Evaporation and the Field Scale Soil Water Diffusivity Function

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Simplifications to the depth-integrated soil water transport equation lead to an Ito stochastic differential equation where the evaporation is related to the stored water by the nonlinear soil water diffusivity function. From the derived equation the diffusivity function was estimated from daily stored water measurements obtained at the field scale using nonlinear filtering theory for a period of 100 days. Comparisons with daily evaporation measured with a sensitive 50-ton lysimeter indicated that the proposed method may be used to determine soil water diffusivity functions at the field scale under natural conditions when applied water and evaporation are the primary controlling physical mechanisms in the hydrologic budget.

1. Introduction

Approximate solutions to the nonlinear diffusion equation have been demonstrated to be in good agreement with measurements obtained from laboratory column experiments of drying soils [Gardner and Hillel, 1962; Gardner and Gardner, 1969]. In nature, however, the simple initial and boundary conditions which can be imposed in laboratory column studies seldom exist. In addition, other variables play a role in the field such as redistribution of water during evaporation, random precipitation, hysteresis, salinity, temperature, and nonuniform initial soil moisture profiles [e.g., Black et al., 1969; Jury et al., 1978; Lima et al., 1990; Dane and Klute, 1977]. Major complications also arise due to the natural variation of soil properties in the field [e.g., Nielsen et al., 1973; Biggar and Nielsen, 1976].

In this study we investigate the applicability of an approximate solution to the nonlinear desorptive diffusion equation proposed by Gardner [1962] to compute evaporation as well as to determine a field diffusivity function from stored water observations and applied water events in the natural environment. There are, of course, a large number of physical transport mechanisms which are not explicitly accounted for in the drying soil model, so that the simplifying assumptions are assumed to generate a sequence of noise disturbances to the transient flow model system [Zielinski, 1991; Shumway, 1988]. Further, an inherent difficulty in field studies is that averaging observations at various spatial locations results in an additional nonstationary noise component that needs to be accounted for when determining the evaporation or the diffusivity function using stored water measurements [White, 1988; Schmugge et al., 1980]. Due to the uncertainties in the model of the physical system, as well as the spatial variability of observations in the field, application of a nonlinear filtering theory is suitable since the two sources of uncertainty can be accounted for in both the evaporation as well as the diffusivity calculation [e.g., Milly, 1986; Milly and Kabala, 1985; Katul et al., 1993; Wendroth et al., 1993].

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Paper number 93WR00094. 0043-1397/93/93WR-00094\$05.00

Irrigation events were scheduled randomly in time over a bare soil field. The field site is equipped with a weighing lysimeter which measures evaporation as well as a network of neutron probe access tubes in which soil stored water profile was monitored on a daily basis [Parlange et al., 1992a]. From the measured stored water time series a field diffusivity function is calculated, and cumulative evaporation predictions are compared against the lysimeter evaporation measurements.

THEORY

2.1. Physical Description

The hydrologic balance in the absence of lateral flow and negligible drainage is

$$\frac{dS}{dt} = P_t - E_t,\tag{1}$$

where S is the depth of stored water between the surface (z = 0) and some depth L, L is the depth of uniform wetting, E_t is the evaporation rate, and P_t is the rate at which water is applied (precipitation or irrigation). The evaporation rate can be calculated using the diffusion equation and assuming isothermal and homogeneous conditions:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left(D(\theta) \frac{\partial \theta}{\partial z} \right), \tag{2}$$

where θ is the volumetric moisture content and D is the soil water diffusivity which is a highly nonlinear function of soil water content [Black et al., 1969; Lisle et al., 1987]. Equation (2) is the well-known nonlinear diffusion equation. Various approximate and exact solutions have been obtained and studied [e.g., Gardner, 1959, 1962; Brutsaert, 1982a, 1979, 1974; Brutsaert and Weisman, 1970; Parlange et al., 1992b, 1993, 1987; Parlange, 1971, 1975; Parlange and Braddock, 1980; Lisle et al., 1987; Heaslet and Alksne, 1961]. Gardner [1962] obtained an approximate solution of the depth-integrated form of (2) for the falling rate stage of soil drying and for an arbitrary diffusivity function,

$$E_t = -\frac{dS}{dt} = \frac{D(S/L)S\pi^2}{4L^2}; \qquad \frac{Dt}{L^2} > 0.3,$$
 (3)

