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PARAMETER ESTIMATION FOR UNSATURATED FLOW AND TRANSPORT MODELS — A REVIEW

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ABSTRACT

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This paper reviews the current status of parameter estimation techniques and their utility for determining key parameters affecting water flow and solute transport in the unsaturated (vadose) zone. Historically, hydraulic and transport properties of the unsaturated zone have been determined by imposing rather restrictive initial and boundary conditions so that the governing flow and transport equations can be inverted by analytical or semi-analytical methods. Contrary to these direct methods, parameter estimation techniques do not impose any constraints on the model, on the stipulation of initial and boundary conditions, on the constitutive relationships, or on the treatment of inhomogeneities via deterministic or stochastic representations. While parameter estimation analyses of subsurface saturated flow are increasingly common, their application to unsaturated flow and transport processes is a relatively new endeavor. Nevertheless, a number of laboratory and field applications currently exist that show the great potential of parameter estimation techniques for improved designs and analyses of vadose zone flow and transport experiments. Several practical examples for determining unsaturated soil hydraulic functions and various transport parameters are presented, and advantages and limitations of the estimation process are discussed. Specific research areas in need of future investigation are outlined.

INTRODUCTION

Increasing demands on groundwater resources have greatly accentuated the need for accurate predictions of subsurface flow and chemical transport to evaluate effects of management practices and alternatives for contaminant remediation. Computer simulations based on numerical models have been increasingly used for these purposes, a trend that undoubtedly will continue as more sophisticated models are being developed and computer costs keep decreasing. However, with greater model sophistication comes a need for more intensive data requirements, and real improvements in precision will eventually hinge on our ability to accurately determine the required model parameters. Difficulties in model calibration are nowhere more evident than in analyses of water and chemical transport in the unsaturated (vadose) zone. Since most groundwater contaminant sources originate in the unsaturated zone, proper understanding and management of this zone is essential to

protecting or improving the quality of groundwater supplies. Model calibration in the vadose zone may be especially difficult because of problems in formulating accurate constitutive relationships for multiphase flow.

Hydraulic and transport properties of the unsaturated zone are commonly determined by imposing rather restrictive initial and boundary conditions so that the governing equations can be inverted by analytical or semi-analytical methods. Such procedures allow direct computation of the specific functional form of deterministic model coefficients. A multitude of laboratory and field methods currently exist (Klute, 1972; Bouwer and Jackson, 1974) that have found great utility in the study of unsaturated flow and transport processes. Unfortunately, these direct inversion methods also have a number of limitations which restrict their practicality, in particular when used for calibrating field-scale models. Experimental analyses based on direct methods are generally quite time-consuming and hence costly owing to the need to meet conditions requisite for the explicit calculation of model coefficients. For example, in some procedures it is necessary to repeatedly achieve steady-state or equilibrium hydraulic conditions for different boundary conditions. Often the governing equations themselves also need to be linearized or otherwise approximated to allow their (semi-)analytical inversion. Another limitation results from the need to impose relatively simple initial and boundary conditions. This is especially problematic for field experiments where accurate control of the boundary conditions on a large scale can be difficult and expensive. Given the inadequacy of most currently available models to describe field-scale behavior, options to deal with spatial heterogeneity in more than a superficial manner are also severely curtailed by the direct inversion requirement. Finally, information concerning parameter uncertainty is not readily obtained from direct inversion techniques.

An alternative and more flexible approach to solving the inverse problem is to employ parameter estimation techniques. In this approach, the direct problem is posed for prescribed but arbitrary initial and boundary conditions, while the physical problem itself can be solved with any appropriate analytical or numerical method. The constitutive relations thought to be applicable to the system are parameterized based on a-priori knowledge, and the coefficients determined by means of an optimization algorithm that extremizes some objective function (e.g., to minimize deviations between observed and model-predicted output). Contrary to direct inversion methods, the optimization approach does not put any inherent constraint on the form or complexity of the model, on the stipulation of the initial and boundary conditions, on the constitutive relationships, or on the treatment of inhomogeneities via deterministic or stochastic representations. Thus, a major advantage is that experimental conditions can be selected on the basis of convenience and expeditiousness, rather than by a need to simplify the mathematics of the direct inversion process. Also, if information concerning parameter uncertainty and effects or model accuracy is desired, it can be obtained from the parameter estimation analysis with little additional effort.

What one sacrifices for the flexibility of the parameter estimation method is an ability to determine the specific form of the constitutive properties of the system. One must assume some model formulation which is presumed to hold to a sufficient degree of approximation. If more than one possible parameterization is deemed feasible, the problem of parameter identification arises which involves performing the estimation analyses for many possible models, and selecting from those models the most accurate or precise one in terms of some objective criterion. Here, we will deal primarily with the parameter estimation problem and only peripherally with the problem of parameter identification. Clearly, if the adopted parametric model does not accurately represent the behavior of the system, then results of the parameter estimation analysis will be of dubious utility.

Other sources of parameter uncertainty are related to the ill-posedness of many inverse problems. A problem is ill-posed when it has either no solution at all, no unique solution, or the solution is unstable (Isaacson and Keller, 1966). In practice, ill-posedness is characterized by non-uniqueness and instability (Yeh, 1986). Non-uniqueness occurs when there are multiple parameter vectors that correspond to extrema of roughly equal magnitude in the objective function, making it impossible to determine the correct solution. As Yeh (1986) points out, the uniqueness problem is closely related to the notion of parameter identifiability, i.e. whether or not it is possible to obtain accurate estimates of the parameters in the mathematical model from available data. Identifiability thus depends on both the assumed model and the experimental data used. A frequent cause for ill-determined parameters is correlation among them. When parameters are highly correlated, a change in one parameter is balanced by a corresponding change in the correlated parameter, with the result that neither can be determined accurately. On the other hand, even when the parameters in a model are completely independent, the available experimental data may lead to an objective function that lacks sensitivity to one or more of the parameters, again with the result that these parameters will have large estimation variances. Instability, on the other hand, occurs when the estimated parameters are excessively sensitive to changes in data. Relatively small measurement errors can then lead to significant errors in estimated parameter values.

The main purpose of this paper is to illustrate the application of parameter estimation techniques to the determination of key parameters affecting flow and transport in the unsaturated zone. Before doing so, a brief review of relevant literature dealing with the parameter estimation process in general will be given, followed with specific applications to the analysis of water flow and solute transport in the vadose zone. A few areas in need of further investigation are outlined at the end of this paper.

PARAMETER ESTIMATION METHODS

This section briefly reviews the general formulation and solution of the parameter estimation problem. The discussion is by no means exhaustive. With

the exception of the penalty function method, only unconstrained parameter estimation is considered. The discussion is further limited to Newton-type optimization techniques. Other methods, such as steepest descent and conjugate gradient methods are left out.

General formulation of the estimation problem

Many parameter estimation problems can be formulated as a weighted least-squares minimization problem:

$$\min_{\mathbf{b}} O(\mathbf{b}) = \frac{1}{2}[\mathbf{q}^* - \mathbf{q}(\mathbf{b})]^T \mathbf{W}[\mathbf{q}^* - \mathbf{q}(\mathbf{b})] + \frac{1}{2}(\mathbf{b}^* - \mathbf{b})^T \mathbf{V}(\mathbf{b}^* - \mathbf{b}) \quad (1)$$

where the objective function (or performance index), $O(\mathbf{b})$, is a function of the model parameters \mathbf{b} , $\mathbf{b} = \{b_1, \dots, b_m\}^T$; $\mathbf{q}^* = \{q_1^*, \dots, q_n^*\}^T$ is the observation vector whose elements represent measured heads, water contents, concentrations or fluxes; $\mathbf{q}(\mathbf{b}) = \{q_1(\mathbf{b}), \dots, q_n(\mathbf{b})\}^T$ represents the predicted response for a given parameter vector \mathbf{b} ; \mathbf{b}^* represents direct estimates or measurements of the parameters b ; and \mathbf{W} and \mathbf{V} are symmetric weighting matrices. The coefficient $\frac{1}{2}$ in eqn. (1) is purely for notational convenience. The objective is to find the parameter vector \mathbf{b}^f that minimizes eqn. (1) or, in other words, results in a best fit between the model and available data. Provided the problem has a unique solution, the final parameter values \mathbf{b}^f are also the best estimates for the unknown model parameters \mathbf{b} .

The second term of eqn. (1) is sometimes called a plausibility criterion (e.g., Carrera, 1984). As Townley (1983) remarks, inclusion of this term in eqn. (1) is equivalent to the penalty function approach for constraining parameters to remain in some feasible region around \mathbf{b}^* . When the parameter estimates \mathbf{b} move away from \mathbf{b}^* , the contribution of the second term of eqn. (1) to the total weighted sum of squares will increase quadratically and minimization of $O(\mathbf{b})$ can only be achieved if \mathbf{b} remains close to \mathbf{b}^* . The weighting matrices \mathbf{W} and \mathbf{V} contain information about measurement accuracy, as well as possible correlations between measurement errors and between parameters. In the absence of any additional information besides the observations \mathbf{q}^* , the simplest and recommended (Beck and Arnold, 1977) approach is to set \mathbf{W} equal to the identity matrix and \mathbf{V} to zero:

$$\mathbf{W} = \mathbf{1}, \quad \mathbf{V} = \mathbf{0} \quad (2)$$

In this case, eqn. (1) reduces to the well-known ordinary least-squares (OLS) problem:

$$\min_{\mathbf{b}} O(\mathbf{b}) = \frac{1}{2}[\mathbf{q}^* - \mathbf{q}(\mathbf{b})]^T [\mathbf{q}^* - \mathbf{q}(\mathbf{b})] = \frac{1}{2} \sum_{i=1}^n [q_i^* - q_i(\mathbf{b})]^2 \quad (3)$$

The OLS formulation has probably been the most popular one for parameter estimation problems. Its attraction is due to its simplicity and because it

requires a minimum amount of information. When observation errors are normally distributed, are uncorrelated and have a constant variance, the OLS estimates possess optimal statistical properties (Bard, 1974). When these conditions are not met, the OLS method will no longer yield optimal parameter estimates in terms of precision and minimum variance. When the normality assumption alone is violated, OLS can still be used with good results (Beck and Arnold, 1977).

More serious difficulties arise due to violation of the constant variance and uncorrelated errors assumptions. These situations often occur in practical problems. For instance, error variances are commonly found to increase with the magnitude of the property being measured. Unequal error variances also result when the observation vector \mathbf{q}^* contains different types of measurements (e.g., pressure heads and water contents) that are expressed in different units. In some cases the remedy is quite simple. In the case of correlated mean and variance, a suitable transformation (e.g., logarithmic) of the measurements may be sufficient to stabilize variances. In general, the weighting is achieved through the matrices \mathbf{W} and \mathbf{V} . In what is generally called the weighted least-squares (WLS) method, \mathbf{W} is a diagonal matrix which corrects for unequal error variances, and \mathbf{V} is taken as zero. The elements of \mathbf{W} are chosen such that the most accurate measurements receive the most weight. The elements of \mathbf{W} and \mathbf{V} may be chosen by the modeler based on knowledge and understanding of the physical system. Since subjective procedures may lead to biased parameter estimates, a preferred method is to base the weighting on statistical considerations. This leads to selection of the inverse of the error covariance matrix as the weighting matrix:

$$\begin{aligned} \mathbf{W} &= \mathbf{C}_q^{-1} \\ \mathbf{C}_q &= E[(\mathbf{q}^* - \bar{\mathbf{q}})(\mathbf{q}^* - \bar{\mathbf{q}})^T] \\ \bar{\mathbf{q}} &= E(\mathbf{q}^*) \end{aligned} \quad \Bigg| \quad (4)$$

where E denotes expectation. The diagonal elements of \mathbf{W} account for unequal error variances, and off-diagonal elements for correlated errors. In case the off-diagonal elements of \mathbf{W} are also taken into account, the method is classified as generalized least-squares (GLS). Often, when a method is described as WLS or GLS, no prior information on the parameters themselves is presumed and the objective function consists of only the first term of eqn. (1).

