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A sequential uncertainty domain inverse procedure for estimating subsurface flow and transport parameters

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Abstract. A parameter estimation procedure, sequential uncertainty domain parameter fitting (SUFI), is presented and has the following characteristics. The procedure is sequential in nature, meaning that one more iteration can always be made before choosing the final estimates. The procedure has a Bayesian framework, indicating that the method operates within uncertainty domains (prior, posterior) associated with each parameter. The procedure is a fitting procedure, conditioning the unknown parameter estimates on an array of observed values. Finally, the procedure is iterative, requiring a stopping rule which is provided by a critical value of a goal function. Performance of the SUFI parameter estimation procedure is demonstrated using three examples of increasing complexity: (1) analysis of a solute breakthrough curve measured in the laboratory during steady state water flow, (2) estimation of the unsaturated soil hydraulic parameters from a transient drainage experiment carried out in a 6-m deep lysimeter, and (3) estimation of selected flow and transport parameters from a hypothetical ring infiltrometer experiment. The procedure was found to be general, stable, and always convergent.

Introduction

During the past several decades, considerable advances have been made in the conceptual understanding and mathematical description of water flow and solute transport processes in variably saturated soils and groundwater systems. A large number of models of different degrees of complexity and dimensionality are now available for predicting subsurface flow and transport [e.g., *National Research Council* (*NRC*), 1990; *Ségol*, 1994]. Still, effective application of these models to practical field situations suffers from two general problems. One issue concerns the inability of models, however complex and sophisticated numerically, to consider all of the important simultaneous physicochemical and hydrologic processes operative in the subsurface, such as the presence of physical and chemical nonequilibrium transport processes, preferential flow, various boundary processes, and spatial and temporal variability in soil hydraulic properties. The second issue is that even if a model were to be developed that would account for all pertinent processes, model users would still have difficulty collecting enough meaningful field data to effectively run the model. The past 30 years or so have probably seen more advances in numerical modeling per se than in the methodology of field data collection and how best to deal with parameter uncertainty in predictive modeling.

Various schemes have been proposed to somehow deal with the problem of uncertainty in model input parameters. The problems of parameter estimation and uncertainty should be addressed in a comprehensive manner using all available information. No experimental work is ever performed in a complete vacuum, and prior information is nearly always available in some manner; such information must be used to advantage by providing direction to further sampling. Nearly every project involves the collection of data of different types and qualities; these data should all be used to improve the understanding of the problem. For example, most environmental problems are spatial in nature, characterized by autocorrelated subsurface flow and transport parameters; autocorrelation in parameters hence must be revealed and taken advantage of. Moreover, measured values of the primary outputs of hydrologic simulation models often reveal the nature of the input fields and hence should also be utilized. While the collection of new or additional data is generally the most direct way of reducing input uncertainty, limiting factors such as cost, time, site destruction, and accuracy may not always permit further sampling. Comprehensive algorithms are needed to link the above seemingly different issues and considerations. An algorithm developed by *Abbaspour et al.* [1996], the Bayesian uncertainty development algorithm (BUDA), can utilize all of the above techniques to achieve a higher reduction in uncertainty in environmental projects. The inverse procedure in this work is part of BUDA.

Of the different options mentioned above the use of measured primary outputs of hydrologic simulation models to estimate model input parameters has received special attention. Much literature is devoted to this process alternatively referred to as inverse modeling, model calibration, parameter fitting, parameter estimation, and history matching. Reviews of the subject are given by *Yeh* [1986] and *Kool et al.* [1987]. The procedure generally involves minimization of the square difference function of some measured and simulated flow or transport variable. *Yeh and Yoon* [1981] studied the parameter identifiability of an aquifer with optimum dimension in parameterization. *Cooley* [1982, 1983] incorporated prior information about the parameters into a nonlinear regression groundwater flow model. *Parker and van Genuchten* [1984] applied an inverse technique to laboratory and field tracer experiments, while *Parker et al.* [1985] used one-step laboratory outflow experiments to estimate the unsaturated soil hydraulic param-

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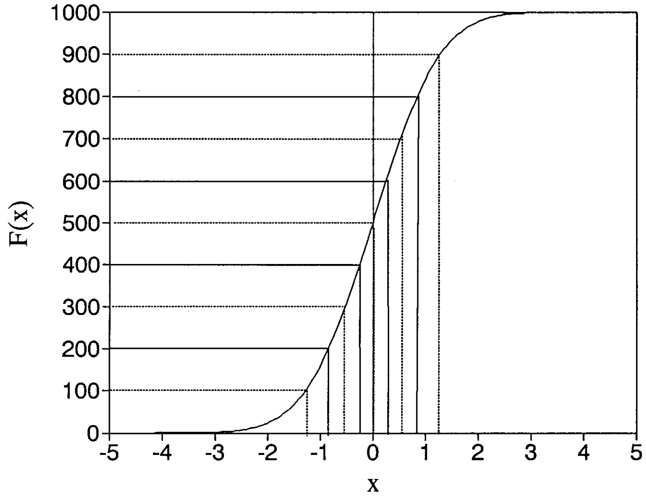

Figure 1. Division of a distributed parameter into equally sized strata for exhaustive stratified sampling. The dashed lines locate the first moments of the strata.

eters. *Carrera and Neuman* [1986] employed a maximum likelihood method and incorporated prior information in their aquifer parameter estimation procedure assuming transient and steady state conditions. *Van Dam et al.* [1990] modified the one-step outflow technique of *Parker et al.* [1985] into a multistep procedure for determining soil hydraulic functions. *Eching and Hopmans* [1993], similarly, studied optimization of the hydraulic functions using both transient outflow and soil water pressure head data. *Dane and Hruska* [1983], *Kool et al.* [1987], and *Sisson and van Genuchten* [1991] determined soil hydraulic properties from in situ water content data during vertical drainage, whereas *Kool and Parker* [1988] applied an inverse procedure to a flow process consisting of ponded infiltration followed by gravity drainage with evaporation at the soil surface. Some studies combined parameter estimation with hydraulic scaling capabilities [*Shouse et al.*, 1992; *Eching et al.*, 1994], while others coupled numerical inverse problems such as heat or mass transport with unsaturated or saturated flow [*Carrera*, 1987; *Mishra and Parker*, 1989; *Sun and Yeh*, 1990]. Yet others introduced geostatistics considerations in the parameter estimation process [*Clifton and Neuman*, 1982; *Kitanidis and Vomvoris*, 1983; *Dagan*, 1985; *Hoeksema and Kitanidis*, 1984; *Kitanidis*, 1995; *Yeh et al.*, 1996].

A common problem with most of the inverse methods is stability and convergence [*Yeh*, 1986], and more robust procedures are desirable. The objective of this work is to describe and demonstrate the use of a very different approach, sequential uncertainty domain parameter fitting (SUFI), for parameter estimation. The procedure is general, forward, sequential, iterative, and Bayesian in nature. The method begins with prior uncertainty domains on the input parameters, usually invoking relatively large uncertainties, and, subsequently, conditions the model parameters on the measured data through an objective or goal function. Ultimately, posterior uncertainty domains are obtained with much reduced uncertainties. The stopping (convergence) rule is dictated by a tolerance imposed on the goal function. On the basis of our experience in working with SUFI with different problems, three of which are discussed later in this work, the proposed procedure was found to be stable, always converging, and also well suited for global optimization.

Sequential Uncertainty Domain Parameter Fitting

The first step in running SUFI is to identify the domain of uncertainty for each parameter. This is achieved by invoking a probabilistic description of the input data. Unfortunately, expressing data in probabilistic forms is not a common practice; still, given the experimental difficulties in determining most inputs, all parameters are subject to some uncertainty and hence projects should benefit from probabilistic rather than absolute statements regarding the input data. The form of the probability function for a given parameter will depend on the information available for that parameter. For example, in depicting hydraulic conductivity, knowledge of a lognormal distribution will speed up the process of convergence. In a worst-

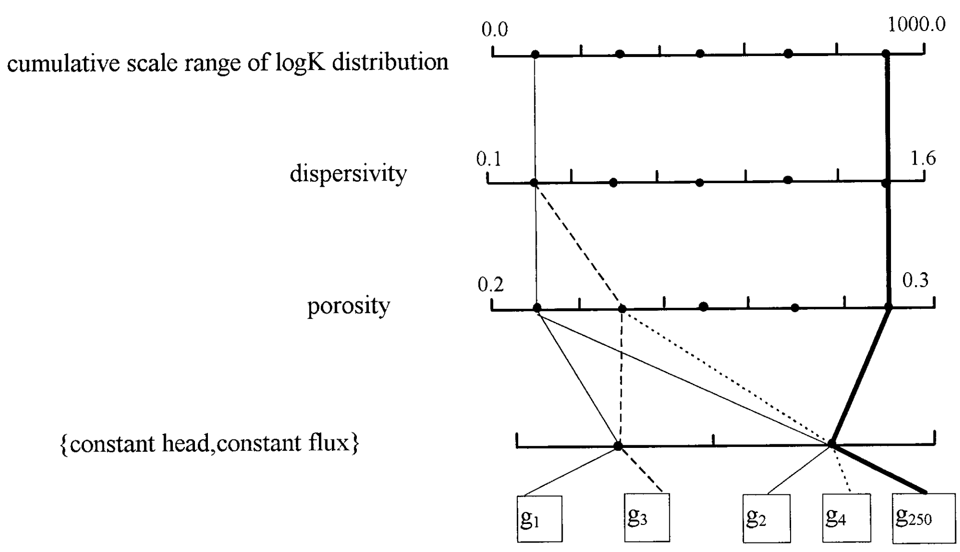

Figure 2. A schematic representation of uncertainty propagation in an exhaustive stratified sampling. The 250 possible values of the goal function are used to build a cumulative frequency distribution of the goal.

