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# Using inverse methods for estimating soil hydraulic properties from field data as an alternative to direct methods

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## Abstract

Water and solute transport in the vadose zone greatly depends on the physical and chemical properties of the soil, which generally exhibit high variability. Additionally, the experimental determination of those properties in the field or laboratory is tedious, time-consuming and involves considerable uncertainty for most practical applications. Recently, inverse modeling has been introduced to estimate effective properties in situ by deducing them from, e.g. a measured time series of soil water content. Inverse methods combine forward soil water flow models with appropriate optimization algorithms to find the best parameter set that minimizes an objective function. Global optimization methods are suitable for locating a global optimum for a given set of conditions (number of parameters, boundary conditions, etc.). In this paper we estimate the soil hydraulic properties of a sprinkler fertigated banana plot in the North of Tenerife (Canary Islands) in a direct and inverse way. For the inverse method, use was made of the measured time series of soil water content at three different depths. The forward model is the numerical solution of the Richards equation as implemented in the agro-environmental model WAVE. Two inverse methods are compared: the traditional “trial and error” method and an inverse method using a global search algorithm referred to as the global multilevel coordinate search combined sequentially with the Nelder–Mead simplex algorithm (GMCS–NMS). The global search is shown to be a relatively efficient procedure for estimating the soil hydraulic properties from measured soil water contents in

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the banana plantation. However, some ill-posedness problems are identified which should be solved by upgrading the quality of the experimental programs in irrigated banana plantations.

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## 1. Introduction

The degradation of groundwater resources in the Canary Islands as a result of agricultural activities suggests the need to design strategies to reduce and control the environmental impact of agriculture. Bananas are the most important crop cultivated in the Archipelago and represent an extreme situation of intensive agriculture. Mean nitrate concentration values of groundwater found in the main agricultural valleys range between 9 and 11 mg/l N-NO<sub>3</sub> (40–50 mg/l NO<sub>3</sub>) and in some areas, exceeding 25 mg/l (110 mg/l NO<sub>3</sub>) (DGA-SPH, 1993).

In this context, numerical, physically based models for water and solute transport are useful tools for analyzing nitrogen leaching as a consequence of fertilizer practices. However, the use of such models is not an easy task, since they contain a large number of parameters that must be identified before the model can be applied to the considered specific situation. The success of predictions and associated uncertainties strongly depends on the identification of the parameters, which is clearly the most critical step in the modeling process.

Some of these parameters can be measured directly in the laboratory or in situ. However, parameters determined from laboratory experiments might not be representative of field conditions. Furthermore, direct methods for the determination of soil hydraulic parameters require the experiments to reach several stages of steady-state conditions and restrictive initial and boundary conditions as well (van Dam et al., 1990). To overcome these problems indirect methods such as inverse modeling can be used to identify the basic flow and transport parameters. This procedure has the advantage that the results are based on a variable, which is observed at a larger time-scale and under natural boundary conditions.

A popular inverse method is manual calibration by a “trial and error” procedure of a soil water and flow model by comparing simulated values of a state variable (e.g. soil water content) with those experimentally measured. From a scientific point of view, the latter is a tricky method that should not be applied by a model user. The main drawbacks of this method are that it is time-consuming and, when several parameters are involved, it is difficult to judge in which direction these should be modified. It is also quite subjective, as the modeler does not know when to stop the calibration process. Finally, the uncertainty on the obtained parameters cannot be quantified in a rigorous way. Consequently, the “trial and error” calibration method cannot ensure that the best parameter set is found.

A more elaborated inverse method combines the numerical model with an algorithm for parameter estimation (e.g. Simunek et al., 1999). Basically, the process searches for the best set of parameters in an iterative way, by varying the parameters and comparing the real response of the system measured during an experiment with the numerical solution given

by the model. Indeed, the search should consist of finding the global minimum of an objective function defined by the error between measured and simulated values. The algorithm minimizes the objective function following its own particular strategy, e.g. by a gradient-based search. Within this framework, many different optimization algorithms have been developed to numerically solve inverse problems. Among others, we may consider the steepest descent method, Newton's method, Gauss method, Levenberg–Marquardt method, Simplex method, global optimization techniques, etc. (Hopmans and Simunek, 1999). Each of these methods has its own advantages and drawbacks, and the success of finding the global minimum depends generally on the presence of multiple local minima in the objective function. Recently Huyer and Neumaier (1999) have developed a global optimization algorithm (multilevel coordinate search) that combines global search and local search capabilities with a multilevel approach that enhances the convergence to the smallest objective function value. In a soil physics context, Lambot et al. (2002) used the global multilevel coordinate search (GMCS) algorithm combined sequentially with the classical Nelder–Mead Simplex algorithm (Nelder and Mead, 1965) to determine subsurface hydraulic properties from a continuously observed soil water content time series obtained from a numerical one-dimensional infiltration-redistribution experiment. The efficiency of the algorithm in finding the global minimum of the objective function depends on the number of parameters to be optimized, the objective function topology, the parameterization of the algorithm, etc.

The success of an inverse parameter determination depends on how well the problem can be posed. Three aspects generally characterize the posedness: identifiability, stability and uniqueness. If more than one parameter set leads to the same model response, the parameters are unidentifiable. Instability means that small errors in the measured variable or in some fixed parameters may result in large changes of the optimized estimated parameters. In contrast to identifiability, uniqueness refers to the inverse relationship; if a given response leads to more than one set of parameters, the inverse solution is non-unique (Russo et al., 1991; Hopmans and Simunek, 1999). The posedness of an inverse method depends on the soil under investigation, the type and range of boundary conditions used, the model structure, and the magnitude of the measurement errors of the input data (Russo et al., 1991; Durner et al., 1999).

The optimization techniques mentioned above are widely used in the context of fundamental soil physics research mostly limited to the estimation of soil hydraulic parameters for uniform soils on small, undisturbed soil columns (see, e.g. Hopmans and Simunek, 1999; Zou et al., 2001). However, they may be considered as powerful engineering tools as they can be applied on field experimental data sets to derive parameters of the system under consideration. The first application of inverse modeling to field data was reported by Dane and Hruska (1983), who optimized van Genuchten's function parameters from drainage data.

In this framework, our study presents a comparison of the performance of two indirect methods for identifying the hydraulic parameters of a stratified soil profile of a banana plot: the traditional “trial and error” method and the inverse modeling method by using the multilevel coordinate search global optimization method. For this purpose the numerical model WAVE (Vanclouster et al., 1996) was used to simulate water fluxes in the stratified soil profile in a sprinkler fertigated banana plantation.