Although the formulation of the parameter estimation problem as a weighted least-squares problem can be arrived at by heuristic arguments, casting the problem in the framework of either maximum likelihood or Bayesian estimation in practice also leads to objective function (1) (Townley, 1983; Carrera, 1984). Whereas the underlying concepts are quite different, each of the latter two methods leads to the same estimator. The maximum likelihood (ML) interpretation is more commonly used, because the ideas it involves are more straightforward (Beck and Arnold, 1977; Townley, 1983). In the ML

method, model parameters are viewed as unknown but deterministic and the objective is to find the parameters that maximize the likelihood of obtaining the measured data, given the joint probability density function of all measurements. A common approach is again to assume errors are normally distributed. This leads to the convenient form of eqn. (1) for the objective function with W and V given by:

$$W = C_q^{-1}, \quad V = C_b^{-1} \quad (5)$$

where C_q was defined previously and C_b is analogously given by:

$$\left. \begin{aligned} C_b &= E[(\mathbf{b} - \bar{\mathbf{b}})(\mathbf{b} - \bar{\mathbf{b}})^T] \\ \bar{\mathbf{b}} &= E(\mathbf{b}) \end{aligned} \right\} (6)$$

Hence, W and V are inverses of the covariance matrices of measurement errors and prior parameter estimate errors, respectively.

If a distribution of errors other than the normal distribution is assumed, the resulting objective function will not have the generalized least-squares form of eqn. (1). Although the true error distribution is frequently unknown, violation of the normality assumption will generally not lead to serious errors (Bard, 1974). Maximum likelihood estimates are asymptotically (i.e. for large samples) unbiased, normally distributed and have minimum variance (Bard, 1974). To achieve the full benefit of the ML method, the covariance matrices C_q and C_b need to be specified. Indeed, Beck and Arnold (1977) recommend simple OLS estimation if these matrices are completely unknown. In general, the weighting matrices will not be known a-priori. In some cases the appropriate weights in the objective function can be estimated along with the model parameters. Examples are given by Bard (1974), Beck and Arnold (1977), Sorooshian and Dracup (1980), and Troutman (1985). A generally applicable procedure is the two-stage least-squares method recommended by Cooley (1982) and Sadeghipour and Yeh (1984). The first stage consists of OLS estimation which utilizes only the available observations \mathbf{q}^* . The OLS solution will generally not lead to optimal parameter estimates, but it will provide unbiased estimates of the error covariances. Let \mathbf{e} be the residual vector at the OLS minimum:

$$O(\mathbf{b}^f) = [\mathbf{q}^* - \mathbf{q}(\mathbf{b}^f)]^T [\mathbf{q}^* - \mathbf{q}(\mathbf{b}^f)] = \mathbf{e}^T \mathbf{e} \quad (7)$$

An unbiased estimate of C_q is then given by:

$$C_q = \frac{1}{n-1} \mathbf{e} \mathbf{e}^T \quad (8)$$

where n is the number of observations. To further improve the parameter estimates, the second stage of the procedure solves the generalized least squares problem using the estimated C_q to provide weights. Based on a number of numerical experiments involving estimation of aquifer transmissivities from hydraulic head data, Sadeghipour and Yeh (1984) concluded that the two-stage approach as compared with OLS estimates led to significantly better parameter estimates.

In cases where prior information on the model parameters is available, the two-stage procedure may be extended to include a plausibility criterion. The parameter error covariance matrix C_b may be estimated at the end of the first stage from:

$$C_b = \frac{\mathbf{e}^T \mathbf{e}}{n - m} \mathbf{H}^{-1} \quad (9)$$

where m is the dimension of the parameter vector and \mathbf{H} is the Hessian, or matrix of second derivatives, of the objective function with respect to the parameters with components:

$$H_{ij} = \frac{\partial^2 O}{\partial b_i \partial b_j} \quad (10)$$

Depending on the algorithm for solving eqn. (1), \mathbf{H} will already be available or can be easily computed at the end of the first stage estimation. Note that regardless of whether or not the second stage estimation is carried out, eqn. (9) may be used to provide an estimate of parameter uncertainty. As an overall index of inversion precision, a norm such as the trace or maximum eigenvalue of C_b may be employed (Yeh, 1986).

Solution methods for least-squares problems

In this section Newton's and related methods for solving least-squares minimization problems will be reviewed. The starting point is the objective function, given by eqn. (1) in the previous section. In order to simplify the notation it is assumed that the weighting matrices \mathbf{W} and \mathbf{V} are diagonal. This allows a new vector of residuals \mathbf{r} to be written, where:

$$\begin{bmatrix} r_1 \\ \cdot \\ \cdot \\ r_n \\ r_{n+1} \\ \cdot \\ \cdot \\ r_{n+m} \end{bmatrix} = \begin{bmatrix} w_1 [q_1^* - q_1(\mathbf{b})] \\ \cdot \\ \cdot \\ w_n [q_n^* - q_n(\mathbf{b})] \\ v_1 (b_1^* - b_1) \\ \cdot \\ \cdot \\ v_m (b_m^* - b_m) \end{bmatrix} \quad (11)$$

with:

$$w_i = (W_{ii})^{1/2}, \quad v_j = (V_{jj})^{1/2}$$

Unequally weighted measurements and prior parameter information are all lumped into \mathbf{r} , so that eqn. (1) becomes:

$$\min_b O(b) = \frac{1}{2} \mathbf{r}^T \mathbf{r} = \frac{1}{2} \sum_{i=1}^N r_i^2 \quad (12)$$

with $N = n + m$. If \mathbf{W} and \mathbf{V} are not diagonal, they must be propagated explicitly in subsequent equations. While this is a straightforward procedure (e.g., Beck and Arnold, 1977; Townley, 1983) the equations become lengthier and salient features of the different solution methods are less clear. Unless the model is linear in all parameters, minimization of eqn. (12) must be carried out iteratively. Initial values, \mathbf{b}^0 , for the parameters must be supplied by the user. At every iteration, a linear system of equations is constructed and solved to give a correction $\Delta \mathbf{b}$ for the current parameter vector \mathbf{b}^i , such that:

$$O(\mathbf{b}^i + \Delta \mathbf{b}) \leq O(\mathbf{b}^i) \quad (13)$$

The iteration continues until some suitable convergence criterion is satisfied. Commonly used stopping criteria are:

$$O(\mathbf{b}^{i+1}) - O(\mathbf{b}^i) \leq \tau_1 \quad (14)$$

and/or:

$$\Delta \mathbf{b}^i \leq \tau_2$$

where τ_1 and τ_2 are set to some small value.

Newton's method can be derived by writing a 3-term Taylor series expansion for $O(b)$ around \mathbf{b}^i :

$$O(\mathbf{b}^i + \Delta \mathbf{b}) = O(\mathbf{b}^i) + \nabla O(\mathbf{b}^i)^T \Delta \mathbf{b} + \frac{1}{2} \Delta \mathbf{b}^T \nabla^2 O(\mathbf{b}^i) \Delta \mathbf{b} + \text{"small"} \quad (15)$$

where "small" contains terms of the order of $\|\Delta \mathbf{b}\|^3$ and smaller. We wish to select $\Delta \mathbf{b}$ so that $O(\mathbf{b}^i + \Delta \mathbf{b})$ is approximately minimized. The correction $\Delta \mathbf{b}$ is determined such that:

$$\Phi(\Delta \mathbf{b}) = \nabla O^T \Delta \mathbf{b} + \frac{1}{2} \Delta \mathbf{b}^T \nabla^2 O \Delta \mathbf{b} \quad (16)$$

has a minimum. A necessary condition for $\Delta \mathbf{b}$ to be a minimizer is that the gradient of $\Phi(\Delta \mathbf{b})$ is zero:

$$\nabla O + \nabla^2 O \Delta \mathbf{b} = 0 \quad (17)$$

and thus:

$$\Delta \mathbf{b} = -(\nabla^2 O)^{-1} \nabla O \quad (18)$$

First and second derivatives ∇O and $\nabla^2 O$ are obtained by differentiating eqn. (12) with respect to \mathbf{b} :

$$\nabla O = \sum_{i=1}^N r_i \nabla r_i = \mathbf{J}^T \mathbf{r} \quad (19)$$

and:

$$\nabla^2 O = \mathbf{H} = \sum_{i=1}^N (\nabla r_i \nabla r_i^T + r_i \nabla^2 r_i) = \mathbf{J}^T \mathbf{J} + \mathbf{S} \quad (20)$$

where \mathbf{J} is called the Jacobian or sensitivity matrix and \mathbf{H} is the Hessian (see eqn. 10). Substitution of eqns. (19) and (20) into eqn. (18) gives Newton's algorithm for updating the unknown parameters b :

$$\Delta \mathbf{b} = -(\mathbf{J}^T \mathbf{J} + \mathbf{S})^{-1} \mathbf{J}^T \mathbf{r} \quad (21)$$

In the so-called full-Newton method, the Hessian (eqn. 20) is evaluated directly. This method is (at least locally) quadratically convergent (Dennis and Schnabel, 1983) and will quickly converge for most problems. A major disadvantage of the full-Newton method is the cost of evaluating the second derivatives:

$$\nabla^2 r_k = \frac{\partial^2 r_k}{\partial b_i \partial b_j} \quad (22)$$

These second derivatives are generally not available analytically. Because approximation by finite differences requires $(m^2 + 3m)/2 + 1$ function evaluations for m parameters, this can greatly add to the overall computational expense. The full-Newton method is for this reason, not commonly used for solving non-linear least-squares problems. More popular are modifications of Newton's method that do not calculate eqn. (20) directly, but use some approximation thereof. These modifications are known as quasi-Newton, Gauss-Newton and Levenberg-Marquardt, respectively. Closest to the full-Newton method is the quasi-Newton method which approximates the Hessian from available first derivative information using a secant update method. A positive definite matrix is constructed and updated at every iteration of the optimization algorithm so that it yields an approximation to \mathbf{H} or \mathbf{H}^{-1} in far fewer steps than a full Hessian evaluation requires. Positive definiteness of the updated matrix ensures that the optimization will proceed in a descending direction. Well-known general methods for updating the matrix include the Davidon-Fletcher-Powell (DFP) and Broyden-Fletcher-Goldfarb-Shanno (BFGS) methods. Equation (20) shows that the least-squares Hessian consists of a first derivative term $\mathbf{J}^T \mathbf{J}$ and a second derivative term \mathbf{S} . Dennis et al. (1981) describe a quasi-Newton algorithm that takes into account this special structure of the least-squares Hessian by approximating only the second derivative term in eqn. (20) with a secant update, and adding this to the directly evaluated first derivative term.

In the Gauss-Newton method it is simply assumed that the first term $\mathbf{J}^T \mathbf{J}$ above is a sufficient approximation to the Hessian. Comparison with eqn. (19) shows that this is a reasonable assumption when the residual vector \mathbf{r} is small. In fact when the residuals are zero at the minimum, the Gauss-Newton method is asymptotic to Newton's method near the minimum and thus locally quadratically convergent. On the other hand, when the solution is far from the minimum or when the residuals remain large at the minimum, the Gauss-Newton method may fail to converge at all. Another problem with the Gauss-Newton

method is its sensitivity to rank deficiency in the Jacobian \mathbf{J} which occurs when one or more of the columns of \mathbf{J} are linear combinations of other columns. This rank deficiency is related to the identifiability problem mentioned in the introduction. Identifiability of the model parameters requires that the Hessian, given by eqn. (20), is non-singular. Otherwise, eqn. (18) will not have a unique solution. For the Gauss–Newton method where \mathbf{H} is approximated by $\mathbf{J}^T\mathbf{J}$, a non-singular Hessian is equivalent to a full rank Jacobian. Exact rank deficiency in the Jacobian occurs when two or more parameters in the model are linearly dependent. Such overparameterization can usually be detected and corrected by inspection of the model that is fitted. Because of finite precision arithmetic, problems will often arise in practice when parameters are highly correlated, e.g., with correlation coefficients exceeding 0.90. This leads to a poorly conditioned Jacobian and slow convergence of the optimization routine. Numerical problems can be alleviated to some extent by using robust techniques (such as orthogonalization) for solving the linear least-squares problem (21), but the final parameter estimates may still have large variances. This latter problem can only be eliminated by choosing a simpler model and/or by including additional information in the objective function.

