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Estimation of in Situ Hydraulic Conductivity Function From Nonlinear Filtering Theory

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A method based on an optimal nonlinear filtering technique is proposed and tested for the determination of the hydraulic conductivity function from a field drainage experiment. Simplifications to Richards's equation lead to a Langevin type differential equation to describe the redistribution of stored water as a function of drainage flux excited by a random initial condition and state forcing. The derived equation is then utilized in an optimal estimation scheme that explicitly accounts for the formulation and observation uncertainty in determining the hydraulic conductivity parameters. A field drainage experiment was carried out to study the usefulness of the proposed method for routine in situ hydraulic conductivity function estimation.

INTRODUCTION

Mathematical description of water flow in the unsaturated zone is complicated by uncertainties in the determination of the hydraulic conductivity–moisture content functional relation (K-θ). In practice, one of the assumptions made in field estimates of hydraulic conductivity is that the observations of moisture content are taken to be error free. Numerous studies on neutron probe scattering techniques indicate that moisture content observations commonly used in field drainage experiments are anything but error free [*Gardner and Kirkham*, 1952; *Hewlett et al.*, 1964; *Haverkamp et al.*, 1984; *Parlange et al.*, 1992*a*; *Schmugge et al.*, 1980; *Sinclair and Williams*, 1979; *Vachaud et al.*, 1977].

The sources of uncertainty in the hydraulic conductivity function at a certain point in the natural environment are the result of (1) simplifying the description of the physical processes that are used indirectly to infer the hydraulic conductivity function; and (2) the measurements used to determine the hydraulic conductivity function [*Flühler et al.*, 1976; *Andersson and Shapiro*, 1983; *Mishra and Parker*, 1989].

One possible approach that can be used to explicitly assess the combined sources of uncertainty in the hydraulic conductivity function is nonlinear filtering. In this approach, an optimal filter is constructed to provide a minimum mean square error estimation solution path to a differential equation describing the redistribution of moisture content [*Gardner*, 1990; *Milly and Kabala*, 1986; *Milly*, 1986]. Then a scheme which accounts for both measurement and system uncertainty is developed for processing real time observations of θ and hydraulic gradient (dH/dz) to obtain the K-θ relation. The proposed methodology presumes that the simplifying assumptions of Richards's equation in drainage experiments generate a stochastic forcing to an initial value differential equation describing the stored water redistribution [*Sobczyk*, 1991, pp. 113–119]. The hydraulic conductivity parameters from discrete stored water and hydraulic gradient measurements can be determined iteratively from a sequence of prediction-updating steps to maximize a defined likelihood function.

Current field methods (CGA (due to Chong, Green, and Ahuja), theta, flux, and classical [see *Libardi et al.*, 1980]), together with the proposed method based on the nonlinear filtering theory, were compared based on a drainage experiment carried out at a field site.

THEORY

Soil Water Transport

The one-dimensional continuity equation for soil water flow can be written

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \tag{1}$$

where θ is the volumetric moisture content, z is the depth (positive downward) and q is the drainage flux. Integrating (1) from $z = 0$ (surface) to a depth b yields

$$-\int_0^b \frac{\partial \theta}{\partial t}\, dz = q_b - q_0 \tag{2}$$

where q_0 is the flux at $z = 0$, and q_b is the vertical flux at $z = b$. A no-flux boundary condition is imposed at $z = 0$ so that $q_0 = 0$.

Equation (2) is rearranged:

$$\frac{\partial}{\partial t}\left[\int_0^b \theta\, dz\right] = \frac{\partial W}{\partial t} = -q_b \tag{3}$$

where W is the stored water (centimeters) between 0 and b. Assuming isothermal and nonhysteretic flow conditions,

$$\frac{\partial W}{\partial t} = K(\theta_b)\, \frac{\partial H_b}{\partial z} \tag{4}$$

where $K(\theta_b)$ and H_b are the unsaturated hydraulic conductivity and the total hydraulic head at depth b, respectively [*Rose et al.*, 1965]. For a vertically homogeneous soil over

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the depth interval $[0, b]$, where the moisture content variation with depth is not large, the average moisture content (θ^*) and θ_b can be related by [*Libardi et al.*, 1980; *Jones and Wagenet*, 1984]

$$\theta_b = A_1\theta^* + B_1 \tag{5}$$

where θ^* is given by

$$\theta^* = \frac{1}{b}\int_0^b \theta\, dz = \frac{W}{b} \tag{6}$$

Various hydraulic conductivity functions with different degrees of freedom and complexity have been proposed in the literature. In this study we use an exponential two-parameter hydraulic conductivity model of the form $K(\theta_b) = U \exp(V\theta_b)$, so $K(\theta_b)$ is related to W at depth b by

$$K(\theta_b) = A \exp(BW) \tag{7}$$

where $A = U \exp(VB_1)$ and $B = VA_1/b$. The soil water transport equation, as a function of stored water only, is given by

$$\frac{\partial W}{\partial t} = -K(W)\left[\frac{\partial H}{\partial z}\right]_{z=b}. \tag{8}$$

Note that in the derivation that follows $K(W)$ need not be limited to an exponential function but can be any smooth function that is differentiable.