The main objectives of the study can be defined as follows:

- (1) To perform a thorough sensitivity analysis to identify the most sensible parameters on which the optimization will be focused. Indeed, it is well known that the efficiency of parameter calibration can clearly be enhanced if the efforts are concentrated on those parameters to which the model simulation results are most sensitive (Beven, 2001).
- (2) To compare the optimized parameter sets of the two above-discussed indirect methodologies and compare them with directly obtained parameter values.
- (3) To investigate the impact of the calibration methodology on the simulated water fluxes that leave the soil profile.

## 2. Materials and methods

### 2.1. Field experimental setup

The experiment was conducted in a 4800 m<sup>2</sup> banana field plot selected within an intensive agricultural area, the valley of Valle de Guerra, in the north of Tenerife (Canary Islands). The valley is enclosed by the Anaga Mountain on its NE side and is open to the Atlantic Ocean on its NW exposure, ending in a cliff 70 m high. Mean annual temperature in this area is 20 °C (minimum of 15 °C in winter), and annual precipitation and crop potential evapotranspiration are around 380 and 1000 mm, respectively. The experimental plot was chosen inside a 42 ha banana plantation (Las Cuevas) owned and operated by a private company. It was selected to represent the average conditions of the area (fertilization and cultural practices) at the time. The plantation, located on a fairly steep ground in the lower part of the valley, is terraced all the way down to the edge of the cliff 70 m above sea level.

The bananas (*Musa acuminata*, cv “Dwarf Cavendish”) were grown in the open air and at a plant density of about 1800 plants/ha. The field was irrigated weekly with a sprinkler fertigation system.

As common practice in the Canary Islands, due to the steep slopes of the landscape, crops grow on “sorribas”, i.e. terraces built across the steep slopes with rock retaining walls, filled with soils imported from the high mountain areas where changes in humidity and temperature have allowed weathering of the volcanic material producing well developed soil. The experimental plot, on a “sorriba” built over 50 years ago, showed an averaged soil depth of 60 cm, with a range of 50–70 cm, below which a net contact with the fractured basaltic rock was found. The soil profile exhibits three different soil horizons (0–20, 20–50 and 50–70 cm). Further details are described elsewhere (Muñoz-Carpena et al., 2002).

Soil water content was measured at six locations uniformly distributed within the field with covered double waveguides TDR probes. At each location, TDR probes were installed at three different depths, 15, 30 and 60 cm, each corresponding to approximately the middle of the three above-mentioned horizons. Between 26 July 1995 and 30 September 1996, soil water content readings were taken on 286 dates resulting in a data set of more than 5000 measurements. A TDR calibration was performed using a packed soil column (∅: 16 cm × 20 cm), that was stepwise dried after saturation. During each

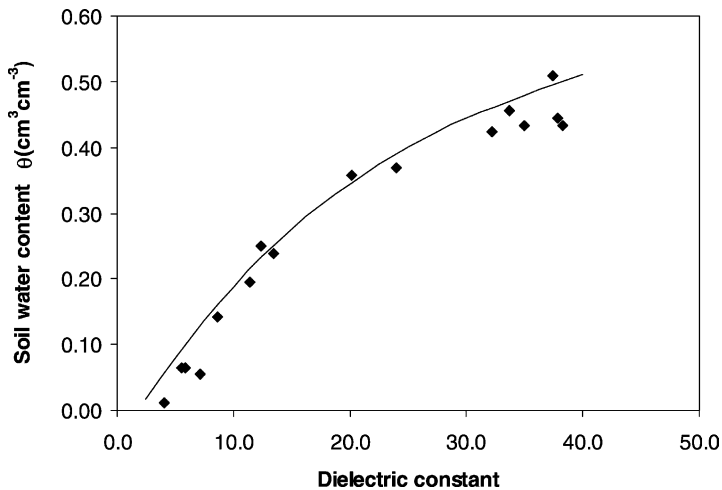


Fig. 1. TDR calibration curve for the considered volcanic soil. Measured data (symbols) and Topp's equation (line).

step, weight and TDR measurements were taken. The relation between the dielectric constant and the soil water content (Fig. 1) followed the commonly used Topp's equation (Topp et al., 1980). Irrigation amounts were measured at the six locations with ground level rain gauges. Six different locations were chosen to account for spatial variability of both soil water content and irrigation, but in the following analyses, we only use the average values for the six locations, considered as representative for the whole experimental field. An automatic weather station was installed on-site (Muñoz-Carpena et al., 1996) to estimate reference evapotranspiration for the crop at intervals of 15 min (1 min data average).

## 2.2. Model description

Developed at the Institute for Land and Water Management of the K.U. Leuven (Belgium), the WAVE model (water and agrochemicals in soil, crop and vadose environment) is a numerical, deterministic model for simulation of the vertical transport of energy (heat) and mass (water, non-reactive solutes, nitrogen species and pesticides) in the soil–plant–atmosphere continuum. It can be applied to soil laboratory columns, field lysimeters and to the field scale if transport is mainly vertical and if effective (1D) parameters are used.

The WAVE model (Vanclouster et al., 1996) integrates several models developed earlier: SWATRE (Belmans et al., 1983), SWATNIT (Vereecken et al., 1990, 1991), the universal crop growth model SUCROS (Van Keulen et al., 1982; Spitters et al., 1988) and subroutines for heat and nitrogen transport based on the LEACHN model (Wagenet and Hutson, 1989). The WAVE model is structured in five modules for determining, respectively, water transport, solute transport, heat balance, nitrogen transformations and crop growth. In this study, only the water transport module was used.

Water transport is modeled by solving a one-dimensional, isothermal Darcian flow equation in a variably, saturated, rigid porous medium, expressed by the following form of Richards equation:

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left[ \frac{\partial h}{\partial z} + 1 \right] \right] - \Gamma(z, h) \quad (1)$$

where  $C(h)$  is the soil water content capacity [ $L^{-1}$ ] equal to the slope of the soil moisture retention curve;  $z$  the vertical distance from the soil surface [L];  $t$  the time [T];  $K(h)$  the soil hydraulic conductivity function [ $LT^{-1}$ ];  $h$  the matric pressure head [L] and  $\Gamma(z, h)$  is the sink term describing water uptake by plant roots. The latter accounts for root water uptake reduction due to water stress and is based on a factor, which reduces linearly the maximal root water uptake ( $S_{\max}$  [ $L^3L^{-3}T^{-1}$ ]) according to four critical matric pressure head:  $h_0$ ,  $h_1$ ,  $h_2$ , and  $h_3$  [L]. Under conditions wetter than  $h_0$ , water uptake ceases due to lack of oxygen in the root zone; below  $h_3$ , it stops due to drought stress, while between  $h_1$  and  $h_2$  water uptake is optimal and  $S_{\max}$  is not reduced. Furthermore, the threshold matric pressure head below which water uptake decreases, depends on whether the atmospheric demand is low or high ( $h_{2l}$  and  $h_{2h}$ , respectively). On the other hand, the atmospheric demand is estimated by splitting the potential crop evapotranspiration into potential transpiration and evaporation using the leaf area index (LAI) as division parameter (Vanclouster et al., 1996).