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where the diffusivity function is given as a function of the stored water. The derivation is based on the assumption that once the rate of evaporation is no longer potential [Brutsaert, 1982b, pp. 237-240; Katul and Parlange, 1992; Jury et al., 1991, pp. 154-156], the evaporation rate becomes independent of the initial drying rate (i.e., when the soil surface is wet) and depends only on the water content of the soil profile [Gardner and Hillel, 1962]. Also, (3) is not valid for short time intervals when $D(S/L)t/L^2 < 0.3$ [Gardner, 1962]. Combining (1) and (3), the hydrologic balance may be written as

$$\frac{dS}{dt} = P_t - \left(\frac{\pi}{2L}\right)^2 SD(S). \tag{4}$$

2.2. State-Space Formulation

For an exponential diffusivity function $D(S/L) = A \exp(BS/L)$ [e.g., Reichardt et al., 1972], (4) may be written in state-space notation as

$$dX_t = \left[P_t - \left(\frac{\pi}{2L}\right)^2 X_t A \exp\left(X_t B/L\right)\right] dt + \nu_s dt, \qquad (5)$$

where $v_s dt$ is a stochastic noise due to uncertainties in the proposed model. The corresponding discrete observation equation at time $t_k (k = 0, 1, 2, 3, \cdots)$ is

$$Z_m(t_k) = X_{t_k} + \nu_m(t_k),$$
 (6)

where X_i is the state variable representing stored water S_i Z_m is the observed amount of stored water at time t_k , and v_m is the observation noise. The state noise $(v_s dt)$ arises due to the various simplifying assumptions invoked in the model of the physical system such as neglecting thermal effects, salinity effects [Lima et al., 1990], clay swelling, hysteresis [Parlange, 1976; Topp, 1971], redistribution within the soil depth L, and so forth. Each of the assumptions given here. as well as all those not included, are too complicated to assess individually at a point. Furthermore, our interest here is to study the combined effects of all these assumptions on the performance of (3) at the field scale. We assume that the simplifications to the system affect (3) in some random manner, and their superposition approaches the Gaussian distribution as suggested by the central limit theorem [Gardiner, 1990, p. 37; Kvanli, 1988, pp. 312-340; Clarke and Disney, 1985, pp. 172-176]. Therefore the state noise is taken to be a zero-mean Gaussian noise sequence with spectral density Q [Arnold, 1974, pp. 202-203; Sobczyk, 1991, pp. 60-61; Gelb, 1974, pp. 72-73]. The observation result is due to both the instrument calibration as well as spatial averaging and is assumed to be zero-mean Gaussian with variance R_t [Vauclin et al., 1984; Haverkamp et al., 1984; Parlange et al., 1992a].

The product $v_s dt$ is defined by the Wiener increment $Q(dW_t)$ of the Wiener process W_t [Gardiner, 1990, pp. 80–82; Gardner, 1990, pp. 124–125] with a mean of zero and a covariance function defined by $\delta(t-\tau)$. Q is the variance per unit time of the state noise process (since the Wiener increment has unit variance) and is an unknown which needs to be solved [Gelb, 1974, p. 73], and δ is the Dirac delta function. We also assume that (5) satisfies the existence and uniqueness conditions for the time interval $[0, \infty]$ [Gardiner,

1990, p. 94]. Given the random nature of the additive noises, the state variable X_t and the water storage observations $Z(t_k)$ are then random variables in time [Zielinski, 1991; Puente and Bras, 1987]. The methodology to determine the evolution of the mean and the variance behavior of X_t in time is discussed next.

2.2.1. Mean behavior of X_t . The ensemble average operator is applied to (5), and after interchanging the differential and expectation operators we obtain

$$\frac{d\langle X_t \rangle}{dt} = P_t - \left(\frac{\pi}{2L}\right)^2 A \langle X_t \exp(BX_t/L) \rangle, \tag{7}$$

where $\langle \ \rangle$ denotes the ensemble average operator. The evaluation of the ensemble average on the right-hand side of (7) requires calculation of all the moments of X_t , thus a closure problem arises since the evaluation of the first moment $d \langle X_t \rangle / dt$ requires all moments of X_t to be known.

