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Inversely estimating soil hydraulic functions using evapotranspiration fluxes

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Abstract

Numerical modelling of the transient moisture fluxes helps in the development of appropriate water management practices, but requires site-specific information on soil hydraulic properties. Forward simulations with a given set of Van Genuchten (VG) model parameters indicate that different soils act differently in their temporal variable evapotranspiration (ET) response under deep-water table/free drainage conditions. Since actual ET fluxes can be recovered from remote sensing measurements, a new possibility is established to derive soil hydraulic functions under actual field conditions for a range of spatial scales. Thus, inverse modelling of ET_a fluxes is a promising way to estimate the so-called *effective* soil hydraulic functions. We numerically explore the possibility of inverse ET modelling to derive VG model parameters for semi-arid regions. The utility of this technique is evaluated using a simulation model to create a 'no error data set' of ET fluxes for cotton crop. Objective functions using actual ET and actual transpiration (T) are defined. Backward simulations are carried out to re-assess selected VG model parameters for the three-soil types, i.e. sand, loamy sand and sandy clay loam. A realistic ET data set is created from the no error data set by incorporating different levels of random error. Seasonal simulated water balance components (ET, deep percolation and change in profile storage) are compared to study the hydrological performance of the inversely estimated soil hydraulic functions. Results indicate that the moisture stress period under fully developed crops is most appropriate for sampling ET fluxes to solve the proposed inverse problem. It is also observed that frequent observations of ET fluxes are desired to reduce undesirable correlation between different fitting parameters. It is observed that when ET fluxes are very accurate, the VG model parameters α, n and θ_s (θ_r, k_s and λ fixed at actual values) are optimised precisely with 12 ET data points. Inverse fitting of these parameters (α, n and θ_s) utilising perturbed data on ET fluxes results in effective soil hydraulic functions, which reliably predict different water balance components for sand and loamy sand soils.

Keywords: Inverse modelling; Soil hydraulic functions; Evapotranspiration; Water management

1. Introduction

India is one of the largest irrigated countries in the world and almost two-thirds of its agricultural production depends on irrigation. However, as a result of inappropriate policies and practices of water management, extensive areas of irrigated lands have been and

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are increasingly facing environmental degradation through water logging and soil salinisation (Agarwal and Jhorar, 1997). On the other hand, some irrigated areas are facing the problem of irrigation water shortage and falling groundwater levels (Agarwal and Roest, 1996). In order to find alternative solutions for these water management related problems, in-depth analysis of interaction between irrigation practices and groundwater dynamics is required. Simulation models have the capability to provide detailed insights into the system under different conditions. Successful application of these models requires estimates of the hydraulic parameters describing the various processes within the system. Effort have been made by different international organisations to develop appropriate database of soil hydaulic properties (Leij et al., 1996; Wösten et al., 1999). However, there is a general lack of available soil hydraulic data bases for simulation model applications to Indian conditions. Considering the paucity of data bases, the scientific meeting cum workshop on Sustainable Irrigation in Saline Environment (Tyagi et al., 1993) recommended that appropriate parameter estimation procedures including inverse techniques should be developed to support water and solute transport models.

Soil water flow in physical–mathematical models is often described by the Richard's equation. Application of unsaturated soil water flow theory requires that the relationships between soil matric pressure head h, hydraulic conductivity k, and volumetric soil water content θ are known. The relationships between h and θ and k and θ are described, respectively, by the water retention curve and the hydraulic conductivity function. These are usually referred to as soil hydraulic functions. The evaluation of the soil water balance of the unsaturated zone using simulation models relies strongly on an appropriate characterisation of the $h(\theta)$ and $k(\theta)$ relationships (Xevi et al., 1996). Therefore, reliable estimates of site and region specific soil hydraulic functions are very crucial to a meaningful application of these models. However, obtaining estimates of these functions can be an onerous task. Our ability to mathematically model water movement in the subsurface seems to be well ahead of our ability to accurately quantify the flow and transport properties of the soils (Wessolek et al., 1994).

Laboratory, as well as field methods have been developed for the measurement of $h(\theta)$ and $k(\theta)$ relationships (Dirksen, 1991) but not a single method has been developed that performs well in a wide range of circumstances and for all soil types. Furthermore, direct measurement of these properties is often extremely difficult, time consuming and expensive (Van Genuchten and Leij, 1992). Alternatively, pedo-transfer functions, which relate the soil hydraulic characteristics to more easily available soil properties, have been developed (Wösten and Van Genuchten, 1988). However, this indirect method to generate soil hydraulic characteristics does not exist without direct methods since only measurements create the required database (Wösten et al., 1995). Moreover, these functions have the limitation of being location specific (Burke et al., 1997). During the past decade, many investigators have proposed estimating simultaneously the $h(\theta)$ and $k(\theta)$ relationships from a transient flow experiment by employing the inverse problem methodology, see Romano and Santini (1999).

Inverse methods use non-linear parameter estimation procedures to derive the soil hydraulic functions from a measured flow event, either in the laboratory or in the field. Certain functions for the hydraulic properties are assumed and the parameters in these functions are estimated by using an optimisation procedure, which minimises the discrepancies between the observed and simulated responses of the system. Inverse modelling has been applied to determine soil hydraulic function for laboratory scale problems (Kool et al., 1987; Van Dam et al., 1994) by fitting a solution of Richard's equation to observations of transient outflow. Unfortunately, laboratory fitted functions are often non-representative, when used for field scale model applications. Once a complex variable like ET can be derived for a given area from remote sensing measurements, ET at known boundary conditions can be used inversely to identify the so-called *effective* soil hydraulic functions (Feddes et al., 1993a,b). This study is an attempt to contribute to this effort.

Recently, estimates of surface soil moisture (Schmugge et al., 1992) and actual evapotranspiration (ET_a) fluxes (Rosema, 1990) for larger flow domains have become available using remotely detectable quantities. Attempts have been made to inversely assess soil hydraulic functions using observations on soil moisture obtained through passive microwave remote sensing techniques (Burke et al., 1997, 1998). Unfortunately, the passive microwave approach refers to only the top few centimetres (~5 cm) of the soil profile. For many application studies involving field, as well as regional water management, knowledge of soil hydraulic properties for the entire root zone is required. The ET_a under unstressed conditions is determined mainly by the atmospheric demand. However, under non-optimal soil moisture conditions, ET_a reflects the integrated effect of moisture distribution over the root zone, which, in turn, depends on the soil hydraulic properties, the root distribution and the drought and salt tolerance of the crop. ET_a can be measured with several field methods. The concept of surface energy balance determinations from satellites has been widely studied during the past few years (Moran and Jackson, 1991; Bastiaanssen et al., 1998). In fact, energy balance for the surface boundary layer is one of the most widely used methods for ET_a estimation (Tan and Shih, 1997).