State-Space Formulation and Model Development

Equation (8) may be written in state-space notation,

$$dX(t) = -Ae^{BX(t)}\left[\frac{\partial H}{\partial z}\right] dt + \varepsilon_s(t)\, dt. \tag{9}$$

The corresponding discrete observation equation at time t_k ($k = 0, 1, 2, 3, \cdots$) is

$$Z_m(t_k) = X(t_k) + v_m(t_k) \tag{10}$$

where $X(t)$ is the stochastic state variable representing the stored water W (between 0 and b) and $Z_m(t_k)$ is the measured amount of stored water at time t_k. The state noise $\varepsilon_s(t)$ results from the various simplifications invoked in the derivation of the soil water transport equation, which we approximate as a zero-mean Gaussian noise [*Arnold*, 1974, pp. 202–203; *Sobczyk*, 1991, pp. 60–61]. As was demonstrated by *Jones and Wagenet* [1984], (8), on the average, reproduces field measured moisture content. It is reasonable to assume that (8) does describe the dynamical characteristics of soil water flow so that the zero-mean state noise assumption is appropriate. The nature of the noise distribution is an arbitrary approximation since the differences found between the model and actual water movement in the field may be site specific, moisture content dependent, etc. Note that the experimental results of *Jones and Wagenet* [1984] suggest relatively uniform scatter of comparable magnitude over a wide range of soil water contents commonly encountered in field studies.

The neutron probe measurement noise $v_m(t_k)$ at time t_k is approximated by a zero-mean Gaussian distribution. The product $\varepsilon_s dt$ defines the Wiener increment dI_t of the Wiener process [*Gardiner*, 1990, pp. 80–82; *Gardner*, 1990, pp. 124–125], with zero mean and covariance function defined by $Q[\delta(t-s)]dt$. Q is the variance per unit time of the Wiener process which is treated as an unknown to be solved in this study, and δ is the Dirac delta function. We also assume that (9) satisfies the existence and uniqueness conditions for the time interval $[0, \infty]$ so that the solution is well behaved and does not "explode" at infinity [*Gardiner*, 1990, p. 94].

The stochastic noise components in the observation equation and state equation permit separate accounting for the measurement errors and the model structure error [*Gelb et al.*, 1974, pp. 105–107]. Given the random nature of the additive noises, the state variable $X(t)$ and the water storage observations $Z(t_k)$ become random variables in time. For the reader's convenience, we adhere in the following derivation to *Gelb et al.*'s [1974] notation since various details and proofs are elaborated upon in this reference. The method used to determine the evolution of the mean and the variance behavior of $X(t)$ in time is discussed next.

Taking the expectation of (9) and using the zero-mean property of the Wiener increment gives

$$\left\langle\frac{dX(t)}{dt}\right\rangle = -\langle Ae^{(BX(t))}\rangle\left[\frac{\partial H}{\partial z}\right] \tag{11}$$

where $\langle\ \rangle$ denotes the expectation operation. Note that $\langle X(t)\rangle$ is defined since (9) satisfies the existence and uniqueness conditions. In (11), the hydraulic gradient is treated as a time-varying deterministic input which excites the state variable of the system. Since the differential and the expectation operators are interchangeable, an expression for the state mean may be obtained as $\langle dX(t)/dt\rangle = d\langle X(t)\rangle/dt$. On the right-hand side of (11) a closure problem arises since all moments of $X(t)$ are required for the evaluation $\langle A \exp[BX(t)]\rangle$, that is, in order to solve for $d\langle X(t)\rangle/dt$ all the moments of $X(t)$ are needed. It is necessary to develop an approximate closure scheme for the given system. One may expand a stochastic function $f(X(t))$ (in this case $f[X(t)] = A \exp[BX(t)]$) around $\langle X(t)\rangle$ with a first-order Taylor series expansion:

$$f(X(t)) = f(\langle X(t)\rangle) + \frac{df}{dx}(X(t) - \langle X(t)\rangle) + O[(X(t) - \langle X(t)\rangle)^2]. \tag{12}$$

By applying the expectation operator on both sides of (12) and neglecting higher-order terms, (11) becomes

$$\frac{d\langle X(t)\rangle}{dt} = -Ae^{B\langle X(t)\rangle}\left[\frac{dH}{dz}\right]_{z=b}. \tag{13}$$

Equation (13) approximates the dynamic evolution of the mean behavior of the stored water in time between 0 and b. If another expression for the hydraulic conductivity function is used, a similar approach can be employed to arrive at a dynamic equation that is dependent on only the mean $\langle X(t)\rangle$ and the hydraulic conductivity parameters (see Appendix B).