To close the equation we let $f(X_t) = X_t \exp(B X_t/L)$ and then expand $f(X_t)$ about $\langle X_t \rangle$ using the Taylor series

$$f(X_{t}) = f(\langle X_{t} \rangle) + \frac{\partial f}{\partial \langle X_{t} \rangle} (X_{t} - \langle X_{t} \rangle)$$

$$+ \frac{1}{2} \frac{\partial^{2} f}{\partial \langle X_{t} \rangle^{2}} (X_{t} - \langle X_{t} \rangle)^{2} + O(X_{t} - \langle X_{t} \rangle)^{3}.$$
 (8)

Taking the second-order approximation for $f(X_t)$, (7) can be written as

$$\frac{d\langle X_t \rangle}{dt} = P_t - \left(\frac{\pi}{2L}\right)^2 A \exp\left(B\langle X_t \rangle/L\right)$$

$$\cdot \left\{ \langle X_t \rangle + \frac{1}{2} \operatorname{Var} X_t \left[\frac{B}{L} \left(2 + \frac{B}{L} \langle X_t \rangle \right) \right] \right\}, \qquad (9)$$

where Var X_t is defined as $\langle (X_t - \langle X_t \rangle)^2 \rangle$. Note that (9) is not closed since it requires the variance behavior of X_t .

2.2.2. Variance behavior of X_t . The time evolution of noisethe variance is given by

$$\frac{d}{dt} \operatorname{Var} X_t = \frac{d}{dt} \langle X_t^2 \rangle - \frac{d}{dt} \langle X_t \rangle^2, \tag{10}$$

where the second term on the right-hand side is $2\langle X_t \rangle d\langle X_t \rangle/dt$. Since X_t satisfies the Ito stochastic differential equation defined as $dX_t = [P_t - (\pi/2L)^2 A X_t \exp(BX_t/L)]dt + QdW_t$, any function $g(X_t)$ satisfies the Ito formula

$$dg(X_t) = \frac{\partial g(X_t)}{\partial t} dt + \frac{\partial g(X_t)}{\partial X_t} dX_t + \frac{1}{2} \frac{\partial^2 g(X_t)}{\partial X_t^2} (dX_t)^2,$$
(11)

where dX_t is given by (5) [Gardiner, 1990, p. 95]. Let $g(X) = X_t^2$. Substituting into (11) and taking the ensemble average gives

$$\frac{d}{dt} \langle X_t^2 \rangle = 2 \left(X_t \frac{dX_t}{dt} \right) + Q. \tag{12}$$

In the above deviation the following properties were used: (1) $\partial g(X)/\partial t = 0$, (2) $dW_t^2 = dt$, $dW_t^{(2+N)} = 0$, and (3) the nonanticipating property of the Wiener increment [Gardiner, 1990, pp. 86-88]. Equation (10) may be rewritten as

$$\frac{d}{dt} \operatorname{Var} X_t = 2 \left[\left\langle X_t \frac{dX_t}{dt} \right\rangle - \left\langle X_t \right\rangle \frac{d\langle X_t \rangle}{dt} \right] + Q. \quad (13)$$

Equation (13) is a special case of the general Riccati type equation originally derived by Kalman and Bucy [1961] for the covariance matrix of the optimal filtering error. Note that (13) is not closed since the evaluation of $\langle X_t dX_t/dt \rangle$ still requires all the moments of X_t . Applying a first-order Taylor series expansion about the mean of the term $[\langle X_t dX_t/dt \rangle]$, taking the ensemble average, and substituting into (13), the time evolution equation for the variance becomes

$$\frac{d}{dt} \operatorname{Var} X_t = Q - \left(\frac{\pi}{2L}\right)^2 A \exp\left(B\langle X_t \rangle / L\right) \left[1 + \frac{BX_t}{L}\right]. \quad (14)$$

Equations (9) and (14) constitute a closed set of predictive equations for the mean and variance in time, respectively. In order to integrate (9) and (14), the diffusivity coefficients A and B, the variance per unit time Q, and some initial conditions for both the mean $\langle X_0 \rangle$ and the variance $\operatorname{Var}(X_0)$ need to be specified.