In this study, we investigate the potential of inverse modelling of ET_a and T_a to derive effective soil hydraulic functions for irrigated soils under arid (Indian) regions having deep groundwater table conditions. Inverse results have been examined for three soil types. Issues that are addressed include: effect of a number of unknown parameters of the selected soil hydraulic function model, effect of measurement frequency of ET_a estimates, and effect of random errors in the ET_a fluxes on the hydrological behaviour of fitted soil hydraulic functions. Fitted soil hydraulic parameters do not necessarily have a physical meaning. Therefore, hydrological behaviour of fitted soil hydraulic functions have been examined with the crop growth and soil water balance simulation model Soil–Water–Atmosphere and Plant (SWAP) to assess the applicability and reliability of using ET_a fluxes to inversely estimate soil hydraulic functions.

2. Methodology

The potential of deriving effective soil hydraulic functions by inverse modelling of ET_a and T_a fluxes is examined by forward, as well as backward simulation of soil water flow by means of the simulation model SWAP (Feddes et al., 1978; Van Dam et al., 1997). Forward simulations are carried out to generate ET_a fluxes as if these were available from independent measurements. Two objective functions are defined to test their suitability during optimisations. Backward simulations are carried out to estimate different parameters of the soil hydraulic function model proposed by Van Genuchten (1980).

2.1. Simulation model

SWAP is based on the implicit finite difference solution of the non-linear partial differential water flow equation given by

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[k(\theta)\left(\frac{\partial h}{\partial z} + 1\right)\right] - A(h) \tag{1}$$

where h is soil water pressure head (L), z is the vertical coordinate (L) indicating depth below the soil surface, $C(h)$ is the differential moisture capacity (L^{-1}), $k(\theta)$ is the hydraulic conductivity (LT^{-1}) as a function of θ, $A(h)$ is a sink term for water uptake by roots (T^{-1}). Input for the upper boundary condition consists of daily precipitation, irrigation and potential ET data. The condition at the bottom of profile depends on the existing geo-hydrological conditions and can be head controlled, flux controlled or a combination of the two. For the present study, free drainage at the bottom of profile is prescribed.

SWAP simulates E_a and T_a, hence ET_a can be taken as their sum. The Penman–Monteith approach (Allen et al., 1994) is used to estimate the potential ET rate ET_p. The partitioning of ET_p into potential soil evaporation E_p and potential transpiration T_p is established according to soil cover fraction.

In the case of a wet soil, E_a is determined by the atmospheric demand and equals E_p. When the soil dries out, the soil hydraulic conductivity decreases, which reduces evaporation. SWAP calculates the maximum possible evaporation rate E_{max} according to Darcy's law and sets E_a equal to the minimum of E_p and E_{max}. Hence, E_{max} is governed by the soil hydraulic functions. The T_a is calculated using the root water uptake reduction due to water and/or salinity stress. In the present study, only water stress is considered. SWAP uses a semi-empirical approach to describe soil moisture uptake by roots:

$$A(h) = \beta(h)A_{max} \tag{2}$$

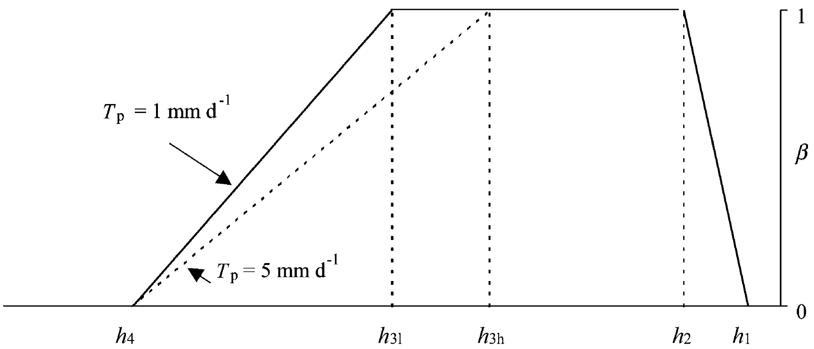

Fig. 1. Schematic of the dimensionless sink-term variable β as a function of the absolute value of the soil water pressure head, h in the SWAP model, after Feddes et al. (1978).

where $\beta(h)$ is a reduction factor and A_{max} is the maximum possible moisture uptake (T^{-1}) by roots under optimum soil moisture conditions and is, in general, a function of the root distribution. However, in the present study, a uniform root density distribution is assumed. The reduction factor β accounts for either too dry or too wet conditions (Fig. 1). It is assumed that under conditions wetter than h_1 (oxygen deficiency) and drier than h_4 (wilting point), water uptake is zero. Limit h_3 also depends on the evaporative demand of the atmosphere, therefore, varies with T_p. For higher T_p, reduction in water uptake occurs already at relatively wetter conditions than that for low T_p (see h_{3h} and h_{3l} in Fig. 1). Between h_1 and h_2 and between h_3 and h_4, a linear variation in β is assumed. In this way, T_a is related to T_p rate by the factor β, which in turn is affected by the soil hydraulic functions. The sink term variables for reduction in root water uptake are crop specific and needs to be defined in advance.

The analytical form of the soil hydraulic functions as proposed by Van Genuchten (1980) is expressed as

$$\theta = \theta_r + [\theta_s - \theta_r]\,[1 + (\alpha h)^n]^{-m} \tag{3}$$

$$k = k_s S^{\lambda}[1 - (1 - S^{1/m})^m]^2 \tag{4}$$

where θ_s and θ_r are, respectively, saturated and residual water content (L^3L^{-3}), α (L^{-1}), n, $m(= 1 - (1/n))$ and λ are empirical shape factors, k and k_s are the unsaturated and saturated hydraulic conductivity (LT^{-1}), respectively, and S_e is the relative saturation defined as

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{5}$$

Table 1
VG model parameters for the three soil types used for forward SWAP simulations

Soil code[a]	θ_s	θ_r	α (cm^{-1})	n	λ	k_s (cm s^{-1})
S1	0.413	0.006	0.0200	2.37	0.500	4.05×10^{-3}
S2	0.473	0.010	0.0130	1.74	0.500	2.89×10^{-3}
S3	0.524	0.010	0.0243	1.53	0.638	0.64×10^{-3}

[a] S1, S2 and S3, respectively, represents a sand, loamy sand and sandy clay loam soil of the USDA classification.