In the Levenberg–Marquardt method the Hessian is approximated as:

$$\mathbf{H} \approx \mathbf{J}^T\mathbf{J} + \lambda\mathbf{D}^T\mathbf{D} \quad (23)$$

where λ is a positive scalar and \mathbf{D} a diagonal scaling matrix. The elements of \mathbf{D} are usually set equal to the norms of the corresponding columns of \mathbf{J} (Moré, 1977). The Levenberg–Marquardt method has a number of advantages over the standard Gauss–Newton method. For non-zero λ , the Hessian approximation is always positive definite which ensures the descent property of the algorithm, even if initial parameter estimates are poor. The Levenberg–Marquardt method can be viewed as an interpolation between the steepest descent and Gauss–Newton methods. When λ is large, the result will be a small step in the steepest-descent direction, while the method degenerates to the Gauss–Newton method as λ approaches zero. The usual strategy is to set λ initially to some large value, and then to decrease its value as the solution approaches the minimum. In principle, the method is also numerically more robust than the Gauss–Newton method. For non-zero λ , $\mathbf{J}^T\mathbf{J} + \lambda\mathbf{D}^T\mathbf{D}$ will have full column rank even if $\mathbf{J}^T\mathbf{J}$ itself does not. In the Gauss–Newton and Levenberg–Marquardt methods, the approximations $\mathbf{J}^T\mathbf{J}$ and are often used to compute \mathbf{H}^{-1} in eqn. (9). This first-order approximation will be accurate to the extent that the second term in eqn. (20) is negligible. The alternative of course is to compute \mathbf{H} in eqn. (9) directly.

All of the methods discussed are expected to work well for many problems. Since parameter estimation problems involving transient flow and/or transport are computationally expensive to solve, it will in many cases be worthwhile to find the most efficient method rather than just use one that is already available. Different optimization algorithms are widely available through software libraries such as IMSL and MINPACK. Comparisons of different algorithms (e.g., Bard, 1974; Beck and Arnold, 1977; Hiebert, 1981; Cooley, 1985) indicate that results can be very problem dependent. While the quasi-Newton method is

preferred for general function minimization, there appears to be little difference between it and Levenberg–Marquardt methods for least-squares problems (Hiebert, 1981; Dennis and Schnabel, 1983). In the problems considered by Hiebert (1981) the Gauss–Newton method performed least well. Hiebert further concludes that the specific implementation of an algorithm can significantly affect performance, and discusses factors that affect efficiency and robustness.

Besides using an efficient optimization algorithm, i.e., one that converges in the least number of iterations, a reduction in overall computational cost can be achieved by reducing cost per iteration. The most expensive part in the solution process is often the evaluation of the Jacobian, i.e., calculation of the parameter sensitivities. These sensitivities are usually evaluated by finite difference approximation. Even when one-sided differences are used, the direct problem must be evaluated $m + 1$ times, in order to obtain the Jacobian for m parameters. Recently, a number of researchers (Neuman, 1980; Carrera and Neuman, 1984, 1986; Townley and Wilson, 1985) have applied adjoint techniques for obtaining the gradient of the objective function in cases where the direct problem is given by a differential equation (e.g., the non-steady flow equation). The technique involves formulation of an adjoint equation to the direct problem. The gradient ∇O sensitivities can then be obtained by solving both direct and adjoint problems once, at a cost that is approximately the same as solving the direct problem twice. Net savings thus result as soon as there is more than one parameter to be estimated. A disadvantage of the adjoint method is that one obtains the gradient ∇O , but not the sensitivity matrix \mathbf{J} . Consequently, no direct approximation of the Hessian is available, and one either has to resort to less powerful optimization methods than the Gauss–Newton or Levenberg–Marquardt method, or combine the adjoint method with a secant Hessian approximation to yield a quasi-Newton algorithm. The adjoint method has thus far been applied to saturated flow problems. A first application to unsteady, unsaturated flow problems is described by Wittmeyer and Neuman (1985).

APPLICATIONS TO UNSATURATED FLOW

Several applications of the parameter estimation method to the determination of unsaturated soil hydraulic properties are discussed in this section. First, the direct problem governed by the saturated–unsaturated flow equation and suitable constitutive relationships for the hydraulic properties will be defined. This is followed by discussion of laboratory and in-situ methods.

The direct problem

The partial differential equation governing transient one-dimensional unsaturated flow in a rigid porous medium is taken as:

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left[K(h) \frac{\partial (h + z)}{\partial x} \right] \quad (24)$$

where x is distance; t is time; $K(h)$ is the hydraulic conductivity as a function of the pressure head h ; $C(h)$ is the soil water capacity, being the slope $d\theta/dh$ of the soil water retention curve $\theta(h)$, where θ is the volumetric water content; and z is the gravitational head such that $dz/dx = 0$ for horizontal flow, $+1$ for vertical flow with x positive upwards and -1 for vertical flow with x positive downwards. The unsaturated hydraulic properties $\theta(h)$ and $K(h)$ are strongly non-linear functions of the pressure head. It is assumed that suitable analytical expressions for these functions are available. Strictly, the problem is one of the model identification as well as parameter estimation since the correct functional forms of $\theta(h)$ and $K(h)$ are generally unknown. Frequently used expressions for the hydraulic functions are those developed by Brooks and Corey (1964) and Van Genuchten (1980). The expressions derived by Van Genuchten are:

$$S_e = \begin{cases} \frac{1}{(1 + |\alpha h|n)^m}, & h < 0 \\ 1, & h \geq 0 \end{cases} \quad (25a)$$

$$K = K_s S_e^{1/2} [1 - (1 - S_e^{1/m})^m]^2 \quad m = 1 - 1/n \quad (25b)$$

where S_e is the effective saturation $(\theta - \theta_r)/(\theta_s - \theta_r)$; θ_s and θ_r are saturated and residual water contents, respectively; K_s is the saturated conductivity and α and n are curve shape parameters. Note that $m = 1 - 1/n$ is not an independent parameter. An expression for $C(h) = d\theta/dh$ is readily obtained by differentiating eqn. (25a).

As written here, eqn. (25) is valid for monotonic wetting or drying only. When the flow process involves both wetting and drying, hysteresis in the $C(h)$ relation will have to be taken into account. Kool and Parker (1987) recently combined Van Genuchten's expressions (25) with an empirical hysteresis model to obtain a set of concise, closed-form expressions describing hysteretic soil hydraulic properties with only one additional parameter. The model was developed with an eye towards application in parameter estimation problems (Kool et al., 1986) where parsimony in the number of model parameters is desirable.

Parameters in eqn. (25) are commonly determined by measuring K_s directly and estimating the remaining parameters by fitting eqn. (25a) to measured (θ, h) data. The (θ, h) measurements are obtained from equilibrium desorption or absorption experiments on laboratory samples or can be measured in-situ using tensiometers and neutron probe. The parameter estimation problem in this case becomes very simple. Disadvantages of such an approach are generally time-consuming data collection and the fact that parameters are fitted to (θ, h) data only, so that any inaccuracy in the assumed hydraulic relationships, as well as effects of measurement error are forced into the predicted $K(h)$ (Parker et al., 1985). Rather than directly measuring only pairs of (θ, h) data, a number of authors have recently tried to estimate the hydraulic properties from transient flow experiments by numerical inversion of eqn. (24). Parameter estimation studies of this type have generally been limited to relatively short laboratory

soil columns, mostly by measuring outflow volumes from initially saturated columns. A comparatively few field-scale experiments involving in-situ measurements of water contents and pressure heads during transient flow have also been attempted. Laboratory approaches will be discussed first.

Laboratory methods

Probably the first attempts to estimate the hydraulic properties from transient flow experiments in the laboratory were those by Zachmann et al. (1981, 1982) who considered hypothetical gravity drainage experiments involving initially saturated columns of sand. Cumulative drainage outflow data were used to estimate by ordinary least-squares two unknown coefficients in a four-parameter model for the hydraulic properties. The direct problem was solved using finite differences, while the objective function for the 1982 study was given by eqn. (3) with the observation vector q^* representing cumulative outflow volumes (Zachmann et al., 1982). Their study shows the importance of selecting correct parametric forms for $K(h)$ and $\theta(h)$ in the estimation process. When incorrect expressions are used, it may still be possible to obtain an acceptable solution to the inverse problem but the hydraulic properties corresponding to that solution may be in error.

This last problem is illustrated in Fig. 1, adapted from Zachmann et al. (1982), in which both the "true" and estimated $\theta(h)$ and $K(h)$ relationships are shown. The "true" parametric functions were represented by Brooks and Corey-type expressions, while in the inverse problem an exponential func-

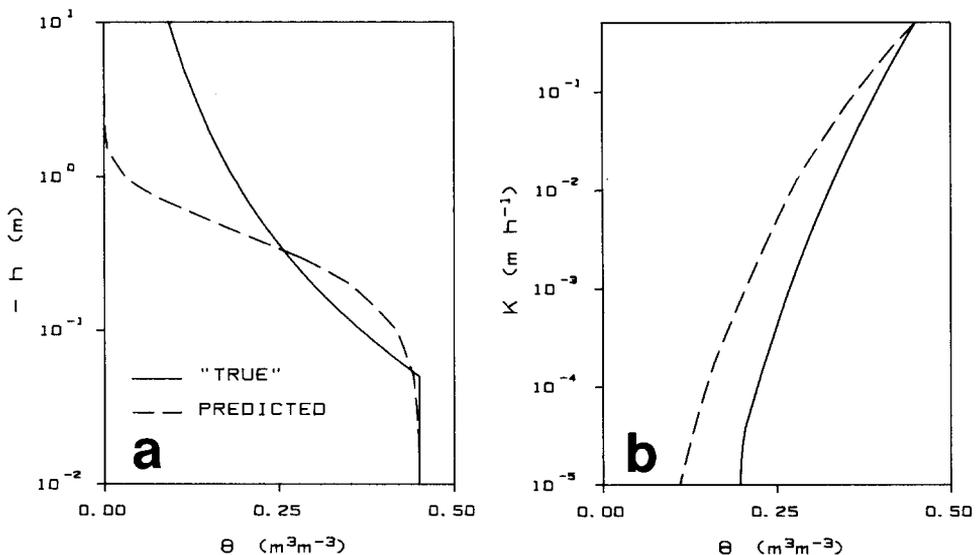


Fig. 1. Actual and predicted hydraulic properties for a hypothetical porous medium (after Zachmann et al., 1982). (a) water retention curve $\theta(h)$; (b) hydraulic conductivity $K(\theta)$.

tion was used for $\theta(h)$ and a power function for $K(\theta)$. Although our own experience, as well as other published results (e.g., Van Genuchten and Nielsen, 1985), suggest that Van Genuchten's expressions (25) are reasonably accurate for many soils, the appropriateness of this or any other model for a particular case will not be known beforehand, and it may be desirable to compare the performance of different functional forms for the hydraulic functions. An obvious criterion for model discrimination is to select the model that has the minimum residual error, under the subjective constraint that the model should predict realistic properties for the medium. A more rigorous criterion involves evaluation of how well a fitted set of hydraulic properties can describe system behavior under initial and boundary conditions that are different from those used in model calibration.