2.2.3. Updating. With an estimate of the state of the system at time t_k , that is, $\langle X(t_k) \rangle^-$ and $\text{Var} [X(t_k)]^-$ obtained from (9) and (14), we wish to update the estimates $(\langle X(t_k) \rangle^+)$ and $\text{Var} [X(t_k)]^+)$ by incorporating the observation $Z(t_k)$, with a variance R_t , when it becomes available at t_k . The updated estimates for the mean and the variance are solved using

$$\langle X(t_k) \rangle^+ = \langle X(t_k) \rangle^- + K_o(Z(t_k) - \langle X(t_k) \rangle^-) \tag{15}$$

$$Var X(t_k)^+ = Var X(t_k)^- (1 - K_g),$$
 (16)

where K_g is the Kalman gain [Gelb, 1974]. The optimum choice of K_g is given by

$$K_g = \left[\frac{\operatorname{Var} X(t_k)^-}{\operatorname{Var} X(t_k)^- + R_t} \right],\tag{17}$$

which defines how to weigh the combination of two sources of information: (1) predictions and (2) observations [Gelb, 1974, pp. 108–109; Arnold, 1974, pp. 205–209]. Note that if $R_t \to \infty$, then $K_q \to 0$, so that the updated mean and variance values are simply $\langle X(t_k) \rangle^-$ and Var $[X(t_k)]^-$, respectively; therefore the observations have no influence on the updating scheme since they are considered completely unreliable. On the other hand, if $R_t \to 0$, then $K_q \to 0$ 1, and the updated mean and variance values are simply the observations $Z(t_k)$ and $R_t(=0)$, respectively. Equations (9) and (14) are conservation equations that respect the physics of the system, while (15) and (16) are statistical corrections which redistribute stored water in a statistical or nonphysical manner [Katul et al., 1993]. The prediction-updating equations (9), (14), (15), and (16) define the structure of the extended Kalman filter (EKF) (see Figure 1).

2.2.4. Determination of the diffusivity function. The parameters required to apply the extended Kalman filter equations are $\langle X_0 \rangle$, $\operatorname{Var}(X_0)$, A, B, R_t , and Q. We assume that the observation variance R_t can be estimated from spatially averaging the neutron probe readings. This is discussed in more detail in the experimental section below. The initial estimate of $\langle X_0 \rangle$ is simply taken to be the initial observation $Z_m(t_0)$. The diffusivity parameters A and B as

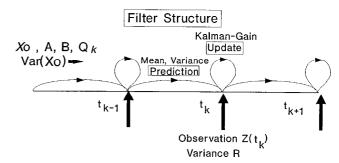


Fig. 1. Structure of the prediction-updating scheme for the extended Kalman filter.

well as Q and $\mathrm{Var}\left(X_{0}\right)$ are then determined with an iterative multivariate optimization scheme for minimizing the least squares objective function (L_{obj}) defined by

$$L_{\text{obj}} = \sum_{k=0}^{k=n} \left[Z(t_k) - \langle X(t_k) \rangle^{-} \right]^2, \tag{18}$$

where n is the span of the record [Gelb, 1974, p. 103]. Note that A, B, Q, and Var (X_0) appear implicitly in (18); therefore an iterative optimization scheme is necessary to minimize L_{obj} for the various combinations of A, B, Q, and Var (X_0). In this study the multidimensional simplex method was used to recursively estimate A, B, Q, and Var (X_0). A complete description of the algorithm is presented by *Press et al.* [1990, pp. 289–293], and more details regarding convergence and other numerical aspects are presented by *Katul et al.* [1993].