2.2. Forward simulations

Forward SWAP simulations are carried out for three soil types, designated as S1, S2 and S3 (Table 1), for deep groundwater table situations by specifying free drainage of the soil profile as the lower boundary condition. The soil S1 (94% sand, 5% clay), S2 (83% sand, 6% clay) and S3 (46% sand, 30% clay) typically represent a sand, loamy sand and sandy clay loam soil of the USDA classification. The Van Genuchten (VG) model parameters for the three soil types, are based on an earlier SWAP calibration against $\theta(z, t)$ observed during field experiments at Hisar and Sirsa, India (Bastiaanssen et al., 1996). Under most field conditions, rootzone soil profiles usually consists of hydraulically different soil layers, whose sequence strongly influences different processes acting in the root zone, viz. infiltration, redistribution, soil water storage, etc. Before a new technique can be applied under such more complex situation, it is important to examine its conceptual feasibility. Accordigly, we have considered uniform soil profiles to examine the possibility of inversely identifying effective soil hydraulic functions using ET fluxes. As a follow up of the study in future, we intend to attempt and prove the fesibility of proposed technique for more complex situation.

All simulations start from the assumed date of sowing (June 26) of cotton. Soil matric pressure head corresponding to -200 cm ($h = 2.3$ pF) was specified as initial condition for all the soils. Meteorological data from the Haryana Agricultural University, Hisar (India), representing an arid climate, are used. The sink term variables required for reduction in ET_a due to moisture stress according to Fig. 1 ($h_1 = -10$ cm; $h_2 = -25$ cm; $h_{3h} = -400$ cm, $h_{3l} = -800$ cm and $h_4 = -16\,000$ cm) used are those calibrated for a cotton crop grown in a field experiment at Sirsa, India (Bastiaanssen et al., 1996). Simulations cover the growing season of cotton crop for 160 days. Five post sown irrigations, each 60 mm, are specified at Day 51, 72, 97, 118 and 143. Day 1 represents the day of sowing.

Examination of temporal ET behaviour for different soils has an important significance in the present investigation. It is required for two specific purposes: whether, under similar conditions, different soils act differently and if so, to decide appropriate crop period, which is suitable to inversely identify soil hydraulic functions.

Daily SWAP outputs of T_a and E_a between Day 100 and 160 were summarised in a time series and sampled to provide ET_a and T_a fluxes for the inverse modelling exercise. The sampling period was selected such that the crop is fully developed and under actual conditions the ET_a fluxes will be affected by maximum depth of soil profile.

2.3. Parameter estimation procedure

Assuming that for any time t_i, $ET_a(t_i)$ and $T_a(t_i)$, can be obtained independently (in our study, we generate by forward model simulations), these data can be employed as input data for the numerical inversion problem. Let $ET_a(b, t_i)$ and $T_a(b, t_i)$ be the numerically calculated values of ET_a and T_a, respectively, corresponding to a trial vector of parameter values $\{b\}$, where $\{b\}$ is the n-dimensional vector containing the parameters that are optimised simultaneously. The inverse problem then is to find an optimum combination of parameters $\{b^o\}$ that minimises either of the following objective functions:

$$O(b) = \sum \{w_i[ET_a(t_i) - ET_a(t_i, b)]\}^2 \tag{6}$$

$$O(b) = \sum \{w_i[T_a(t_i) - T_a(t_i, b)]\}^2 \tag{7}$$

where w_i is a weighting function. Eqs. (6) and (7) will be, hereafter, referred as ET- and T-based objective functions, respectively. PEST (Watermark Computing, 1994) was used to determine $\{b^o\}$. PEST is a model independent parameter estimation program, based on the Gauss–Marquardt–Levenberg method of non-linear optimisation. It adjusts the model parameters until the fit between model outputs and or field observations is optimised in the weighted least square sense. PEST does this by taking control of the model and running it as many times as is necessary in order to determine the optimal set of adjustable parameters. This optimisation method was selected, because it is very efficient in the number of model calls while searching. This is a pre-requisite for optimisation problems in which computation intensive numerical models are used.

The parameter estimation procedure has been examined for all the three soils in Table 1 with deep groundwater table conditions. The data set on ET_a and T_a for the selected days of the SWAP model output as generated with the forward simulations constituted input to the objective functions (Eqs. (6) and (7)) of the inverse problem. In practice, such data on ET_a could be acquired from advanced field measurement techniques or from satellite images. The data on T_a are considered anticipating their availability in future, for instance by suitably partitioning remotely sensed ET_a into E_a and T_a. Rather sparse sampling strategy is chosen to represent the constraints of limited dependency on independent ET_a measurements. One of the scenarios investigated for improving the accuracy of soil hydraulic parameter estimations is more frequent sampling of ET_a and T_a fluxes.

A standard inverse method require that the inverse problem be well posed and well conditioned, so that the solution exists and is unique and stable (Romano and Santini, 1999). General

Table 2
Summary of different soil hydraulic VG model parameter sets used for backward simulations

Parameter set	Description
Set-1	All parameters optimised
Set-2	All parameters, except θ_s and k_s optimised
Set-3	All parameters except k_s and λ optimised
Set-4	Only α, n and θ_s optimised

information on ill-posedeness and parameter identifiability can be found in Hopmans and Simunek (1999). In general, parameter identifiability can be increased by reducing the number of optimised parameters. A number of parameter estimation runs were carried out with different combinations of VG model parameters (Table 2) to explore the possibility as to which parameters can be estimated using $\mathrm{ET_a}$ or T_a fluxes. For parameter set-1, all the VG model parameters are allowed to be optimised. Realising that at least two parameters (θ_s and k_s) of the VG model have a clear physical meaning and can be obtained from field measurements, the parameter set-2 is designed by setting θ_s and k_s at the known values of Table 1. It is important to note that, k_s varies strongly between soil types (Clapp and Hornberger, 1978; Cosby et al., 1984; Wösten et al., 1995) and also with the scale (Quintard and Whitaker, 1988; Stam et al., 1989). The Darcy parameterisation prescribes a linear relationship between the flux density and the hydraulic potential gradient. Unlike the unsaturated conductivity, the saturated hydraulic conductivity does not depend on flux density or the soil water potential. In the case of k_s, the averaging in both horizontal and vertical directions can be done without explicit a priori knowledge of the small scale solutions of the soil water fluxes. In principle, large scale vertical k_s of multi-layer profiles can be determined as harmonic mean in the vertical direction of the arithmatic mean of small scale conducitvity in the horizontal (spatial) direction (Kabat et al., 1997). The parameter set-3 is designed to estimate only the $h(\theta)$ relationship by setting k_s and λ at known values. For parameter set-4, an additional parameter θ_r is also set at known values, as θ_r represents the residual moisture content which for many soils can be assigned a value near to zero (Russo, 1988). A uniform initial guess of different VG model parameters is specified for all the three soils. The initial values of VG model parameters as specified during backward simulations are: $\theta_s = 0.40\ (\mathrm{cm^3\ cm^{-3}})$; $\theta_r = 0.0\ (\mathrm{cm^3\ cm^{-3}})$; $\alpha = 0.01\ \mathrm{cm^{-1}}$; $n = 2.5$; $\lambda = 0.5$ and $k_s = 2.31 \times 10^{-3}\ \mathrm{cm\ s^{-1}}$.