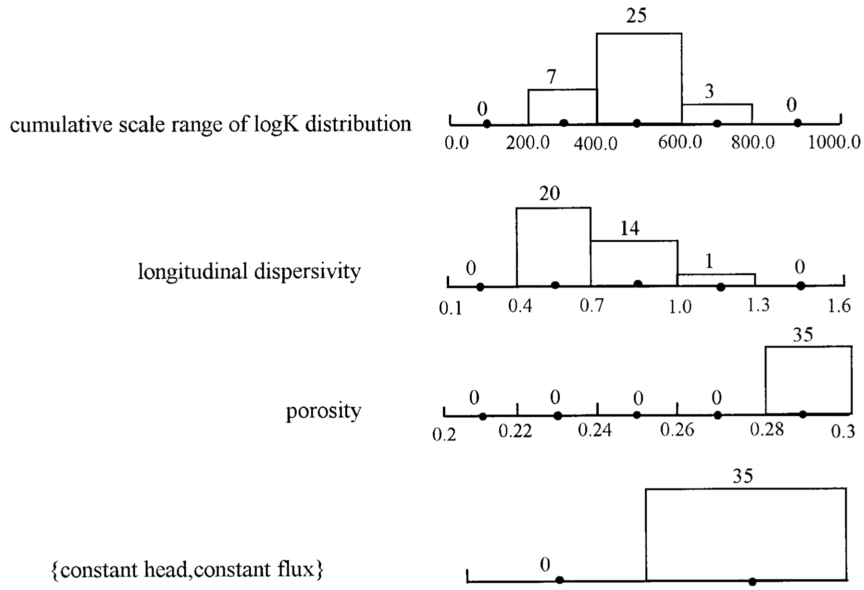

Figure 3. Frequency distribution of the number of hits in each stratum. The strata with the largest number of hits are most likely to contain the desired estimates.

case scenario the uncertain domain of a parameter can be depicted as a finite interval, i.e., a uniform probability distribution between physically realistic lower and upper bounds of that parameter. In addition, nominal parameters can be considered in the analysis. For example, if the type of boundary condition to be imposed is uncertain, a variable A can consist of A = {constant head, constant flux}. Similarly, a variable H could depict uncertainty in the type of chemical equilibrium or nonequilibrium model to be adopted, i.e., H = {local equilibrium, first-order kinetics, two-site sorption kinetics}.

During the second step, uncertainty in each parameter must be propagated through a simulation model to a goal function. Some of the commonly used goal functions in parameter estimation procedures are of the form

Absolute error

$$g = \sum_{i=1}^{N} |x_m - x_s|_i \tag{1}$$

Root-mean-square error (RMSE)

$$g = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_m - x_s)_i^2} \tag{2}$$

Logarithmic form of RMSE (LRMSE)

$$g = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\log x_m - \log x_s)_i^2} \tag{3}$$

where x_m is a measured value, x_s is a simulated value, and N is the number of measurements. We emphasize here that different goal functions can lead to quite different values for the estimated parameters. While a suitable goal function must always be formulated, its form may depend also on the objectives of the problem being investigated. The potentially very important effects of different goal functions on the results have not yet been given due attention in the literature. This issue is further discussed at the end of this paper.

If measured values (x_m^i, $i = 1, \cdots, N$) contain error, then we treat each measured point as a random variable and obtain the Bayesian distribution [*Benjamin and Cornell*, 1970] of the goal function as

$$f_G^b(g) = \int_1 \cdots \int_N f_G(g|x_m^1, \cdots, x_m^N) f(x_m^1) \cdots f(x_m^N)\, dx_m^1 \cdots dx_m^N \tag{4}$$

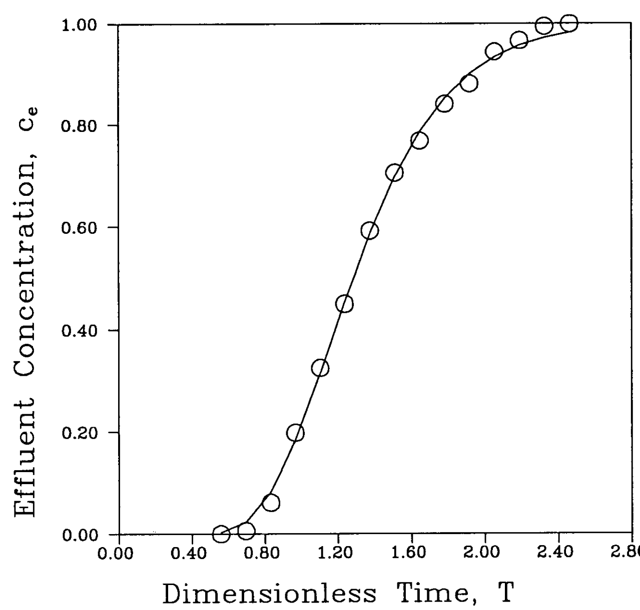

Figure 4. Comparison of measured (circles) effluent and simulated (solid line) concentrations using parameters obtained by both *van Genuchten and Wierenga* [1986] and the sequential uncertainty domain parameter fitting (SUFI) estimation approach.

Table 1. Parameters of Chromium Column Displacement Experiment in Example 1

Parameters	Values Obtained by *van Genuchten and Wierenga* [1986]	Values Obtained by SUFI*
Peclet number *P*	19.65	19.66†
Retardation factor *R*	1.349	1.348‡
Value of goal function expressed as (2)	0.01406	0.01398

*SUFI is defined as the sequential uncertainty domain parameter fitting.
†The range of uncertainty is (19.659–19.665).
‡The range of uncertainty is (1.34766–1.34772).

SUFI employs a Latin hypercube procedure [*McKay*, 1979] to obtain a solution of (4).

To propagate uncertainty in the parameters, SUFI can invoke either an exhaustive stratified sampling scheme or a random stratified sampling scheme. The stratified sampling procedure is based on a division of the cumulative probability scale range into equal probability strata for each uncertain input parameter. The first moment of each stratum on the parameter scale range is taken to represent that stratum. The procedure is illustrated in Figure 1 for a lognormally distributed parameter such as the saturated hydraulic conductivity. For parameters having uniform probability distributions the interval depicting the range of the parameter is simply divided into equal strata and the midpoint of each stratum is chosen to represent that stratum. Categorical or nominal parameters are already discretized and need no further treatment. In the exhaustive stratified sampling a hydrologic simulation program is subsequently run for all possible combinations of strata for all input parameters, and for each run the goal function is calculated (Figure 2). For the case of the random stratified sampling, only a random subset of the exhaustive case is used for simulation. This exercise allows uncertainties in the input parameters to be propagated to the goal function. The choice of the exhaustive stratified sampling or the random stratified sampling depends on the number of parameters and the speed of the simulation program. If there are too many parameters or the simulation program is too slow, then the random stratified sampling should be invoked.

Each parameter stratum in the SUFI analysis carries a score which is initially set to zero. After each simulation the goal function is calculated, and if it meets a certain tolerance criterion (e.g., when $g < 0.2$), a hit is obtained and a positive point is added to the score of each of the strata of that run. For the case where the goal function possesses a distribution as the result of measurement errors, if the tolerance is greater than the lower limit on the 95% confidence interval of the goal, then we obtain a hit. When all runs are completed, a frequency distribution of hits is constructed for each stratum as illustrated in Figure 3, where the numbers on the horizontal axes indicate the range of the parameters and the numbers on each column refer to the number of hits. Next, strata having zero or a small number of hits at both ends of each interval are eliminated, thus providing an updated uncertainty domain for the next iteration. If the initial estimate of the uncertainty range for a parameter was too small and the actual value was to the right of the interval, then all hits would fall on the rightmost stratum as shown in Figure 3 for the porosity. For the next iteration therefore we would select the interval to be [0.28, 0.32], for example. With each iteration the uncertainty domain for each parameter should get smaller, while the goal function will also decrease.