The variance $P(t)$ is given by

$$P(t) = \langle(X(t) - \langle X(t)\rangle)^2\rangle. \tag{14}$$

A dynamic equation for $P(t)$ may be constructed by differentiating (14) and interchanging the expectation and differentiation operators,

$$\frac{dP(t)}{dt} = \left\langle \frac{d(X(t) - \langle X(t)\rangle)^2}{dt} \right\rangle. \tag{15}$$

Linearization of the right-hand side of (15) around the mean given in (12) yields

$$\frac{dP(t)}{dt} = -2\,\frac{dH}{dz}\,\frac{df(X(t))}{dx}\,P(t) + Q \tag{16}$$

where Q is the state spectral density function or error variance per unit time [*Gelb et al.*, 1974, p. 122]. The derivative $df(X(t))/dx$ in (16) is evaluated at $\langle X(t)\rangle$. Using the exponential hydraulic conductivity formulation, the extended Kalman filter equations (EKF) for continuous dynamic and discrete observations become

$$\frac{d\langle X(t)\rangle}{dt} = -Ae^{B\langle X(t)\rangle}\,\frac{dH}{dz} \tag{17}$$

$$\frac{dP(t)}{dt} = -2\left[\left(\frac{dH}{dz}\right)ABe^{B\langle X(t)\rangle}\right]P(t) + Q \tag{18}$$

which constitute coupled predictive equations for both $\langle X(t)\rangle$ and $P(t)$. These equations are also presented for a power law hydraulic conductivity function in Appendix B.

In order to integrate (17) and (18) for $\langle X(t)\rangle$ and $P(t)$, the coefficients A, B, and Q as well as the initial conditions for the mean $\langle X(t_0)\rangle$ and the variance $P(t_0)$ need to be provided. Once the initial conditions are specified, (17) and (18) can be simultaneously integrated to yield a prediction of $\langle X(t)\rangle$ and $P(t)$ at time t_k when an observation $Z(t_k)$ is available. At time t_k, predictions of $\langle X(t)\rangle$ and $P(t)$, denoted by $\langle X(t_k)\rangle^-$ and $P(t_k)^-$, respectively, may be corrected by employing the information contained in the neutron probe measurement $Z(t_k)$. Because of the measurement error variance R in $Z(t_k)$, the predictions and measurements have to be weighted according to their respective variances in the updating steps. As shown by *Gelb et al.* [1974, pp. 107–110], the optimal solution path requires the updating equations to be given by

$$\langle X(t_k)\rangle^+ = \langle X(t_k)\rangle^- + K_g(Z(t_k) - \langle X(t_k)\rangle^-) \tag{19}$$

$$P(t_k)^+ = P(t_k)^-(1 - K_g) \tag{20}$$

where $\langle X(t_k)\rangle^+$ and $P(t_k)^+$ are the updated mean and variance. K_g is the Kalman gain,

$$K_g = \frac{P(t_k)^-}{P(t_k)^- + R} \tag{21}$$

which defines how to weigh the two sources of information: predictions and observations. The structure of the nonlinear extended Kalman filter defined by (17), (18), (19), (20), and (21) is shown in Figure 1. The procedure is stable in practice because the linearization trajectory is being computed throughout the calculations [*Puente and Bras*, 1987]. It should be noted that (17) and (18) are conservation equations which respect the "physics" of the model while (19) and (20) are "statistical" corrections, which redistribute water content in a statistical (nonphysical) manner.

Determination of the Hydraulic Conductivity Parameters

The parameters needed to apply the extended Kalman filter equations are $\langle X(0)\rangle$, $P(0)$, A, B, R, and Q. The initial mean $\langle X(0)\rangle$ was taken as the water storage between 0 and h at field saturation, and the observation error variance R was determined from the neutron probe calibration curve which is discussed below in the experimental setup. The hydraulic conductivity parameters A and B as well as Q and $P(0)$ were determined following an iterative multivariate optimization scheme. This optimization procedure computes the unknown parameters $\hat{U} = [A, B, P(0), Q]^T$ by maximizing the joint distribution of all observations. This likelihood function is defined by [*Shumway*, 1988, pp. 178–180; *Gelb et al.*, 1974, p. 103].

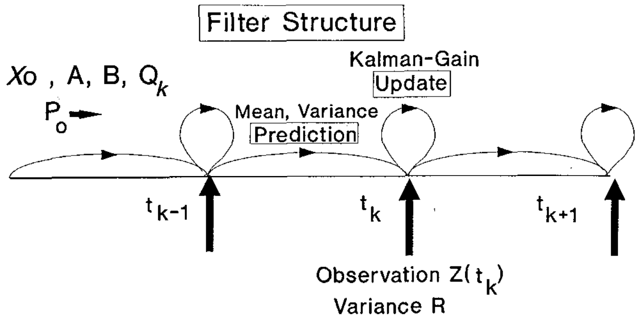

Fig. 1. Structure of the extended Kalman filter displaying the sequence of prediction-updating steps as neutron probe measurements become available.

$$l(\hat{U}, Z(t_1), Z(t_2), \cdots, Z(t_n)) = \prod_{k=1}^{k=n} p(Z(t_k)|\langle X(t_k)\rangle^-, \hat{U}) \tag{22}$$

where

$$p(Z(t_k)|\langle X(t_k)\rangle^-, \hat{U}) = \frac{1}{[2\pi P(t_k)^-]^{1/2}} \exp\left(-\frac{1}{2P(t_k)^-}(Z(t_k) - \langle X(t_k)\rangle^-)^2\right) \tag{23}$$

