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INPUT DATA FOR AGROHYDROLOGICAL SIMULATION MODELS: SOME PARAMETER ESTIMATION TECHNIQUES

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ABSTRACT

The use of simulation models implies the need for model parameters, which are not always easy to assess. Therefore different parameter estimation techniques are discussed in this paper and their applications for determining the key-parameters affecting soil water and solute flow in the unsaturated zone are analysed. Although a number of well established direct methods to determine soil hydraulic parameters have found great utility, they have unfortunately a number of limitations for their applicability in the field. Contrary to these common direct methods, parameter estimation techniques do not put any constraints on the basic model nor its boundary conditions. The capabilities of parameter estimation techniques combined with the inverse problem are shown for the water retention and hydraulic conductivity function of a loamy sand.

Spatial variability of soil hydraulic properties can be described by scaling techniques. The combination of scaling and parameter estimation procedures makes it possible to arrive at stochastically representative soil hydraulic characteristics needed to feed simulation models on a regional scale.

The required accuracy of model parameters is a function of the type of application and the scale of the problem. When properly interpreted, sensitivity analysis as presented in this paper could help to establish criteria on the required accuracy of model parameters.

Parameter estimation techniques offer a solution when a gap between data requirements and data availability exists. As such they are regarded in this paper as a tool to ease the use of agrohydrological simulation models.

INTRODUCTION

During the last decade a number of complex simulation models describing the dynamics of the soil-water-plant-atmosphere system have been developed. Simulation models have become indispensible tools for quantifying soil physical, chemical and biological processes in the unsaturated and saturated zone.

Dynamic simulation models (Feddes et al., 1988) can be used to assess the effects of water management measures, such as drainage, irrigation and soil improvement on the terms of water balance of agricultural as well as nature conservation areas. The yield of a crop well supplied with nutrients can be directly related to its water use, i.e. to its transpiration. The combination of simulating water balance terms and a crop growth model offers the opportunity to evaluate long-term effects of alternative soil and water management practices on crop production and agricultural income. When transport of solutes in the unsaturated/saturated system is linked to water flow simulation, the long-term impact on pollution of groundwater reservoirs and on salinization of the soils can be studied.

Agrohydrological simulation models can also be applied to predict effects of future changes in the environment (e.g. increase of CO2 concentration in the atmosphere) on the land and water resources.

In quantitative land evaluation, use of deterministic agrohydrological simulation models is considered to be essential. Van Wijk and Feddes (1986) used a soil water/crop production simulation model to evaluate effects of drainage on timing of farming operations and on related crop yield on a daily basis. The procedure has been extended (Van Lanen and Bouma, 1988; Hack-ten Broeke et al., 1988; Hack-ten Broeke and Kabat, 1988) and used to evaluate soil-water related land qualities , i.e. soil moisture deficit, soil aeration and workability using detailed site-specific data.

Reliable application of simulation modelling requires a large number of model parameters to be quantified. The accuracy of simulation depends on the accuracy of parameters appearing in the model. Model parameters usually have the form of a functional relationship between one or more variables. These functions are often not unique (for example: hysteresis of the soil water retention curve) and need to be specified a priori. In this paper the discussion is restricted to the main parameters affecting one-dimensional vertical water flow and solute transport in the unsaturated zone: the soil water retention curve (pF-curve) and hydraulic conductivity function. These parameters should be preferably determined from field-experiments. Because of the limitations of direct methods (discussed later in this paper), especially indirect methods to estimate these soil characteristics are the key-topics of the paper.

When using one-dimensional models on a regional scale, scaling as an alternative approach to deal with spatial variability of soil hydraulic properties can be used (Hopmans, 1987). In this study different combinations of indirect methods and parameter estimation techniques with scaling, to arrive at statistically representative sets of soil physical properties, are proposed.

Finally, a few examples of simple sensitivity analysis interpreted in terms of land qualities are presented. We also include a short comment on the required accuracy of the soil hydraulic parameters in terms of applications to the land evaluation studies.

BASIC RELATIONS

The one-dimensional transport of water and solutes in the unsaturated zone can be generally described by the following two equations:

$$\frac{\delta h}{\delta t} = \frac{1}{C(h)} \frac{\delta}{\delta z} \left[K(h) \left(\frac{\delta h}{\delta z} + 1\right)\right] - \frac{S}{C(h)} \qquad (1)$$

$$\frac{\delta \rho s}{\delta t} + \frac{\delta \Theta c_r}{\delta t} = \frac{\delta}{\delta z} \left(\Theta D \frac{\delta c_r}{\delta z} - q c_r\right) - \Theta \mu c_r + \Theta \gamma \qquad (2)$$

In equation 1 (for transient soil water flow) t is time, z is vertical coordinate (positive upwards), $K(h)$ is the hydraulic conductivity as a function of the soil water pressure head h, $C(h)$ is the soil water capacity, being the slope $d\Theta/dh$ of the soil water retention curve $\Theta(h)$, where Θ is the volumetric soil water content and S is the sink term describing water uptake by the plant roots. In equation 2 c_r is the resident solution concentration, s is the adsorbed concentration, ρ is the dry soil bulk density, D is a dispersion coefficient, q is the Darcian flux, μ is a first order degradation coefficient and γ is a production coefficient.