Choosing the number of strata for each parameter should be problem dependent. While having more strata may promote faster convergence because of possibly fewer iterations, too many strata could result in an unacceptable number of simulations for each iteration, especially when the simulation model runs slowly and many parameters are to be estimated. For example, if 10 parameters are present and each parameter range is divided into 3 strata, then the total number of simulations required would be 59,049 for the exhaustive stratified sampling case. For this scenario, as mentioned above, SUFI allows random stratified sampling which selects randomly a subset of simulations to be performed. For example, if we limit the number of simulations to 1% of the above exhaustive case, then each of the 59,049 simulations would be performed with a probability of 1%. This would reduce the number if simulations to about 590. Another option in SUFI for obtaining a faster result is to run the program in parallel. For example, if we would like to perform 4000 runs in an iteration, we could submit simultaneously 10 jobs of 400 runs each.

Test Cases and Parameter Estimation Results

The performance of the sequential uncertainty domain parameter fitting (SUFI) procedure is illustrated below by means of three examples of increasing complexity: (1) analysis of a solute breakthrough curve measured in the laboratory during steady state water flow, (2) estimation of unsaturated soil hydraulic pa-

Table 2. Progression to Convergence for Example 1

Number of Iterations	Parameters	Parameter Value		Number of Strata	Number of Hits in Each Stratum	Tolerance
		Minimum	Maximum			
1	*P*	5.0	50.0	10	0, 1, 2, 3, 2, 1, 1, 1, 0, 0	0.06
	R	1.0	2.0	10	0, 0, 2, 7, 2, 0, 0, 0, 0, 0	
2	*P*	9.5	41.0	10	0, 0, 2, 2, 0, 0, 0, 0, 0, 0	0.02
	R	1.2	1.5	10	0, 0, 0, 0, 2, 2, 0, 0, 0, 0	
3	*P*	15.8	22.1	10	0, 0, 0, 0, 0, 2, 2, 0, 0, 0	0.0144
	R	1.32	1.38	10	0, 0, 0, 0, 2, 2, 0, 0, 0, 0	
4	*P*	18.32	20.21	20	10 × 0, 4, 6, 7, 7, 6, 6, 5, 3, 0, 0	0.0141
	R	1.338	1.356	20	8 × 0, 5, 7, 8, 8, 7, 6, 3, 0, 0, 0, 0, 0	
5	*P*	19.265	20.021	20	7 × 0, 1, 2, 1, 10 × 0	0.0140
	R	1.3452	1.3515	20	9 × 0, 2, 0, 2, 8 × 0	
6	*P*	19.492	19.73	40	28 × 0, 1, 11 × 0	0.01398
	R	1.347	1.3492	40	12 × 0, 1, 27 × 0	

Table 3. Distribution of the Number of Hits for Iteration 1 in Table 2 as a Function of Tolerance

Number of Iterations	Parameters	Parameter Value		Number of Strata	Number of Hits in Each Stratum	Tolerance
		Minimum	Maximum			
1	*P*	5.0	50.0	10	2, 3, 3, 3, 3, 3, 3, 3, 3, 2	0.10
	R	1.0	2.0	10	0, 0, 9, 10, 9, 0, 0, 0, 0, 0	
	P	5.0	50.0	10	0, 3, 3, 3, 3, 3, 2, 2, 2, 1	0.08
	R	1.0	2.0	10	0, 0, 8, 9, 5, 0, 0, 0, 0, 0	
	P	5.0	50.0	10	0, 1, 2, 3, 2, 1, 1, 1, 0, 0	0.06
	R	1.0	2.0	10	0, 0, 2, 7, 2, 0, 0, 0, 0, 0	
	P	5.0	50.0	10	0, 0, 1, 1, 1, 1, 0, 0, 0, 0	0.04
	R	1.0	2.0	10	0, 0, 0, 4, 0, 0, 0, 0, 0, 0	
	P	5.0	50.0	10	0, 0, 0, 1, 0, 0, 0, 0, 0, 0	0.02
	R	1.0	2.0	10	0, 0, 0, 1, 0, 0, 0, 0, 0, 0	
	P	5.0	50.0	10	0, 0, 0, 0, 0, 0, 0, 0, 0, 0	<0.02
	R	1.0	2.0	10	0, 0, 0, 0, 0, 0, 0, 0, 0, 0	

rameters from a transient drainage experiment carried out using a large 6-m deep lysimeter, and (3) estimation of selected flow and transport parameters from a hypothetical ring infiltrometer experiment. We also used example 1 to show the effect of a 50% error in measured data, and we performed example 3 with both exhaustive and random stratified sampling schemes.

Example 1: Analysis of Observed Solute Breakthrough Curve

The first example deals with a column experiment treated previously by *van Genuchten and Wierenga* [1986]. In this experiment, transport of chromium was studied through a 5-cm long column of sand. Figure 4 shows the observed effluent curve. The governing transport model for this example is the one-dimensional convection dispersion equation

$$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \tag{5}$$

subject to the initial and boundary conditions

$$C(x, 0) = 0 \tag{6}$$

$$\left(-D \frac{\partial C}{\partial x} + vC\right)\Big|_{x=0} = vC_0 \tag{7}$$

$$(\partial C/\partial x)(\infty, t) = 0 \tag{8}$$

where C is the volume-averaged concentration, R is the retardation factor accounting for linear sorption, D is the dispersion coefficient, x is the distance, t is the time, v is the pore water velocity, and C_0 is the inlet concentration. The analytical solution of this transport problem for the flux-averaged relative effluent concentration c_e at the end of the column $x = L$ is given by

$$c_e(T) = \frac{1}{2} \operatorname{erfc}\left[\frac{\sqrt{P}}{2\sqrt{RT}}(R - T)\right] + \frac{1}{2} e^P \operatorname{erfc}\left[\frac{\sqrt{P}}{2\sqrt{RT}}(R + T)\right] \tag{9}$$

$$T = vt/L \tag{10}$$

$$P = vL/D \tag{11}$$

where T is dimensionless time (pore volume) and P is the column Peclet number. Measured $c_e(T)$ data are plotted in Figure 4.

Several methods for estimating the unknown parameters P and R in (9), i.e., trial and error, analysis of the slope of the effluent curve, analysis of a lognormal plot of the data, and using a nonlinear least squares analysis based on *Marquardt*'s [1963] maximum neighborhood method, are discussed by *van Genuchten and Wierenga* [1986]. Of these four methods the least squares approach was shown to be the most accurate and objective method. The least squares approach minimized the following goal function

$$g = \sum_{i=1}^{N} (c_e - c)^2 \tag{12}$$

where c_e is the calculated concentration from (9), c is the observed effluent concentration, and N is the number of observed data points. The residual sum of squares, g, was minimized using the least squares program of *van Genuchten* [1980], leading to the values for P and R listed in Table 1. The results obtained with SUFI are also listed in Table 1 and shown in Figure 4 as the solid curve which is the same as the curve

Table 4. Progression to Convergence for Example 1 for the Case With Measurement Errors

Number of Iterations	Parameters	Parameter Value		Number of Strata	Number of Hits in Each Stratum	Tolerance
		Minimum	Maximum			
1	*P*	5.0	50.0	10	3, 2, 3, 1, 1, 0, 0, 0, 0, 0	0.215
	R	1.0	2.0	10	0, 0, 0, 0, 1, 5, 3, 1, 0, 0	
2	*P*	5.0	27.5	10	1, 3, 3, 3, 3, 3, 0, 0, 0, 0	0.208
	R	1.3	1.7	10	1, 0, 3, 4, 4, 3, 1, 0, 0, 0	
3	*P*	5.0	20.75	10	1, 1, 3, 5, 5, 6, 3, 3, 2, 1	0.208
	R	1.3	1.58	10	1, 0, 0, 3, 5, 5, 4, 5, 4, 3	

Table 5. Soil Hydraulic Parameters of Crushed Bandelier Tuff Used in the Caisson Drainage Experiments (Example 2)

Hydraulic Parameters	Values Obtained by *van Genuchten et al.* [1987]		Values Obtained by SUFI		
	Method 1	Method 2	Scenario 1	Scenario 2	Scenario 3
θ_r	0.0*	0.0255	0.0*	0.0*	0.043083
θ_s	0.331*	0.3320	0.331*	0.331*	0.36975
α, cm^{-1}	0.01433	0.01545	0.005025	0.011915	0.00595
n	1.506	1.474	1.79	1.579	1.8675
K_s, cm d^{-1}	25.0	33.71	9.85	12.45	28.167
l	0.5*	0.4946	0.5*	0.5*	0.5*
Value of goal function	0.011623 (equation (16))	0.015655 (equation (2))	0.0096 (equation (2))	0.004945 (equation (16))	0.007238 (equation (2))

Parameters were estimated using method 1, estimating three parameters using water content θ and pressure heads h; method 2, estimating six parameters using θ and h; scenario 1, estimating three parameters using θ only; scenario 2, estimating three parameters using θ and h; and scenario 3, estimating five parameters using θ only.