2.4. Evaluation criteria

Traditionally, reliability of estimated parameters is evaluated based on statistical properties (e.g. bias, standard deviation) of fitted values (Wagner and Gorelick, 1986). However, these parameter estimates may be meaningless if the model fails to reliably reproduce salient features of particular interest. The ultimate objective of this study is to derive soil hydraulic functions appropriate to develop and test alternative water management practices in an irrigation context. A water budget for unsaturated zone consists of principal inflows and outflows for depth of interest, such as root zone and resulting change in storage ΔS that occurs if inflows and outflows are not balanced. For irrigated arid and semi-arid regions with deep groundwater table, the principal inflows are rainfall R and irrigation I and the principal outflows are $\mathrm{ET_a}$ and deep percolation Q. The water balance for such areas can be described by

$$\Delta S = R + I - \mathrm{ET_a} - Q \tag{8}$$

Fundamental to the adopted inverse procedure is that VG model parameters are fitted in such a way that the ability of the model to reproduce $\mathrm{ET_a}$ (or T_a) fluxes is optimised. It is well recognised that the fitted parameters do not have physical meaning. A possible correlation between them means that many combinations of the parameters could fit the data (in our case $\mathrm{ET_a}$ or T_a fluxes) equally well (Snow and Bond, 1998), so casting doubt on the values of simultaneously optimised parameters. Therefore, it is important to know how fitted VG model parameters will reproduce other water balance components, such as ΔS and Q. Accordingly, we do not intend to derive precise parameter values, rather we will derive effective soil hydraulic functions, which can be reliably used for simple water balance computations. It may also be potentially dangerous to use inversely estimated parameters to forward model flow conditions beyond those present in the original inversion experiment (Hollenbeck and Jensen, 1998). Therefore, we evaluate the

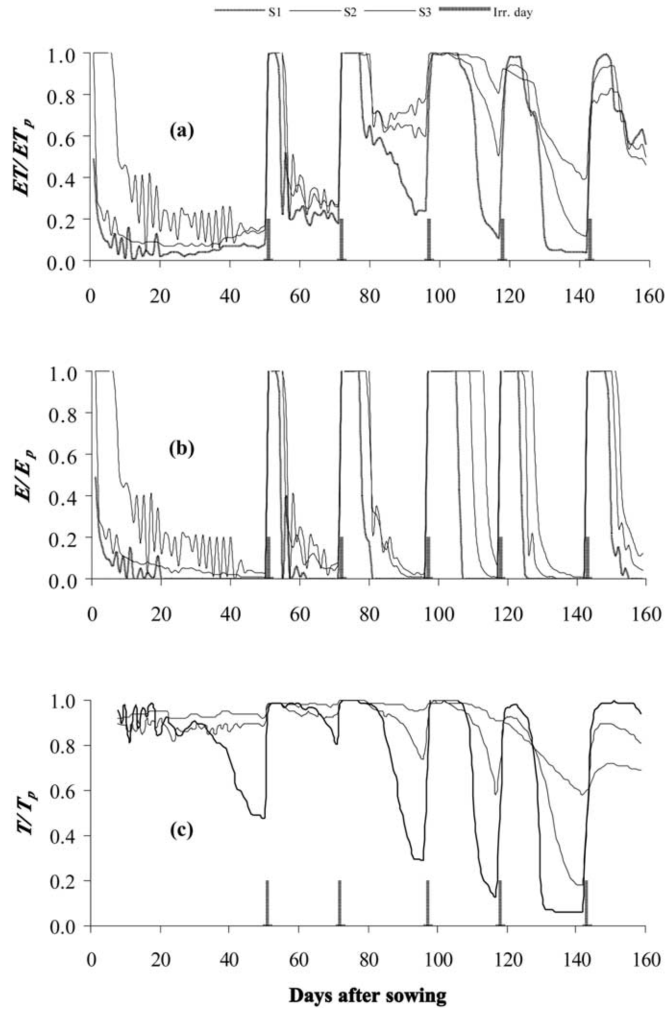

Fig. 2. Results of forward SWAP simulations for the three soil types as in Table 1. (a) Relative evapotranspiration (ET/ET_p), (b) relative soil evaporation (E/E_p) and (c) relative transpiration (T/T_p) for cotton crop under deep groundwater conditions.

performance of fitted soil hydraulic functions by studying the overall hydrological consequences of these functions for a different irrigation regime than that was used during parameter optimisation.

3. Results and discussion

3.1. Sampling strategy

The time series of simulated ET_a/ET_p, E_a/E_p and T_a/T_p for cotton crop on the three soils (Table 1) under deep groundwater table condition is depicted in Fig. 2(a)–(c). The five peaks in the simulated ET fluxes are the result of specification of five irrigation events during the growing season. Although the same initial and boundary conditions were specified, the simulated ET_a, E_a and T_a behaviour for all the three soils is quite different except immediately after an irrigation event, when soil moisture conditions are sufficient to meet nearly potential demand. Note the ET_a, E_a and T_a behaviour after Day 100, particularly during the intervening period of different irrigation events, i.e. between Day 107–117 (irrigation being at Day 97 and 118) and Day 130–142 (irrigation being at Day 118 and 143). This suggests that during moisture

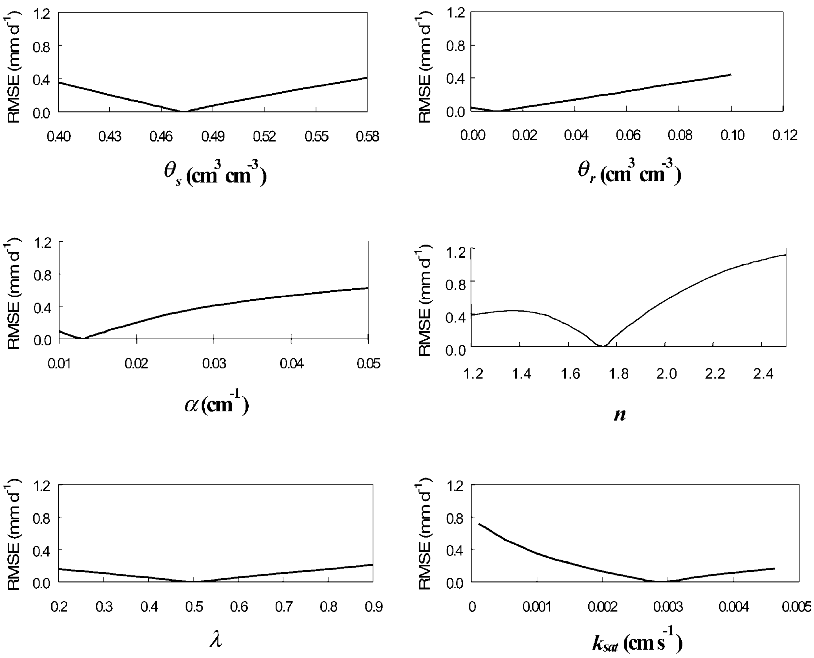

Fig. 3. The RMSE of the simulated transpiration as a function of the VG model parameters.