In the most general simulation model of water and solute transport in the soil, equation 1 is solved along with equation 2. This implies that parameters involved in the equation 1 directly influence the solution of equation 2. Hence, the pF-curve and K(h) function have a key role in the entire model.

DIRECT METHODS TO ESTIMATE SOIL HYDRAULIC PARAMETERS

Whereas direct measurements of pF-curve do not usually represent a major problem, the common direct methods to estimate unsaturated hydraulic conductivity are still extremely difficult to implement and remain costly and time consuming. Most of these methods are based on so-called direct solution of the inverse problem in the laboratory or field conditions (Green et al., 1986). Recent developments in direct methods are also given by Klute and Dirksen (1986). Well established direct field methods are for instance the instantaneous profile method, different unit-gradient type methods, sorptivity methods and the crust method. For a review see Van Genuchten et al. (1988).

The direct methods are based on the direct solution of Darcy's equation or on different approximations and simplifications of equation 1, which is then inverted and simplified in such a way, that K can be expressed in terms of directly measurable variables. This procedure is often called the direct inverse problem. There is a principal difference between the direct inverse problem and the inverse problem combined with parameter estimation techniques together with optimization techniques. In practice these approaches are still often mixed up.

Although a number of well established direct methods have found great utility in the studies of unsaturated flow and transport processes, they have unfortunately a number of limitations which restrict their applicability. In some direct procedures it is necessary to periodically achieve steady-state or hydraulic equilibrium for different boundary conditions. The need to impose even relatively simple initial and boundary conditions (saturated soil profile, free drainage) represents a problem especially for field experiments. Furthermore direct inversion techniques do not readily provide information about statistical value of the estimated parameters.

INDIRECT METHODS TO OBTAIN SOIL HYDRAULIC PARAMETERS

Difficulties in obtaining reliable data on unsaturated hydraulic conductivity have been often regarded as a major obstacle when using deterministic simulation models. Consequently the same problem arises often in the context of quantitative land evaluation. An outcome could be the so-called indirect methods. These methods predict the soil hydraulic properties from more easily measured data, i.e. from soil water retention data, soil texture or other soil properties. The most recent approach to predict soil hydraulic parameters is based on the solution of the inverse problem by parameter estimation techniques combined with optimization procedures (Kool et al., 1987; Kabat et al., 1989).

Predicting the K(h) function from soil water retention data

The soil water retention data are more easily measured than hydraulic conductivity data. Methods for predicting the hydraulic conductivity function from soil water retention data are usually based on statistical pore size distribution models (Mualem, 1986). The most frequently applied predictive conductivity models are from Mualem and Burdine (Van Genuchten et al., 1988). Van Genuchten (1980) combined Mualem's model with an empirical S-shaped curve for the soil water retention function to derive a closed-form analytical expression for the unsaturated hydraulic conductivity curve.

The empirical Van Genuchten equation for the soil water retention curve reads:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m} \qquad \begin{matrix} (\theta_r \le \theta \le \theta_s) \\ m = 1 - 1/n \end{matrix} \qquad (3)$$

where θ_r and θ_s are the residual and saturated water contents respectively; α, n and m are parameters determining the shape of the pF-curve. The residual water content is the soil water content where the pressure head becomes indefinitely small. In practice, θ_r is the water content corresponding to some large negative value of soil water pressure head. The parameter n determines the steepness of the curve while α is approximately the inverse of the pressure head at the inflection point (Wösten and van Genuchten, 1988).

After combination of equation 3 with the Mualem's model, the final Van Genuchten analytical function describing the unsaturated hydraulic conductivity in terms of soil water pressure head is written as:

$$K(h) = K_s \frac{[(1 + |\alpha h|^n)^m - |\alpha h|^{n-1}]^2}{(1 + |\alpha h|^n)^{m(l+2)}} \qquad (4)$$

K_s is the saturated hydraulic conductivity and should be either measured (i.e. in case of "pure" prediction of the K(h) from pF-curve) or can be treated as an additional unknown in case of simultaneous fitting procedures. Although Mualem (1976) concluded that l should on the average equal 0.5, it is apparently a soil-specific parameter and it is recommended to treat l as an additional unknown. Hence, the Van Genuchten model in its most general form contains a total of 6 unknown parameters: θ_r,θ_s,α,n,l and K_s. Computer software has been developed (Van Genuchten, 1986, unpublished) to fit simultaneously the analytical functions of the model to some observed (measured) θ(h)- and K(h)-data. The same program allows to predict K(h)-data from observed pF-curves. Kabat and Neefjes (1988) extended the mentioned program and developed a PC user-friendly package with different possibilities to fit and to predict retention and conductivity data.

For calibration of the deterministic simulation models, it is essential to have an idea how the parameters in the Van Genuchten model affect the actual shape of the soil water retention curve and unsaturated hydraulic conductivity curve. As an example, the sensitivity analysis reported by Wösten and van Genuchten (1988) is reproduced in Figure 1 and 2. In these figures the relative hydraulic conductivity is defined as K/K_s. The different combinations of model parameters involved in the sensitivity analysis are given in Table 1.