Another common cause for erroneous parameter estimates, even when a correct parametric model is used, occurs when different combinations of parameters lead to roughly the same minimum in the objective function. This type of uniqueness problem was investigated by Hornung (1983) and Kool et al. (1985). In both studies, soil hydraulic properties were represented by Van Genuchten's model. Hornung assumed the parameters K_s , θ_s and θ_r to be known and attempted to determine α and n from a column drainage experiment. A vertical column, initially at hydrostatic equilibrium, was subjected to a constant infiltration flux at the surface and the column outflow rate measured. No unique solution could be found using only these measurements. The non-uniqueness problem could be resolved when additional information was included, in Hornung's case the final steady pressure head at some fixed position inside the column. Kool et al. (1985) estimated the three parameters θ_r , α and n in eqn. (25) also from a column drainage experiment. Unlike the gravity drainage studies of Zachmann et al. (1982) and Hornung (1983), the experimental set-up in their study was that of a "one-step" pressure outflow method where desorption was initiated by a step change in air pressure at the upper column boundary. Kool et al. (1985) concluded that the ability to uniquely solve the three-parameter estimation problem is a function of the difference between the average initial and final water content in the column. Uniqueness was not a problem when this difference was at least 50% of the difference between θ_s and θ_r . This suggests that in gravity drainage experiments the desired resolution can only be achieved by using unrealistically long soil columns, except for extremely coarse materials such as those used by Zachmann et al. (1982). The one-step outflow method is much more convenient to use since the water content difference depends on the imposed step change in potential, which is directly controlled by the experimenter.

Parker et al. (1985) used the one-step outflow procedure to determine hydraulic properties of undisturbed soil cores taken from four different field soils ranging from sandy loam to clay. Soil cores were assembled in pressure cells, saturated and then subjected to a step change in the pressure head, Δh , of 10 m by increasing the external gas pressure. The parameters θ_s and K_s were independently measured, while α , n and θ_r were estimated from the cumulative

outflow versus time measurements. Predicted $\theta(h)$ and $K(h)$ relationships were then compared with independently determined hydraulic properties for the same soil cores. Good agreement was found for all soils in the range $-10 < h < 0$ m, i.e. the same range of pressure heads over which the outflow measurements were taken, but extrapolation to lower pressure heads outside the measurement ranges proved to be less reliable. Predicted $\theta(h)$ curves generally overestimated water contents at pressure heads < -10 m, indicating poor estimates of θ_r . This problem could be alleviated by including additional information in the objective function, in this case a direct measurement of θ at $h = -150$ m. Thus, their objective function was of the form:

$$O(\mathbf{b}) = w \sum_{i=1}^N [q_i^* - q_i(\mathbf{b})]^2 + v \sum_{j=1}^M [\theta_j^* - \theta_j(\mathbf{b})]^2 \quad (26)$$

where q_i^* is measured cumulative outflow at times t_i ($i = 1, \dots, N$); $q_i(\mathbf{b})$ represent outflow at times t_i , computed by solving eqn. (24) for the trial parameter vector \mathbf{b} with \mathbf{b} having elements $(\alpha, n, \theta_r)^T$; θ_j^* is the measured water content at pressure head h_j ; and $\theta_j(\mathbf{b})$ is the corresponding predicted water content obtained from eqn. (25a). Measurement errors were assumed to be uncorrelated and to have constant variance. Weights w and v account for the different scales of measurement for outflow volumes and water contents. Since only the ratio w/v is of interest, w was set equal to 1.0 and v calculated as:

$$v = M \sum_{i=1}^N q_i^* / N \sum_{j=1}^M \theta_j^* \quad (27)$$

The one-step outflow method is a convenient procedure for obtaining input data for the inverse problem because it is experimentally simple and quick, Jennings et al. (1985) describe another parameter estimation procedure based on a pressure outflow test. Their experiment involves a stepwise desorption test in which each step is not necessarily continued until equilibrium. Jennings et al. use spline functions to describe the retention and relative permeability functions, with "knots" on the spline acting as parameters obtained by matching the observed stepwise outflow curve.

A disadvantage of these and most other parameter estimation procedures based on transient, unsaturated flow data, is the computational expense associated with the numerical solution of eqn. (24). During iterative optimization, the direct problem given by eqn. (24) may have to be solved 30 or more times. As discussed in the previous section, a large part of total computational cost is associated with the finite difference approximation of the Jacobian. A reduction in computer costs can likely be obtained by using adjoint-state techniques for evaluating the gradient of the objective function (Wittmeyer and Neuman, 1985). An alternative is to use an experimental design that permits a (semi-) analytical solution for the direct problem. For horizontal flow eqn. (24) can be written as:

$$\frac{\partial}{\partial x} \left(D_h \frac{\partial \theta}{\partial x} \right) = \frac{\partial \theta}{\partial t} \quad (28)$$

where $D_h = K dh/d\theta$ is the hydraulic diffusivity. Philip (1955) gave a simple iterative solution of eqn. (28) for adsorption into a semi-infinite column subject to a first-type inlet boundary condition. The solution was recently modified by Van Grinsven et al. (1985) for desorption. Using these solutions, eqn. (28) can be solved much more cheaply than eqn. (24). Input data for the inverse problem could consist of measurements of cumulative absorption (desorption), and/or moisture content distribution inside the column at one or more times. W. Bouten (University of Amsterdam, Netherlands, unpublished results) applied the modified Philip solution to estimate D_h from cumulative evaporation measurements. Using Van Genuchten's expressions, the parametric form for $D_h(\theta)$, written for simplicity in terms of the effective saturation S_e , is:

$$D_h(S_e) = \frac{(1 - m)K_s}{\alpha m(\theta_s - \theta_r)} S_e^{1/2 - 1/m} [(1 - S_e^{1/m})^{-m} + (1 - S_e^{1/m})^m - 2] \quad (29)$$

with $m = 1 - 1/n$. Note that K_s and α appear in eqn. (29) as a ratio and therefore cannot be determined simultaneously from horizontal flow experiments only. For laboratory soil columns, direct measurement of K_s is a simple procedure, so that this should not present a problem. Richie et al. (1987) outline a parameter estimation procedure for determining hydraulic properties from measured pressure head distributions along an unsaturated horizontal soil column during steady-state flow, and using additional measurements of total mass of water in the column, steady flow rate and saturated water content. Depending on the functional relationships for $\theta(h)$ and $K(h)$, the direct problem is given in closed or semi-closed form, and the inverse problem could thus be solved very cheaply. Richie et al. (1987) obtained very good results for two hypothetical soils but did not test the procedure on real soils. A disadvantage of their experimental set-up is that it requires a considerable number of tensiometers to be installed in the column. In the hypothetical experiments 16 tensiometers were installed along a 30 cm long column. As compared with the transient outflow procedures of Kool et al. (1985) and Jennings et al. (1985), the method of Richie et al. (1987), as well as those based on eqn. (30), sacrifice some experimental convenience for reduced computational expense.

In-situ methods

Whereas laboratory experiments have the advantage of being easy, quick and precise, a major disadvantage is that they lead to soil properties that are often non-representative of field conditions. Main reasons for this are the typically small size of laboratory samples, and the fact that collection of soil cores invariably introduces some disturbance that may affect flow and transport properties. Since analyses of the soil hydraulic functions are ultimately directed towards field-scale processes, determination of in-situ properties is

more relevant than data obtained from laboratory analyses. The application of parameter estimation techniques to determination of in-situ soil hydraulic properties is, at least in principle, a straightforward matter. Restricting ourselves to vertical one-dimensional flow, input data for the inverse problem can consist of measured water contents and/or pressure heads at different depths and times during infiltration and/or drainage events. Solution of the direct problem (24) further requires the stipulation of suitable initial and boundary conditions. Having instrumented the site with equipment for measuring water contents and/or pressure heads, initial conditions can be determined directly, while boundary conditions can be treated as additional unknowns in the estimation problem as needed.

To date, only one study has been published (Dane and Hruska, 1983) in which parameter estimation methods were employed to determine the water retention and hydraulic conductivity functions simultaneously from a transient field experiment. In this study, Dane and Hruska studied gravity drainage from a clay loam soil. Initial water content profiles and profiles after 7 and 25 days of drainage were measured with a neutron probe. The soil surface was covered to provide a zero-flux upper boundary condition, while a first-type lower boundary condition was determined from tensiometer readings at a depth of 0.9 m. Parameters α and n in Van Genuchten's model (25) were determined by numerical inversion of eqn. (24) while other parameters in the model were assumed known. θ_s and K_s were determined from the maximum water content and steady-state infiltration rate, respectively, both measured during wetting of the soil prior to drainage. A guessed value, obtained by inspection of available $\theta(h)$ data, was assigned to θ_r . Dane and Hruska obtained good agreement between the predicted and independently obtained $\theta(h)$ relation for the clay loam soil, but found that the predicted $K(\theta)$ relation overestimated independently determined conductivities by approximately one order of magnitude. Much better agreement was achieved when the value of K_s was arbitrarily taken to be 10 times lower than its measured value; this produced only small changes in the optimum values for α and n . Use of a much lower than measured K_s value was justified by arguing that macropore flow probably occurred during ponded infiltration, leading to an inflated value for K_s .

A more general procedure than that followed by Dane and Hruska (1983) would be to not fix θ_r and K_s , but to take these as additional unknowns in the inversion problem. As indicated by the results of Dane and Hruska and others (see the discussion by Van Genuchten and Nielsen, 1985), a reliable value for K_s is difficult to obtain, especially in structured media. A value for θ_r could be obtained by determining the water content at some suitably low pressure head, e.g., -150 m. This is a somewhat arbitrary definition of θ_r . However, experience shows that when input data for the inverse problem do not include measurements at very low pressure heads, as is the case for gravity drainage, inversion results are not very sensitive to the value of θ_r . On the other hand, it also implies that predicted $\theta(h)$ and $K(h)$ relations cannot be reliably extrapolated to dry conditions.

Next, an example of parameter estimation for a drainage problem similar to the study of Dane and Hruska (1983) is considered, but with K_s and θ_r taken as additional unknowns. The example involves drainage from a 3 m diameter by 6 m deep lysimeter, filled with crushed Bandelier Tuff, a material with silty sand texture. The in-situ experiment was carried out at the Los Alamos National Laboratory and is described in detail by Abeele (1984). The lysimeter was instrumented with neutron probe access tubes and tensiometers at depths of 0.4, 1.16, 1.91, 2.71, 3.47 and 4.23 m. The average water content following ponded infiltration for more than one month provided a value for θ_s of 0.331. The saturated conductivity, K_s , computed from the steady-state flux exiting the bottom of the lysimeter was $0.1244 \text{ m day}^{-1}$. After saturation, the lysimeter was allowed to drain for 100 days during which period water content and pressure head profiles were monitored. The surface of the lysimeter was covered during the drainage period. In the present analysis of the problem Van Genuchten's model (25) is used to describe hydraulic properties with θ_s the only known parameter.

