

## Estimation of root water uptake parameters by inverse modeling with soil water content data

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[1] In this paper we have tested the feasibility of the inverse modeling approach to derive root water uptake parameters (RWUP) from soil water content data using numerical experiments for three differently textured soils and for an optimal drying period. The RWUP of interest are the rooting depth and the bottom root length density. In a first step, a thorough sensitivity analysis was performed. This showed that soil water content dynamics is relatively insensitive to RWUP and that the sensitivity depends on the texture of the considered soil. For medium-fine textured soil, the sensitivity is particularly low due to relatively high unsaturated hydraulic conductivity values. These ones allow a “compensating effect” to occur, i.e., vertical unsaturated water fluxes overshadowing in some way the root water uptake. In a second step, we analyzed the well-posedness of the solution (stability and nonuniqueness) when only RWUP are optimized. For this case, the inverse problem is clearly ill-posed except for the estimation of the rooting depth parameter for coarse and the very fine textured soils. In a third step, we addressed the case where RWUP are estimated simultaneously with additional parameters of the system (i.e., with soil hydraulic parameters). For this case, our study showed that the inverse problem is well-posed for the coarse and very fine textured soils, allowing for the estimation of both RWUP of interest provided that a powerful global optimization algorithm is used. On the contrary, the estimation of RWUP is unfeasible for medium-fine textured soil due to the “compensating effect” of the vertical unsaturated water flows. In conclusion, we can state that the inverse modeling approach can be applied to derive RWUP for some soils (coarse and very fine textured) and that the feasibility is strongly improved if the RWUP are simultaneously optimized with additional parameters. Nevertheless, more detailed research is needed to apply the inverse modeling approach to real cases for which additional issues are likely to be encountered such as soil

heterogeneity and root dynamics. *INDEX TERMS*: 1866 Hydrology: Soil moisture; 1875 Hydrology: Unsaturated zone; 1818 Hydrology: Evapotranspiration; *KEYWORDS*: root water uptake, inverse modeling, soil water content, parameter estimation

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### 1. Introduction

[2] The correct modeling of evapotranspiration fluxes at different spatiotemporal scales remains an important challenge for hydrologists. Numerous evapotranspiration models have been developed such as those derived from land surface energy balances [e.g., Dickinson *et al.*, 1993; Ducoudré *et al.*, 1993] or found in agrohydrological simulation models describing more in detail the soil water, the

soil vapor, and energy balance in the soil-crop-atmosphere continuum [e.g., Jarvis, 1994; van Dam *et al.*, 1997]. This latter type of model generally contains various components representing different physical processes such as, e.g., soil water flow and root water uptake (RWU). The RWU process is of paramount importance, as in relatively moist systems most water leaves the soil through root water uptake and plant transpiration rather than by direct evaporation at the soil surface [Chahine, 1992].

[3] For modeling purposes, RWU in agrohydrological models is often conceptualized by a macroscopic approach in which a depth-dependent soil water sink term is defined,

which is then added to the soil water mass conservation equation for a representative elementary soil volume [Whisler et al., 1968; Molz, 1981]. Actual RWU is calculated as the product of a maximum possible RWU and a reduction function taking into account water stress, salinity stress, or both [Homaei, 1999]. Maximum RWU is time and depth dependent and is generally defined by some parameters characterizing the rooting depth and the root density distribution. These root water uptake parameters (RWUP) have to be identified before using the agrophysical hydrological model in predictive mode. A straightforward method to generate RWUP is to combine a soil water and energy transport model of the soil-plant-atmosphere system with a vegetation growth model [see, e.g., Van den Broek and Kabat, 1995]. However, this approach is uncommon in the field of surface hydrology as it relies on elaborate crop-specific parameterization schemes which depend both on the crop phenotypology and genotypology. Hence there is a need to evaluate the robustness of alternative RWUP identification strategies such as the method based on hydrological tracers [e.g., Brunel et al., 1995], or the method based on a simplified water balance [e.g., Hupet et al., 2002], or the use of an inverse modeling procedure [e.g., Vrugt et al., 2001a]. This latter approach is an estimation method in which parameters are optimized by minimizing a predefined objective function which measures discrepancies between observations, i.e., measurements of a state variable (e.g., soil water contents) and the corresponding outputs of the model. Inverse procedures for parameter estimation have been widely used in the field of vadoze zone hydrology [see Hopmans and Simunek, 1999] but have almost exclusively been confined to the estimation of soil hydraulic properties from outflow experiments [e.g., van Dam et al., 1994], evaporation experiments [e.g., Romano and Santini, 1999], or infiltration and redistribution experiments [e.g., Si and Kachanoski, 2000]. Quite recently, the inverse procedure was also applied to the whole soil-plant-atmosphere system to infer RWUP from soil water content observations by coupling appropriate numerical models with a parameter optimization algorithm [Musters and Bouten, 1999; Vrugt et al., 2001a, 2001b; Zuo and Zang, 2002]. This inverse approach is becoming more popular because only a few restrictions are imposed on the experimental conditions. In addition, it results in effective parameter estimates for which the uncertainty ranges can be quantified. Nevertheless, the use of inverse techniques has some well-known limitations which are mainly related to the nonuniqueness and instability of the optimized parameter set. Nonuniqueness leads to several parameter sets describing the data, each yielding equivalent minimum values for the objective function [Gupta and Sorooshian, 1983; Duan et al., 1992]. Non-unique parameter estimates may occur when the parameter sensitivity is low or when the parameters are mutually dependent. Instability is related to the fact that errors on measurements, fixed parameters, or boundary conditions may result in considerable changes in optimized parameter sets. Instability generally occurs when high measurement noise characterizes the data for the inversion and/or when the sensitivity of the parameters to the input data is too low. The well-posedness, the uniqueness, and the stability of the identification of soil hydraulic properties have been exten-