TABLE 1 Parameters of the Van Genuchten model used in the sensitivity analysis as presented in Figure 1 and 2.

Figure	θ_s	θ_r	α	n	l
1a	0.5	0.1	0.005	1.5,2.5,3.5,4.5	0.5
1b	0.5	0.1	0.005,0.015, 0.025,0.035	2.5	0.5
2a	0.5	0,0.1, 0.2,0.3	0.005	2.5	0.5
2b	0.5	0.1	0.005	2.5	0.5,-2.0,2.0

Predictive models for K(h) based on soil water retention data perform reasonably well for most coarse and many medium textured soils, but for fine textured soils the results are usually less satisfactory.

The Van Genuchten model is valid for monotonic wetting or drying only. Kool and Parker (1987) extended the model for hysteresis in pF-curves and K(h) functions, adding only one parameter.

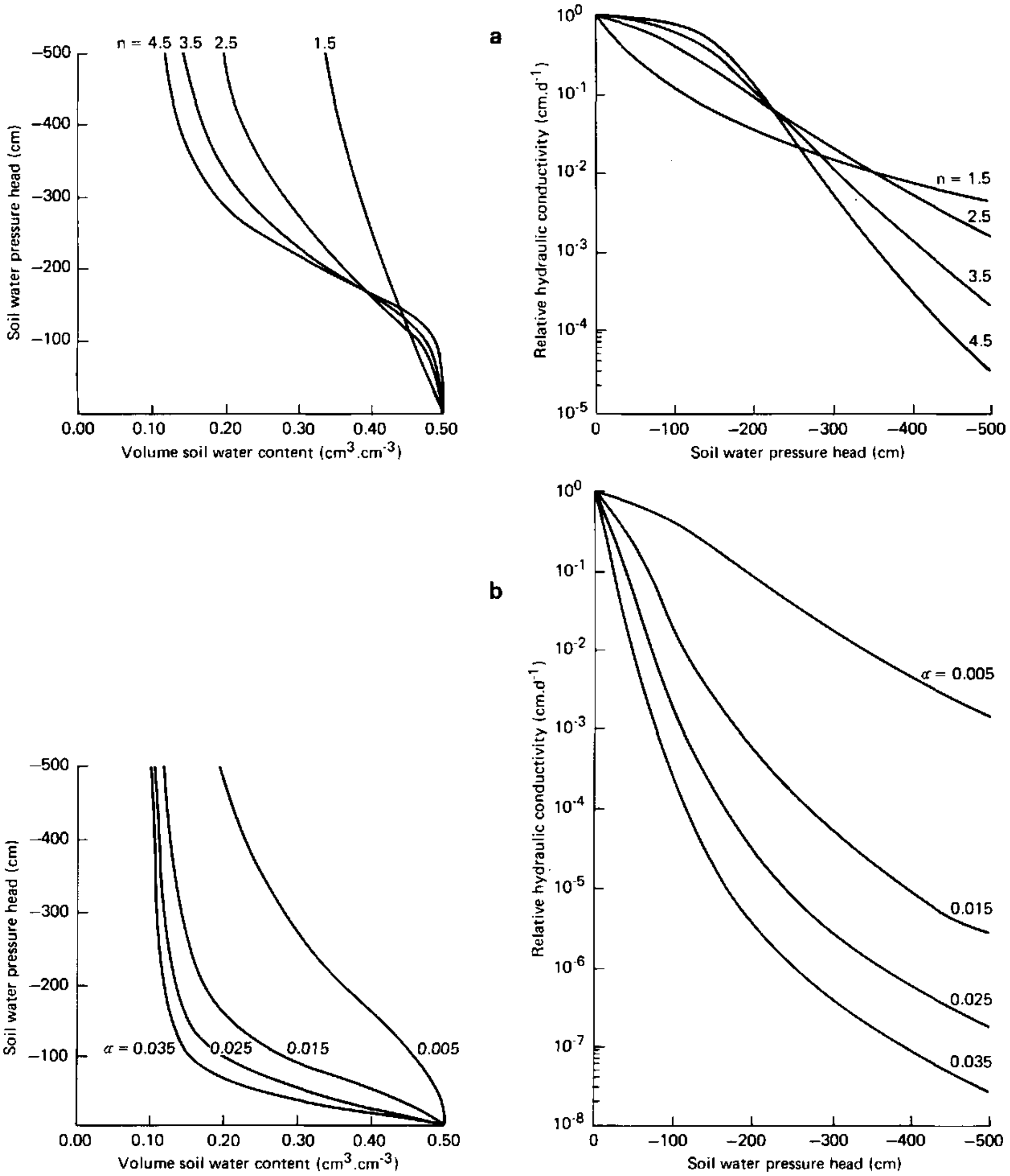

Fig. 1 Effect of the parameters *n* and α (a and b respectively) of the Van Genuchten model on the predicted water retention and relative hydraulic conductivity functions (after Wösten and Van Genuchten, 1988).