Preliminary analyses of hypothetical data sets showed that the parameter estimation problem for the two parameters α and n can be solved uniquely using only information on water content profiles during drainage, but that the simultaneous estimation of three or more parameters requires additional information. For this reason, measured water contents, and additionally, measured pressure head at one depth (0.4 m) were used as input data for the inverse problem. Observed water contents and pressure head at $t = 1, 4, 10, 20, 40$ and 100 days after the start of drainage were used in the objective function. Observed pressure heads at depth $x = 4.23 \text{ m}$ were used to provide the lower boundary condition for the solution of the direct problem. Observed water contents at this depth were not used, so that simultaneous information on water contents and heads at $x = 0.4 \text{ m}$ only was employed. The initial condition was $h(x) = 0$, while the upper boundary condition was that of a zero flux. The direct problem (24) was solved using an efficient fully implicit, mass-lumped Galerkin-type, linear finite-element code with a variable time step and constant node spacing Δx of 5 cm. As a check on numerical accuracy, a computer run for the same problem with $\Delta x = 2.5 \text{ cm}$ was made, which gave essentially identical results. The inverse problem was formulated as a weighted least-squares problem with suitable weighting to account for the different scale of measurement of water contents and pressure head:

$$O(\mathbf{b}) = \sum_{i=1}^5 \sum_{j=1}^6 [\theta_{ij}^* - \theta_{ij}(\mathbf{b})]^2 + v \sum_{j=1}^6 [h_j^* - h_j(\mathbf{b})]^2 \quad (30)$$

where θ_{ij}^* represents measured water contents at depths x_i and times t_j , h_j^* is the measured pressure head at depth 0.4 m and times t_j , and \mathbf{b} is the four-parameter vector $(\alpha, n, \theta_r, K_s)^T$. After Parker et al. (1985), relative weights for pressure heads are computed as the ratio of mean observed water content to mean observed pressure head:

$$v = 6 \sum_{i=1}^5 \sum_{j=1}^6 \theta^*(x_i, t_j) / 30 \sum_{j=1}^6 h^*(t_j) \quad (31)$$

With pressure heads expressed in m H₂O, this gave a weighting of $v = 0.160$. The non-linear least-squares problem for the four parameters (α , n , θ_r , K_s) was solved using the Levenberg-Marquardt method. Error variances were computed with eqn. (8) as a check on the correctness of the weighting coefficient (31). Weighting the residuals in the objective function by reciprocals of error standard deviations would have given a relative weight of $v = 0.124$ to the pressure head observations. This was considered sufficiently close to the actual weight so that the analysis was not repeated.

Estimated parameter values and their statistics are given in Table 1. Since the estimated value for θ_r is identically zero, there are no error estimates for this parameter. Of the remaining parameters, the estimated K_s is the least accurate with a 95% confidence interval of $\pm 50\%$ of the estimated value. Observed and fitted water content profiles at $t = 1, 10, 40$ and 100 days are shown in Fig. 2. For pressure heads at 0.4 m depth, the mean deviation between observed and fitted values was 0.07 m H₂O. Fig. 2 shows good overall agreement between observed and fitted water contents, with poorer results for $t = 1$ day and for the 3.47 depth at $t = 4$ days. Computed water content profiles show a more rapid initial decrease than observed. This is related to the high estimated value for K_s (Table 1) which is about 2 times higher than the observed value of 0.124 m day^{-1} . A too high K_s value will result in overly rapid initial drainage, but will have less of an effect where the soil has become unsaturated. Consequently, the estimated value of K_s is determined mainly by observations at small times. The wide 95% confidence region further indicates the poor identifiability of K_s . As discussed previously, the remedy for this is to include prior information on K_s in the least-squares function. In practice, determining a good value for in-situ K_s is quite difficult. Alternatively, the early time observations could have been assigned higher weights to obtain a more accurate estimate for K_s . If an experiment contains no observations at saturated or near-saturated conditions, K_s will be very ill-determined, as for example in the experiment of Dane and Hruska (1983) who observed little sensitivity to K_s when it changed by an order of magnitude. To verify accuracy of parameter estimates, predicted

TABLE 1

Van Genuchten parameters for Bandelier Tuff estimated from in-situ drainage

| Parameter | Initial value | Estimated value | Std. dev. | 95% confidence limits | |
|------------------------------|---------------|-----------------|-----------|-----------------------|-------|
| | | | | lower | upper |
| α (m ⁻¹) | 2.00 | 1.433 | 0.15 | 1.13 | 1.74 |
| n | 2.00 | 1.506 | 0.052 | 1.40 | 1.61 |
| θ_r | 0.05 | 0.0 | — | — | — |
| K_s (m day ⁻¹) | 0.25 | 0.250 | 0.063 | 0.124 | 0.376 |

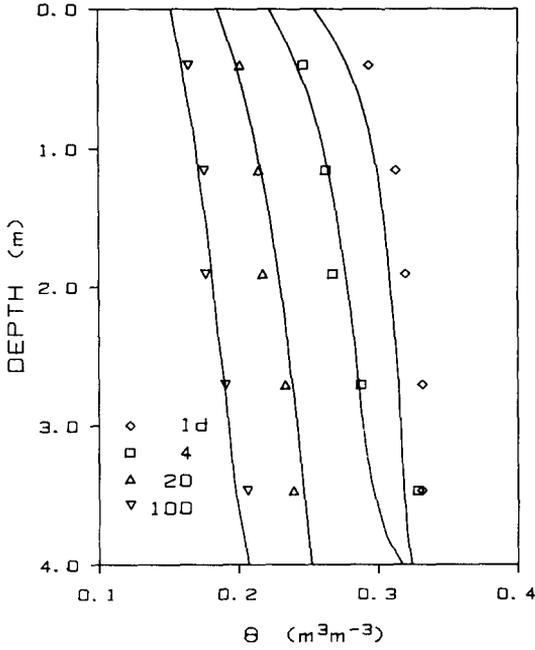


Fig. 2. Observed and fitted water content profiles during drainage of Bandelier Tuff. Observed data from Abeele (1984).

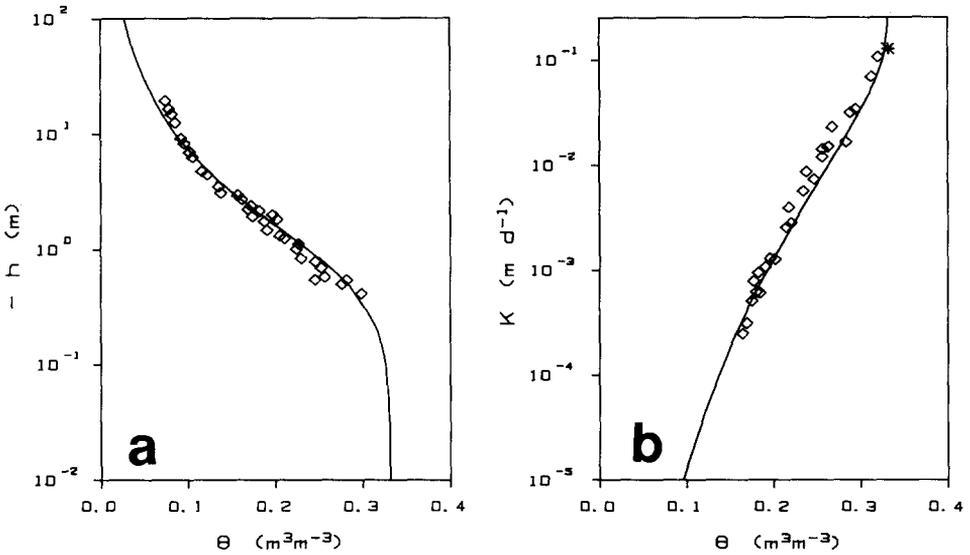


Fig. 3. Hydraulic properties of Bandelier Tuff. (a) water retention curve $\theta(h)$; (b) hydraulic conductivity $K(\theta)$. Data points from Abeele (1984), * is the measured saturated conductivity.

and independently determined $\theta(h)$ and $K(\theta)$ relations for the Bandelier Tuff are compared in Fig. 3. The $\theta(h)$ data points in Fig. 3a represent in-situ measurements from the lysimeter as well as from the laboratory at the lower pressure heads. The $K(\theta)$ data points shown in Fig. 3b were calculated from the lysimeter drainage experiment (Abee, 1984) using the instantaneous profile method (Watson, 1966). Both figures show excellent agreement.

The results of Fig. 3 as well as those by Dane and Hruska (1983) clearly illustrate the potential of parameter estimation techniques for determination of in-situ soil hydraulic properties. We acknowledge that the lysimeter experiment was carried out in a very homogeneous medium, whereas field soils may exhibit marked heterogeneity (e.g., layering) at this scale of observation. Nevertheless, the type, intensity and accuracy of measurement in the lysimeter example are those of a typical field situation. In this case, measurements were taken over a 100 day period. While this is quite long, the frequency with which measurements need to be taken should decrease quickly as the duration of the experiment increases. The lysimeter data changed little after approximately 20 days. In the present study no attempt was made to determine the minimum required experimental duration. Experience with laboratory outflow tests indicate that the important factor is change in water content and pressure head between beginning and end of the experiment rather than duration of the experiment per se. This means that measurements would have to be taken over a longer period of time for a slowly draining heavy-textured soil as compared with a more quickly draining light-textured soil. Alternatively, the desired effect may be obtained more rapidly by not covering the soil surface during drainage and allowing simultaneous evaporation and gravity drainage. Unfortunately, unless the generally variable evaporation rate is known a-priori, this will lead to additional unknowns in the parameter estimation process. A practical solution would be to take periodic measurements of the surface moisture content during the experiment and use this information to obtain a prescribed first-type surface boundary condition. Another alternative would be to use transient infiltration data in the inversion problem, either instead of or in addition to drainage data. An infiltration test, especially when the soil is initially dry and infiltration is continued until the medium is saturated, should lead to better resolution in the input data, and hence to more accurate estimates for K_s . The simultaneous use of both infiltration and drainage data also leads to a better definition of the parameters. As shown by Kool et al. (1986) for laboratory data, an additional advantage of the latter approach is that it can be used quite effectively to determine the soil's hysteretic hydraulic properties.

APPLICATIONS TO SOLUTE TRANSPORT

The common representation of subsurface transport employs the convection–dispersion equation that includes terms for solid–liquid partitioning and irreversible kinetics. Thus, the general one-dimensional transport equation is taken to be of the form:

$$\frac{\partial \rho s}{\partial t} + \frac{\partial \theta c_r}{\partial t} = \frac{\partial}{\partial x} \left(\theta D \frac{\partial c_r}{\partial x} - q c_r \right) - \theta \mu c_r + \theta \gamma \quad (32)$$

where c_r is the resident solution concentration, s is the adsorbed concentration, ρ is the dry soil bulk density, D is a dispersion coefficient, q is the Darcian fluid flux density, μ is a first-order degradation coefficient and γ is a zero-order production coefficient. Other symbols are the same as before. Most parameter estimation studies of solute transport thus far have assumed steady-state flow or some equivalent steady-state system using a transformation that avoids the solution of the transient flow equation (eqn. 24) along with eqn. (32). For steady-state flow in a homogeneous profile, the transport equation reduces to:

$$\frac{\rho}{\theta} \frac{\partial s}{\partial t} + \frac{\partial c_r}{\partial t} = D \frac{\partial^2 c_r}{\partial x^2} - v \frac{\partial c_r}{\partial x} - \mu c_r + \gamma \quad (33)$$

where $v = q/\theta$ is the mean pore water velocity.

Application of parameter estimation techniques to the determination of various unknown coefficients in eqn. (33) are discussed below. For convenience, a distinction will be made between transport models involving local equilibrium and non-equilibrium conditions. Spatial variability of medium properties often limits the applicability of deterministic approaches based on eqn. (33) to mass transport predictions at the field-scale. Thus, a stochastic formulation that explicitly considers the effects of areal variations in hydraulic fluxes on field-scale solute transport will also be discussed.

Equilibrium transport

Consider the special case where adsorption is described by a linear isotherm of the form $s = kc_r$, where k is an empirical distribution coefficient. Equation (33) reduces then to:

$$R \frac{\partial c_r}{\partial t} = D \frac{\partial^2 c_r}{\partial x^2} - v \frac{\partial c_r}{\partial x} - \mu c_r + \gamma \quad (34)$$

where $R = 1 + \rho k/\theta$ is the retardation factor. Inspection of eqn. (34) shows that the equilibrium transport model contains five unknown parameters: R , D , v , μ and γ . Of these five parameters, a maximum of four can be fitted simultaneously to a set of observed $c_r(x, t)$ data. This dependency of at least one of the coefficients follows immediately by noting that division of eqn. (34) by a constant permits one of the coefficients to be eliminated. Consequently, at least one of the non-zero coefficients R , D , v , μ or γ must be known independently. Because values of D , μ and γ are not easily measured independently, in practice either v or R (or both) must be known beforehand. For non-adsorbing chemicals, $R = 1$ and v can be fitted to the data. This may be opportune if, for example, uncertainty exists about the hydraulic flux or the effective water content in the system. For adsorbing chemicals, R can at least in principle be estimated directly using batch equilibration techniques.