It should be noted that $\hat{U}$ appears implicitly in (22) and (23). Equations (22) and (23) require that the coefficients A, B, $P(0)$, and Q result in a path of state means $\langle X(t_k)\rangle$ which maximizes the probability of occurrence of the measurements $Z(t_k)$. Maximization of (22) may be achieved by minimizing the quantity $\sum[(Z(t_k) - \langle X(t_k)\rangle^-)^2]/P(t_k)^-$ whose individual term appears in the exponential bracket in (23). This results in an objective function (L) defined by the weighted least squares

$$L = \sum_{k=0}^{k=n}\left[\frac{(Z(t_k) - \langle X(t_k)\rangle^-)^2}{P(t_k)^-}\right] \tag{24}$$

in which the weights of the residuals are $[P(t)^-]^{-1}$, and n is the number of stored water observations sampled during the experiment.

Starting with initial estimates of A, B, $P(0)$ and Q, (17) and (18) are integrated from t_k until t_{k+1} for $k = 0, 1, 2, \cdots, n - 1$. The predicted $\langle X(t_{k+1})\rangle^-$ is compared to the measurement $Z(t_{k+1})$ to compute one term of the summation defining L; then the updating procedure is performed using

(19) and (20) to obtain $\langle X(t_{k+1})\rangle^+$. Since four parameters [A, B, Q, and $P(0)$] are required to minimize one objective function, a multidimensional optimization scheme was necessary. In this study, the multidimensional simplex method [see *Press et al.*, 1990, pp. 289–293] was used to recursively estimate A, B, Q, and $P(0)$. Since the multidimensional simplex method is a simple unconstrained optimization, the objective function L was artificially penalized to insure that A, B, Q, and $P(0)$ were positive. The filtering computation scheme is outlined in Appendix A.

Other Field Methods

Four other methods are considered, namely the so-called flux, theta, CGA, and classical methods [*Libardi et al.*, 1980; *Jones and Wagenet*, 1984]. The flux, theta, and CGA methods assume unit hydraulic gradient and require moisture content observations only, while the classical method also requires matric potential observations. A major disadvantage of all four methods is the fact that an arbitrary smoothed monotonically decreasing relation between θ and t is required.

EXPERIMENTAL SETUP

A field plot, 1.22 m × 1.22 m, was used to investigate the applicability of the proposed methodology to determine the in situ hydraulic conductivity function. The soil is a Yolo light clay the properties of which are described by *Buchter et al.* [1991]. A steel sheet 20 cm in depth was used to define the plot square. The sheet was inserted 10 cm into the ground, and the soil outside the sheet was compacted against the wall to minimize lateral flow near the soil surface. An average ponding depth of 3–5 cm was maintained for 10 days until no changes in moisture contents were noted in the top 50 cm. The infiltration rate after 10 days of ponding, with an applied head of 5 cm, was 0.06 cm min^{-1} which corresponds to a field-saturated infiltration rate of 17 cm d^{-1}. The surface was then covered with a plastic sheet to insure the no-flux surface boundary condition assumed. One neutron probe access tube and three tensiometers per depth, located at 15 cm and 30 cm below the soil surface were used to monitor the stored water in the top 22.5 cm and the hydraulic gradient at 22.5 cm. Neutron probe and tensiometric observations were recorded every 6 hours for the first day and every 12 hours afterward for a total period of 43 days. The matric potential was recorded using a Soil Measurement Systems Tensimeter (pressure transducer) that offsets the barometric pressure and is accurate to within ±1 mbar.

Since the accuracy of the neutron probe affects the observation noise, a study on the instrument and calibration was required. Generally, the noise in volumetric moisture content measurements obtained from neutron probe soundings is the result of two sources [*Haverkamp et al.*, 1984; *Schmugge et al.*, 1980]: (1) instrumental noise, which depends on the radioactive source (type and strength), the detector type, and count time (for more details, see *Dickey* [1990], *Stone* [1990], and *Cuenca* [1989], and (2) calibration noise due to the instrumental noise, access tubing, air gap between the probe and the access tube, and the soil sampling method used to obtain the volumetric moisture content.