Predicting the K(h) function from soil texture and some additional soil properties

These methods, for example pedotransfer functions (Bouma and van Lanen, 1987), are based on statistical correlations between soil hydraulic properties and particle size distribution and other soil data, such as organic matter content, bulk density, clay mineralogy and cation exchange capacity (Bloemen, 1980; De Jong, 1982; Haverkamp and Parlange, 1986; Vereecken et al., 1988).

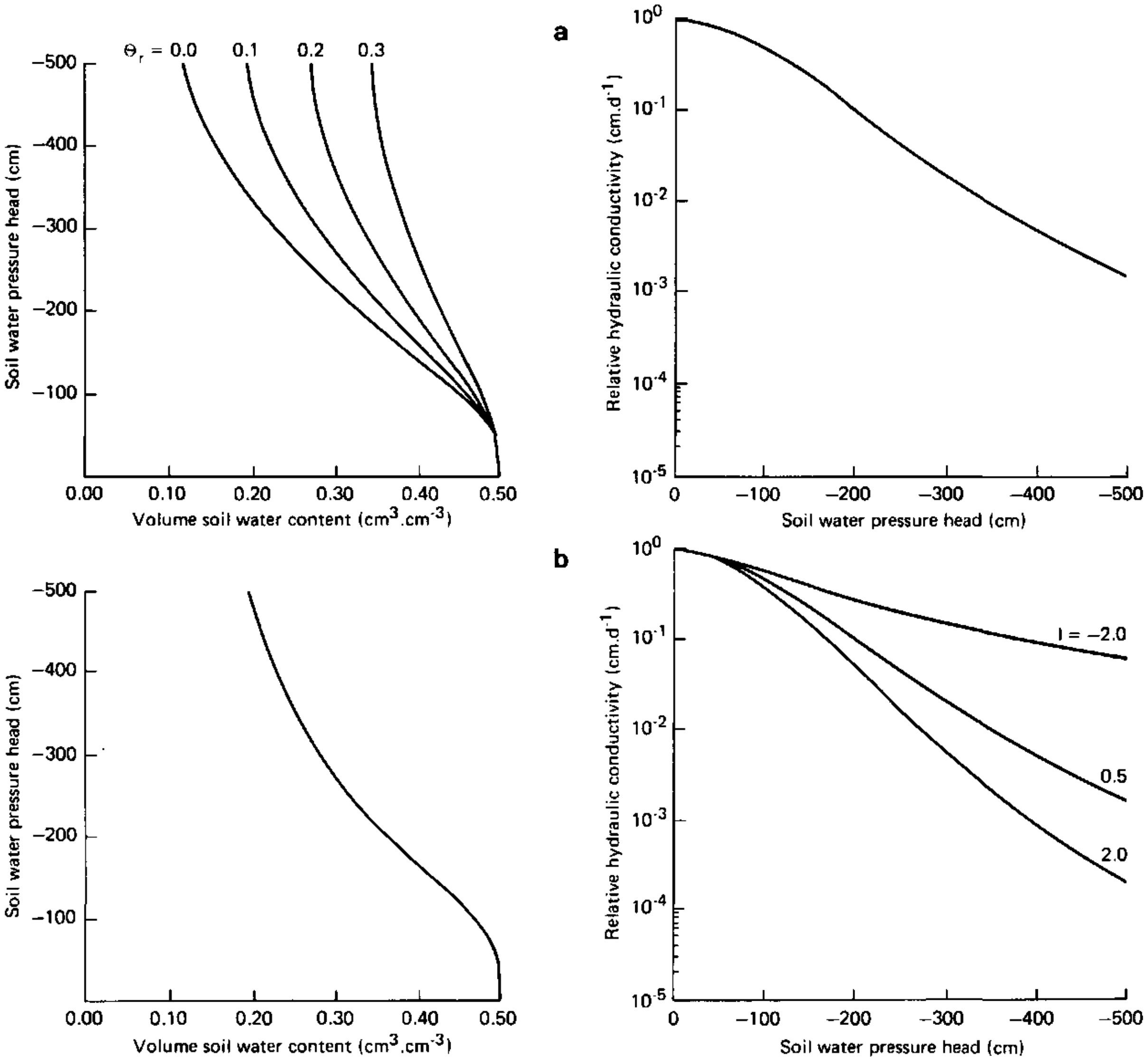

Fig. 2 Effect of the parameters θ_r and *l* (a and b respectively) of the Van Genuchten model on the predicted water retention and relative hydraulic conductivity functions (after Wösten and Van Genuchten, 1988).

Wösten et al. (1987a) classified water retention and hydraulic conductivity characteristics of representative Dutch soils according to their texture and some additional properties. K(h) and Θ(h) functions, selected from this classification can be obtained by the earlier mentioned package (Kabat and Neefjes, 1988) either in the table-form or in the form of fitted parameters of the Van Genuchten model.