The soil water retention function is given by (van Genuchten, 1980):

$$Se(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = [1 + \alpha|h|^n]^{-m} \quad (2)$$

where  $Se$  is the effective saturation;  $\theta(h)$  the soil water content [ $L^3L^{-3}$ ] at matric pressure head  $h$ ;  $\theta_s$  and  $\theta_r$  are the saturated and residual soil water content [ $L^3L^{-3}$ ], respectively;  $\alpha$  is the inverse of the air entry value of  $h$  [ $L^{-1}$ ];  $m$  and  $n$  are curve shape parameters. The former characterizes the asymmetry and is assumed to be  $m = 1 - 1/n$ , while the latter is related to the slope of the curve (van Genuchten, 1980).

The hydraulic conductivity can be described in WAVE with several model equations. In this study, the following expression for the unsaturated hydraulic conductivity function was chosen. It results when combining Eq. (2) with the pore-size distribution model of Mualem (1976):

$$K(Se) = K_s Se^\lambda [1 - (1 - Se^{-m})^m]^2 \quad (3)$$

where  $K(Se)$  and  $K_s$  are the unsaturated and saturated hydraulic conductivity [ $LT^{-1}$ ], respectively and  $\lambda$  is the pore connectivity parameter, which accounts for tortuosity and correlation between pore sizes (Durner et al., 1999).

In the vertical direction, the model considers the existence of heterogeneity in the form of horizons or layers within the soil profile. These layers are subdivided in space intervals called soil compartments. Halfway in each soil compartment, a node is identified for which the state variables are calculated using finite difference techniques, space implicit and time explicit.

To model less dynamic processes (crop growth) a fixed daily time step is used, while for strongly dynamic processes, such as water, solute and heat transport and solute transformations, a smaller variable time step can be chosen to limit mass balance errors induced by

solving the flow equation. The model inputs are given on a daily basis and outputs can be obtained at daily intervals or higher (e.g. Muñoz-Carpena et al., 2001).

### 2.3. Direct estimation of model parameters

Concerning the high number of parameters required by the model, although there was the possibility to obtain them from the literature, it was decided to measure as many of them as possible. Thus, the effort spent on parameter determination was hoped to be regained in terms of minimal calibration work. Model inputs and parameters used in this work and also the methodology applied for their determination is described in Muñoz-Carpena et al. (1999a,b). Hydraulic properties were determined on undisturbed USDA 7.62 cm soil cores using Tempe cells and laboratory constant head permeameters (Klute, 1986). The undisturbed samples were taken at the six different locations and the three above-mentioned depths. Thus, average values for each depth were used. The soil moisture retention curves were then fitted (Table 1) to van Genuchten's water retention model (van Genuchten, 1980), which is available in WAVE. Table 1 shows also the saturated hydraulic values obtained with the constant head permeameters, and Mualem's pore connectivity parameter ( $\lambda$ ), which can be assumed equal to the most commonly accepted value of 0.5 (Mualem, 1976). The maximum root water uptake rate ( $S_{\max}$ ) was considered constant within the root zone and was fixed at  $0.023 \text{ cm}^3 \text{ cm}^{-3} \text{ day}^{-1}$  (Vancloster et al., 1996). In addition, the matric pressure head values, which characterize the root water uptake for bananas, were obtained from Simunek et al. (1998). The leaf area index (*LAI*) function and the crop coefficients ( $K_c$ ) were taken from (Muñoz-Carpena et al., 1999a,b). The yearly evolution of both parameters,  $K_c$  and *LAI* is presented in Fig. 2, where linear interpolation between values is considered.

### 2.4. Sensitivity analysis

Model parameter estimation is an arduous task, which can be done efficiently if the parameters most influencing the model response are previously identified. For this purpose, a sensitivity analysis provides information about the sensitivity of the model to its parameters, i.e. it indicates those parameters whose variation has large effects on the model outputs. This analysis is usually based on coefficients, which express the proportion of variation ( $\partial q/\partial b_j$ ) in a model output variable ( $q$ ) relative to an infinitesimal change in a particular parameter ( $b_j$ ). According to Yeh (1986), sensitivity coefficients can be calculated with the "influence method" (finite differences). In an attempt to optimize van Genuchten's

Table 1  
Hydraulic parameters selected for the sensitivity analysis

Depth (cm)	van Genuchten parameters					
	$\theta_s$ ( $\text{cm}^3/\text{cm}^3$ )	$\theta_r$ ( $\text{cm}^3/\text{cm}^3$ )	$\alpha$ ( $\text{cm}^{-1}$ )	$n$	$K_s$ (cm/day)	$\lambda$
15	0.549	0.322	0.278	1.377	311	0.5
30	0.520	0.315	0.220	1.406	201	0.5
60	0.495	0.250	0.189	1.292	199	0.5

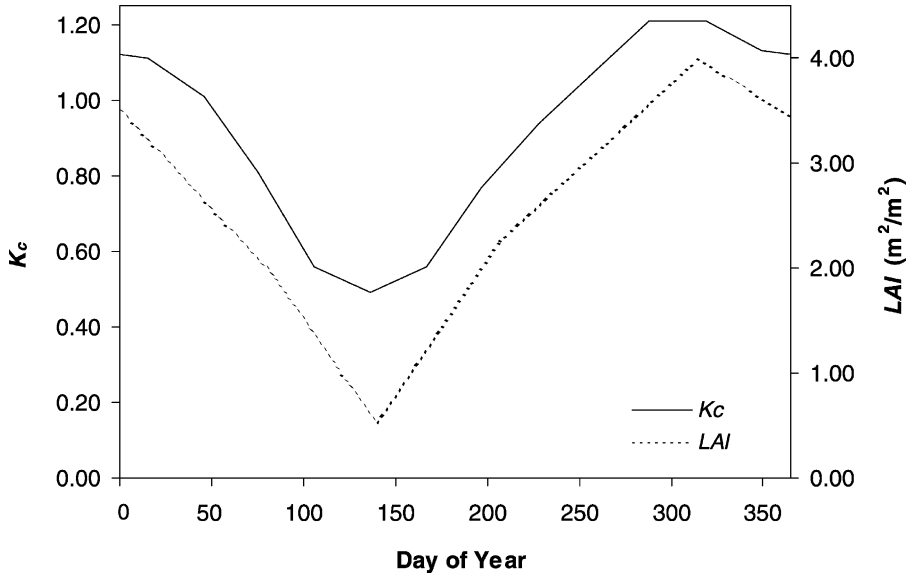


Fig. 2.  $K_c$  and LAI functions used in the simulations.

hydraulic parameters from actual evapotranspiration and actual transpiration, [Jhorar et al. \(2002\)](#) used the root mean square error between reference and modeled values of cumulative actual transpiration as a sensitivity estimator. Furthermore, they varied the parameters over a particular range. However, as a common practice, the “influence method” is used and only a 1% parameter change is considered ([Simunek and van Genuchten, 1996](#)).

