frac{Rx - vt}{\sqrt{4DRt}}\right] \qquad [11]$$

for negligible c_i. The solution presented in Eq. [11] may be derived by either neglecting molecular diffusion, or by considering an infinite system ($-\infty < x < \infty$).

The laboratory exercise involves changing the inlet solution salt concentration to a soil column during saturated, steady vertical flow. The electrical conductivity (a rapidly and easily obtained measure of salinity) is monitored for discrete fractions of the column outflow, to produce the breakthrough curve for the saline solution. Transport parameters D, R, and v are then estimated based on optimization of the measured data to Eq. [11]. Figure 4 shows a portion of a student's worksheet which addresses this problem. Cassel and Elrick (1992; Example 3) illustrated the use of MathCAD for nonlinear optimization of a similar miscible breakthrough problem.

Visual Feedback Concerning the Impacts of Nonlinear Coefficients

Visual feedback concerning the specific effects or impacts of individual or combinations of equation parame-

ters is an effective means of communicating the *feel* of often complex nonlinear equations integral to the natural and physical sciences. This may be easily accomplished as part of the sort of instructional exercises noted above. Students may choose to interactively alter the value of single or multiple equation parameters, and view the resulting changes in one or more embedded graphic charts. Alternatively, a number of predicted graphic series may be produced by copying the range of cells containing the model equation, and referencing a specific set of nonlinear parameters for each series. An example of the latter approach as applied to the CDE is presented in Fig. 4, where predictions based on two values for the retardation factor (R), which bracket the optimal solution have been included, and their effects on the resulting predicted chemical breakthrough curve are visually evident.

SUMMARY AND CONCLUSIONS

Many commercial spreadsheet software programs offer convenient and effective means to perform nonlinear parameter estimation. Among the advantages of the spreadsheet approach to nonlinear optimization and parameter estimation are its relative ease of use, general applicability, demonstration or reinforcement of least-squares principles, and the ability to interactively alter selected parameter values and immediately view the results via embedded graphics.

Our experiences indicate that our students are able to learn rudimentary and advanced spreadsheet techniques more easily than for often specialized mathematical or statistical programs, and that very few possess requisite programming skills to develop their own parameter estimation routines. Several former students have indicated that their exposure to basic and advanced spreadsheet skills, including nonlinear parameter estimation, have proven to be among the most valuable tools gleaned from our courses. They have gainfully applied these tools in other university courses, in their own research, and in a variety of employment opportunities following graduation.

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