The Van Genuchten model can be fitted simultaneously to observed water retention and hydraulic conductivity data and then the fitted parameters can be used in a multiple regression analysis to investigate relationships between these parameters and soil bulk density, texture and organic matter content (Wösten and van Genuchten, 1988; Vereecken et al., 1988). Established regression functions can then be used to predict soil hydraulic parameters from basic soil properties.

Inverse problem combined with optimization techniques to estimate water retention and hydraulic conductivity functions

In this approach the direct flow problem may be formulated for any set of initial and boundary conditions and solved with any analytical or numerical method. Input data to be measured for the method are water contents and/or pressure head profiles in time. Certain constitutive functions for the hydraulic properties are assumed (Van Genuchten, 1980) and then the parameters in those functions are estimated by using an optimization procedure to minimize an objective function (e.g. the sum of the square deviations between observed and calculated pressure heads, water contents etc.). This method can be applied in both laboratory and field conditions. A disadvantage of the laboratory procedure is that we cannot explore the full potential of this method, due to the always limited size of the soil sample. Moreover, collection of soil samples always introduces some disturbance that may affect flow properties. Thus, application of the method in-situ seems to be more appropriate.

To demonstrate the capacities of the method, data were used from the experiment described by Kool et al. (1987) and by Abeele (1984) to estimate soil water retention and hydraulic conductivity functions of a loamy sand. Though we have principally followed the steps of the inverse problem for the same data set (Kool et al., 1987), differences between the procedures lie in the total number of measured data used (we were restricted to only published data) and in the way of solving the direct problem (equation 1). While Kool et al. (1987) used a finite element Galerkin type of simulation model, we applied the transient finite difference simulation model SWACROP (Wesseling et al., 1988). Parameters of the Van Genuchten functions can be given directly as input for the SWACROP model. Nodal spacing of 1 cm was used along with a convergence criterion within a variable time step, so a high numerical accuracy could be achieved.

The in-situ experiment (Abeele, 1984) involved drainage from a lysimeter (diameter: 3 m, depth: 6 m) filled with a loamy sand. The soil profile had been initially saturated and the surface was covered during the entire drainage period (zero flux condition). The volumetric water contents θ and pressure heads h were measured at 6 depths during the drainage period of 100 days. Pressure heads measured at the bottom of the considered profile provided the lower boundary conditions.

The constitutive functions used were those of Van Genuchten with a vector of unknown parameters $b = [\alpha, n, \theta_r, K_s]$. The remaining two parameters θ_s and l were assumed to be known and values 0.331 and 0.5 respectively (Kool et al., 1987) were assigned to them.

The optimization problem, that minimizes the objective function $O(b)$, is formulated as a weighted least-squares problem:

$$O(b) = \sum_{i=1}^{5} \sum_{j=1}^{6} [\theta'_{ij} - \theta_{ij}(b)]^2 + \sum_{j=1}^{6} W [h'_j - h_j(b)]^2 \qquad (5)$$

where θ'_{ij} represents measured water content at depth i and time j, h'_j is the measured soil water pressure head at time j at the constant depth of 1.16 m, $\theta_{ij}(b)$ and $h_j(b)$ are calculated water content and pressure heads obtained with the model SWACROP. Weighing factor W was chosen according to Parker et al. (1985) to equal 0.16.

The result of the predictions are presented in Figure 3, where estimated pF- and K(h)-curves are compared with independently determined functions as reported by Abeele (1984). Furthermore, the estimated curves are merely duplicates of those estimated by Kool et al. (1987). Since the accuracy and frequency of measurements in the lysimeter were similar to common field situation, these results clearly illustrate the potentials of this method to determine in-situ soil hydraulic properties. The only special restriction in this aspect was covering of the soil surface to