*Parameter values assumed to be known.

obtained by *van Genuchten and Wierenga* [1986]. The value of the goal function based on the RMSE formulation (equation (2)) using estimated parameters obtained by SUFI was essentially the same as that obtained using the least squares approach of *van Genuchten and Wierenga* [1986].

Table 2 shows the progression of SUFI to convergence using as initial parameter estimates uniform distributions in the intervals $P = [5.0, 50.0]$ and $R = [1.0, 2.0]$. The minimum and maximum parameter values in Table 2 depict the lower and upper limits of the parameter uncertainty domains; notice that these intervals become smaller and smaller as the iterative search proceeds. As mentioned earlier, no exact rules exist for choosing the number of strata. A large number of strata are possible in this example because of the small number of parameters and the simple analytical model involved (equation (9).

We emphasize that the value of the goal function during each iteration can be adjusted by a tolerance, $g <$ tolerance, allowing us to choose prior uncertainty domains for the next iteration. Table 3 demonstrates this point for iteration 1 in Table 2 and for different tolerance levels. As the magnitude of the tolerance is decreased, the number of hits decreases until there are no hits in any of the strata for each parameter. Our experience indicates that it is better to be relatively conservative. For example, in the present case it is better to use for the second iteration the domain having a tolerance of 0.06 rather than domains having tolerances of 0.04 or 0.02. Having a higher tolerance will avoid the possibility of falling into local minima as the iterative process continues. The data in Table 3 also reveal that for the given uncertinty domains, the goal function is far more sensitive to the retardation factor R than to the Peclet number P since the strata for R are much better discriminated (leading to narrower intervals with hits) than for P.

In a second run we assumed that each measured datum could be in error by 50%. In other words, the actual value of

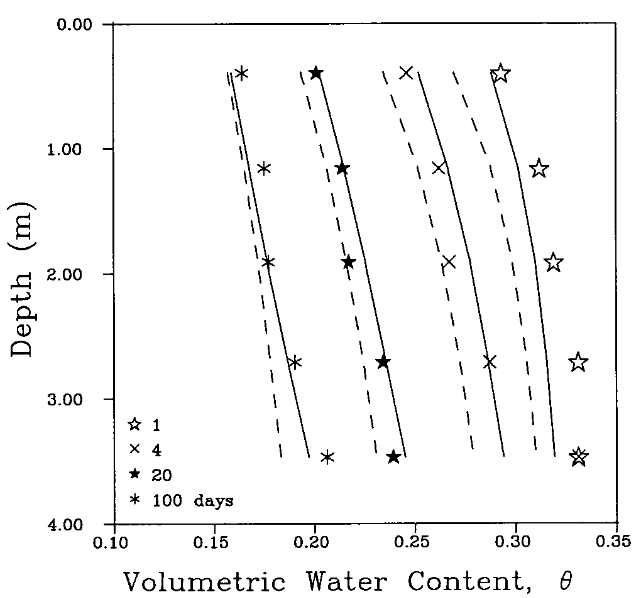

Figure 5. A comparison of measured water contents (data points) with simulated values using parameters obtained with the three-parameter method 1 approach of *van Genuchten et al.* [1987] (dashed line) and the three-parameter (θ only) SUFI scenario 1 approach (solid line).

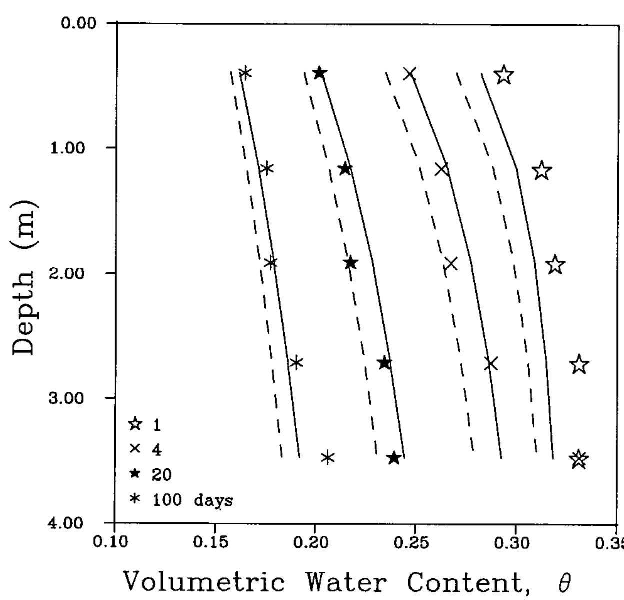

Figure 6. A comparison of measured water contents (data points) with simulated values using parameters obtained with the three-parameter method 1 approach of *van Genuchten et al.* [1987] (dashed line) and the three-parameter (θ and h data) SUFI scenario 2 approach (solid line).

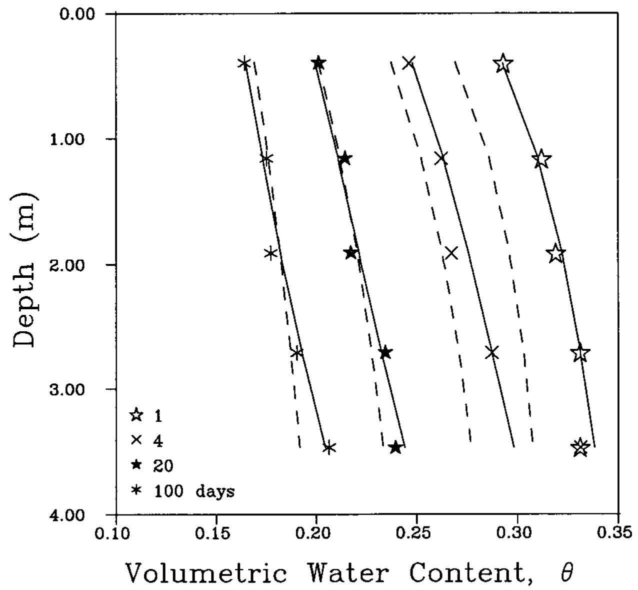

Figure 7. A comparison of measured water contents (data points) with simulated values using parameters estimated with the six-parameter method 2 approach of *van Genuchten et al.* [1987] (dashed line) and the five-parameter (θ only) SUFI scenario 3 approach (solid line).

each x_m^i was uniformly distributed in the interval $[0.5x_m^i, 1.5x_m^i]$, where $i = 1, \cdots, N$. The results of this example are shown in Table 4. We notice the larger values of the tolerances as compared with the previous case and the inability to reduce the tolerance after the third run. In general, measurement errors have the effect of producing more hits, and this limits the resolution with which we can choose the posterior interval. The overall effect of the measurement errors, based on our definition of a hit, is to give a larger uncertainty interval for each parameter. Given the 50% error in the measurements, we cannot get more precise values for the parameters than the intervals (5.0, 20.75) for P and (1.3, 1.58) for R. This constitutes the uncertainty in these parameters after fitting. Compare these values with (19.659, 19.665) for P and (1.34766, 1.34772) for R obtained in the case without measurement errors.