The final aim of the modeling analysis is to obtain good predictions of the flux at the bottom of the soil profile as this strongly influences the mass of nitrogen leaving the soil profile. Unfortunately, the flux at the bottom was not measured and time series of soil water content were the only available data for the model calibration. Hence, we performed two different sensitivity analyses. The first was carried out to check the sensitivity of soil water content to change in a range of soil and plant parameters. The selection of the soil and plant parameters was based on previous global sensitivity analysis done with the model (e.g. [Diels, 1994](#); [Vanclouster et al., 1995](#)). This analysis was done to identify the most sensitive parameters on which the calibration process should be focused. The second one was performed to check the sensitivity of the flux at the bottom of the soil profile, as it is ultimately the predictive variable of interest.

Sensitivity coefficients for soil water content were formulated with the “influence method” following [Simunek and van Genuchten \(1996\)](#). These coefficients were normalized according to [Simunek et al. \(1999\)](#) to allow for comparison of sensitivities between different parameters, independent of their magnitudes (see [Eq. \(4\)](#)):

$$\begin{aligned}
 SC_{\theta}(z, t, b_j) &= \Delta b_j \frac{\partial \theta(z, t, b_j)}{\partial b_j} \approx \left| 0.1 b_j \frac{\theta(\mathbf{b} + \Delta \mathbf{b} \cdot \mathbf{e}_j) - \theta(\mathbf{b})}{1.1 b_j - b_j} \right| \\
 &= |\theta(\mathbf{b} + \Delta \mathbf{b} \cdot \mathbf{e}_j) - \theta(\mathbf{b})|
 \end{aligned} \tag{4}$$



where  $SC_{\theta}(z, t, b_j)$  represents the soil water content change at time  $t$  and depth  $z$  due to a variation of the parameter  $b_j$ . The magnitude of variation was set here to 10% ( $\Delta \mathbf{b} \cdot \mathbf{e}_j = 0.10b_j$ ) to avoid possible disturbances associated to the numerical solving process used for the simulation. Thereby,  $\mathbf{b}$  is the parameter vector, while  $\mathbf{e}_j$  is the  $j$ th unit vector.

Table 1 shows the hydraulic parameters selected for the sensitivity analysis, while some of the crop parameters are presented in Fig. 2. The hydraulic parameters considered include saturated and residual soil water contents ( $\theta_s$  and  $\theta_r$ ), inverse of the air entry value of the matric pressure head ( $\alpha$ ), van Genuchten's shape parameter  $n$ , Mualem's pore connectivity parameter ( $\lambda$ ) and saturated hydraulic conductivity ( $K_s$ ). As described before, the van Genuchten parameter values were estimated by fitting matric pressure head versus soil water content data obtained with Tempe cells. The crop parameters chosen were leaf area index ( $LAI$ ), crop coefficient ( $K_c$ ) and maximum root water uptake rate ( $S_{max}$ ).

The sensitivity coefficients of each parameter were calculated for the whole simulation period (432 days) and for the three different depths at which soil water content was measured (15, 30 and 60 cm). Variation of hydraulic parameters was considered independently layer by layer. To compare the sensitivity coefficients among parameters, time-average coefficients were calculated according to the following expression (Inoue et al., 1998):

$$SC_{\theta}(z, b_j) = \frac{1}{t_{end} - t_0} \int_{t_0}^{t_{end}} SC_{\theta}(z, t, b_j) dt \quad (5)$$

with  $t_0 > t > t_{end}$ .

In a similar way as in Eq. (4), the formulation of the sensitivity coefficients for the cumulative flux at the bottom of the soil profile will lead to:

$$SC_F(b_j) = |F(\mathbf{b} + \Delta \mathbf{b} \cdot \mathbf{e}_j) - F(\mathbf{b})| \quad (6)$$

where  $SC_F(b_j)$  is the accumulated bottom flux change corresponding to a variation of the parameter  $b_j$  of the parameter set  $\mathbf{b}(\Delta \mathbf{b} \cdot \mathbf{e}_j = 0.10b_j)$ .

## 2.5. Indirect parameter estimation

The calibration process was performed with only one part of the available data set in order to leave the rest for model validation. The period between 1 October 1995 and 31 March 1996 was selected for the calibration as this period seems to contain useful information and explores a large range of soil water content conditions.

### 2.5.1. The "trial and error" procedure

The strategy used consisted of performing a first simulation run with the parameter sets obtained from direct measurements (Table 1 and Fig. 2). The modeled soil water contents were then compared with the measured ones. Then we tuned progressively some parameters selected for calibration according to the sensitivity analysis, until an adequate fit was achieved. The goodness of the fit was based on the calculated root mean square error (RMSE) and the visual inspection of the time series of measured and simulated soil water contents. The simulated flux at the bottom of the profile was also considered.

### 2.5.2. The inverse modeling procedure

This technique consisted of calibrating selected parameters using an iterative process of three basic steps: (i) parameter perturbation; (ii) forward modeling; and (iii) objective function evaluations. For the third step the error between the forward simulation results and field measurements is considered as objective function. The optimal parameter set is the one, which produces the minimum objective function. To minimize the objective function, the forward model was combined with a global optimization algorithm. In this study the global multilevel coordinate search, GMCS, algorithm was used. The latter combines a global minimum search and local minima search with a multilevel approach (Huyer and Neumaier, 1999). Basically, using the GMCS, the parameter search space is split into smaller “boxes”. Each box is characterized by its midpoint, whose function value is known. A box can be split into smaller ones. As a rough measure of the numbers of times a box has been split, a level is assigned to each box. The fact that the algorithm starts with the boxes at the lowest levels (i.e. less split) constitutes the global part of the algorithm. The local part of the algorithm is characterized by the fact that at each level the box with the lowest function value is selected. The GMCS is a good alternative to other optimization algorithms: initial values of the parameters to be optimized are not needed and it is very robust, because it can deal with discontinuous nonlinear multimodal objective functions. To enhance the minimization of the objective function the GMCS is combined sequentially with the Nelder–Mead Simplex algorithm (NMS) (Nelder and Mead, 1965). Indeed, the GMCS algorithm needs only to find an approximate solution, which is supposed to be in the basin of attraction of the global minimum. By using this solution as initial guess for the NMS, fast convergence towards the global minimum is ensured (Lambot et al., 2002).