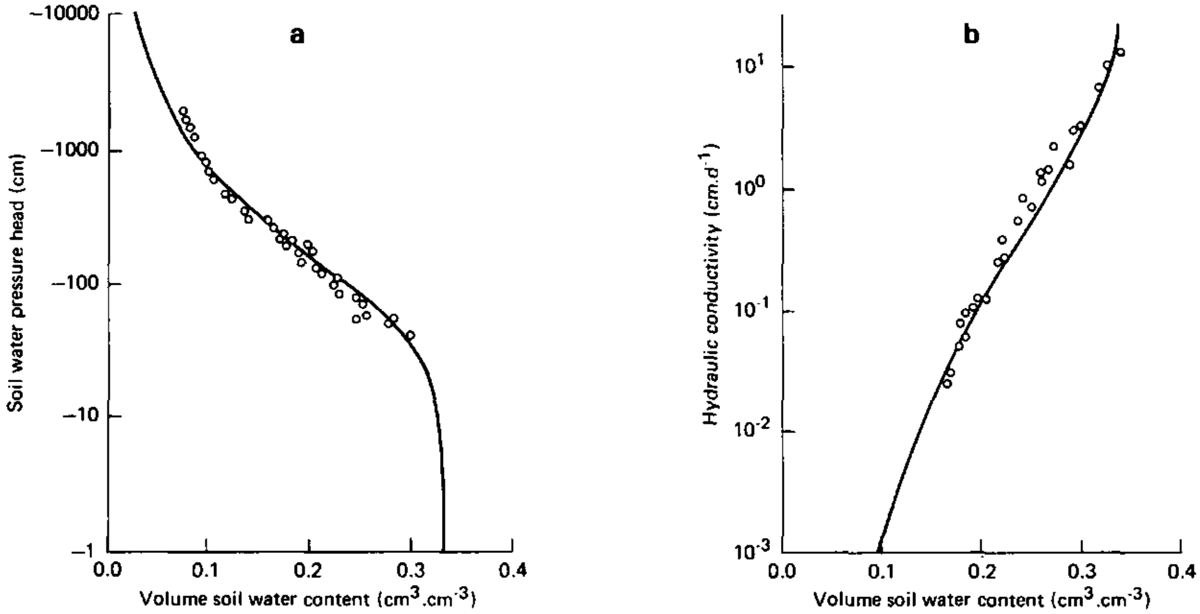

Fig. 3 Water retention curve (a) and hydraulic conductivity curve (b) estimated by the inverse problem combined with optimalization techniques (solid lines) as compared with measured curves (points).

assure a zero flux condition. However, the actual evaporation flux can be measured nowadays with reliable techniques as for instance the Bowen ratio energy balance method. An alternative solution could be recording moisture content near the soil surface and use it as the prescribed upper boundary condition.

The inverse problem combined with optimization is receiving gradually more and more attention. The newest variation of the methodology is represented by simplified Kalman filtering techniques (Karvonen, 1988; Kabat et al., 1989).

USING SCALING IN ESTIMATION OF SOIL HYDRAULIC PARAMETERS

The purpose of scaling (Hopmans, 1987) is to simplify the description of spatial variation of soil hydraulic properties. By this simplification, the pattern of spatial variability is described by a set of scale factors α_r which relate the soil hydraulic properties at each location r to a representative mean (m):

$$h_r = h_m/\alpha_r \tag{6}$$

$$K_r = K_m \alpha_r^2 \tag{7}$$

These equations are valid for all h_r and K_r measured at different water contents (concept of similar media). To cope with the variable soil porosity h and K are expressed as a function of degree of saturation Θ/Θ_s rather than Θ. Using different scaling techniques (Hopmans, 1987) one can determine a reference (representative) mean of soil water retention and hydraulic conductivity curves (see Figure 4).

The combination of scaling with indirect techniques to estimate soil physical parameters represents one of the challenges of future investigations. In the following section we elaborate on some possibilities.

a) Soil water retention data of all the locations r considered could be collected. Then, the Van Genuchten analytical model can be fitted for each water retention data set at location r. Obtained pF-curves can be scaled and using Van Genuchten parameters of the scaled soil water retention function, representative soil hydraulic conductivity can be predicted.

b) Soil water retention data could be collected for only a limited number of profiles. Regression between these data (or coefficients of fitted functions) and easy to measure soil properties (Wösten and van Genuchten, 1988) can be established. The regression models can be used to predict $\Theta(h)$-data at all the remaining sampling locations. In the following step the set of pF-curves could be scaled and K(h) functions predicted.

c) Scaling procedures could be combined with the optimization problem. In such a case reference $\Theta(h)$ and K(h) functions could be directly estimated by optimization. An easier way would be to use a known distribution function of the scale factors to "process" the estimated pF- and K(h)-curves in a stochastic way (Hopmans, 1987).

The above mentioned set of possibilities is by no means exhaustive and several variations on these combinations are to be anticipated. Although it is still difficult to apply these combined methods, they could