sively studied by means of both experimental and numerical experiments [see, e.g., Kool et al., 1985; Carrera and Neuman, 1986; Simunek and Van Genuchten, 1996]. In contrast, only a few studies have dealt with the identification properties of RWUP parameters. *Musters and Bouten* [1999] and *Vrugt et al.* [2001a, 2001b] identified RWUP for a field experiment but did not investigate the feasibility of the procedure by means of numerical experiments. Yet this preliminary “testing” step is necessary to claim that the inverse problem is well-posed and that the approach can be robustly applied for identification of RWUP. Using a combined numerical and experimental approach, *Hupet et al.* [2002] identified nonuniqueness and stability problems in the estimation of RWUP through inversion.

[4] The general purpose of this study was to investigate numerically the feasibility of estimating RWU parameters from soil water content observations by an inverse modeling approach. We chose a numerical analysis since in such an analysis everything is known, i.e., the chosen model is correct, and all parameters and measurement errors are known beforehand [Simunek et al., 1998]. This is obviously an optimal situation for testing the potential and the limitations of the inverse procedure. In this study, preference is given to the use of soil water content data in the objective function since advanced soil moisture probing technology such as time domain reflectometry (TDR) is now readily available to monitor this state variable with a high spatio-temporal resolution. Furthermore, to be able to compare our results, we chose the same state variable, i.e., soil water content, as that used in the previous studies dealing with the inverse estimation of RWUP [Musters and Bouten, 1999; Vrugt et al., 2001a, 2001b]. Numerical experiments were generated for a long dry period in three differently textured soils. The two target RWUP of interest are the rooting depth (*RD*) and the bottom relative root length density (*BRLD*), which together fully characterize the maximum RWU profile. First, we analyze the sensitivity of *RD* and *BRLD*, as instability and nonuniqueness may be strongly related to the sensitivity of the optimized parameters. Second, we address the uniqueness and stability of the solution when only RWUP are optimized. In this case, Monte Carlo simulations are performed to test the stability of the solution to errors in input data, to errors in some fixed parameters, and to errors in both. Finally, we investigate uniqueness and stability of the solution when RWUP and some additional parameters are optimized simultaneously.

## 2. Material and Methods

### 2.1. The Forward Problem

#### 2.1.1. Root Water Uptake Model

[5] Water flow and root water uptake were simulated using the water transport module of the SWAP model [van Dam et al., 1997]. Description of the one-dimensional vertical transient water flow is based on Richards' equation combined with a sink term:

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

where  $C(h) = \partial\theta/\partial h$  is the soil water capacity [ $L^{-1}$ ],  $h$  is the soil water pressure head [ $L$ ],  $t$  is time [ $T$ ],  $z$  is the vertical

coordinate [L] defined as positive upward,  $K(h)$  is the hydraulic conductivity [ $L T^{-1}$ ], and  $S(z)$  is the sink term describing water uptake by plant roots [ $T^{-1}$ ]. In this study, we assume the soil water relations can be described by the closed-form *Van Genuchten* [1980] relations:

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

$$K(\theta) = K_s S_e^\lambda \left[ 1 - (1 - S_e^{1/m})^m \right]^2 \quad (3)$$

where  $\theta_r$  and  $\theta_s$  are the residual and saturated volumetric water content, respectively [ $]$ ;  $\alpha$  [ $L^{-1}$ ],  $n$ ,  $m = (1 - 1/n)$  and  $\lambda$  [ $]$  are empirical parameters;  $K_s$  is the saturated conductivity [ $L T^{-1}$ ]; and  $S_e = (\theta - \theta_r) / (\theta_s - \theta_r)$  is the relative saturation [ $]$ . Soil water flow was simulated with equation (1) with specified lower and upper boundary conditions. For a dry period with no rainfall, the upper boundary condition is governed by crop potential evapotranspiration ( $ET_p$ ).  $ET_p$  is obtained by multiplying the reference evapotranspiration ( $ET_o$ ) calculated according to *Allen et al.* [1994] by an appropriate crop coefficient considered here as a constant for the selected period. Afterward,  $ET_p$  is partitioned between the potential soil evaporation ( $E_p$ ) and transpiration ( $T_p$ ) by

$$E_p = ET_p \exp^{-0.6LAI} \quad (4)$$

where  $LAI( )$  is the leaf area index. Potential transpiration ( $T_p$ ) is then calculated by subtracting  $E_p$  from  $ET_p$ . In the SWAP model, the maximum possible RWU rate,  $S_{max}(z)$ , integrated over the rooting depth, is equal to the potential transpiration and is defined as follows:

$$S_{max}(z) = \frac{RLD(z)}{\int_{-RD}^0 RLD(z) dz} T_p \quad (5)$$

where  $RLD(z)$  is the root length density at depth  $z$  ( $L L^{-3}$ ) and  $RD$  is the rooting depth (L). Note that this formulation of the  $S_{max}$  function is in fact an extension of the model by *Feddes et al.* [1978] and *Prasad* [1988] allowing a more flexible distribution of the maximum RWU according to the root density profile. In this study, only a linear root density profile will be considered, requiring therefore the specification of three parameters, i.e., the top root length density ( $TRLD$ ), the bottom root length density ( $BRLD$ ), and the rooting depth ( $RD$ ). In this study, we decided to fix  $TRLD$  equal to 1 in order to characterize the linear RWU profile with only two parameters ( $BRLD$  and  $RD$ ). The sink term  $S(z, h)$  of equation (1) is then calculated as proposed by *Feddes et al.* [1978] as follows:

$$S(z, h) = \gamma(h) S_{max}(z) \quad (6)$$

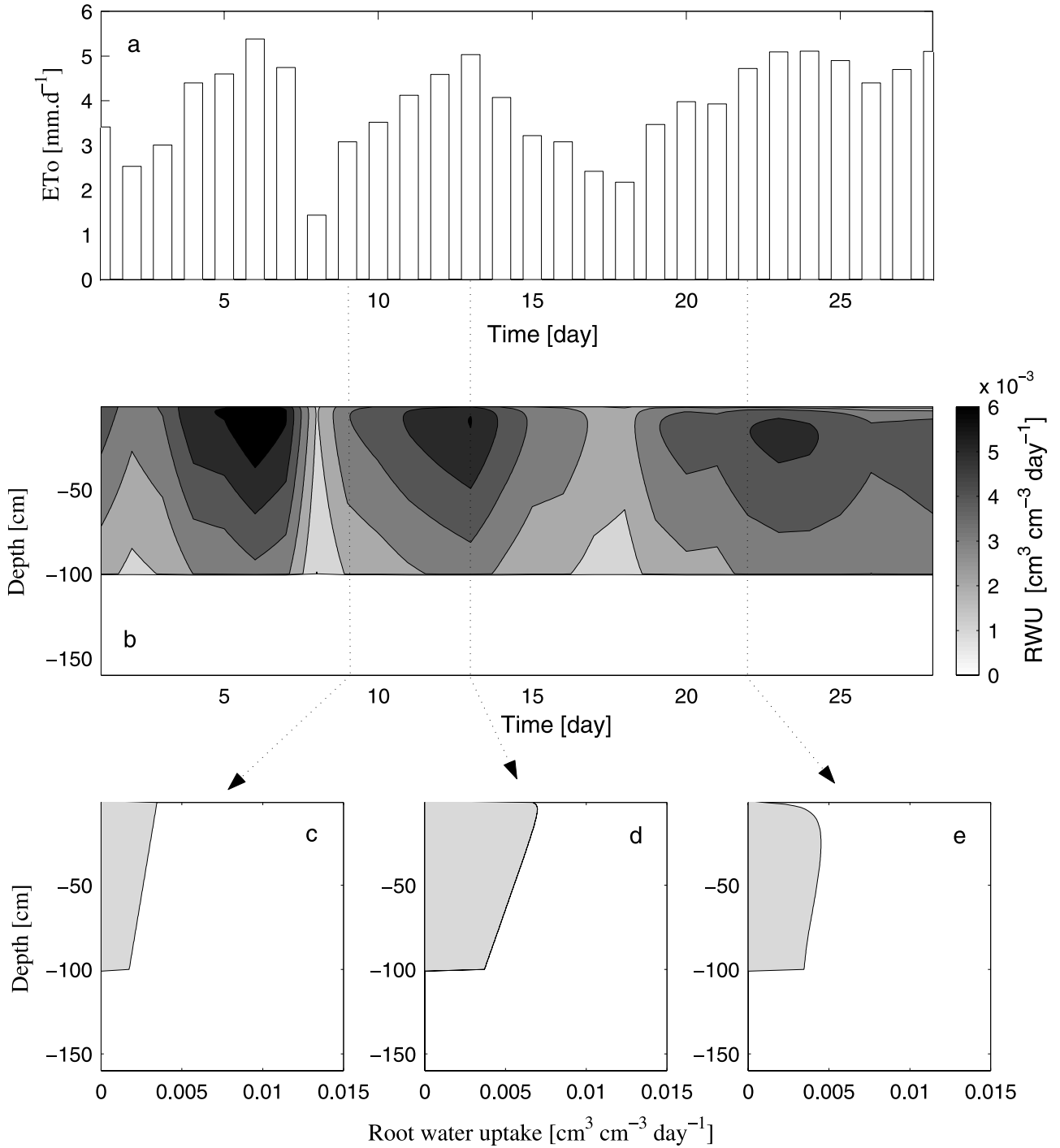
where  $S_{max}(z)$  is the maximal RWU as a function of depth [ $T^{-1}$ ] and  $\gamma(h)$  is a dimensionless reduction function that simulates the effects of soil water stress. The reduction function  $\gamma(h)$  is characterized by different pressure head