Since the parameter calibration by inverse modeling can be considered as a nonlinear optimization problem and can be solved as a generalized least-squares problem, we defined the objective function by:

$$\text{OF}(\mathbf{b}) = W \sum_{i=1}^N [\theta_{\text{mea}}(t_i) - \theta_{\text{sim}}(t_i, \mathbf{b})]^2 \quad (7)$$

where  $\text{OF}(\mathbf{b})$  is the objective function of the parameter vector  $\mathbf{b}$ ;  $\theta_{\text{mea}}$  and  $\theta_{\text{sim}} [\text{L}^3\text{L}^{-3}]$  are the measured and simulated soil water content, respectively;  $t$  the time [T] and  $N$  is the number of measurements available. The normalizing coefficient,  $W$  is set equal to  $(Ns^2)^{-1}$ , where  $s$  denotes the standard deviation of the measurement data (Lambot et al., 2002).

Parameter uncertainty was estimated using linear regression analysis. Although, restrictive and only approximately valid for nonlinear problems, it allows comparing confidence intervals between parameters (Hopmans and Simunek, 1999). This analysis implies the estimation of the parameter covariance matrix, which allows calculating both 95% parameter confidence intervals, based on Student’s  $t$ -distribution, and parameter correlation matrix. Details of the formulation can be found elsewhere (Hopmans and Simunek, 1999; Lambot et al., 2002).

The selected parameters were first optimized, within the calibration period, layer by layer using only soil water content data of the corresponding layer ( $N = 125$ ). Next, all available soil water content measurements ( $N = 375$ ) in the profile were used, but again the parameters of each horizon were determined independently. Finally, due to the clear

interactions between the layers, it was decided to optimize simultaneously the parameters of the three different horizons. Values of the flux at the bottom of the profile predicted by the model with the optimized parameters were also considered.

As mentioned above, the RMSE was used to evaluate the goodness of fit. Indeed, the RMSE is a useful single measure of the prediction capability of a model, since it indicates the precision with which the model estimates the value of the depended variable. The smaller the RMSE, the better the simulated values fit the observed data (Eching and Hopmans, 1993). Accordingly to the notations described above, RMSE was calculated as follows:

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N [\theta_{\text{mea}}(t_i) - \theta_{\text{sim}}(t_i, \mathbf{b})]^2} \quad (8)$$

## 2.6. Validation process

For the validation process, two periods were used: the first between 26 July and 30 September 1995 and the second between 1 April and 30 September 1996. Three simulation runs were performed: first with the parameter set identified directly from the measurements; second with parameter set obtained by the trial and error method; and finally with the parameter sets obtained by the inverse procedure. The goodness of the fit was based on the RMSE and the visual inspection of simulated and observed soil water contents.

## 3. Results and discussion

Results of the sensitivity analysis for soil water content (Tables 2 and 3), showed that soil water content, predicted by WAVE, was more sensitive to the hydraulic than to the crop

Table 2

Average sensitivity coefficient (% soil water content),  $SC_{\theta}(z, b_j)$ , for the hydraulic parameters corresponding to the variation of those of the first, second and third layer, respectively

Depth	$\theta_s$	$\theta_r$	$n$	$\alpha$	$K_s$	$\lambda$
First layer (0–20 cm)						
15	$3.0 \times 10^{-3}$	$6.0 \times 10^{-4}$	$3.8 \times 10^{-3}$	$2.3 \times 10^{-4}$	$1.7 \times 10^{-4}$	$7.7 \times 10^{-5}$
30	$2.4 \times 10^{-4}$	$1.0 \times 10^{-4}$	$2.2 \times 10^{-4}$	$7.3 \times 10^{-5}$	$4.9 \times 10^{-5}$	$3.2 \times 10^{-5}$
60	$1.4 \times 10^{-4}$	$6.0 \times 10^{-5}$	$1.9 \times 10^{-4}$	$3.7 \times 10^{-5}$	$2.4 \times 10^{-5}$	$2.3 \times 10^{-5}$
Second layer (20–50 cm)						
15	$5.6 \times 10^{-5}$	$1.9 \times 10^{-5}$	$9.4 \times 10^{-5}$	$2.7 \times 10^{-4}$	$1.0 \times 10^{-4}$	$3.7 \times 10^{-5}$
30	$2.8 \times 10^{-3}$	$6.6 \times 10^{-4}$	$3.4 \times 10^{-3}$	$7.3 \times 10^{-5}$	$2.2 \times 10^{-4}$	$7.0 \times 10^{-5}$
60	$2.5 \times 10^{-4}$	$6.8 \times 10^{-5}$	$1.0 \times 10^{-4}$	$1.1 \times 10^{-5}$	$3.6 \times 10^{-5}$	$1.4 \times 10^{-5}$
Third layer (50–70 cm)						
15	$5.6 \times 10^{-5}$	$3.7 \times 10^{-6}$	$4.2 \times 10^{-5}$	$2.4 \times 10^{-5}$	$3.6 \times 10^{-5}$	$8.8 \times 10^{-6}$
30	$2.8 \times 10^{-3}$	$3.3 \times 10^{-6}$	$4.2 \times 10^{-5}$	$4.2 \times 10^{-5}$	$3.5 \times 10^{-5}$	$9.9 \times 10^{-6}$
60	$2.5 \times 10^{-4}$	$3.3 \times 10^{-4}$	$4.4 \times 10^{-3}$	$3.2 \times 10^{-5}$	$2.4 \times 10^{-4}$	$5.0 \times 10^{-5}$

Table 3

Average sensitivity coefficient (% soil water content),  $SC_{\theta}(z, b_j)$ , for the crop parameters

Depth	$K_c (\times 10^{-5})$	$LAI (\times 10^{-5})$	$S_{\max} (\times 10^{-6})$
15	2.9	2.8	3.1
30	2.7	2.7	3.1
60	1.8	2.1	1.6

parameters. These results are consistent with the findings of [Musters et al. \(2000\)](#) who applied inverse modeling to a forest ecosystem (pine stand) and [Hupet et al. \(2002\)](#) who analyzed parameter sensitivity of the WAVE model in a maize-cropped field. At any depth, sensitivity of the soil water content to  $\theta_s$ ,  $\theta_r$  and  $n$  parameters was high. The sensitivity coefficient of the saturated hydraulic conductivity ( $K_s$ ) was low, but still relatively significant. Among the hydraulic parameters, Mualem's pore connectivity parameter ( $\lambda$ ) presented the smallest coefficient. It is also worth mentioning that parameter change in one layer affected specially soil water content of the corresponding layer.