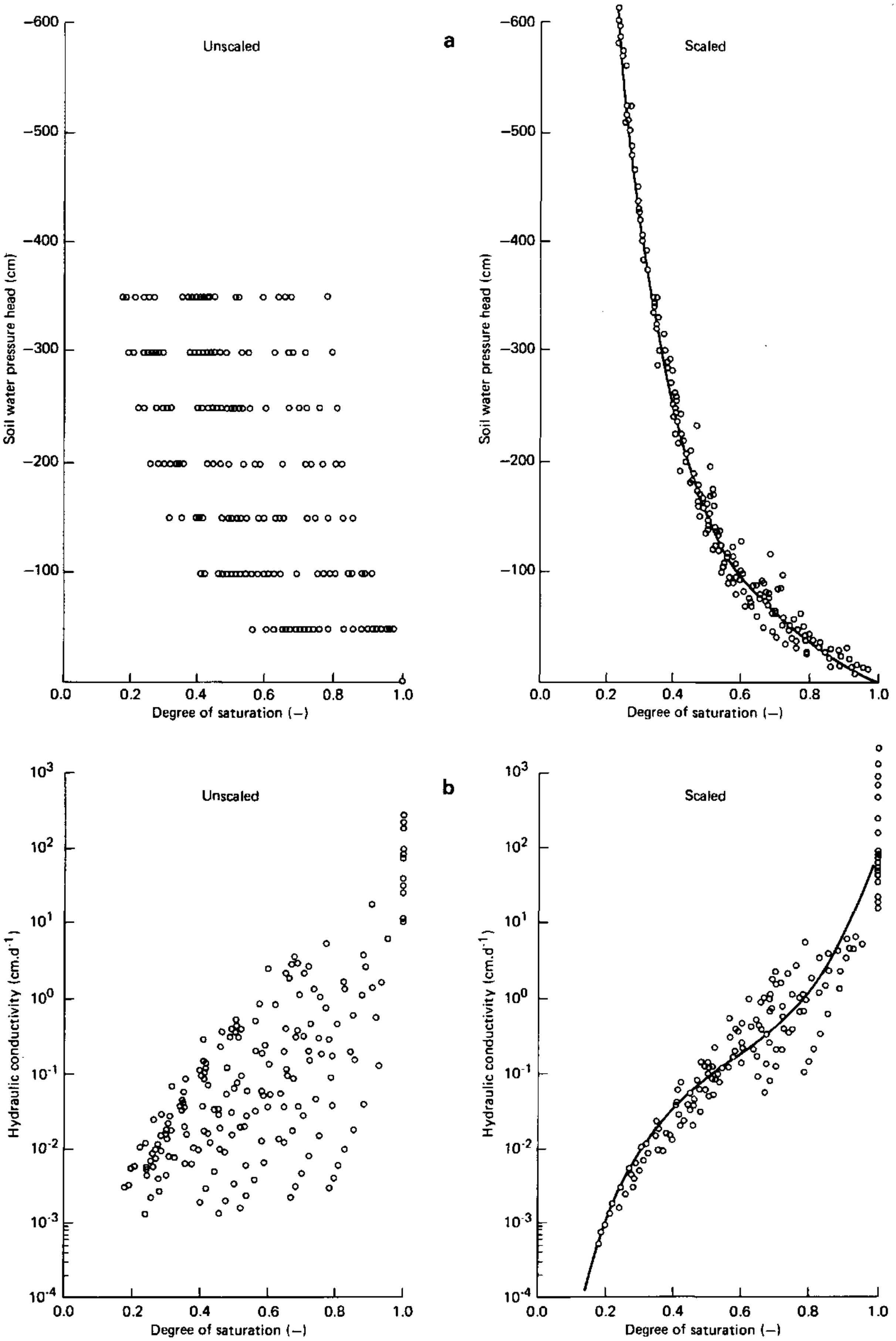

Fig. 4 Unscaled and scaled water retention (a) and hydraulic conductivity data (b) (after Hopmans, 1987).

lead to statistically and spatially representative soil hydraulic parameters needed to feed simulation models.

REQUIRED ACCURACY OF SOIL PHYSICAL PARAMETERS FOR SIMULATION MODELS

The reliability of simulation results depends on the accuracy of parameters appearing in the model. Firstly, the required accuracy should be relevant to the type of application and type of problem to be solved (Wösten et al., 1987b). It is a function of the scale of the problem. When dealing with site-specific studies, a high accuracy of the parameters is requested.

As an example how to use sensitivity analysis to get an idea about the needed accuracy, we used the same simulation concept as Hack-ten Broeke and Kabat (1988) to investigate the sensitivity to the soil hydraulic parameters. Data collected for a maize crop over 1985 and 1986 were used. After calibration of the model with the independently measured pF- and hydraulic conductivity curves (dashed line in Figure 5), two new sets of the curves were generated using slightly varying parameters of the Van Genuchten model. A noise was introduced to the generated curves so that they resembled the real curves with the irregularities introduced by the measuring techniques. Then the model was run with the generated parameters. Some of the results are presented in Figure 5 and are interpreted in terms of water-related land qualities. Simulated pressure heads at 5 cm depth are the measure for workability and trafficability (Hack-ten Broeke et al., 1988). From simulated pressure heads for both years it can be concluded that mainly for the wet periods (h > -100 cm) the deviations are minor. Moreover, all three pressure head curves show almost the same trend.

The difference between actual crop transpiration and potential transpiration (not shown in the figure) characterizes the land quality soil moisture deficit. Analyzing the curves of actual cumulative transpiration only small differences were found. Finally the cumulative actual dry matter production curves (in fact an integrated land quality) are plotted in Figure 5. Again, differences between the curves are acceptable. For the wet year of 1985 there is even no difference at all between the curves.

Wösten and van Genuchten (1988) presented a sensitivity study comparing the accuracy of predicted and measured hydraulic functions in