values  $h_1, h_2, h_3$  (low and high according to the climatic demand), and  $h_4$ . Above  $h_1$  and below  $h_4$ ,  $\gamma(h)$  is zero; between  $h_2$  and  $h_3$  (l or h),  $\gamma(h)$  is 1; and between the range  $h_1-h_2$  and  $h_3-h_4$  the value of the reduction function is linearly interpolated.

[6] The actual root water uptake given by equation (6) is subsequently integrated over the whole rooting depth and yields the actual transpiration rate  $T_a$ . For illustration purpose (see Figure 1) the RWU pattern was generated with this conceptualization for a dry period of 28 days (see numerical runs). We used a rooting depth of 100 cm, a  $TRLD$  of 1, and a  $BRLD$  of 0.5 corresponding to a trapezoidal root length density pattern. Note that although RLD patterns generally decrease exponentially with depth for most vegetation types [*Canadell et al.*, 1996], we chose a trapezoidal pattern for this case study. Figure 1b illustrates that for this conceptualization the depth over which the RWU takes place is constant (for a period when crop growth is neglected) and independent of the climatic demand. On the other hand, for a certain depth the maximum possible RWU is variable according to the climatic demand as shown in Figures 1c, 1d, and 1e. Finally, in this RWU conceptualization, water stress appears as soon as the pressure head drops below a critical value in any layer of the soil (Figures 1d and 1e).

### 2.1.2. Reference Run

[7] For the identification of RWUP, a reference run was generated for a long dry period of 28 days (without any significant rainfall) corresponding to actual climatic conditions in Belgium encountered between 6 July and 2 August 1999 in the field experiment described by *Hupet and Vanclooster* [2002]. This period was characterized by a moderate potential evapotranspiration (see Figure 1a) with a mean value of  $3.93 \text{ mm d}^{-1}$ . The reference run and subsequent numerical simulations were generated for a homogeneous soil profile, 160 cm deep with free drainage as the lower boundary condition. The flow domain was discretized into 40 compartments using, as suggested by *van Dam and Feddes* [2000], a nodal distance of 1 cm for the first 10 compartments and a nodal distance of 5 cm for the remaining soil profile. The initial condition was selected as a pressure head profile corresponding to field capacity, considered here as the state of "equilibrium" reached after 3 days of water redistribution within a saturated soil profile with zero flux as top boundary condition. We used soil hydraulic properties corresponding to the average of those measured within a small loamy experimental field at 28 different locations (for further details, see *Hupet and Vanclooster* [2002]). The soil was assumed to be covered with a fully developed and nongrowing maize crop characterized by a LAI of 4, a crop coefficient of 1.1, and a rooting depth of 100 cm [*Girardin*, 1999], and a top root length density of 1 and a bottom root length density of 0.5. Note that the value of this latter parameter was selected quite arbitrarily, although it is located just in the middle of the defined parameter space (i.e., 0–1, see below), which is an advantage for the study under consideration. The critical pressure heads of the water stress function were assigned to values listed by *Wesseling* [1991] for maize, i.e.,  $h_1 = 15 \text{ cm}$ ,  $h_2 = 50 \text{ cm}$ ,  $h_{3l} = 600 \text{ cm}$ ,  $h_{3h} = 325 \text{ cm}$ , and  $h_4 = 8000 \text{ cm}$ . To extend the results of this study, two additional reference runs were also generated for two differently textured soils