Example 2: Estimating the Unsaturated Soil Hydraulic Properties

The second example involves transient drainage of water from a large caisson 6 m deep and 3 m in diameter. The experimental study was conducted by *Abeele* [1984] at Los Alamos National Laboratory for the purpose of measuring the unsaturated soil hydraulic properties of Bandelier Tuff in connection with studies of radionuclide migration from waste disposal facilities. The initially dry tuff in the caisson, instrumented with tensiometers and neutron probe access tubes, was first saturated with water and then allowed to drain under gravity for 100 days. The experimental data were previously analyzed by *van Genuchten et al.* [1987] and *Kool et al.* [1987] using nonlinear least squares optimization methods based on the Levenberg-Marquardt method [*Marquardt*, 1963]. The data were used to estimate the hydraulic parameters in the following model for the unsaturated soil hydraulic parameters [*van Genuchten*, 1980]:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{(1 + |ah|^n)^m} \tag{13}$$

$$K = K_s S_e^l [1 - (1 - S_e^{1/m})^m]^2 \tag{14}$$

where θ is volumetric water content, θ_r is residual water content, θ_s is saturated water content, h is pressure head, α and n are shape factors, $m = 1 - 1/n$, K_s is saturated hydraulic conductivity, l is a pore connectivity parameter, and S_e is effective fluid saturation:

$$S_e(\theta) = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{15}$$

The drainage data were analyzed by *van Genuchten et al.* [1987] and *Kool et al.* [1987] using two different methods with different goal functions and input data. In the first method (method 1) three parameters, α, n, and K_s, were estimated using the following goal function

$$g(\mathbf{B}) = \sum_{i=1}^{M} \sum_{j=1}^{P} [\theta_{ij}^* - \theta_{ij}(\mathbf{B})]^2 + W^2 \sum_{j=1}^{P} [h_j^* - h_j(\mathbf{B})]^2 \tag{16}$$

where θ_{ij}^* represents measured water contents at $M = 5$ depths and $P = 6$ different times, h_j^* is the measured pressure head at $x = 0.4$ m, $\theta_{ij}(\mathbf{B})$ and $h_j(\mathbf{B})$ are model-predicted θ and

Table 6. Progression to Convergence for Example 2, Scenario 2

Number of Iterations	Parameters	Parameter Value Minimum	Parameter Value Maximum	Number of Strata	Number of Hits in Each Stratum	Tolerance
1	α, cm^{-1}	0.005	0.05	10	0, 1, 1, 2, 0, 0, 0, 0, 0, 0	0.01
	n	1.0	2.0	10	0, 0, 0, 2, 1, 1, 0, 0, 0, 0	
	K_s, cm d^{-1}	1.0	100.0	10	0, 1, 1, 0, 1, 1, 0, 0, 0, 0	
2	α, cm^{-1}	0.0095	0.023	10	0, 3, 4, 4, 2, 1, 0, 0, 0, 0	0.007
	n	1.3	1.6	10	0, 0, 0, 1, 1, 2, 2, 3, 2, 2	
	K_s, cm d^{-1}	10.9	60.4	10	6, 4, 2, 1, 0, 0, 0, 0, 0, 0	
3	α, cm^{-1}	0.0108	0.0176	10	1, 6, 5, 3, 1, 0, 0, 0, 0, 0	0.0054
	n	1.39	1.6	10	0, 0, 0, 0, 1, 1, 4, 4, 3, 3	
	K_s, cm d^{-1}	10.9	30.7	20	2, 3, 4, 2, 2, 2, 0, 1, 12 × 0	
4	α, cm^{-1}	0.0108	0.0142	10	0, 0, 1, 1, 0, 0, 0, 0, 0, 0	0.005
	n	1.474	1.6	10	0, 0, 0, 0, 0, 0, 0, 1, 1, 0	
	K_s, cm d^{-1}	10.9	18.8	30	0, 0, 0, 0, 1, 0, 1, 23 × 0	
5	α, cm^{-1}	0.0112	0.0125	10	0, 0, 0, 0, 0, 1, 0, 0, 0, 0	0.004945
	n	1.54	1.6	10	0, 0, 0, 0, 0, 0, 1, 0, 0, 0	
	K_s, cm d^{-1}	11.2	14.2	30	12 × 0, 1, 17 × 0	

Table 7. Progression to Convergence for Example 2, Scenario 3

Number of Iterations	Parameters	Parameter Value Minimum	Parameter Value Maximum	Number of Strata	Number of Hits in Each Stratum	Tolerance
1	θ_r	0.001	0.1	4	1, 1, 2, 1	0.0085
	θ_s	0.3	0.4	4	0, 0, 3, 2	
	α, cm^{-1}	0.005	0.05	6	3, 1, 1, 0, 0, 0	
	n	1.0	2.0	6	0, 0, 0, 2, 2, 1	
	K_s, cm d^{-1}	1.0	100.0	6	0, 1, 2, 1, 1, 0	
2	θ_r	0.001	0.1	4	3, 2, 1, 0	0.008
	θ_s	0.36	0.4	4	1, 2, 3, 0	
	α, cm^{-1}	0.005	0.0275	6	5, 1, 0, 0, 0, 0	
	n	1.4	2.0	6	0, 1, 2, 0, 2, 1	
	K_s, cm d^{-1}	18.0	83.0	6	0, 3, 2, 0, 1, 0	
5	θ_r	0.0092	0.0505	6	0, 0, 0, 0, 4, 4	0.00729
	θ_s	0.3675	0.375	4	0, 4, 4, 0	
	α, cm^{-1}	0.00542	0.00625	4	0, 1, 4, 3	
	n	1.75	1.9	6	0, 0, 0, 1, 4, 3	
	K_s, cm d^{-1}	28.0	34.0	6	4, 3, 1, 0, 0, 0	
6	θ_r	0.0367	0.0505	6	0, 1, 0, 2, 1, 0	0.007258
	θ_s	0.369	0.373	4	1, 2, 1, 0	
	α, cm^{-1}	0.0056	0.00625	4	0, 1, 3, 0	
	n	1.82	1.9	6	0, 0, 0, 2, 2, 0	
	K_s, cm d^{-1}	28.0	34.0	6	4, 0, 0, 0, 0, 0	
7	θ_r	0.039	0.046	6	0, 0, 0, 1, 0, 0	0.007238
	θ_s	0.369	0.371	4	0, 1, 0, 0	
	α, cm^{-1}	0.0057	0.0061	4	0, 0, 1, 0	
	n	1.86	1.89	6	0, 1, 0, 0, 0, 0	
	K_s, cm d^{-1}	28.0	30.0	6	1, 0, 0, 0, 0, 0	

h values corresponding to parameter vector $\mathbf{B} = (\alpha, n, K_s)$, and $W = 0.0016$ is a weighting coefficient chosen such that the two terms of (16) attain roughly the same value [*Kool et al.*, 1987]. The estimation method involved an inverse solution of the one-dimensional unsaturated flow (Richards) equation for an initially saturated soil profile, i.e., $h(x) = 0$, subject to a no flow boundary condition at $x = 0$ and a first-type lower boundary condition at $x = 4.23$ m by linearly extrapolating between observed pressure head data at that depth.

In the second method (method 2), six parameters, $\mathbf{B} = \{K_s, \alpha, n, \theta_r, \theta_s, l\}$, were estimated directly from reported laboratory and caisson $\theta(h)$ and $K(h)$ data [*Abeele*, 1979, 1984] using the following goal function

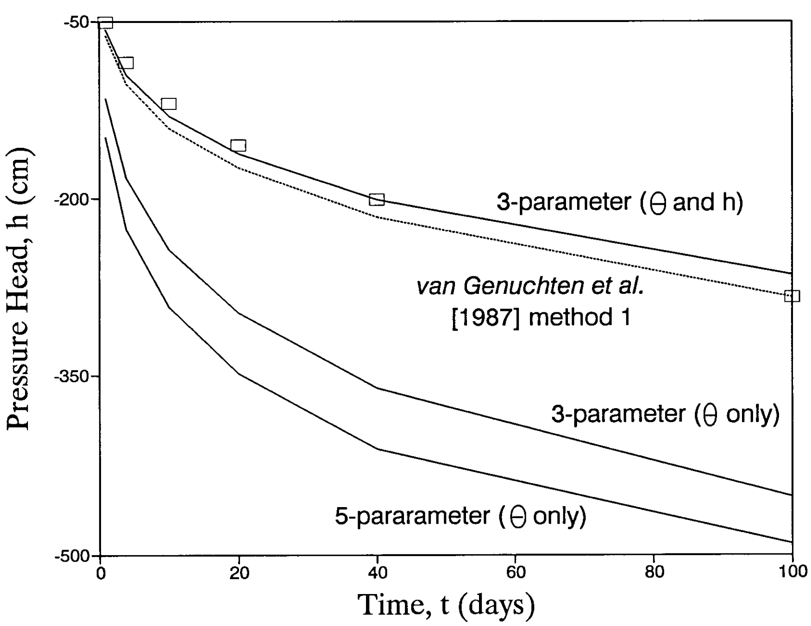

Figure 8. A comparison of measured pressure heads (data points) with simulated values using parameters estimated by method 1 of *van Genuchten et al.* [1987] (dashed line) and scenarios 1, 2, and 3 of SUFI (solid lines).