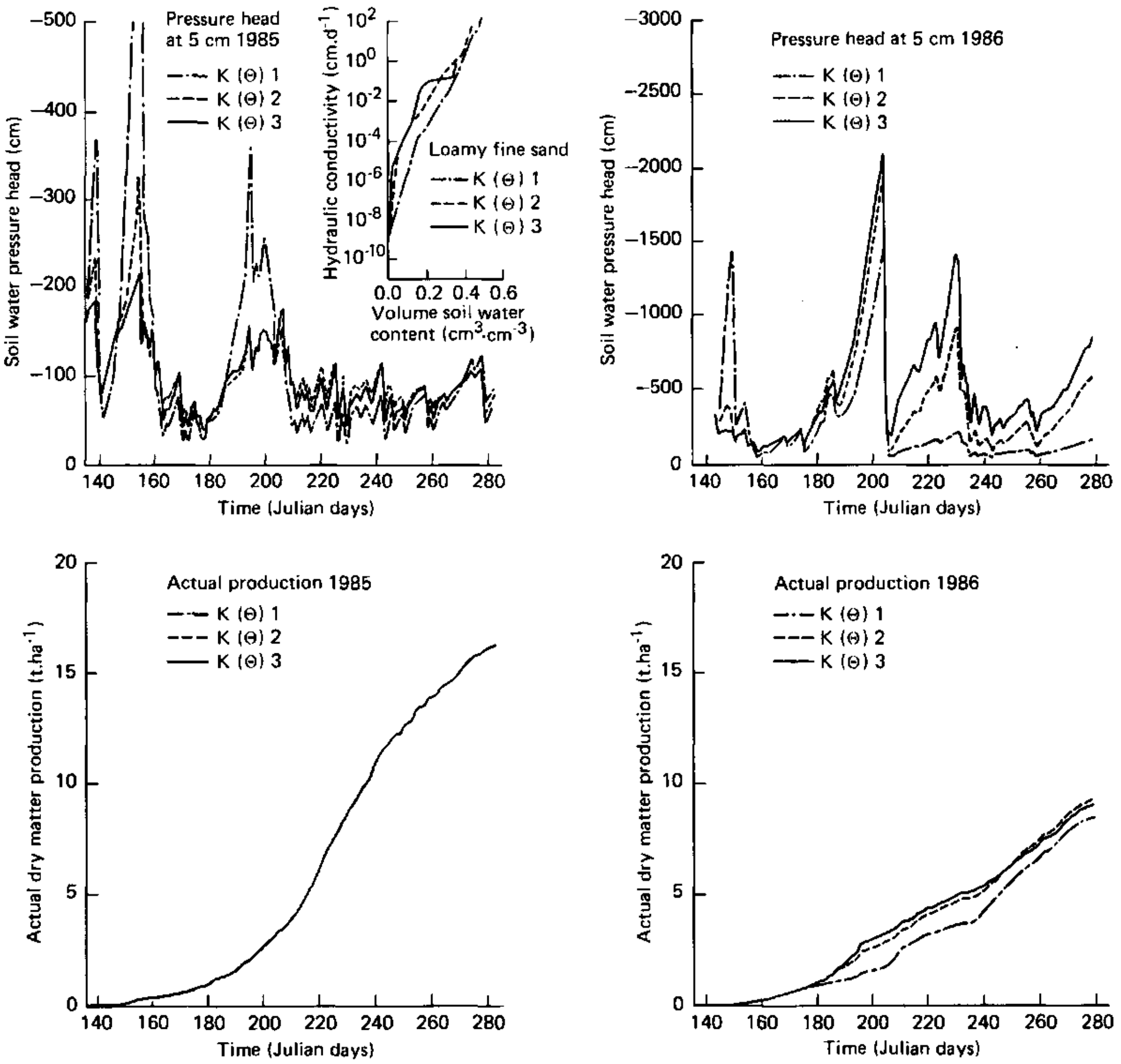

Fig. 5 Sensitivity of the model SWACROP to the soil hydraulic parameters interpreted in terms of simulated soil water pressure heads at 5 cm depth and actual dry matter production.

terms of functional criteria typical for several applications, i.e. travel time through the unsaturated zone, depth of the water-table sustaining a given rate of capillary rise and downward flux. The predicted conductivity functions were obtained with the Van Genuchten equation using parameter values correlated with soil texture and some additional soil properties. They concluded that the predictive regression models can be used to estimate soil hydraulic functions when working on scales 1:50 000 or smaller.

There are many ways to test the model sensitivity and to interpret model outputs using stochastic methods. Mainly for the regional problems the stochastic treatment of the model input as well as stochastic presentation of the results is important and should receive more attention.

CONCLUSIONS

Application of agrohydrological simulation models requires quantification of model parameters. Soil hydraulic characteristics, as the key-parameters for the simulation models of soil water balance and solute transport, can be estimated using standard direct methods. However, these methods have restrictions in their applicability. Since field measurements always give more relevant information, a number of indirect methods have been discussed in this paper as an attempt to show their capabilities to estimate in-situ soil hydraulic parameters. It is shown that the inverse problem combined with mathematical optimization techniques can give a good estimate of soil water retention and hydraulic conductivity curves. On a regional scale, estimation of model parameters must be concerned with the spatial variability. The easiest way to deal with this phenomenon at this moment is scaling, which can be combined with parameter estimation procedures to get stochastically representative soil hydraulic parameters for one-dimensional simulation models.

Required accuracy of soil hydraulic parameters to feed models depends on the type of application and on the scale of the problem to be solved. Sensitivity analysis must be interpreted in terms of applications. For instance, the results presented in Figure 5 show how the sensitivity to soil hydraulic parameters can decrase when more integrated land qualities are considered.

Different parameter estimation procedures along with application directed sensitivity analysis makes the application of deterministic models on regional scale more feasible.

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