stress period, which is often encountered in the arid regions, these fluxes have the potential to be utilised for the inverse problem. However, E_a, like surface soil moisture, is usually controlled by only the top few cm's of soil. Any parameter estimated by utilising E_a alone would represent the soil hydraulic functions of only top few centimetres of the soil. Moreover, applicability of Eq. (1) for top few centimetres of soil is also questionable due to the effects of splashing rain, dry crust formation and cultivation practices on the soil hydraulic functions. Note the difference between ET_a (Fig. 2(a)) and T_a (Fig. 2(c)) behaviour for the period covering Day 143–160. During this period, it is difficult to identify soil type based on ET_a behaviour, but the T_a behaviour is quite different for the three soils. This suggests that the use of T_a fluxes may be more appropriate to identify soil hydraulic functions. The following conclusions regarding sampling strategy may be drawn at this stage. Either T_a fluxes are used for the inverse mode or crop period is selected in such a way that the ET_a component is mainly due to T_a, which happens when the crops are fully developed, i.e. fully covering the soil. Therefore, T_a and ET_a data for the present inverse problem (Eqs. (6) and (7)) are sampled from the period covering 100 days after sowing.

3.2. Sensitivity of T_a to VG model parameters

Having established that different soils act differently with respect to ET fluxes, the next logical step is to study the sensitivity of these fluxes to different parameters of the selected Eqs. (3) and (4) of soil hydraulic functions. Considering the problems associated with the simulation of E_a under actual field conditions, the sensitivity of simulated T_a to θ_r, θ_s, α, n, k_s and λ is studied by varying each parameter in turn. The root mean square error (RMSE) between the reference and modelled T_a for the selected sampling period (Day 100–160) is estimated to get an indication of T_a sensitivity to VG model parameters. The reference parameter set for this sensitivity analysis is that of loamy sand soil (Table 1). The range over which the parameters are varied is set considering the three soil types considered in the forward

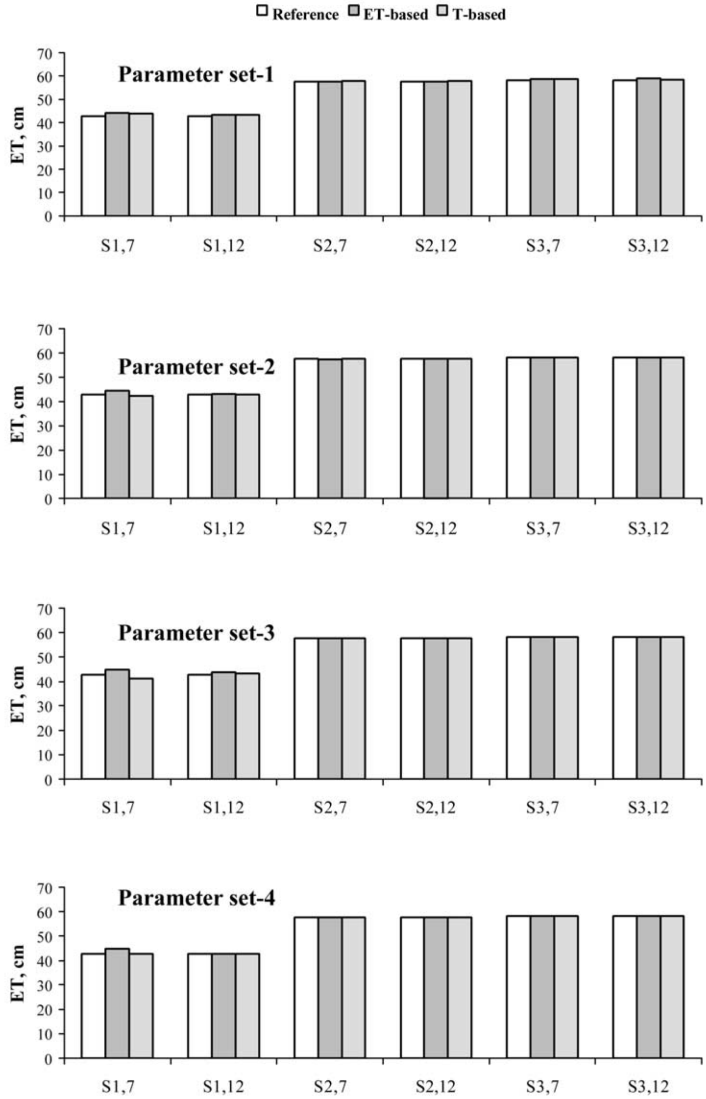

Fig. 4. Simulated *evapotranspiration* (ET) for reference, as well as inversely estimated soil hydraulic functions using ET- and *T*-based objective function for S1, S2 and S3 soils. For different parameter sets (1, 2, 3 and 4), see Table 1. The digits 7 and 12 indicates the number of observations.

simulations. The results of sensitivity of T_a to the VG model parameters is shown in Fig. 3. T_a is sensitive to all the VG model parameters with maximum sensitivity to parameter n and minimum to parameter λ. Fortunately, the parameter λ for most of the soils can be taken as 0.5 (Van Genuchten, 1980; see also Table 1). This sensitivity analysis indicates the possibility of estimation the VG model parameters using ET fluxes.

3.3. Estimation of soil hydraulic parameters

3.3.1. No error in ET_a

The adopted parameter estimation methodology was tested, using exact (forward simulated) ET_a and T_a observations. First, we used ET_a and T_a fluxes for seven selected days ($t = 115, 125, 130, 135, 140, 150, 159$) as input to the objective functions Eqs. (6) and (7). It was only possible to exactly fit parameter set-4