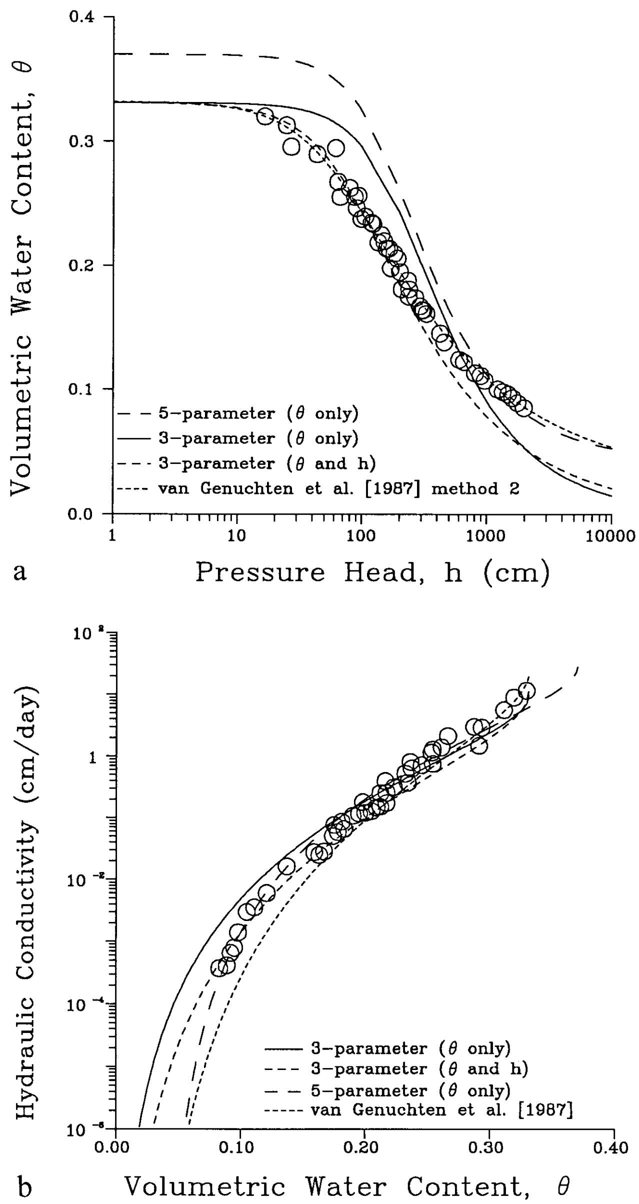

Figure 9. Hydraulic properties of Bandelier Tuff. (a) Water retention $\theta(h)$ and (b) hydraulic conductivity $K(\theta)$ curves are shown using different methods. Data points are measured values from *Abeele* [1984].

$$g(\mathbf{B}) = \sum_{i=1}^{M} [\theta_i^* - \theta_i(\mathbf{B})]^2 + V \sum_{j=1}^{N} \{\log (K_j^*) - \log [K_j(\mathbf{B})]\}^2 \tag{17}$$

where θ_i^* and $\theta_i(\mathbf{B})$ are observed and predicted water contents at M values of the pressure head, K_j^* and $K_j(\mathbf{B})$ are observed and predicted conductivities at N values of h, and V is a weighting factor that makes the two terms of (17) of roughly equal value. The results obtained by *van Genuchten et al.* [1987] for the two runs are shown in Table 5.

We ran three different scenarios with SUFI. First, the goal function (2) with observed water contents only was used to perform a three-parameter (α, n, and K_s) estimation. Second, the goal function (16) was used with measured water contents and pressure heads to again estimate α, n, and K_s. Third, a five-parameter (θ_r, θ_s, α, n, and K_s) estimation was carried out, again with goal function (2) and again using only water contents as the conditioning data. The latter scenario was used to examine the observation by *Kool et al.* [1987] that simultaneous estimation of three or more parameters required more information than just water content data. The HYDRUS [*Vogel et al.*, 1996] code was used in each case to obtain simulated water content and pressure head data. Initial and boundary conditions were similar to those used by *Kool et al.* [1987].

Hydraulic parameters estimated by SUFI using the three scenarios above are also listed in Table 5 and compared with the results obtained by *van Genuchten et al.* [1987] (see also *Kool et al.*, 1987). Figures 5, 6, and 7 show the measured water contents as a function of depth after 1, 4, 20, and 100 days for scenarios 1, 2, and 3, respectively. For scenarios 1 and 2 the curves based on the three-parameter (method 1) estimation results obtained by *van Genuchten et al.* [1987] are also shown for reference, while for scenario 3 (Figure 7) curves based on the six-parameter method 2 estimation are shown. In all cases the parameters estimated by SUFI lead to a closer fit to the data. Tables 6 and 7 show the progression of SUFI toward convergence for scenarios 2 and 3, respectively. We note here that the measured value of K_s as obtained by *Abeele* [1984] was 12.4 cm d^{-1}.

Two important observations can be made for this test case. First, contrary to the observation of *Kool et al.* [1987] with respect to their nonlinear least squares analysis, SUFI was capable of a five-parameter inversion using only observed water content values. Actually, SUFI was found to have no limitation in this regard, and any number of parameters can be fitted using any pertinent observed data. As previously mentioned, the only limitation of SUFI may be the total number of simulations that need to be carried out as a function of the stratification of the parameters and the speed of the simulation code. Second, Figures 5, 6, and 7 seem to suggest that the best fit was obtained with the five-parameter case (θ data only) followed by the three-parameter case without h data, and finally the three-parameter case using both θ and h data. However, this conclusion is correct only if we consider water content as the output. The five-parameter estimation is highly conditioned on the 30 observed water content data and provides the best fit because of more degrees of freedom in the fitting process. This conditioning on only one variable, in this case water content, may not necessarily provide better estimates for other output variables such as pressure heads, drainage rates, or concentrations if measured. This point is further illustrated in Figures 8, 9a, and 9b.

Figure 8 compares the observed pressure head data with predicted values when the parameter sets of scenarios 1, 2, and 3, as well as those of method 1 of *van Genuchten et al.* [1987] (Table 5), are used in the forward problem. Clearly, goal functions which included observed pressure head values provided the best estimates. The same is evident when the calculated hydraulic properties (equations (13) and (14)) using SUFI-derived parameters (scenarios 1, 2, and 3) are compared with the measured hydraulic data (data points) and the method 2 curves [*van Genuchten et al.*, 1987] fitted to those data (Figures 9a and 9b). The data points in Figures 9a and 9b are a composite of data derived from the caisson drainage experiment using a standard instantaneous profile (gravity drainage) analysis in the wet range ($\theta > 0.164$) and independently measured retention and conductivity data in the dry range ($\theta < 0.164$) obtained in the laboratory using small cores [*Abeele*, 1979,

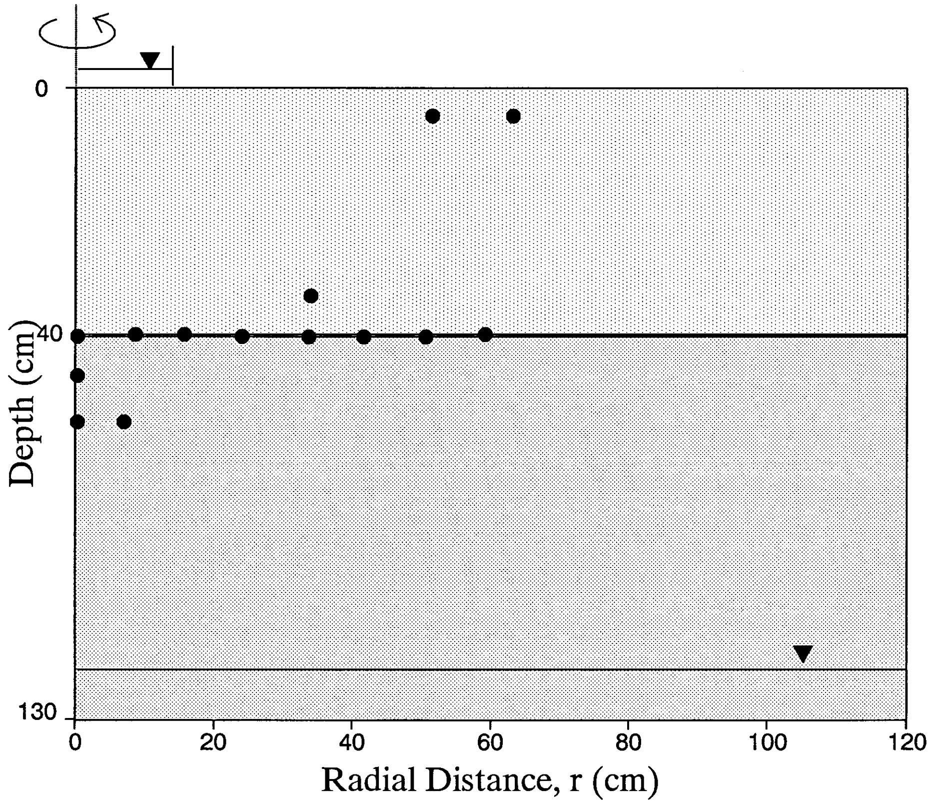

Figure 10. Schematic of the system considered in test example 3. Points indicate locations of the 14 concentration sampling points.