Concerning the flux at the bottom of the profile, the sensitivity coefficients ([Table 4](#)) showed that this model output variable was also most sensitive to  $\theta_s$  and  $n$ . However, it is interesting to note that it was very sensitive to the crop coefficient ( $K_c$ ) too, illustrating that the model sensitivity to a particular parameter depends on the objective function (output variable) considered. [Vanclooster et al. \(1995\)](#) presented similar results, but by contrast to values in [Table 4](#), they found WAVE to be relatively sensitive to  $K_s$ . This can be explained by the fact that they analyzed the sensitivity of the model for wet conditions. The next most sensitive parameters were  $\theta_r$  and  $LAI$ , while  $\lambda$  had the smallest coefficient.

Consequently, the van Genuchten hydraulic parameters were selected for calibration based on soil water content data measured experimentally. Among these parameters,  $\theta_s$  has a clear physical significance and can rather be determined directly. Thus, the number of parameters for optimization was reduced to  $\theta_r$ ,  $\alpha$  and  $n$ .

The parameters estimated by the "trial and error" method are shown in [Table 5](#). Soil water content simulations at 15, 30 and 60 cm depth corresponding to these parameters are presented in [Fig. 3](#). The simulated values approximate the measured values in the field rather well and the model responded satisfactorily to drought periods and rain and irrigation events. Simulations and measurements compared better during rain and irrigation

Table 4

Sensitivity coefficient (mm),  $SC_F(b_j)$ , for the hydraulic and crop parameters

$n$	63.50
$K_c$	40.60
$\theta_{\sigma}$	38.20
$LAI$	9.50
$\theta_p$	8.10
$\alpha$	2.30
$K_s$	2.20
$S_{\max}$	0.30
$\lambda$	0.20

Table 5  
Calibrated hydraulic parameters with 95% confidence intervals (for inverse optimization only)

Depth (cm)	$\theta_r$ (cm <sup>3</sup> /cm <sup>3</sup> )	$\alpha$ (cm <sup>-1</sup> )	$n$
Experimental determination			
15	0.322	0.278	1.377
30	0.315	0.220	1.406
60	0.250	0.189	1.292
The “trial and error” method			
15	0.200	0.018	1.45
30	0.220	0.019	1.55
60	0.220	0.023	1.35
Inverse optimization			
15	0.254 ± 0.040	0.0191 ± 0.007	2.653 ± 0.893
30	0.256 ± 0.038	0.0234 ± 0.010	2.471 ± 0.830
60	0.269 ± 0.041	0.0565 ± 0.024	1.643 ± 0.270

periods than during drought ones. The average coefficients of variation among sampling locations for each soil depth TDR reading were 24, 17 and 21%, respectively. The model prediction in the calibration period was better than in the validation one. During May 1996, the simulation did not fit the field data, probably due to sampling errors, because there was no response of the measured values to the irrigation events during this period.

Concerning the inverse simulation methodology applied to this stratified soil profile, as the experimentally determined soil moisture retention curves at the three depths were not so different, an initial strategy was adopted. This strategy consisted of optimizing the three parameters,  $\theta_r$ ,  $\alpha$  and  $n$ , layer by layer and iteratively applying the inverse procedure on the different layers until the parameter values obtained were stable. However, this strategy failed due to the strong interactions between the three horizons. Hence, the inverse procedure was changed to determine the above-mentioned parameters of the three layers simultaneously, resulting in nine parameters to optimize.

First, we started the inverse optimization procedure using broad parameter intervals, i.e.  $\theta_r[0.01-0.350]$ ;  $\alpha[0.005-0.300]$  and  $n[1.05-3.30]$ . No acceptable results were obtained, because the search space defined by those intervals was too large. Thereby, we decided to reduce the parameter intervals trying four new alternatives: *Inv. Opt. 1*  $\{\theta_r[0.15-0.30]$ ;  $\alpha[0.050-0.200]$ ;  $n[1.05-2.00]\}$ ; *Inv. Opt. 2*  $\{\theta_r[0.01-0.270]$ ;  $\alpha[0.005-0.050]$ ;  $n[1.10-3.00]\}$ ; *Inv. Opt. 3*  $\{\theta_r[0.15-0.320]$ ;  $\alpha[0.005-0.050]$ ;  $n[1.10-3.3]\}$ ; *Inv. Opt. 4*  $\{\theta_r[0.15-0.320]$ ;  $\alpha[0.010-0.070]$ ;  $n[1.10-3.30]\}$ . All of them, except *Inv. Opt. 1*, yielded acceptable parameters according to RMSE and visual inspection of goodness of fit. Although, different parameter estimations were obtained, 95% confidence intervals of the optimized parameters overlapped for the distinct inverse simulations carried out. The best solution (corresponding *Inv. Opt. 3*) is presented in Table 5. As can be seen in this table, the  $\alpha$  value for the third layer was outside of the *Inv. Opt. 3*  $\alpha$  interval. This can be explained by the fact that the GMCS solution serves as initial guess to initialize the NMS algorithm. The latter performs an additional local search without limitations of iterations and parameter space, which may force the optimal value to be out of the predefined interval. Each inverse