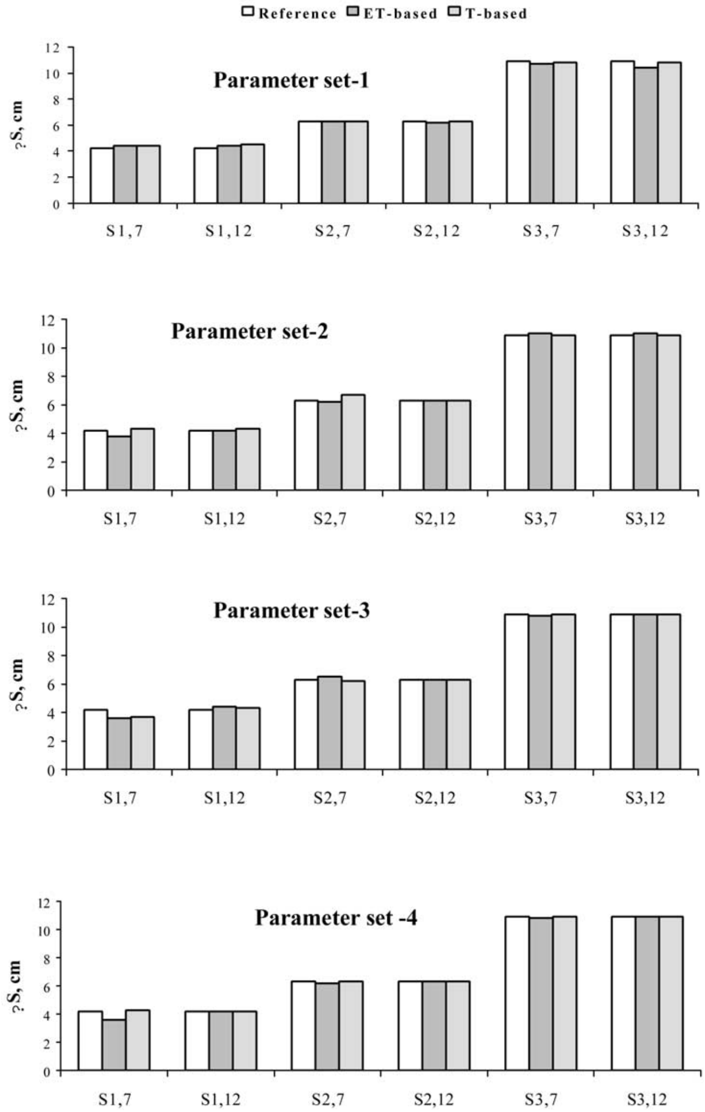

Fig. 5. Same as Fig. 4 but for *change in soil moisture storage* ΔS over 150 cm depth between days 1 and 160.

(see Table 2 for details about different parameter sets) for loamy sand and sandy clay loam soils, when T_a based objective function (Eq. (7)) was used. Next, we increased the number of observations to 12 by including five more ET_a and T_a fluxes for days $t = 100, 105, 110, 120$ and 145. With this increased frequency of observations, the parameters set-4 was fitted exactly for all the three soils, when either ET_a or T_a based objective functions were used. This increased frequency of observations could not exactly fit other parameter sets. However, the bias, defined as the difference between actual value and fitted value, for different VG model parameters got reduced with the increased number of observations in the objective function.

As outlined in Section 2.4, we do not intend to derive exact parameter values but rather to attempt to fit effective soil hydraulic functions capable of reproducing the hydrologic behaviour of soils. A verification numerical experiment, therefore, tested the

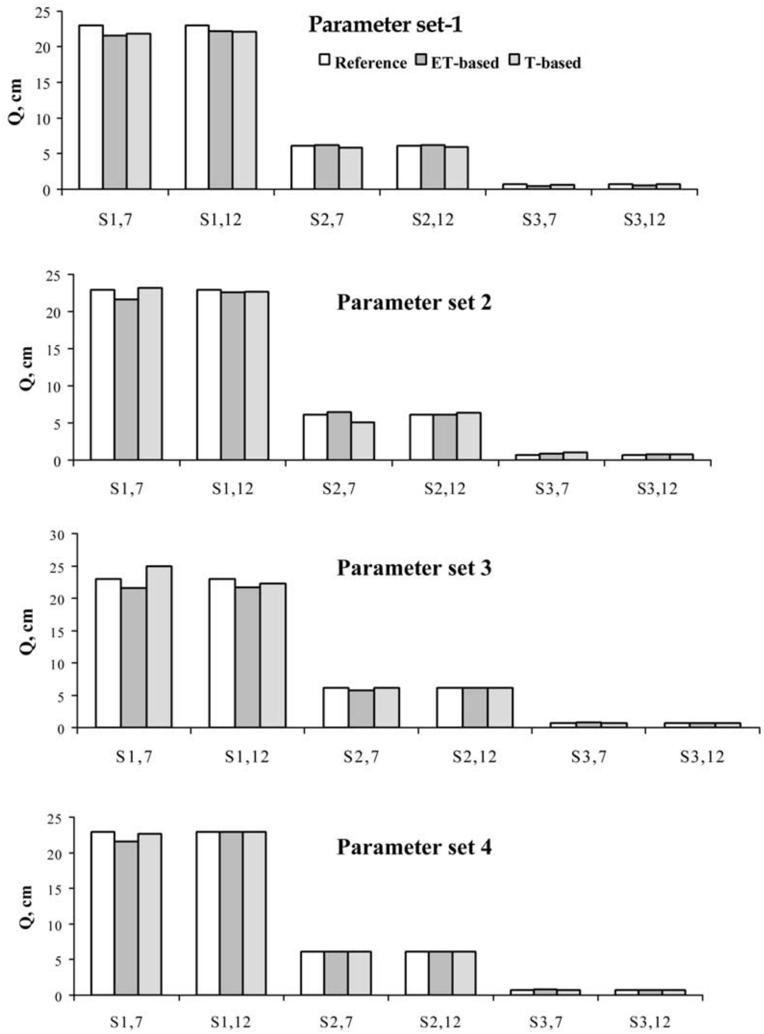

Fig. 6. Same as Fig. 4 but for simulated *deep percolation* (Q) at 150 cm depth.

hydrological behaviour of different fitted parameter sets through simulation of seasonal water balance of cotton crop. Care was taken to minimise any discrepancies, resulting due to initial conditions, in the simulated hydrological behaviour, particularly deep drainage. The initial profile condition specified for each verification experiment was such that for zero flux condition at the soil surface, the cumulative drainage past 150 cm depth was just negligible (= 0.009 cm) for a period of 160 days. Thereafter, simulations were performed for cotton crop by specifying 20 cm irrigation on Day 1 and 5 post sown irrigation each of 10 cm (instead of 6 cm during inverse optimisation). Seasonal simulated water balance components (ET, ΔS and Q) for the reference and fitted soil hydraulic functions are presented in Figs. 4–6. The figures show the effect of ET- or T-based objective function, frequency of observations and different parameter set on the hydrological behaviour of fitted soil hydraulic functions. Not much difference is observed in the simulated ET (Fig. 4) and ΔS (Fig. 5). However, considering simulated Q (Fig. 6), the T-based objective function performs better than ET-based objective function, particularly for soil S1,

Table 3
Correlation coefficients for different VG model parameters as affected by the number of observation