1984]. Notice that the simultaneous use of observed pressure heads and water contents in the caisson (scenario 2) now provides a much better fit than when only water content data are used (scenarios 1 and 3). These results indicate that in general, it is best to somehow include data of different types in the goal function for an all-purpose simulation. Such an approach requires selection of proper coefficients, such as W in (17), for the different data types used in the goal function. As discussed in more detail later, this task is not a trivial one.

Example 3: Hypothetical Water and Solute Infiltration Test

The third example considered here is a hypothetical case involving the radially symmetric three-dimensional infiltration of water and a dissolved solute from a single-ring infiltrometer into a variably saturated, layered soil profile (Figure 10). This problem was previously used to mathematically verify part of the SWMS_2D code version 1.12 [*Simunek et al.*, 1994]. The layered soil profile was assumed to be that of the Hupselse Beek watershed in the Netherlands, consisting of a 40-cm thick A horizon on top of a 300-cm B/C horizon. The hydraulic parameters describing the observed mean-scaled hydraulic functions and the assumed transport parameters of the two soil layers [*Cislerova*, 1987; *Hopmans and Stricker*, 1989] are given in Table 8. For our purposes these parameters are treated here as true parameters.

Calculations were carried out for a period of 5 days using the SWMS_2D code with the true parameters as listed in Table 8. The soil profile was assumed to be initially free of any solute. All sides of the flow region were considered to be impervious except for a ponded region ($h = 0$) inside the ring infiltrometer around the origin at the surface (Figure 10). Figure 11 presents calculated pressure head and concentration profiles at two different times. Calculated concentrations after 2 days at 14 arbitrary locations (Figure 10) were chosen to represent the measured values.

We assumed that six of the hydraulic and solute parameters in Table 8 were unknown: the saturated hydraulic conductivities of the two soil layers (K_{s1} and K_{s2}), the longitudinal and transverse dispersivity coefficients (D_L and D_T), the adsorption coefficient (κ), and a first-order rate constant for solute degradation in the liquid phase (μ_w). The adsorption coefficient appears in the retardation factor R as follows

Table 8. Soil Hydraulic Parameters of the Hupselse Beek Area Used in the Verification Example of the SWMS_2D Code

Hydraulic and Transport Parameters	True Values Used in SWMS_2D Forward Simulation		Values Obtained by SUFI	
	Layer 1	Layer 2	Layer 1	Layer 2
θ_s	0.399	0.339	0.399*	0.339*
θ_r	0.0001	0.0001	0.0001*	0.0001*
α, cm^{-1}	0.0174	0.0139	0.0174*	0.0139*
n	1.3757	1.6024	1.3757*	1.6024*
K_s, cm d^{-1}	0.0207	0.0315	0.0209	.031666
D_L, cm	0.5	0.5	0.500025	0.500025
D_T, cm	0.1	0.1	0.101	0.101
κ cm^3 g^{-1}	0.1	0.1	0.1032	0.1032
μ_w, min^{-1}	−3.472E-5	−3.472E-5	−3.625E-5	−3.625E-5

Read −3.472E-5 as -3.472×10^{-5}.
*Parameters assumed to be known.

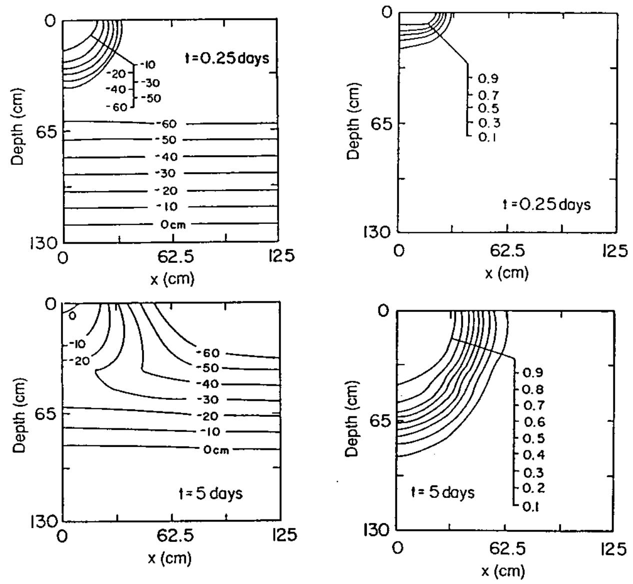

Figure 11. Simulated (left) pressure head profiles and (right) concentration profiles at (top) $t = 0.25$ and (bottom) $t = 5$ days for test example 3.

$$R = 1 + \frac{\rho \kappa}{\theta} \tag{18}$$

where ρ is the soil bulk density. The dispersion, adsorption, and degradation parameters were assumed to be the same for the two soil layers. We subsequently used SUFI with (2) as the goal function to estimate the 6 unknowns using the 14 "measured" concentration values as the conditioning information.

The initial parameter values used to start SUFI were assumed to contain large uncertainties and were depicted with uniform distributions within the following intervals: K_{s1} = [0.001, 0.1], K_{s2} = [0.001, 0.1], D_L = [0.15, 0.75], D_T = [0.01, 0.4], κ = [0.05, 0.5], and $\mu_w = [-1.0 \times 10^{-4}, -1.0 \times 10^{-6}]$. The final estimates of these parameters as obtained with SUFI using the exhaustive stratified sampling option are given in Table 8. Table 9 shows the progression to convergence. The predicted concentration distributions using the final estimates were essentially identical to those shown in Figure 11.

Since the true parameters for this hypothetical example were known, the simulation model should be able to fully explain the measured concentrations; that is, we should be able to achieve a value of zero for the goal function. Such a scenario is highly unlikely in reality since measurements are always subject to some error. Also, the selected simulation model with its limited number of invoked processes and associated parameters will hardly ever correctly describe the true physical processes operating in the subsurface, thus leading to additional approximations or inaccuracies for the estimated parameters in that simulation model. Numerical approximations in the simulation model itself may also further limit the final accuracy of the parameter estimation process. To obtain a goal function of zero in this example, SUFI requires that the true values of the six parameters all fall in the middle of an interval in their respective strata. The data shown in Table 9 suggest that a goal function of zero eventually would be obtained if the iterative process were continued. Since having a goal function of zero is not the objective, the iterative process was terminated after the eighth iteration when the tolerance reached a very small value.

An interesting observation in Table 9 is that during the first and second iterations, SUFI could not discriminate among the different strata of D_L and D_T despite the relatively large uncertainty domains used for these two parameters. This result indicates that the goal function was insensitive to these parameters for the given level of uncertainty in the other parameters. When the other parameters became more defined during the

Table 9. Progression to Convergence for Test Example 3

Number of Iterations	Parameters	Parameter Value Minimum	Parameter Value Maximum	Number of Strata	Number of Hits in Each Stratum	Tolerance
1	D_L, cm	0.15	0.75	2	2, 2	0.04
	D_T, cm	0.01	0.4	2	2, 2	
	κ, cm^3 g^{-1}	0.05	0.5	2	4, 0	
	μ_W, d^{-1}	−1.0E-4	−1.0E-6	2	4, 0	
	K_{s1}, cm d^{-1}	0.001	0.1	2	4, 0	
	K_{s2}, cm d^{-1}	0.001	0.1	2	4, 0	
3	D_L, cm	0.25	0.65	4	0, 0, 1, 0	0.005
	D_T, cm	0.01	0.4	2	1, 0	
	κ, cm^3 g^{-1}	0.05	0.16	3	0, 1, 0	
	μ_W, d^{-1}	−1.0E-4	−1.0E-5	2	0, 1	
	K_{s1}, cm d^{-1}	0.017	0.026	2	0, 0, 1, 0, 0, 0	
	K_{s2}, cm d^{-1}	0.025	0.05	2	1, 0	
4	D_L, cm	0.45	0.55	3	1, 1, 0	0.003
	D_T, cm	0.01	0.205	3	1, 1, 0	
	κ, cm^3 g^{-1}	0.087	0.123	4	1, 1, 0	
	μ_W, d^{-1}	−5.5E-5	−1.0E-5	3	0, 2, 0	
	K_{s1}, cm d^{-1}	0.02	0.0215	3	1, 1, 0	
	K_{s2}, cm d^{-1}	0.025	0.037	3	1, 1, 0	
8	D_L, cm	0.45	0.5167	2	0, 1	0.0002
	D_T, cm	0.01	0.14	5	0, 0, 0, 1, 0	
	κ, cm^3 g^{-1}	0.087	0.105	5	0, 0, 0, 0, 1	
	μ_W, d^{-1}	−4.0E-5	−1.0E-5	4	1, 0, 0, 0	
	K_{s1}, cm d^{-1}	0.02	0.021	5	0, 0, 0, 0, 1	
	K_{s2}, cm d^{-1}	0.025	0.033	3	0, 0, 1	

Read −1.0E-4 as -1.0×10^{-4}.