The neutron probe used in this experiment was a Campbell Pacific Nuclear hydroprobe (Model 503) with a radioactive source of 50 mCi americium 241/beryllium located at the midpoint of the detector with a preset count time of 32 s. Generally, for a specific hydroprobe configuration the instrumental noise may be reduced by averaging an increasing number of readings per depth [*Parlange et al.*, 1992, 1993]. In order to select a reasonable number of readings per depth and to determine the instrumental noise during calibration and soundings, 214 unshielded readings at 75 cm soil depth were recorded during a separate experiment as a function of observation identification number; these are presented in Figure 2 [*Parlange et al.*, 1992]. During the 214 unshielded readings, the moisture content was assumed to be constant. The unshielded counts were uncorrelated in time as demonstrated by the autocorrelation function in Figure 3. The raw data of Figure 2 were transformed to a standardized series with a zero mean and a unit variance. A moving average was performed on the standardized series in order to assess the reduction in instrument variance gained by averaging more soundings [*Parlange et al.*, 1992]. A window, whose width is determined by the number of readings averaged, was passed through the standardized series and the computed variances were plotted versus the corresponding window width (Figure 4). It was desirable to reduce the instrument noise as much as was practically possible. We decided to take three readings per depth. Averaging three observations the instrumental variance component was reduced by 70% (Figure 4) and diminished in importance relative to the neutron probe calibration variance.

The calibration of the neutron probe was performed by inserting six aluminum access tubes (outer diameter, 5 cm; wall thickness, 1.3 mm; pressure rating, 825 kPa) of length 1.1 m into the ground. Aluminum tubing was optimal in this experiment since aluminum is more transparent to fast and thermalized neutrons than polyvinyl chloride [*Allen and Segura*, 1990] yielding more thermalization of fast neutrons by the soil medium which results in a better performance and calibration [*Stone*, 1990]. The drilling/sampling was performed using a Madera sampler (volume of sample, 60 cm^3) using the Soil Conservation Service (SCS) method discussed by *Dickey* [1990]. The standard count prior to each set of subsurface readings was obtained by averaging 10 shielded counts [*Dickey*, 1990] over the casing of the neutron probe. Figure 5 shows the calibration curve (26 samples) and the best fit regression line ($r^2 = 0.85$). The standard error of estimate of the calibration curve was 2.1% equivalent volumetric moisture content, which was considered to be the standard deviation of the instrument calibration. During the drainage experiment three soundings per depth were averaged so that the error in the volumetric soil moisture content measurement was mainly due to the calibration curve standard error of estimate, equal to 2.1%. Therefore, the observation noise standard deviation is $R^{1/2} = 0.021 \times 22.5$ cm.

RESULTS AND DISCUSSION

The nonlinear filtering approach was applied to determine the hydraulic conductivity function. The initial mean $\langle X(0)\rangle$ and R used in the multidimensional optimization scheme were 47.8% × 22.5 cm and $(2.1\% \times 22.5 \text{ cm})^2$ which correspond with the measured saturation moisture content and the observation noise, respectively. The measured field saturated water content in this experiment was close to the value reported by *Buchter et al.* [1991]. The raw data for θ^*

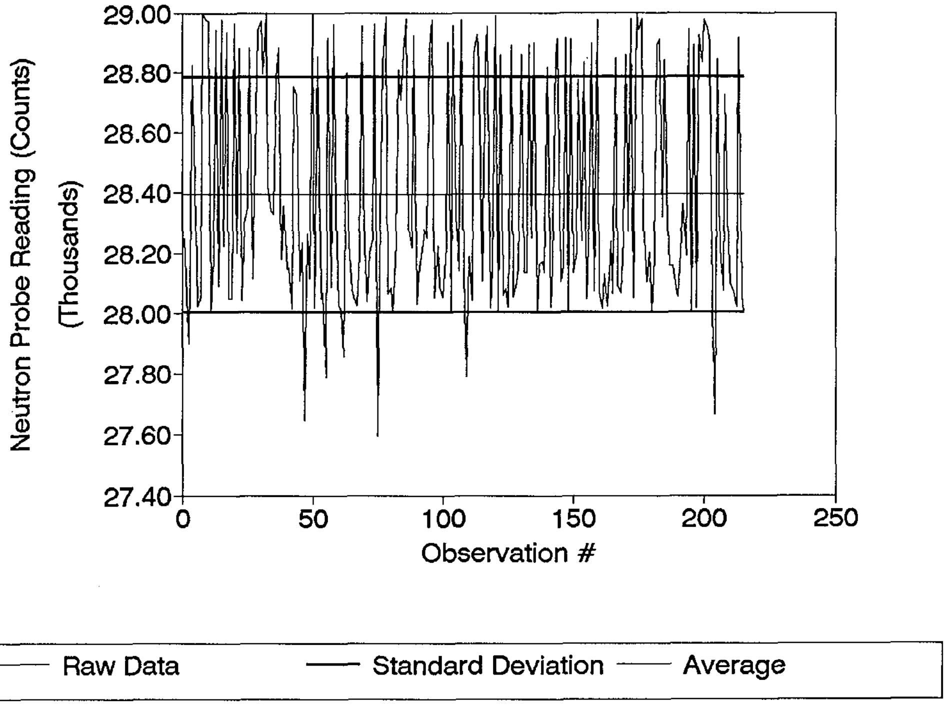

Fig. 2. Unshielded neutron probe soundings at 75 cm soil depth. The 214 displayed readings were taken over a 2 hour span during which the moisture content was assumed to be constant.

and the hydraulic gradient dH/dz are displayed in Figure 6 for the 43 day period. The estimated A, B, Q, and $P(0)$ that resulted in the maximum likelihood estimate were 1.244×10^{-8} cm d^{-1}, 1.625 cm^{-1}, 2.413×10^{-2} cm^2 d^{-1}, and 1.504 $\times$ 10^{-2} cm^2, respectively. With the final estimates of A, B, Q, and $P(0)$, the predicted average moisture contents and their standard deviations $\pm(P(t))^{1/2}$ are also shown in Figure 6, which indicates that all the probability mass is contained within ±1 standard deviation.