Parameter	α	n	θ_r	θ_s	k_s	λ
Number of observations = 7						
α	1.00					
n	7.7×10^{-14}	1.00				
θ_r	0.92	0.32	1.00			
θ_s	0.96	0.23	0.99	1.00		
k_s	0.94	0.26	0.99	0.99	1.00	
λ	0.95	0.24	0.99	0.99	0.99	1.00
Number of observations = 30						
α	1.00					
n	0.20	1.00				
θ_r	0.62	0.01	1.00			
θ_s	0.39	0.82	0.27	1.00		
k_s	0.27	0.17	0.34	0.11	1.00	
λ	0.75	0.21	0.42	0.27	0.26	1.00

when the number of input observations on ET fluxes are seven. When the number of observations are increased to 12, both the forms of objective function performs equivalently. This has very important implications: when the number of observations are sufficient, the total ET is sufficient to solve the inverse problem. This greatly simplifies the data collection for inverse modelling experiments from independent data sources. The frequency of observations have significant effect on the simulated hydrological behaviour of fitted soil hydraulic functions. When the frequency of observations is increased from 7 to 12, the simulated hydrological behaviour (ET, ΔS and Q) of fitted soil hydraulic functions tends to become closer to that of the reference set. This suggests the necessity of more frequent sampling of ET fluxes to inversely identify effective soil hydraulic functions. Among the different parameter sets, as defined in Table 2, the hydrologic behaviour of parameter set-4 is closest to the reference set. In fact, it is the only parameter set, which is fitted exactly. This means that if k_s and θ_r can be estimated independently, the ET fluxes are most suitable to derive rest of the VG model parameters (i.e. α, n and θ_s).

Encouraged by the favourable effects of increased number of observations, we further investigated the effect of more intensive sampling by including alternate day ET_a fluxes into the objective function. This sampling strategy resulted in 30 observations of ET_a fluxes for the period covering days 100–160. Now, the parameter set-1 was also fitted closely. Under ideal conditions such intense measurements may be available, for instance NOAA satellite scans earth daily. However, there may be constraints in realistic situations, such as cloud coverage. Therefore, in further analysis, we will deal only with the limited (i.e. 12) number of observations. But, we would like to share an important implication of frequency of sampling. Table 3 shows the correlation between different VG model parameters as affected by the frequency of observations. The correlation coefficients, which are unacceptably large, when seven observations are used, reduce considerably when number of observations are increased to 30. It is important to note that, if two or more parameters are simultaneously estimated then it is desirable that correlation between the optimised parameters should be small. This further stresses the need to have more observation on ET fluxes from independent measurements to inversely identify soil hydraulic functions.

Two conclusions can be drawn at this stage. When the number of independent observations on ET fluxes are sufficient, there is no significant effect of utilising T_a fluxes in the objective function meaning that ET fluxes are sufficient to solve proposed inverse problem. The increased frequency of observations improves the precision of parameter estimation and the hydrological behaviour of different parameter sets.

3.3.2. Effect of random error in ET_a fluxes

In reality, exact correspondence between model predictions and observed data never occur, partly due to simplifications inherent in the parametric model, as well as to the measurement errors (Kool et al., 1987). Further, errors in observations may make the inverse procedure ill posed (Hollenbeck and Jensen, 1998). We now consider the effect of random error in the input data (ET_a flux) on the fitted functions in order to show the accuracy required in the measurement/estimation of ET_a fluxes for the proposed parameter estimation procedure. We do it by adding different levels of random error in the no error ET_a fluxes. The ET_a fluxes with error, ET_{ae}, were calculated as

$$ET_{ae} = ET_a\{1 + n(0,1)p\} \quad (9)$$

where $n(0,1)$ represents a number drawn at random

Table 4
Statistical properties (mean, μ, bias, B and 99% CI) of estimated water balance components for different parameter sets fitted on perturbed ET_a data. Incorporation of random errors (re) of 10 and 20% to the no-error data set generated the perturbed data. The results are based on 10 generated data sets each having 12 data points

Parameter set	ET (cm)						ΔS (cm)						Q (cm)					
	10% re			20% re			10% re			20% re			10% re			20% re		
	μ	B	CI	μ	B	CI	μ	B	CI	μ	B	CI	μ	B	CI	μ	B	CI
S1																		
Reference	42.8	–	–	42.8	–	–	4.2	–	–	4.2	–	–	23.0	–	–	23.0	–	–
Set-1	43.6	0.8	1.0	43.2	0.4	2.2	4.4	0.2	0.1	4.4	0.2	0.1	22.0	1.0	1.0	22.5	0.5	2.3
Set-2	42.6	0.2	0.9	42.1	0.7	2.6	4.3	0.1	0.2	4.1	0.1	0.2	23.2	0.2	0.8	23.8	0.8	2.6
Set-3	43.2	0.4	1.0	43.1	0.3	2.9	4.3	0.1	0.1	4.1	0.1	0.2	22.5	0.5	1.1	22.8	0.2	3.0
Set-4	42.7	0.1	0.9	42.4	0.4	2.0	4.3	0.1	0.1	4.2	0.0	0.2	23.0	0.0	1.0	23.5	0.5	2.0
S2																		
Reference	57.6	–	–	57.6	–	–	6.3	–	–	6.3	–	–	6.1	–	–	6.1	–	–
Set-1	57.8	0.2	1.0	57.6	0.0	1.2	6.4	0.1	0.1	6.1	0.2	0.5	5.8	0.3	0.9	6.4	0.3	1.4
Set-2	57.9	0.3	1.0	58.1	0.5	0.8	6.3	0.0	0.1	6.1	0.2	0.2	5.9	0.2	1.0	5.9	0.3	0.8
Set-3	58.0	0.4	0.2	57.6	0.0	0.8	6.3	0.0	0.2	6.0	0.3	0.3	5.7	0.5	0.4	6.4	0.2	0.9
Set-4	57.9	0.3	0.4	58.0	0.4	0.6	6.2	0.1	0.1	6.1	0.2	0.2	5.9	0.2	0.5	5.9	0.2	0.5
S3																		
Reference	58.3	–	–	58.3	–	–	10.9	–	–	10.9	–	–	0.8	–	–	0.8	–	–
Set-1	56.8	1.5	2.8	56.6	1.7	3.0	8.6	2.3	2.3	10.0	0.9	2.6	4.7	3.9	4.1	3.4	2.6	3.3
Set-2	56.9	1.4	2.2	56.2	2.1	3.2	11.0	0.1	1.0	11.3	0.4	2.0	2.1	1.3	1.4	2.5	1.7	2.6
Set-3	56.9	1.4	2.4	56.4	1.9	2.8	10.6	0.3	1.2	10.9	0.0	2.1	2.6	1.8	1.8	2.7	2.0	2.6
Set-4	56.7	1.6	2.8	55.8	2.5	3.0	11.1	0.2	1.1	11.7	0.8	2.0	2.2	1.4	2.2	2.5	1.8	3.1

from a normally distributed population with a mean of 0 and a variance of 1. Random numbers greater than 1 and less than -1 were set equal to 1 and -1, respectively, to control error level. p represents relative error. To simulate measurement errors of 10 and 20%, we successively set p to 0.10 and 0.20, respectively. At each error level, we generated 10 series of ET_{ae} fluxes, each consisting of 12 data points, to incorporate any variation that might occur at a given error level. Thereafter, we repeated the inverse procedure for all the three soils. We studied two options for the assignment of weights w_i to different observations. First, we assigned equal weights ($w_i = 1.0$) to each observation. Another option tried was assignment of weight, w_i, inversely proportional to the magnitude of the observation (i.e. $w_i = 1/ET_{ae}$). Assignment of weight in this way implies that every observation have equal contribution to the objective function, irrespective of its magnitude. This is particularly important for erroneous data. The second option resulted into better results. The simulation results, with weight assigned inversely proportional to the magnitude of the observation, are discussed further.