3. Experiment

The experiments were carried out from September 4 to December 12, 1990, at the University of California, Davis. Some aspects of the field experimental setup have been presented by Katul and Parlange [1992] and Parlange and Katul [1992]. For completeness the field details pertinent to this study are presented. The soil is a uniform Yolo clay loam with no layering in the top first meter. The soil physical properties are described by *Buchter et al.* [1990]. The site is equipped with a sprinkler irrigation system which covers a surface area of 150 m by 130 m with a gross application rate of 0.5 cm h⁻¹ [see Parlange et al., 1992a]. The daily evaporation rate was measured by a 50-t capacity weighing lysimeter on a 20-min time step and integrated over the full day to obtain total daily evaporation. The weighing lysimeter used in this study is circular in design, with a diameter of 6 m and a depth of 1 m [Pruitt and Angus, 1960]. The volumetric moisture content is monitored by a Campbell Nuclear Pacific hydroprobe, model 503. Five aluminum access tubes, spaced 18 m apart along a transect from west to east, were drilled using the Soil Conservation Service method, and the samples obtained were used for the neutron probe calibration [Parlange et al., 1992a; Dickey, 1990; Cuenca, 1989]. Neutron probe soundings were taken at 15 cm (assumed to represent stored water between 0-22.5 cm) and at 30-, 45-, 60-, and 75-cm depths at 0800 (PST) at the five locations described in Figure 2a. A comparison between the lysimeter-measured evaporation and evaporation obtained from the neutron probe is presented by Parlange et al.

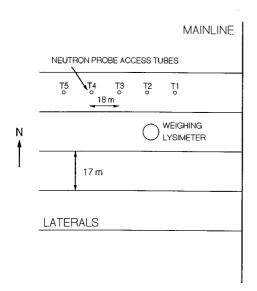


Fig. 2a. Location of the neutron probe access tubes $(T_i, i = 1, 2, \dots, 5)$ and the weighing lysimeter.

[1992b]. The gross application rate results in net application rates varying from 0.4 to 0.48 cm h⁻¹. These sprinkle irrigation rates are gentle enough that no surface runoff occurs. The total water applied during each irrigation wets a depth of 15–25 cm. The irrigations have a relatively insignificant influence on the deeper soil profiles. Notice in Figure 2b, where the time variation of the spatially average stored water at each depth is presented in conjunction with the applied water, that the deeper soil moisture changes are small compared to the variability in the top 22.5 cm for the full study period. Evaporation and the applied water events are the primary physical processes that affect the stored water change with time near the land surface. In this study we set L equal to 225 mm.

The wetting of the 22.5-cm soil horizon is not uniform as assumed in (3), and L changes with each irrigation. It is important to note that the neutron probe spatially averages the stored water within the top 22.5 cm [see *Cuenca*, 1989, pp. 183–184]. In part, this is due to the calibration of the

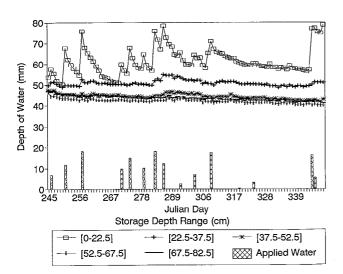


Fig. 2b. Neutron probe measured stored water time series at each location in the field.

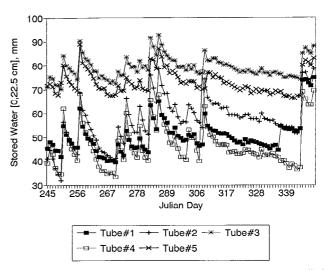


Fig. 2c. Field average time series of stored water and applied water events.

neutron probe which relates measured neutron counts to the average moisture content obtained from soil samples of 22.5-cm length [Parlange et al., 1992a]. Even though the wetting depth L may be less than 22.5 cm and varies with each irrigation, the neutron probe is sensitive enough to measure stored water changes within the top 22.5 cm. The variation of stored water in time between 0 and 22.5 cm for each access tube location is displayed in Figure 2c.

4. RESULTS AND DISCUSSION

The nonlinear filtering approach was used to determine the diffusivity function parameters (A and B), the state variance per unit time Q, and the initial variance. The $\langle X_0 \rangle$ was set equal to the first mean observation value $Z_1(t_0)=57.4$ mm (Julian day equals 245). The observation variance R_t as a function of time was obtained by computing the variance from the spatially averaged stored water using all of the access tubes (see Figure 3). Note that the variance of the field-measured stored water is much larger than the neutron

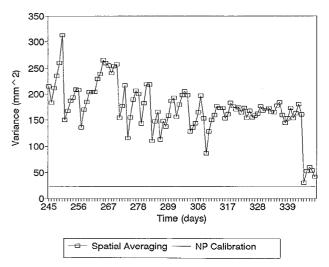


Fig. 3. Time variation of the observation variance due to spatial averaging of measured stored water as well as the neutron probe calibration variance for the top 22.5 cm.