The variation of the standard deviation in time indicates that the proposed dynamic equation performs better during rapid drainage (Figure 6), which is consistent with other studies [*Flühler et al.*, 1976]. Also in this near-saturated range, most of the water content fluctuation is due to drainage, and the instrumental error noise is not critical. However, the instrumental noise becomes more noticeable as the drainage flux (at b = 22.5 cm) becomes smaller when steady state conditions are approached (Figure 6). This is described well by an increase in the predicted variance. The computed initial standard deviation $(P(0)^{1/2}/b)$ around the field saturation value is 0.55%, indicating that the assumed value of the initial mean $\langle X(0)\rangle/b$ = 47.8% was very reasonable in the multidimensional optimization scheme.

In this study, the variance per unit time (Q) of the state noise (ε) was assumed to be stationary and treated as a fitting parameter in the multidimensional optimization scheme. An equivalent water content variation of 0.69% d^{-1} was obtained for $Q^{1/2}/b$, indicating that the model prediction un-

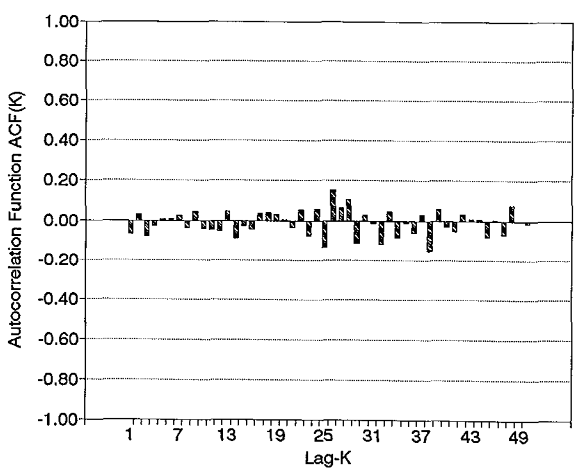

Fig. 3. Autocorrelation function of the unshielded neutron probe counts from Figure 2.

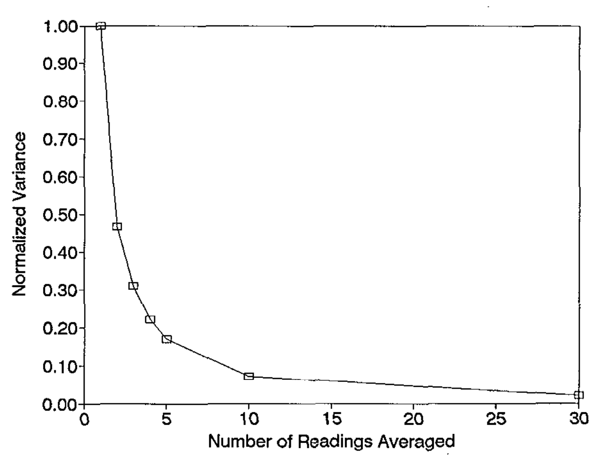

Fig. 4. Reduction in normalized instrument variance as a function of readings averaged.

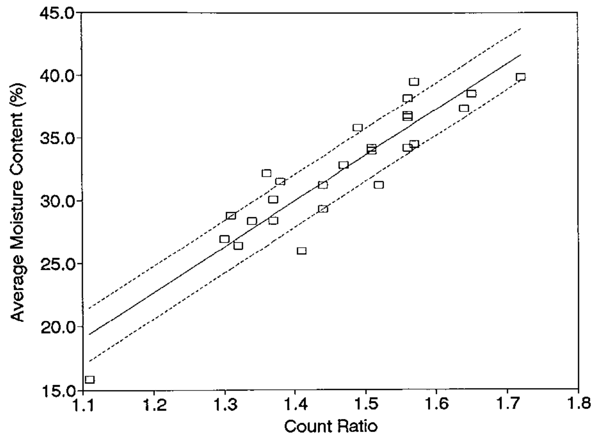

Fig. 5. Neutron probe calibration curve. The coefficient of determination $r^2 = 0.85$, and the standard error of estimate SEE = 2.10% volumetric moisture content. The count ratio is defined as the ratio of the actual count to the standard count.

certainty for quantifying daily stored water due to drainage is 0.69%. Note that the observation uncertainty is 2.1%.