Proper stipulation of boundary conditions for the solution of eqn. (34) can be critical to the parameter estimation problem. Choice of boundary conditions depends on the method of solute introduction into the system and on the mode of observation of concentrations in time and/or space. If solute of concentration c_0 is injected at a constant flow rate, then the appropriate boundary condition is:

$$\left(vc_r - D \frac{\partial c_r}{\partial x}\right)_{x=0^+} = \begin{cases} vc_0, & 0 \leq t \leq t_0 \\ 0, & t > t_0 \end{cases} \quad (35)$$

where t_0 is the duration of pulse c_0 . The solution of eqn. (34) subject to eqn. (35) and to the additional conditions:

$$c_r = c_i \quad x \geq 0, \quad t = 0 \quad (36a)$$

$$\partial c_r / \partial x = 0 \quad x \rightarrow \infty, \quad t > 0 \quad (36b)$$

may be used to describe resident concentrations in effectively semi-infinite systems or in finite systems of length L when $P = vL/D \geq 5$ (Van Genuchten and Parker, 1984). Subject to some additional constraints, the solution of eqns. (34)–(36) may suffice for smaller P in a finite system when D is due to mobile-immobile zone interactions (Parker, 1984; Parker and Valocchi, 1986). Detection of resident solutions may be obtained by sectioning soil cores and extracting the solution via a suction apparatus or, for non-adsorbed species, by repeated washing with tracer-free solution.

Another mode of solute detection, pertinent to certain experimental conditions, involves flux concentrations which represent hydraulic flux-weighted mean concentrations on a cross section of the porous medium. Such concentrations arise naturally from observations of effluent from a soil column, a lysimeter, or an extraction well. Macroscopically, the flux concentration c_f may be defined as a ratio of solute flux density to hydraulic flux density which indicates (Kreft and Zuber, 1978):

$$c_f = c_r - \frac{D}{v} \frac{\partial c_r}{\partial x} \quad (37)$$

Using eq. (37) we find that eqns. (34) and (36) transform to expressions of identical form in c_f while eqn. (35) becomes:

$$c_f = \begin{cases} c_0, & 0 \leq t \leq t_0 \\ 0, & t > t_0 \end{cases} \quad (38)$$

If boundary conditions are improperly formulated, appreciable errors in parameter estimates may arise for the inverse problem. As an example, consider a problem discussed by Parker and Van Genuchten (1984a). Resident solutions were generated using an analytic solution to eqns. (34)–(36) for medium coefficients given in Table 2. The initially solute-free medium ($c_i = 0$) is subjected to a pulse input of $c_0 = 100 \mu\text{g cm}^{-3}$ for a duration $t_0 = 5$ days.

TABLE 2

Comparison of fitted transport parameters using correct and erroneous detection modes for hypothetical problem

| | D | R | μ | γ |
|-----------------------|--------|--------|--------|----------|
| True values for c_r | 100.00 | 2.5000 | 0.2500 | 0.5000 |
| Fit to c_r solution | 100.28 | 2.5006 | 0.2496 | 0.4971 |
| Fit to c_f solution | 85.6 | 2.52 | 0.34 | 0.76 |
| Fit to c_f solution | 161.7 | 3.00 | (0.25) | (0.50) |

D in $\text{cm}^2 \text{day}^{-1}$, γ in $\mu\text{m cm}^{-3} \text{day}^{-1}$, values in parentheses was assumed known.

Resident solutions were predicted for 11 depths from 0–100 cm at $t = 5$ and 10 days. Parameters were estimated by a non-linear least-squares regression procedure with equal weights for all observations and using only the $t = 5$ days data. Initial guesses for all parameters were taken to be unity. Using the correct solution for resident concentrations, parameter estimates were found to be very close to their true values whereas for the erroneous flux concentration boundary conditions, significant errors in parameter estimates occurred. When μ and γ were fixed at their correct values, a two-parameter fit greatly overestimated D and R . This overestimation is a characteristic occurrence when resident concentrations are misinterpreted as flux concentrations (Parker and Van Genuchten, 1984b). The converse will be found when flux concentrations are misinterpreted as resident concentrations.

Non-equilibrium transport

Although the linear equilibrium convection–dispersion model represented by eqn. (34) is the most common approach to describing transport, many circumstances arise for which it may be inadequate. Limitations arise due to kinetic control of adsorption reactions disregarded by eqn. (34). One approach to the extension of eqn. (31) has been to consider two types of adsorption sites, one governed by equilibrium adsorption and one by reversible first-order kinetics. Such two-site models have been discussed by Selim et al. (1976), Cameron and Klute (1977), Rao et al. (1979), De Camargo et al. (1979), Van Genuchten (1981), Flühler and Jury (1983) and others. If type-1 sites are regarded as equilibrium-controlled, then R in eqn. (34) may be considered the retardation due to adsorption on type-1 sites (R_1). For kinetically-controlled type-2 sites, the term:

$$\frac{\partial \bar{c}_2}{\partial t} = \alpha(k_2 c_r - \bar{c}_2) \quad (39)$$

must be added to the LHS of (34), where \bar{c}_2 is the amount of solute adsorbed on type-2 sites expressed as an equivalent solution concentration, α is a rate coefficient, and k_2 is the slope of the equilibrium isotherm for type-2 sites

TABLE 3

Initial and fitted parameter values and associated residual SSQ's for the two-site model fit to boron effluent data from Glendale clay loam

| | D | R_t | β | ω | SSQ |
|----------------|-------|-------|---------|----------|-------|
| Initial values | 1.0 | 1.00 | 0.500 | 0.200 | |
| Final values | 216.0 | 3.58 | 0.564 | 14.2 | 0.142 |
| Initial values | 2.00 | 10.00 | 0.200 | 0.200 | |
| Final values | 47.7 | 4.30 | 0.600 | 0.424 | 0.53 |

Units of D in $\text{cm}^2 \text{day}^{-1}$, other values dimensionless.

$d\bar{c}_2/dc_r$. Analytic solutions for the two-site model may be obtained for both resident and flux detection modes if adsorption/exchange is linear (Coats and Smith, 1964; Van Genuchten and Wierenga, 1976b; Parker and Van Genuchten, 1984a), while for non-linear adsorption numerical solutions may be employed (e.g., Van Genuchten and Wierenga, 1976a; Flühler and Jury, 1983).

As an application of the parameter estimation method to the two-site model, consider an experimental breakthrough curve for boron in a Glendale clay loam described by Van Genuchten (1974). A boron tracer of pulse duration $t_0 = 5.06$ days and having a concentration $c_0 = 20 \mu\text{g cm}^{-3}$ was leached through an initially solute-free 30 cm long column. The measured pore water velocity was 38.5 cm day^{-1} . Four parameters were fitted to the data: the dispersion coefficient D , total retardation factor $R_t = 1 - R_1 + R_2$ where $R_2 = 1 + k_2$, a site distribution factor $\beta = R_1/R_t$, and a reduced rate constant $\omega = \alpha(1 - \beta)R_t L/v$ where L is the column length (for more details see Van

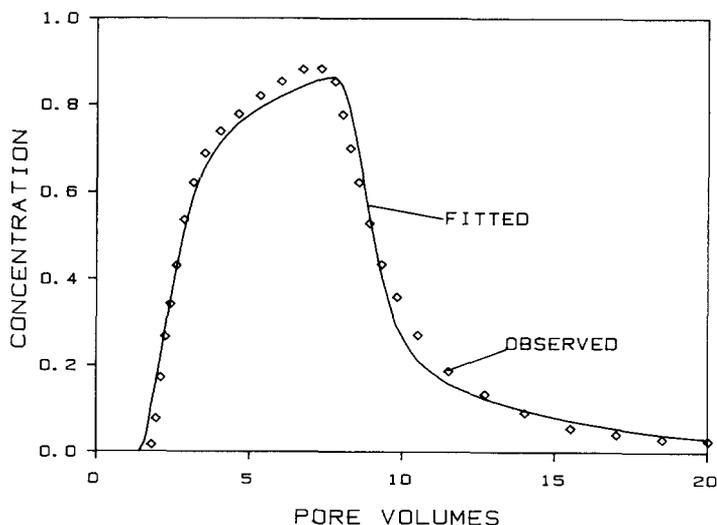


Fig. 4. Experimental boron effluent curve for Glendale clay loam and fitted curve using linear two-site kinetic model (from Parker and Van Genuchten, 1984a).

Genuchten, 1981 or Parker and Van Genuchten, 1984a). Final parameter estimates and sums of squared residuals (SSQ) for two different sets of initial parameter estimates using the solution for flux concentrations are shown in Table 3. The results of the first example yielding the lowest SSQ are compared with the experimental data in Fig. 4. For the second set of initial parameter estimates, the inversion program converged to a set of parameter values having a larger SSQ using the stopping criteria that all parameters change by a factor of less than 0.0005 from the previous iteration and allowing a maximum of 50 trials with no residual decrease at an iteration. In this instance a local minimum or plateau occurs in the response surface, which prevents convergence to the global minimum. This points to the need for realistic initial estimates of parameter values. Some specific guidelines for selecting initial values for the two-site model are discussed by Parker and Van Genuchten (1984a).

As pointed out by Van Genuchten (1981) and Nkedi-Kizza et al. (1983), a mathematical problem of identical form to that of the two-site kinetic model may be obtained when apparent non-equilibrium in the system is attributed to diffusional limitations between mobile and immobile pore regions, provided that diffusion is approximated by an apparent first-order exchange process. In non-dimensionalized form, the two-site and two-region models become identical, thus leading to difficulty in ascribing proper physical significance to fitted model parameters (e.g., β and ω in the preceding example). Further complications relevant to the parameter identification problem arise owing to relationships between the first-order two-site/two-region model, and to interrelationships between the first-order two-site/two-region model and the equilibrium convection–dispersion model on the simpler side, or a true diffusional kinetic model on the more complex side. It may be demonstrated that under certain conditions, the true diffusion kinetic analysis will degenerate to the form of the first-order kinetic model or to the local equilibrium model (Passioura, 1971; Raats, 1981; Bolt, 1982; De Smedt and Wierenga, 1984; Van Genuchten, 1985; Valocchi, 1985; Parker and Valocchi, 1986). In such circumstances, the parameter identification problem will be essentially indeterminate and model selection should be governed by parsimony (e.g., Parker, 1984).