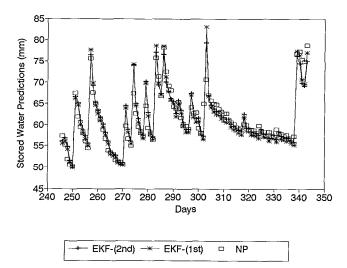


Fig. 4. One-step predictions of the simple extended Kalman filter (first-order closure EKF-1st, second-order closure EKF-2nd, and neutron probe spatially averaged observations).

probe calibration variance. The neutron probe calibration curve variance is $(0.021 \times 225 \text{ mm})^2$ [see Parlange et al., 1992a]. Using the R_t time series and $\langle X(0) \rangle$ preset to the first measured value, the multidimensional optimization scheme calculates the diffusivity parameters to be $A=0.0292 \text{ mm}^2 \text{ d}^{-1}$, B=32.59, $Q=18.87 \text{ mm}^2 \text{ d}^{-1}$, and Var $(X_0)=5.38 \text{ mm}^2$, corresponding to the minimum value of L_{obj} . The state variance per unit time (Q) is of the same order as the neutron probe calibration variance, while the model uncertainty for stored water prediction on a daily basis is within the neutron probe noise (see Figure 3).

To investigate the influence of the variance $\text{Var } X_t$ on the mean behavior of $\langle X_t \rangle$ we compare the results obtained using (9) with a simpler first-order closure approximation

$$\frac{d\langle X_t \rangle}{dt} = P_t - \left(\frac{\pi}{2L}\right)^2 A \exp\left(B\langle X(t)\rangle/L\right)\langle X(t)\rangle. \quad (19)$$

Equation (19) was obtained by replacing $\langle f(X_t) \rangle = \langle X_t | \exp$ (BX_t/L) by $\langle X_t \rangle$ exp $(B\langle X_t \rangle B/L)$. Using (19) instead of (9) and solving the system, the optimum values for A, B, Q, and Var (X_0) are 2.95 mm² d⁻¹, 18.82, 9.25 × 10⁻³ mm² d⁻¹, and 1.75 mm², respectively. The one-step predictions of stored water using the first-order approximation (EKF-1), the second-order approximation (EKF-2), and the neutron probe stored water measurements are plotted in Figure 4. The second-order approximation is closer to the actual measurements than the first-order approximation (Figure 4) for the day of year interval 310-340; however, the difference is not very large between the two predictions. The predicted standard deviation about the predicted mean values is shown in Figure 5a for both the first-order approximation (19) as well as the second-order approximation (9). Clearly, the variance predictions obtained from the first-order closure scheme are unrealistically small and essentially lie on the predictions themselves. For standard deviation comparisons, Figure 5b compares the spatial standard deviation about the mean measured stored water and that predicted by the second-order closure. The second-order standard deviation is within the spatial variability measured in the field.

The cumulative evaporation predictions using the second-order closure scheme are compared with the lysimeter cumulative evaporation in Figure 6. The good agreement found with the second-order (EKF) predictions and cumulative lysimeter measurements ($r^2=0.98$, Figure 7) indicates that the estimated diffusivity function provides a good description of evaporation and soil water transport processes. Thus the approximate solution to the transient flow equation of Gardner may be extended to actual field situations with variable soil water content.

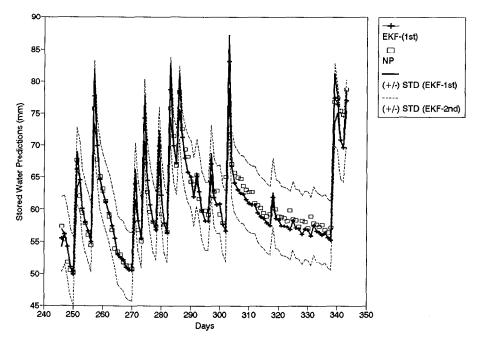


Fig. 5a. Predicted standard deviations about the mean stored water from first- (STD-1) and second-order closure (STD-2) schemes as well as measured spatially averaged stored water.