The parameters A and B estimated by the nonlinear filtering approach were then compared to those estimated by the theta, flux, CGA, and classical methods (Table 1). The raw moisture content and matric potential data were smoothed by eye prior to the application of the latter four methods. The smoothing insured a monotonic decrease in moisture content with time, and an attempt was made to preserve local trends observed in the data. With the exception of the CGA, all the methods provided comparable estimates of A and B, with the classical method estimates' being well within the 67% confidence band of the extended Kalman filter predictions of $P(t)$ for all of the observed moisture content ranges (Figure 7). The CGA, theta, and flux methods resulted in higher conductivity values than the nonlinear filtering approach and the classical method, especially for $\theta^* > 0.43$. This can be attributed to the deviations from the unit-gradient assumption (see Figure 6).

TABLE 1. Parameters A and B of the Hydraulic Conductivity Function Estimated by Various Methods

Method	A, cm d^{-1}	B, cm^{-1}
Nonlinear filter	1.24×10^{-8}	1.625
Classical	1.20×10^{-9}	1.872
Flux	1.56×10^{-9}	1.865
Theta	2.45×10^{-9}	1.818
CGA	8.13×10^{-11}	2.212

Here $K(W) = A \exp(BW)$.

CONCLUSIONS

A nonlinear filtering approach for the determination of the in situ hydraulic conductivity function from drainage experiments was developed and tested in the field. The method permits separate accounting of measurement error and model structure error through the incorporation of two independent noises: observation noise and state noise. The continuous nonlinear filter was linearized about the state mean trajectory to obtain a simple description of the time evolution of the mean stored water and variance propagation. Unlike current field methods which provide $K(\theta)$ relations in the mean from arbitrarily smoothed field observations, the nonlinear filtering approach provides estimates of $K(\theta)$ in the mean and variance based on raw measurements. This is important for uncertainty analysis of water and solute transport in the field. The nonlinear filtering approach also allows the quantitative assessment of the validity of the dynamical equation on a daily basis, based on the state variance per unit time (Q). In this study, the estimated state standard deviation per unit time per depth b was 0.69% d^{-1} moisture content variation, which is small compared to the neutron probe calibration error (2.1%). For a daily time step, the isothermal and nonhysteretic assumptions invoked were not inappropriate for this transient field experiment.

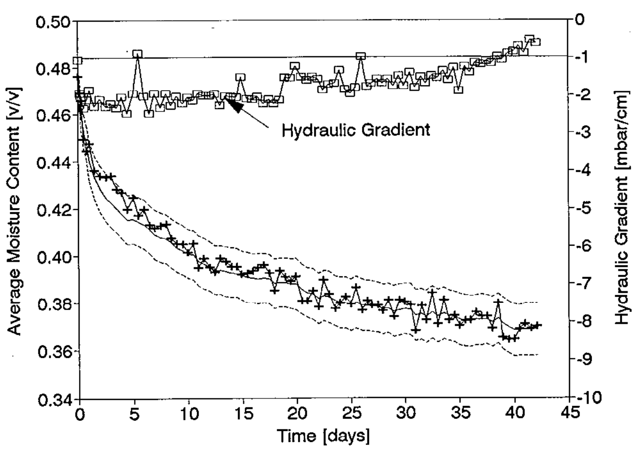

Fig. 6. Observed average moisture content as a function of time (plus), hydraulic gradient (open square), predicted moisture content (single solid line). The predicted time variation of standard deviation $[\langle X(t)\rangle \pm P(t)^{1/2}]b^{-1}$ is also shown (dashed lines).

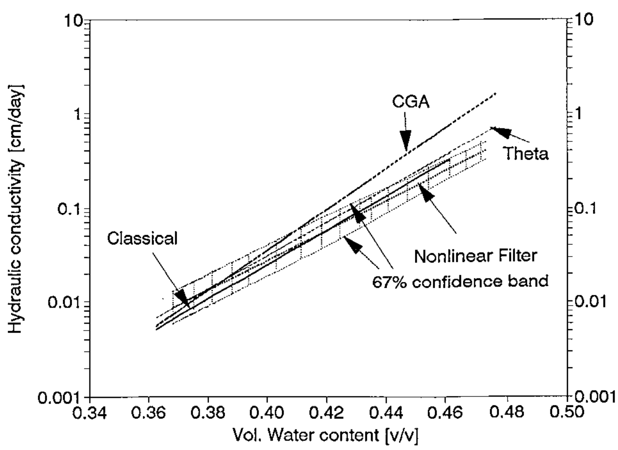

Fig. 7. $K(\theta)$ functions estimated by the CGA, theta, flux, classical, and proposed nonlinear filtering methods. The predicted standard deviation by the proposed method is also shown.

APPENDIX A: OPERATIONAL PROCEDURE TO DETERMINE PARAMETERS OF HYDRAULIC CONDUCTIVITY FUNCTION

Once the water content and hydraulic gradient measurements have been carried out and the variance of the neutron probe calibration (R) is known, the following procedure can be used to determine the optimal hydraulic conductivity parameters A and B, the initial variance $P(0)$, the state spectral density Q and the time evolution of the standard deviation $P(t)^{1/2}$.