Further difficulties in the parameter estimation problem may arise due to non-linearity and/or non-uniqueness in the adsorption isotherm, and hence in R (or R_1 and R_2), and to similar complications for the production and decay coefficients μ and γ . A number of modelling approaches have been developed which incorporate more complex equilibrium chemistry, ranging from the use of empirical non-linear isotherms with or without hysteresis (Van Genuchten and Cleary, 1979) to more detailed geochemical analyses (Rubin and James, 1973; Jennings et al., 1982; Cederberg et al., 1985). The use of overly simplified chemical models to describe complex systems can lead to difficulties when predictions are extrapolated to situations that are different from those used in the calibration process. For example, Jardine et al. (1985) found that a linear two-site non-equilibrium transport model closely described observed Al breakthrough curves for a soil in which Ca–Al exchange and Al polymerization

TABLE 4

Effect of influent Al concentration ($\mu\text{g ml}^{-1}$) on calculated and fitted parameters for a linear two-site kinetic model (after Jardine et al., 1985)

| Influent concentration | R | | β | | fitted α (h^{-1}) |
|------------------------|-------|--------|---------|--------|-------------------------------------|
| | calc. | fitted | calc. | fitted | |
| 0.73 | 40.2 | 51.8 | 0.632 | 0.620 | 0.132 |
| 1.51 | 25.2 | 42.2 | 0.415 | 0.417 | 0.124 |
| 2.37 | 16.8 | 49.6 | 0.216 | 0.261 | 0.127 |
| 4.85 | 13.6 | 17.1 | 0.325 | 0.363 | 0.262 |
| 7.75 | * | 12.0 | 0.329 | 0.385 | 0.330 |

* Data not available from isotherm.

controlled transport. An acceptable fit was obtained in spite of highly non-linear adsorption-precipitation relations. For experiments run at different influent Al concentrations, values of D , R_t , β and α for the linear two-site model were estimated from breakthrough curves using a least-squares regression analysis. Independent estimates of linearized distribution coefficients, allowing calculation of R_t and β , were made from batch equilibrium data. Comparisons of fitted and calculated values indicated good correspondence for β , while R_t values were less consistent (Table 4). Notable variations in the apparent rate constant α occurred with influent concentration, which should not arise if the reaction strictly followed first-order chemical kinetics or was diffusionally controlled. Higher-order chemical kinetics may be suggested. An equally plausible explanation is that at lower influent Al-levels, increasing non-linearity in the isotherm produces greater tailing in the breakthrough curves. This tailing is then simulated by the model as a kinetic effect yielding lower fitted α .

In more recent studies, potassium transport subject to non-linear K-Ca exchange in a heterogeneous medium with equilibrium and kinetic adsorption sites has been simulated. To evaluate parameter interactions, the linear two-site kinetic model was fitted to a series of hypothetical breakthrough curves that were generated numerically with a similar kinetic model that also accounted for non-linear adsorption. While keeping the rate coefficients α fixed at the original values used in the non-linear model, the fitted (linear) retardation factors were found to decrease significantly with increasing α . This interaction occurs because the linear model will simulate tailing, due actually to non-linearity in the isotherms, through adjustments in the relative proportion of equilibrium versus non-equilibrium adsorption sites, as well as through changes in the dispersion coefficient. Interactions between D and observed chemical-kinetic effects were also noted by Van Genuchten (1981) for non-linear boron displacement through a clay loam soil. Thus, when a strongly non-linear displacement model is linearized or when important kinetic mechanisms are neglected in the parameter estimation analysis, the results may

become physically meaningless, even for parameters that are not directly affected by the approximation.

Field-scale transport

The question of field-scale variability effects on both the formulation of the direct problem and on the inverse problem solution will now be considered. To evaluate the effects of field-scale heterogeneities, a stochastic approach must generally be taken. Here, discussion will be restricted to a relatively simple model discussed by Parker and Van Genuchten (1984a) which is similar to the one-dimensional stochastic transport models of Bresler and Dagan (1981), Amoozegar-Fard et al. (1982) and Simmons (1982). Conceptually, the transport region is regarded as being composed of numerous independent parallel soil columns (denoted as the "local" scale), each having specific properties and being subject to specific local boundary conditions. Additionally, it is assumed that transport within each column can be described by the one-dimensional convection-dispersion eqn. (34) with constant coefficients. Lateral flow, transverse dispersion, and vertical inhomogeneities are conveniently ignored.

To approximate transient flow, hydraulic fluxes and water contents are averaged over the time and space domains of interest. At the local scale, mean local surface hydraulic fluxes q_0 and water contents θ are defined as (Parker and Van Genuchten, 1984a):

$$\bar{q}_0 = \frac{1}{t_m} \int_0^{t_m} q_0(t) dt \quad (40)$$

$$\bar{\theta} = \frac{1}{x_m t_m} \int_0^{t_m} \int_0^{x_m} \theta(x, t) dx dt \quad (41)$$

where $(0, t_m)$ and $(0, x_m)$ are the time and distance intervals for averaging and q_0 is the hydraulic flux at the soil surface. The time-averaged local velocity is then taken as:

$$\bar{v} = \bar{q}_0 / \bar{\theta} \quad (42)$$

At the global- or field-scale, means over the areal domain A of the time-averaged velocity are defined as:

$$\langle \bar{v} \rangle = \frac{1}{A} \int_{(A)} \bar{v} dA \quad (43)$$

of the time-averaged surface flux \bar{q}_0 :

$$\langle \bar{q}_0 \rangle = \frac{1}{A} \int_{(A)} \bar{q}_0 dA \quad (44)$$

and of the instantaneous surface flux q_0 at time t as:

$$\langle q_0 \rangle(t) = \frac{1}{A} \int_{(A)} \bar{q}_0(t) dA \quad (45)$$

The equivalent steady-state time variable is then defined by the transformation:

$$t^*(t) = \int_0^t \langle q_0 \rangle(\tau) d\tau / \langle \bar{q} \rangle \quad (46)$$

Variations in local pore water velocities \bar{v} are assumed to be lognormally distributed with probability density function $\rho(\bar{v}) = N(\mu_{\ln}, \sigma_{\ln}^2)$ where μ_{\ln} and σ_{\ln}^2 are the mean and variance of $\ln \bar{v}$, respectively. The local dispersion coefficient is assumed to be perfectly correlated to \bar{v} such that $D = \varepsilon \bar{v}$ for deterministic apparent dispersivity ε . Ignoring R , μ and γ leads then to a three-parameter field-scale transport model described by ε , σ_{\ln} and μ_{\ln} .

Field-scale resident concentrations \hat{c}_r are given as areal means over domain A as:

$$\hat{c}_r(x, t^*) = \frac{\int_{(A)} c_r(x, t^*) dA}{\int_{(A)} dA} \quad (47)$$

where c_r is the local-scale concentration. Since \bar{v} is the only random variable on A , $\rho(\bar{v}) d\bar{v}$ may be substituted for dA :

$$\hat{c}_r(x, t^*) = \frac{\int_0^\infty c_r(x, t^*; \bar{v}) \rho(\bar{v}) d\bar{v}}{\int_0^\infty \rho(\bar{v}) d\bar{v}} \quad (48)$$

Ignoring variations in θ in the field as small compared to q , field averaged flux concentrations are obtained as:

$$\hat{c}_f(x, t^*) = \frac{\int_0^\infty c_f(x, t^*; \bar{v}) \bar{v} \rho(\bar{v}) d\bar{v}}{\int_0^\infty \bar{v} \rho(\bar{v}) d\bar{v}} \quad (49)$$

The integrals in eqns. (48) or (49) may be evaluated by numerical quadrature once local boundary conditions are stipulated. As appropriate, these may be defined by invoking a constant pulse duration t_0 for the field or by imposing a constant local mass loading which leads to local values of t_0 varying inversely with \bar{v} . For purposes of model calibration, note that for n random measurements of local concentration c_r or c_f in the field, the field-average values \hat{c}_r or \hat{c}_f may be calculated by replacing the integrals in eqns. (48) or (49) by sums with weighting coefficients $\rho(\bar{v}) = 1/n$ assigned to each observation. To obtain \hat{c}_r , local velocities must be known.

Application of the above model to a field experiment described by Jury et al.

TABLE 5

Parameter estimates and their standard errors of estimation (\pm) for the field-scale bromide tracer experiment of Jury et al. (1982), values fixed on input are shown in parentheses

| Trial | ε (mm) | $\langle v \rangle$ (mm day ⁻¹) | σ_{in} | SSQ |
|-------|-----------------------|--|-------------------|-----------|
| 1 | 1.0 \pm 227 | 30.5 \pm 21.0 | 0.800 \pm 0.943 | 0.0005177 |
| 2 | (0.01) | 30.5 \pm 1.8 | 0.803 \pm 0.060 | 0.0005185 |
| 3 | (1.0) | 30.5 \pm 1.8 | 0.800 \pm 0.060 | 0.0005177 |
| 4 | (10.0) | 29.7 \pm 1.7 | 0.763 \pm 0.063 | 0.0005182 |
| 5 | (100.0) | 24.7 \pm 1.6 | 0.373 \pm 0.143 | 0.00056 |
| 6 | 123 \pm 22 | 23.6 \pm 1.4 | (0.0) | 0.00061 |

(1982) involving measurements of bromide transport in a 0.64 ha field under transient hydraulic conditions is considered. Concentrations were determined with solution samplers at various depths taken at different times after addition of the tracer. Areal-averaged resident concentrations at a depth of 30 cm versus transformed time t^* were used as input to the inverse problem to estimate ε , (note that $\langle \bar{v} \rangle$ is a known function of σ_{in} and μ_{in}). The results indicate large uncertainty in ε (Table 5). Using a two-parameter fit with ε fixed at various values, little sensitivity of the model to ε for $\varepsilon \leq 10$ mm was found. For larger ε , the mean error increases slightly, but compensation between ε and σ_{in} is observed as the fitted values of σ_{in} decrease for larger ε . Thus, field-scale dispersion is reduced as local-scale dispersion increases. Note from Table 5 that even when $\sigma_{in} = 0$, which corresponds to the deterministic convection–dispersion model, SSQ is only moderately larger than for the three-parameter stochastic model.

Fitted concentration–time curves using trial 1 and trial 6 parameter estimates from Table 5, corresponding to the three-parameter stochastic model and the two-parameter deterministic model, are compared to observed data for $x = 30$ cm in Fig. 5a. Using the same parameter estimates, breakthrough curves were predicted for 60–90 cm depths and are compared to observed data in Fig. 5b and c. It is apparent that while the two models are virtually indistinguishable at the calibration depth, they yield increasingly divergent predictions at greater depths. Jury and Sposito (1985) presented a detailed comparison of the deterministic convection–dispersion model (denoted as the CDE model) and a “transfer function model” (TFM, Jury, 1982) which corresponds to the stochastic model described above with $\varepsilon \rightarrow 0$ (local piston flow). Results of their analyses for calibration of the two models to breakthrough curves for each depth are shown in Fig. 6. Error ellipses computed by partitioning squared deviations between model predictions and observations by the χ^2 theorem indicate better clustering for the TFM than the CDE model, but both models are clearly too simplistic to fully describe the observed transient transport of bromide. While the CDE tends to underpredict the rate of spreading of the solute distribution due to the assumption of homogeneity, the TFM tends to

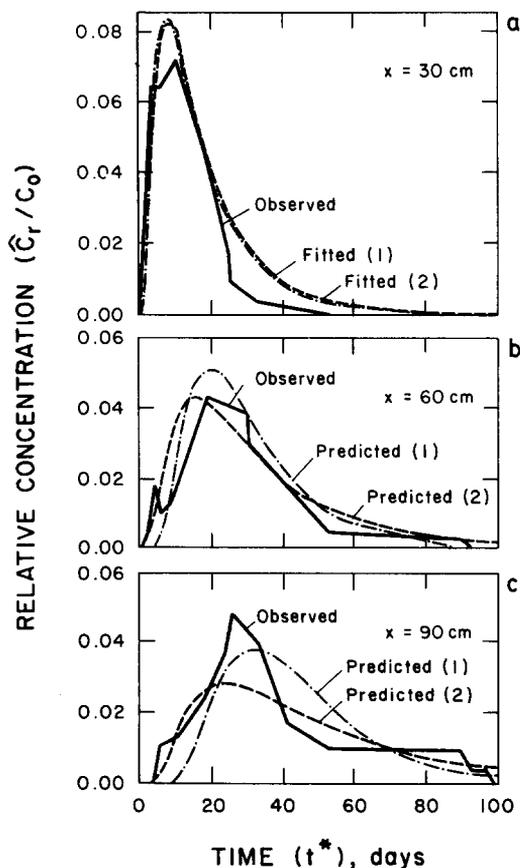


Fig. 5. Experimental areally-averaged resident concentrations at three depths as a function of transformed time t^* for bromide transport in a field soil (data from Jury et al., 1982). (a) data for 30 cm depth and fitted curve using the deterministic convection–dispersion model and a three-parameter stochastic model; (b) data for 60 cm depth and predicted curves for the two models using parameters fitted to the 30 cm depth data; (c) same as (b) for the 90 cm depth data.

overpredict spreading due to the assumption of zero lateral transport and of perfect correlation of velocity distributions with depth. These results emphasize the caution which must be exercised when a calibrated model is used to extrapolate to conditions and particularly to travel distances which differ greatly from those employed for the inverse problem solution.