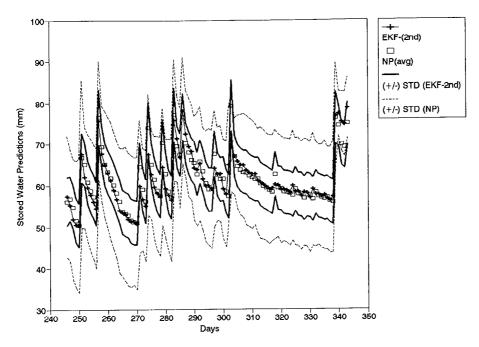


Fig. 5b. Comparison between predicted mean stored water using second-order closure (EKF-2) and measured field scale stored water. The ±1 standard deviation band around the mean values for second-order closure predictions (±STD EKF-2nd) and measurements (±STD NP) is also shown.

The diffusivity function obtained from the extended filtering scheme (EKF-2), along with laboratory diffusivity measurements carried out using Yolo clay soil by Lima et al. [1990] based on the procedure proposed by Bruce and Klute [1956] and Klute and Dirksen [1986], is presented in Figure 8. The Lima et al. [1990] soil water diffusivity measurements were sorption type measurements with different sodium absorption ratios (SAR) and concentrations of NaCl-CaCl₂ solution [Cuenca, 1989, pp. 94–95]. Because of the nature of the laboratory experiments the diffusivity values are generally higher than the diffusivity values from the field-drying experiments.

Fig. 6. Comparison of predicted using EKF (second-order closure) and measured cumulative evaporation as a function of time.

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5. Conclusions

Based on field scale experiments, the application of a simplified flow theory of drying soils was found to provide a useful method for obtaining soil water diffusivity function parameters, that is, water storage and evaporation. Based on simplifications to the soil water transport equation, evaporation was described as a nonlinear function of the soil water profile storage. The simple model described the field scale water transport well on the average and proved to be useful for field hydrologic budget calculations when the applied water was known. Due to the model uncertainty and field scale spatial variability in moisture content, a nonlinear filter was constructed and applied to data collected over a period

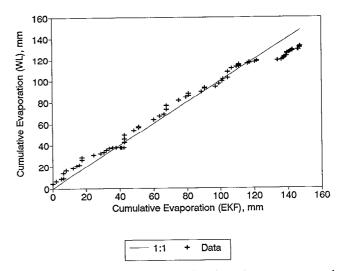


Fig. 7. Predicted (EKF second-order closure) versus measured (weighing lysimeter) cumulative evaporation ($r^2 = 0.98$).

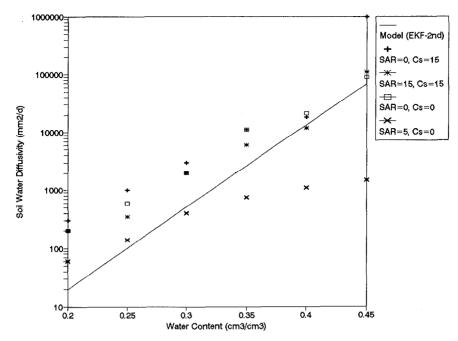


Fig. 8. Comparison between computed soil water diffusivity function using the EKF (second-order closure) for desorptive conditions and laboratory (sorptive) measurements for various sodium adsorption ratios (SAR) and various concentrations of $CaCl_2$ and NaCl (meq L^{-1})^{1/2} mixture solutions (Cs).

of 99 days to aid in the determination of the diffusivity function, prediction of the stored water in the top 22.5-cm soil layer, and prediction of the cumulative evaporation. The one-step prediction of stored water reproduced the observed spatially averaged stored water measurements as well as the cumulative lysimeter evaporation measurements. The state or model variance per unit time is of the order of the uncertainty involved in the neutron probe calibration. More field experiments for different soil textures are required to further assess the validity of this approach.

Acknowledgments. The authors would like to thank Mike Mata and Rick Snyder for their assistance; Ken Tanji, M. Levent Kavvas, and Carlos Puente for their helpful discussions; and P. C. D. Milly for his suggestions. This work is supported in part by the USGS (92G-2266), UC Salinity/Drainage Task Force (90-14), Water Resources Center (W-774), and the INCOR cooperative grant.

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(Received April 24, 1992; revised December 12, 1992; accepted January 7, 1993.)