Table 10. Progression to Convergence for Test Example 3 Using Random Stratified Sampling Procedure

Number of Iterations	Parameters	Parameter Value Minimum	Parameter Value Maximum	Number of Strata	Number of Hits in Each Stratum	Tolerance
1	D_L, cm	0.15	0.75	6	0, 6, 9, 4, 8, 0	0.08
	D_T, cm	0.01	0.4	6	5, 0, 3, 8, 0, 10	
	κ, cm^3 g^{-1}	0.05	0.5	6	0, 9, 8, 0, 0, 7	
	μ_W, d^{-1}	−1.0E-4	−1.0E-6	6	4, 4, 0, 8, 0, 8	
	K_{s1}, cm d^{-1}	0.001	0.1	6	4, 21, 12, 0, 0, 0	
	K_{s2}, cm d^{-1}	0.001	0.1	6	3, 5, 6, 9, 3, 0	
3	D_L, cm	0.32	0.65	6	9, 0, 6, 0, 0, 5	0.012
	D_T, cm	0.075	0.4	6	1, 9, 8, 0, 0, 0	
	κ, cm^3 g^{-1}	0.05	0.5	6	1, 8, 0, 0, 0, 0	
	μ_W, d^{-1}	−1.0E-4	−1.0E-6	6	12, 7, 0, 0, 3, 0	
	K_{s1}, cm d^{-1}	0.0175	0.045	6	1, 8, 0, 0, 0, 0	
	K_{s2}, cm d^{-1}	0.0285	0.056	6	7, 4, 0, 0, 0, 0	
4	D_L, cm	0.32	0.65	6	0, 9, 3, 4, 0, 0	0.0078
	D_T, cm	0.075	0.1833	6	4, 7, 0, 0, 0, 0	
	κ, cm^3 g^{-1}	0.05	0.2	6	4, 0, 0, 11, 0, 0	
	μ_W, d^{-1}	−1.0E-4	−1.17E-5	6	0, 0, 0, 4, 11, 4	
	K_{s1}, cm d^{-1}	0.0175	0.0267	6	4, 0, 0, 13, 0, 0	
	K_{s2}, cm d^{-1}	0.0285	0.0376	6	0, 3, 7, 3, 0, 3	
10	D_L, cm	0.498	0.515	6	2, 2, 2, 1, 2, 5	0.0005
	D_T, cm	0.0985	0.106	6	2, 1, 3, 1, 5, 1	
	κ, cm^3 g^{-1}	0.097	0.103	6	1, 0, 2, 10, 0, 0	
	μ_W, d^{-1}	−3.5E-5	−3.2E-5	6	0, 0, 1, 1, 5, 5	
	K_{s1}, cm d^{-1}	0.02054	0.0209	6	0, 1, 0, 2, 5, 4	
	K_{s2}, cm d^{-1}	0.0313	0.0317	6	1, 3, 3, 3, 3, 0	

third iteration, D_L and D_T started to exert more effect on the goal function. This example hence shows that the sensitivity of an objective function to a certain parameter may depend on the invoked or calculated uncertainty domains of the other parameters. The example also indicates that SUFI is a very appropriate tool for carrying out sensitivity analyses. Most traditional methods of carrying out sensitivity analyses invoke systematic changes in a certain parameter of interest while keeping all other parameters constant. Such an approach assumes exact (true) knowledge of the other parameters and hence is not appropriate for cases where the true values of parameters are not known. By contrast, SUFI provides a method for situations where the parameters are treated with uncertainty.

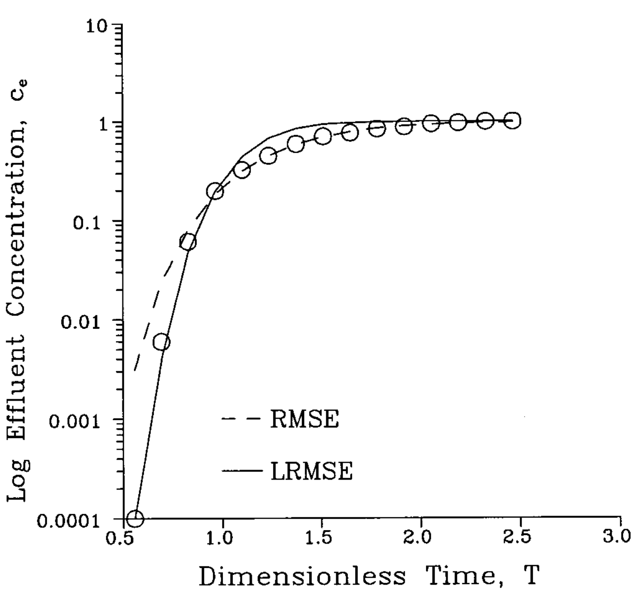

Figure 12. A comparison of measured effluent concentrations (data points) with simulated values using parameters estimated by SUFI assuming a logarithm-based root-mean-square error (LRMSE) objective function and a regular root-mean-square error (RMSE) objective function.

The results with the random stratified sampling which was also performed for this example are shown in Table 10. In this example we divided the uncertainty intervals of the parameters into six strata. This produces an exhaustive sample space of 46,656 combinations. We allowed only 0.3% of the combinations to be simulated, and this resulted in about 140 simulations in each iteration. We stopped after the tenth iteration, where a goal value of 0.0005 was obtained. The random stratified sampling also worked well for this example, and on the basis of our experience it is better to use this sampling scheme when many parameters are involved.

Influence of the Goal Function

A detailed analysis of different goal functions is beyond the scope of this paper. Still, we would like to show briefly the potentially important implications of formulating and using different goal functions. The implications are illustrated for the first test example which we analyzed also using the logarithm-based (LRMSE) goal function as given by (3). In this case we obtained the results $P = 57.16$ and $R = 1.153$. Figure 12 shows that the LRMSE-fitted effluent curve differs substantially from the previously obtained RMSE curve. The pronounced differences between the two cases is caused by a scale phenomenon. When the RMSE is used, the contributions of relatively small concentrations to the value of the goal function are essentially ignored. By comparison, LRMSE puts more weight on the smaller concentrations at the expense of the higher values.

Proper definition of the goal function can become even more difficult, and somewhat subjective, when different types of data are represented in the goal function, such as was the case with (16) for the caisson drainage example 2. When we repeated the second scenario for this example using W rather than W^2 in (16), the estimates for the three unknowns became quite different: $\alpha = 0.0224$ (cm^{-1}), $n = 1.12576$, and $K_s = 85.5$ (cm d^{-1}). Given that the measured K_s was 12.4 cm d^{-1}, the parameter estimates using W should be relatively inaccurate. Using W instead of W^2 in this case leads to a goal function whose value is dominated by pressure heads solely because of their numerically larger values; this occurs in spite of the fact that in situ pressure head measurements often yield less accurate data than water content measurements.

Conclusions

The acronym SUFI was coined to represent a parameter estimation procedure which is sequential, operates within parameter uncertainty domains, employs only forward calculations, and is iterative in nature. The procedure is general, stable, always convergent, and has no inherent limitations in terms of the number of parameters that can be considered simultaneously. The number of function calls can be limited by invoking a less exhaustive sampling scheme, or the program can be made to run faster by parallel submission of smaller jobs. The sequential uncertainty domain parameter estimation procedure performed well in three different examples involving a wide range of flow and transport parameters. The procedure begins with a prior and concludes with a posterior state of belief of the value of the parameters being estimated. The states of belief are expressed as uncertainty domains, with the posterior uncertainty domain being much smaller than the prior one. Although not discussed in great detail, the importance of the goal function on the results is demonstrated.

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