Data specification and data error

Given a suitable parametric model, the most critical factor for successful parameter estimation analysis becomes specification of a data set which will lead to a unique and well-behaved solution of the inverse problem. In practice, experimental design will be a compromise between optimum conditions for the

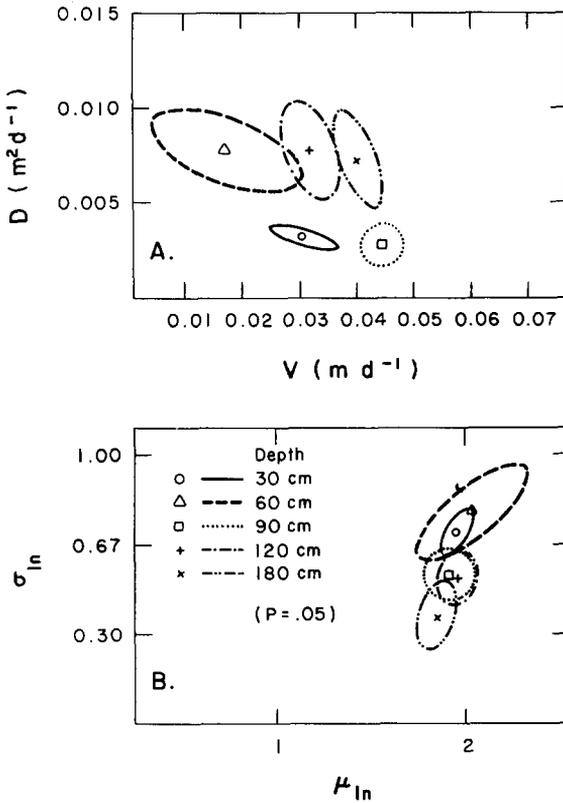


Fig. 6. Mean and 0.05 probability error ellipses for parameters fitted to breakthrough curves at different depths for (a) CDE model, and (b) TFM model (from Jury and Sposito, 1985).

inverse problem and technological and economic constraints. In other words, we would like to obtain a well-behaved inverse problem but not pay too dearly in computational and experimental costs. The assumed model will dictate to some extent the type of data which must be collected. Data sufficient to define the hydrologic conditions will be necessary, although the requirements may range from stipulation of (quasi)-steady-state hydraulic fluxes or water balances for simple hydrologic models, to complete specification of soil hydraulic properties and flow boundary conditions for explicit modelling of transient variably-saturated flow. Irrespective of the flow model, observations of tracer concentrations must be made at various locations and/or times. Frequency and spatial distribution of observations will impact the feasibility of the inverse problem.

As an example of the effects of data set composition on the inverse problem, consider a hypothetical data set generated with the linear two-site/two-region model consisting of 12 concentration observations versus time at two depths each. Such a situation is not atypical of field experiments where the data may be obtained from suction solution samplers (Parker and Van Genuchten,

TABLE 6

Statistics for inverse problems on 240 realizations of a data set subject to random error (after Wagner and Gorelick, 1986)

| | D | v | μ | γ |
|-------------------------------|-------|-------|--------|----------|
| True values | 100.0 | 25.00 | 0.2500 | 0.500 |
| <i>Time and distance data</i> | | | | |
| Mean | 100.9 | 24.98 | 0.2495 | 0.487 |
| Bias | 0.9 | 0.02 | 0.0005 | 0.013 |
| Standard deviation | 7.6 | 0.29 | 0.0164 | 0.227 |
| <i>Distance-only data</i> | | | | |
| Mean | 101.7 | 25.06 | 0.2471 | 0.389 |
| Bias | 1.7 | 0.06 | 0.0029 | 0.111 |
| Standard deviation | 12.4 | 0.73 | 0.0258 | 0.941 |
| <i>Time-only data</i> | | | | |
| Mean | 95.3 | 25.15 | 0.2599 | 0.901 |
| Bias | 4.7 | 0.15 | 0.0099 | 0.401 |
| Standard deviation | 27.9 | 0.44 | 0.0635 | 1.926 |

D in $\text{cm}^2 \text{day}^{-1}$, v in cm day^{-1} , μ in day^{-1} , γ in $\mu\text{g cm}^{-3} \text{day}^{-1}$.

1984a). Using data for both depths, a five-parameter inversion for v , D , R , β , ω and t_0 successfully converged to the true values. Using concentration data for only one depth, convergence could not be obtained for the five-parameter inversion. Convergence for the smaller data set was feasible if t_0 was assumed known and only four parameters were estimated.

In actuality, exact correspondence between model predictions and observed data will never occur, due in part to simplifications inherent in the parametric model as well as to measurement errors. Wagner and Gorelick (1986) studied the effects of the latter via a Monte Carlo approach. Twenty concentration observations were generated for two times each at 25 depths using the simple one-dimensional convection–dispersion model for the same problem as discussed previously in conjunction with Table 2. Each concentration value was assumed to be subject to random measurement error such that the probability of a given observed value is normally distributed with standard deviation equal to 20% of the true concentration. Parameter estimation analyses for 240 realizations of the data, with random error overlain, were carried out to determine D , v , μ and γ . Means, variances and biases of the parameter estimates from the 240 replications were computed using a weighted least-squares procedure with weights inversely proportional to the estimated concentration values. The results (Table 6) indicate that parameter estimates are essentially unbiased. This may be attributed in part to the adopted weighting scheme which corresponded to the assumed model for distributions of measurement error. Sensitivity to data error varied markedly with parameters. For v , the standard deviation of estimates for the 240 realizations was only 1% of the mean value, for

D and γ they were approximately 7%, and for μ the standard deviation was 45% of the mean. The difficulty in accurately determining μ would be evident in individual inversion analyses from a large standard error of estimation in the parameter.

To compare the suitability of concentration observations in time or space, similar Monte Carlo analyses were performed using either observations in time at single points in space or observations versus distance at single times. The results (Table 6) indicate less satisfactory parameter estimates than when both time and distance data were used. Use of spatially distributed observations led to results with markedly lower biases and standard errors than the use of temporally distributed observations. Additionally, better agreements between parameter confidence limits, obtained from individual inversion analyses and those estimated from the Monte Carlo analyses, were obtained using spatially distributed data, indicating that the linear error analysis is more suitable for spatial data.

Similar preference of spatially over temporally distributed data appear to be indicated also by analyses of Jury and Sposito (1985) for field-scale tracer movement. Parameter estimation variances for their transfer function model calibrated using soil core data (spatial distributions) were lower than when model calibration was carried out using suction solution sampler data (temporal distributions) at single depths. The interpretation of these results is, however, confounded by differences in experimental procedures. In the soil core experiments, 36 replicates were available. The solute was moved into the ground by daily sprinkler irrigation, and the entire experiment took only two weeks. In contrast, the solution sampler experiment was irrigated by rainfall with long periods of evaporation in between and had only 14 sites for solution sampler analysis (W.A. Jury, pers. commun., 1986).

The results above indicate that the form and accuracy of data for the inverse problem can incur varying degrees of estimation error in the parameters and in some instances impede convergence. Data uncertainty may affect the sensitivity of the results to different parameter estimation methods as well. In weighted least-squares regression, the weighting coefficients may be very significant in this respect. In the parameter estimation studies of Jury and Sposito (1985), three different objective functions were studied based on an ordinary least-squares procedure, a least-squares minimization of observed and predicted time moments to fourth-order, and a maximum likelihood analysis. Significant differences in the parameter estimates by the three methods were observed with the moments method giving greater weight than the other methods to low-concentration observations at longer times and the ordinary least-squares procedure giving them the least weight.

FUTURE DIRECTIONS

As unsaturated zone flow and transport simulations become increasingly common due to heightened concerns with the prevention and remediation of

groundwater contamination, the need for efficient and accurate methods of model calibration will become more crucial. Also, because of inherent limitations of any modelling effort, it is important that probable errors associated with model parameters and ultimately with model predictions, be quantifiable. Parameter estimation methods offer the most suitable means of meeting these requirements. Such methods have been widely applied in surface hydrology and lately also in saturated subsurface flow and transport modelling; they have only recently begun to be applied to vadose zone flow and transport model calibration. In this paper, we have summarized the basic methodology involved in parameter estimation and reviewed recent applications pertinent to vadose zone flow and transport modelling. It is clear that while certain progress has been made, a great deal of work remains to be done.

To date, the majority of studies have involved laboratory-scale experiments and rather simple parametric models. The few reported field-scale parameter estimation studies have involved simple model formulations, boundary conditions and/or soil conditions. Efforts are needed to extend parameter estimation methods to more complex field conditions using models capable of accommodating soil heterogeneity, variable and uncertain boundary conditions, simultaneous flow and transport, complex biochemical processes and other phenomena. Parameter identification and parameter estimation studies will need to be carried out in conjunction to meet these needs. Parametric formulations for the direct problem incorporating different processes in varying degrees of sophistication will need to be studied to determine the most efficient representations which do not excessively compromise accuracy and precision. For example, to accommodate effects of soil heterogeneity, investigations must address the development of concise parametric representations of soil variability, perhaps employing scaling analyses in conjunction with geostatistical methods and incorporating prior information to facilitate blocking of statistically homogeneous zones.

Given that a variety of approaches to the direct problem will be possible, explicit methods of dealing with the parameter identification problem will need to be addressed. To do this, accuracy and precision associated with different parametric representations must be considered simultaneously to evaluate the point at which increased complexity and accuracy of the model is counteracted by loss in precision due to an inability to estimate a larger number of parameters with confidence.

The analysis of optimum experimental design and optimum input data requirements for unsaturated flow and transport model inversion via parameter estimation methods has not been investigated in a systematic manner for field-scale problems. Attention must be given to the selection of the most suitable measurements (e.g., water contents, heads, solution concentrations, solid phase concentrations), the most appropriate methods of measurement (e.g., concentrations via suction samples or cores), and optimum distributions of observations in time and space. Consideration of optimum initial and boundary conditions for experiments when these are wholly or partially controlled, suitability of ambient environmental conditions, and sensitivity to uncertain-

ties in boundary and initial conditions will be important in the development of field calibration methods.

Finally, the importance of improving the efficiency and robustness of numerical methods for both the direct problem and the inverse problem is emphasized. Because parameter estimation involves repeated solution of the direct problem, efficiency of the latter becomes increasingly crucial to the practicality of parameter estimation especially when spatial variability effects are explicitly considered in the direct problem and dimensionality and model complexity increase. Because parameter values are under automatic control in the inversion analysis, robustness of the direct problem solution, in the sense of insensitivity of model accuracy to parameter values, will be of fundamental importance. Although much research on optimization methods has been done, this is still an active field and gains may be anticipated from improved efficiency and robustness of optimization techniques. The development and application of adjoint state methods to evaluate parameter gradient vectors would appear to be a particularly fruitful endeavor, which should yield substantial benefits especially when a large number of parameters must be estimated. Because the choice of objective function formulation can have significant effects on the computed results, particularly when data uncertainty is large, the objective function selection must be given suitable attention. For conclusion, much work remains to be done in the development of parameter estimation methods for unsaturated zone flow and transport models, but as the quest for field-scale predictive capability and the need for efficient calibration becomes increasingly great, these methods will be of ever increasing utility.

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