1. Set the initial mean $\langle X(0)\rangle = Z(0)$, the stored water neutron probe reading at $t = 0$.
2. Assume initial values for A, B, $P(0)$, and Q (see discussion below).
3. With $[A, B, P(0), Q]$ known, integrate numerically (17) and (18) from $t = 0$ to $t = t_1$ to determine $\langle X(t_1)\rangle^-$ and $P(t_1)^-$.
4. Using the neutron probe measurement $Z(t_1)$, compute $L_1 = (Z(t_1) - \langle X(t_1)\rangle^-)^2/P(t_1)^-$.
5. Compute the Kalman gain K_g from (21).
6. Determine the updated values $\langle X(t_1)\rangle^+$ and $P(t_1)^+$ from (19) and (20) using $\langle X(t_1)\rangle^-$, $P(t_1)^-$ and K_g.
7. These updated values serve as initial values to (17) and (18) at t_1 and hence steps 3 to 6 are repeated to obtain L_2, $\langle X(t_2)\rangle^+$ and $P(t_2)^+$.
8. Carry out the above procedure until time t_n. Compute the objective function L from (24).
9. Try another set of initial conditions $[A, B, P(0), Q]$ and determine another value for L using steps 3 to 8.
10. Continue step 9 until L cannot be minimized further. The values computed $[A, B, P(0), Q]$ are the optimal values.

Since the minimization of L is based on four parameters, it is computationally inefficient to use a trial and error approach. Alternatively, one may use a multidimensional optimization scheme such as the multidimensional simplex method (see *Press et al.* [1990, pp. 289–293] for a description of the algorithm) in order to efficiently search for the optimum combination of A, B, $P(0)$, and Q that minimizes the objective function L. This method requires only function evaluation, not derivatives. A diagram of the computational scheme showing the implementation of the multidimensional optimization algorithm is shown in Figure 8.

Note that if a hydraulic conductivity function with more than two parameters is selected (say, four), then the value of L is affected by six parameters, and therefore the optimization scheme is applied in six dimensions. In this case, other optimization schemes such as Powell's method [*Press et al.*, 1990, pp. 294–301] or the conjugate gradient methods [*Press et al.*, 1990, pp. 305–307] could be more efficient, but require derivative calculation.

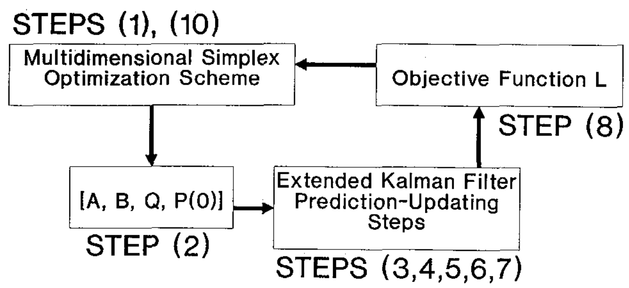

Fig. 8. Computational scheme for determining the optimal parameters $[A, B, Q, P(0)]$.

All the methods described above may not provide a global minimum for L, and hence the starting values for $[A, B, \cdots, P(0), Q]$ may become important. It is suggested that the hydraulic conductivity function also be estimated using another technique (i.e., CGA, flux, theta, or classical method) as the starting parameters for the optimization scheme.

An alternate optimization approach is the use of a simulated annealing algorithm that is not easily "fooled" by unfavorable local minima of L [see *Press et al.*, 1990, pp. 331–334].

APPENDIX B: EXTENSION TO POWER LAW HYDRAULIC CONDUCTIVITY FUNCTION

An alternative derivation of (17) and (18) for a hydraulic conductivity function of the form $K(W) = AW^B$ is presented [*Campbell*, 1974]. The procedure in Appendix A is not altered; however, (17) and (18) are replaced by a new set of equations given below. Taking the expectation of (9) gives

$$\left\langle \frac{dX(t)}{dt} \right\rangle = -\langle A(X(t))^B \rangle \left[\frac{\partial H}{\partial z}\right]. \quad \text{(B1)}$$

Expanding $AX(t)^B$ with a first-order Taylor series expansion about $\langle X(t)\rangle$ yields

$$A(X(t))^B = A\langle X(t)\rangle^B + AB\langle X(t)\rangle^{B-1}(X(t) - \langle X(t)\rangle) \quad \text{(B2)}$$

Taking the expectation of (B2), and noting that $\langle X(t) - \langle X(t)\rangle\rangle = 0$,

$$\langle A(X(t))^B \rangle = A\langle X(t)\rangle^B. \quad \text{(B3)}$$

Substituting (B3) into (B1),

$$\frac{d\langle X(t)\rangle}{dt} = -A\langle X(t)\rangle^B \left(\frac{\partial H}{\partial z}\right)_{z=h}, \quad \text{(B4)}$$

which depends on $\langle X(t)\rangle$ only.

Similarly for the variance,

$$\frac{dP(t)}{dt} = -2\left[\left(\frac{dH}{dz}\right)_{z=b} AB\langle X(t)\rangle^{B-1}\right]P(t) + Q. \quad \text{(B5)}$$

In Appendix A, (17) and (18) can be replaced by (B4) and (B5), respectively.

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