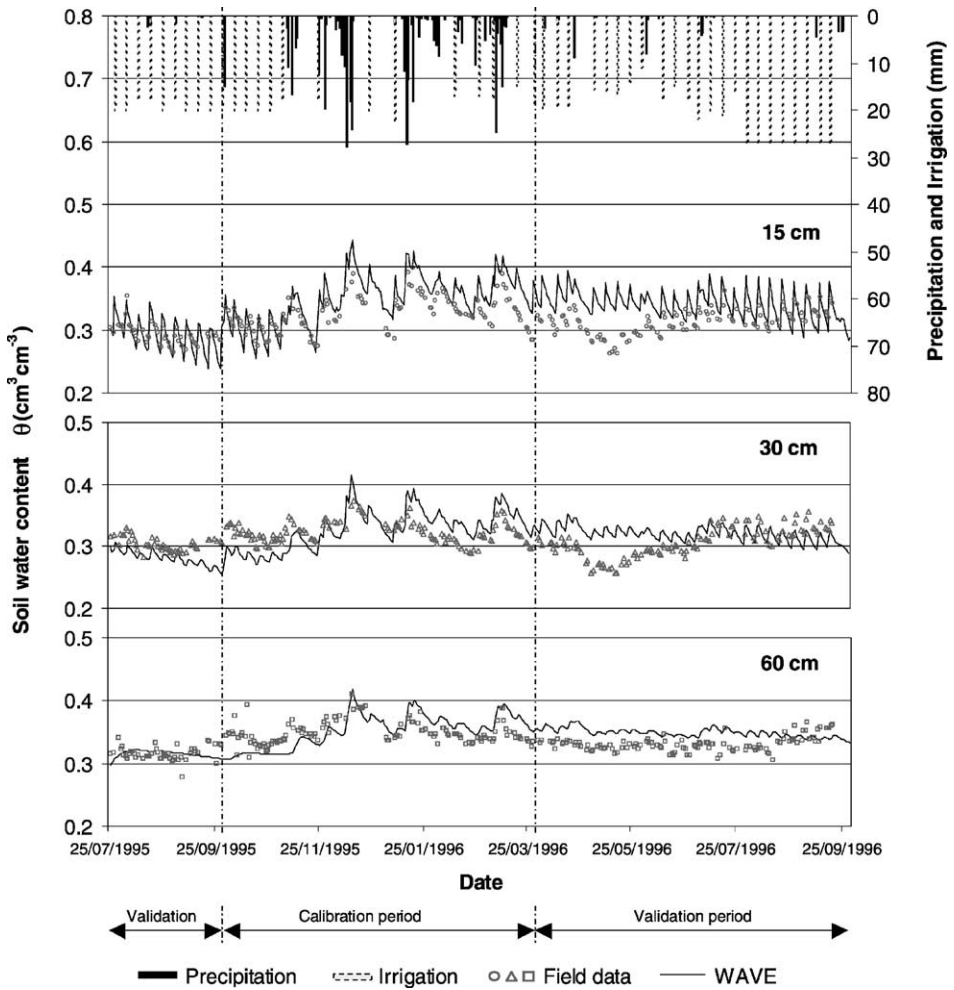


Fig. 3. Soil water content simulation with parameters calibrated by the “trial and error” method. Measured data (symbols) and WAVE prediction (lines).

optimization included 4095 iterations and took around 2 h using a PC Pentium 4 at 1.4 GHz.

Fig. 4 shows the soil water content simulation at the three depths for the optimized parameters presented in Table 5. Like in Fig. 3, predictions in the calibration period were more successful than in the validation one. Graphical comparison between model predictions with the parameters estimated by the “trial and error” method (Fig. 3) and between those resulting from the set of parameters optimized in each inverse simulation procedure (Fig. 4 and others not included), showed that inverse optimization yielded better results than the “trial and error” method. RMSEs for the calibration, validation and whole period (Table 6) confirmed the conclusions obtained from the visual inspection above-mentioned.

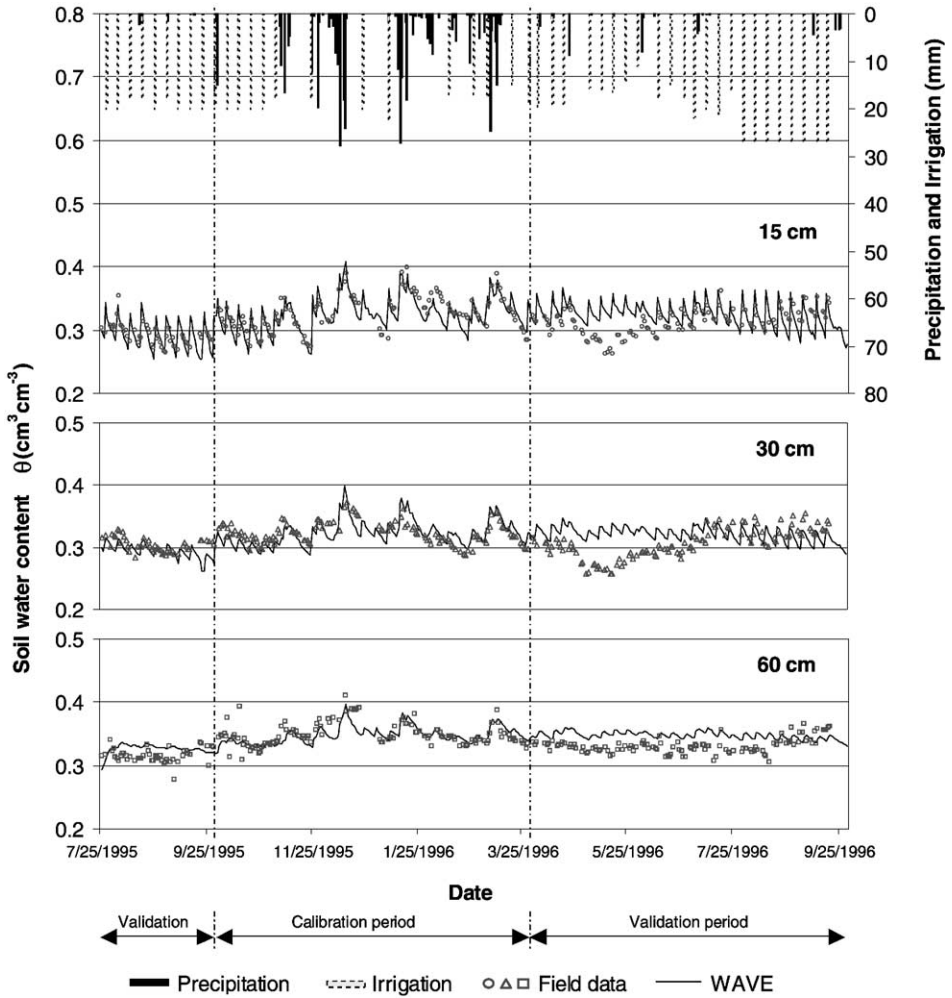


Fig. 4. Soil water content simulation using the parameters of Table 5 estimated by inverse optimization. Measured data (symbols) and WAVE prediction (lines).

Table 6  
Root mean square errors (RMSEs) and predictions of flux at the bottom of the profile

Estimation method	RMSE			Cumulative bottom flux (mm)		
	Calibration	Validation	Whole	Calibration	Validation	Whole
Experimental determination	0.0417	0.0490	0.0447	511.7	339.7	851.4
The “trial and error” method	0.0288	0.0341	0.0319	163.6	56.9	220.5
Inverse optimization	0.0175	0.0305	0.0257	246.1	178.1	424.2

Concerning model predictions for the flux at the bottom of the profile, there were little differences between the values obtained for each inverse simulation procedure carried out (ranging 410.4–429.2 mm). Table 6 shows the simulated bottom flux values for the three periods using the parameter sets of Table 5. Extremely large differences were observed when comparing the three estimation methods. The direct estimation of parameters yielded very large amount of water leaving the soil profile, while the value obtained from the “trial and error” method was much smaller. Furthermore, it is interesting that small RMSE differences (0.0319 versus 0.0257) had a large effect on the cumulative bottom flux (220.5 versus 424.2 mm). This illustrates that even with an acceptable model calibration uncertainties in flux predictions could be extremely large.

Consequently, although, the “trial and error” method is more flexible and popular in modeling water balances in agricultural soils, it has some disadvantages: (i) it is more time-consuming; (ii) it is difficult to know in which directions the parameters should be tuned (particularly if they interact among each other); (iii) the result depends on the initial values; (iv) it is a subjective process; (v) it does not assure to find the best solution; and (vi) it does not allow the parameter uncertainty to be quantified objectively. Moreover, from a scientific point of view it is not an appropriate method.