For each of the four-parameter sets, the inverse problem is solved repetitively, each time with a different realisation of random measurement error incorporated into the exact ET fluxes. There were 10 repetitions of parameter inversion each for both the error levels. Each repetition yields a single realisation of parameter estimates. Hydrological behaviour of each of the fitted parameter set is then quantified as outlined in Section 3.3.1. The results are then used to evaluate the statistical properties of the simulated hydrological behaviour of fitted parameters by averaging different water balance components over all the 10 realisations of parameter estimates. The statistical properties for different water balance components are the bias B and 99% confidence interval (CI), which measure systematic and random error, respectively. The B of the kth water balance component is the absolute difference between the mean expected value of the component $E[x_k]$ and the true value of the component x_k.

$$B = |E[x_k] - x_k| \quad (10)$$

The 99% CI for estimate $E[x_k]$ is given by

$$\mathrm{CI} = t_{0.005}\frac{\mathrm{sd}(x_k)}{\sqrt{n}} \quad (11)$$

where $t_{0.005}$ is the value of t-distribution associated with the 0.005 probability level, $\mathrm{sd}(x_k)$ is the standard deviation of kth water balance component estimated by different ($= 10$) realisations and n is the number of random realisations.

The results of the statistical analysis are presented in Table 4. It is desirable that both B and the CI of the water balance components be small. The estimates of mean water balance components, bias and CI (Table 4) indicates that both the systematic and random error increases with increase in random error incorporated in ET fluxes. The results further indicate that the parameter set-4 is fitted most reliably with bias (<5%) and 99% CI (<10%) of different water balance components within acceptable limits. For soil S3, none of the four-fitted parameter set predicts acceptable water balance components, very high bias and 99% CI, particularly for ΔS and Q (Table 4). We speculate that this is due to the fact that soil S3 showed minimum drought stress to ET (Fig. 2) under prescribed irrigation regimes. It means that periods with prolonged and severe stress are the most suitable for selecting the satellite overpass dates, because the effect of VG model parameters is more pronounced under such situations. Further if the expected error in the ET fluxes is proportional to the magnitude of true value, as incorporated in this paper, then selection of severe drought stress periods means less absolute deviation in ET fluxes.

3.4. General discussion

We anticipate that the proposed inverse procedure may invite some criticism, particularly prior knowledge of sink term variable. Though it is beyond the scope of this paper to deal with this problem, we do suggest a simple framework to solve the same. The sink term variables (h_1–h_4) are crop dependent. For uniform cropping pattern, these can be derived locally from field or laboratory experiments or may be derived from available information. In case of mixed cropping patterns, the following strategy may be adopted. Kabat et al. (1997) have demonstrated that scaling techniques may be used to derive effective parameters. From satellite images, pixels representing similar vegetation cover may be grouped. Representative pixels from each group may be selected and effective parameters derived by scaling techniques. With known hydraulic functions for these pixels, ET fluxes may be used to inversely identify sink term variables. The sink term variables determined in this way may then be employed to derive effective hydraulic functions for other pixels belonging to the representative groups. In this way, much of the tedious and time consuming work involved in the conventional methods of determining soil hydraulic functions may be avoided.

In this study, we assigned similar initial guesses, independent of soil type, for different VG model parameters. When dealing with an actual system, however, two favourable situations may occur. A few measurements at representative sites may provide not only a better initial guess of θ_r, θ_s and k_s but more importantly, it may provide a narrower allowed range of these parameters as compared to those considered during this investigation. For example, θ_r was allowed change from 0.0 to 0.10, θ_s from 0.40 to 0.58 and k_s from 0.12 to 5.79×10^{-3} cm s^{-1}. Alternatively, the pedo-transfer function approach may be used for obtaining reasonable initial guess of the soil hydraulic parameters to initialise the optimisation procedure (Burke et al., 1998).

It must also be noted that during this study the ET was affected only by water stress, i.e. there was no effect of other stresses, such as salinity and pest/diseases. As such the present findings may not be applicable to situations, where other stresses are dominant, until and unless properly accounted for during backward simulations. Further studies are needed to test the present approach for spatially variable fields, but if the conclusions hold, a relatively simple method is available to parameterise soil variability at large scales.

The application of the proposed inverse modelling approach to estimate soil hydraulic functions requires that information on timing and amount of rainfall/irrigation is known. This is also a pre-requisite for the successful application of any simulation model to study appropriate water management strategies.

Thus, it does not demand additional data collection. The findings are applicable only to regions, where strong moisture depletion is experienced during the growing season (thereby making soil hydraulic characteristics an important factor affecting ET). This is often the case in arid and semi-arid regions having deep groundwater.

4. Conclusions

1. Provided the root water extraction function is known, ET fluxes can be used to inversely identify effective soil hydraulic functions for arid and semi-arid regions. The ET-based fitted functions are suitable to make simple water balance computations required for water management related decisions.
2. Simulated temporal ET fluxes for three soil types suggest that moisture stress period of fully developed crops is most appropriate for sampling ET fluxes to solve proposed inverse problem.
3. Under ideal conditions (no error in ET fluxes), when number of ET data are sufficient, it is possible to inversely identify all the parameters of VG model. However, when number of observations are limited, it is necessary to reduce the number of fitting parameters in order to obtain exact soil hydraulic functions.
4. Frequent measurement of ET fluxes is desired not only to precisely estimate soil hydraulic functions by the inverse technique, but also to reduce the undesirable correlation between different fitting parameters.
5. If the expected errors in the ET fluxes are proportional to the magnitude of the true value of ET fluxes, as incorporated in this paper, the weight assigned to the observations must be inversely proportional to the magnitude of ET fluxes.
6. Although the results described in this paper are promising, they are only applicable to a number of prevailing conditions, such as homogeneous soil and crop conditions, free drainage, moisture stress during growing season and root water extraction function known. There are many situations in arid and semi-arid regions, where the conditions of free drainage and severe moisture stress are often met. Nevertheless, the effect of other conditions, such as spatially variable field conditions still needs further investigation.

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