On the contrary, the use of the inverse optimization algorithm makes the calibration process faster, because it does not depend on initial values and within the search space (defined by the given parameter intervals) it does not test all the possible combinations, just those sets with more likelihood to be the solution. This technique is less subjective and due to its working procedure, it is more efficient in finding the best solution. However, its flexibility depends on the number of parameters to optimize, which is limited by convergence problems.

As illustrated in this study, the inverse optimization method is a promising parameter estimation procedure, but it requires the inverse problem to be well-posed. Our situation suffers from ill-posedness, since nine parameters were estimated simultaneously. In addition, the optimization algorithm was shown by Huyer and Neumaier (1999) and Lambot et al. (2002) to be effective when no more than four parameters were identified. Fig. 5 shows the different soil moisture retention curves corresponding to the distinct sets of parameters calibrated by the “trial and error” methodology and by some of the inverse simulations performed, as well as those determined by the direct approach (Table 5). From this figure, we can see that the algorithm was not able to find the global solution. Coefficients of correlations between several estimated parameters were high. This means that different parameter combinations can equally well describe the experimental measurements. On the other hand, the soil water content input data used for the optimization might not contain enough information for a unique identification of the hydraulic parameters. Thus, an increase in the number of optimized parameters entails the need for further measurements of different types (Hopmans and Simunek, 1999), such as tensiometric and/or outflow data. Yet, it must also be taken into account that additional data require more time and make the experimental setup more difficult (Zou et al., 2001). Moreover, it must be considered that, as shown by Carrera and Neuman (1986), when input data are subject to measurement errors, the convergence of the minimization algorithm at several points in the parameter space may be very slow due to instability. Inverse optimization techniques should be complemented with direct methods, especially when



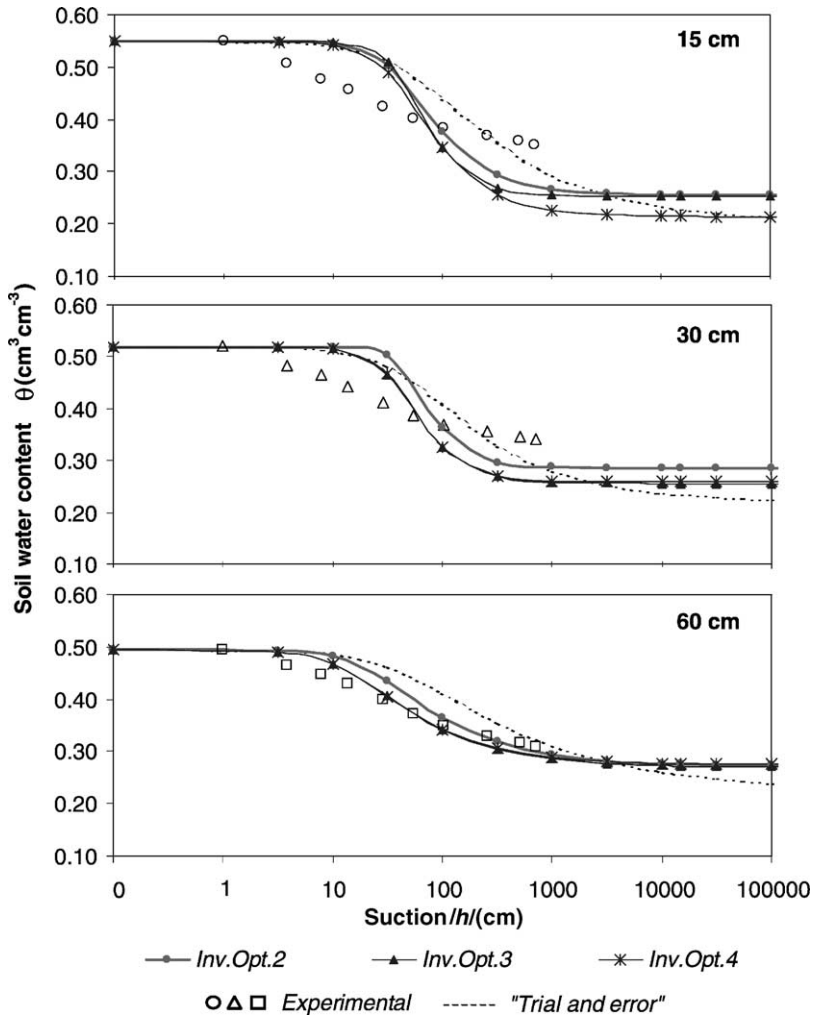


Fig. 5. Soil moisture retention curves for the different parameter estimation methods. Measured data (symbols) and obtained from calibration (lines).

over-parameterized models are used. Indeed, Russo et al. (1991), analyzing infiltration events to determine soil hydraulic properties by inverse simulation, concluded that the use of prior information of the model parameters reduces the degree of ill-posedness of the inverse problem and might lead to a stable and unique solution, even when the input data are associated with considerable measurement errors.

In addition, it should be taken into account that, although, laboratory determinations are more precise and in general more convenient than field measurements, the use of soil properties determined in small cores is questionable (Russo et al., 1991). In this work there is a considerable deviation between the directly determined and inversely estimated soil

moisture retention curves in particular for the top soil layer. This may be explained by the fact that the soil structural phenomena, which generally drives soil water flow at the field scale, are poorly represented at the core scale on which soil retention curves are directly determined.

#### 4. Conclusions

The use of the WAVE model applied to a sprinkler fertigated banana plantation in the North of Tenerife (Canary Islands) showed that using laboratory-determined soil hydraulic properties to simulate the field water balance at field scale in a stratified soil profile can produce inaccurate results. Although, there are many other uncertainties (e.g. semi-empirical crop parameters, spatial variability within the field, determination of irrigation amounts, representation of a 3D situation with a 1D model), it is generally well accepted that some of the soil parameters experimentally determined should be further calibrated with an observed data set.

The study also pointed out the issues related to the “trial and error” calibration procedure, which, besides being a tricky and non-scientific method, it is not really objective (certainly not for a cropped three-layered soil) and it can lead to relatively poor fit of the measured data, even if time is not a limiting factor. An alternative method is the use of an optimization algorithm, like GMCS–NMS that, combined with the numerical model, results in a relatively efficient parameter estimation technique. However, under certain boundary conditions of the inverse problem, it may yield different solutions, that lead to the same response for the model variable used in the calibration process (i.e. soil water content), but with different results for other variables such as the cumulative bottom flux. This clearly illustrates the problem of ill-posedness, which, in this study, can be partially explained due a large number of parameters to optimize and to errors or insufficient information in the measured input data set used for calibration. Nevertheless, ill-posedness is an intrinsic problem of parametric models suggesting the necessity of additional experimental data to identify the more realistic optimized solution.

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