**Figure 1.** Spatiotemporal patterns of root water uptake illustrated for the considered RWU conceptualization. Figure 1a shows daily ET<sub>0</sub> for the reference run, and Figure 1b shows the corresponding RWU patterns. RWU for days 9, 13, and 22 are illustrated in Figures 1c, 1d, and 1e.

corresponding to a coarse and a very fine soil whose respective soil hydraulic properties were derived from *Wösten et al. [1998]* (see Table 1 and Figure 2).

## 2.2. The Inverse Problem

### 2.2.1. Objective Function

[8] Identification of RWUP by an inverse procedure is a nonlinear optimization problem which consists in finding the parameter vector  $\mathbf{b}$  (containing the RWUP to be optimized) by minimizing an objective function  $OF(\mathbf{b})$ .

Considering incorporation of only soil water content observations in the OF (hereinafter called OF), and assuming that residuals, i.e., errors between “measured” and simulated soil water contents are normally distributed, independent and homoscedastic, the unweighted maximum likelihood OF yields

$$OF(\mathbf{b}) = (\boldsymbol{\theta}^* - \boldsymbol{\theta})^T \cdot (\boldsymbol{\theta}^* - \boldsymbol{\theta}) = \mathbf{e}^T \cdot \mathbf{e} \quad (7)$$

**Table 1.** Mualem-Van Genuchten Parameters Corresponding to the Loamy Soil of the Experimental Field (Medium-Fine) and the Other Two Soils Considered (Coarse and Very Fine) [Wösten *et al.* 1998]

|  | Coarse | Medium-Fine | Very Fine |
|--|--------|-------------|-----------|
| $\Theta_r, \text{cm}^3 \text{cm}^{-3}$ | 0.025  | 0.00        | 0.01      |
| $\Theta_s, \text{cm}^3 \text{cm}^{-3}$ | 0.366  | 0.392       | 0.538     |
| $n(\ )$                                | 1.52   | 1.22        | 1.07      |
| $\alpha, \text{cm}^{-1}$               | 0.043  | 0.003       | 0.0168    |
| $K_{sat}, \text{cm d}^{-1}$            | 70     | 5           | 8.235     |
| $\lambda(\ )$                          | 1.25   | 0.5         | 0.0001    |

where  $\mathbf{b}$  is the model parameter vector;  $\theta^* = \theta^*(z_j, t_j)$  and  $\theta = \theta(z_j, t_j, \mathbf{b})$  are the vectors containing, respectively, the “measured” and the simulated soil water content data relative to depth  $z_j$  and time  $t_j$ ; and  $\mathbf{e} = \theta^* - \theta$  is the vector of residuals. In the present study, we considered a hypothetical intensive sampling scheme where soil water content is measured with a daily time step ( $n = 28$ ) each 10 cm between 0 and 160 cm, i.e., at 10, 20, ..., 150 cm depth ( $n = 14$ ), resulting in 420 soil water content data points in the OF.

### 2.2.2. Optimization Algorithms

[9] For the minimization of equation (7), we used two different optimization algorithms. The first one is derived from the Gauss-Marquardt-Levenberg (GML) method, which starts by searching mainly along the steepest gradient of the OF surface and gradually switches to a direction based on a first-order approximation of the OF surface. This optimization algorithm is included in PEST [Doherty *et al.*, 1995], which is a nonlinear parameter estimation program which can be linked via templates to any model. As the GML algorithm is very efficient in terms of the number of model calls to find the global minimum [e.g., Finsterle and Pruess, 1995], we used it when the number of parameters to be optimized was small, typically in our case for one or two RWUP. Nevertheless, it is well known that efficiency of local optimization algorithms to find the global minimum becomes very limited when the number of parameters increases, e.g., in our case when RWUP are simultaneously optimized with some soil hydraulic parameters. In this case, we used a second optimization algorithm based on a global search procedure. This is the global multilevel coordinate search (GMCS) algorithm [Huyer and Neumaier, 1999] combined sequentially with the classical Nelder-Mead simplex (NMS) algorithm. This global optimization algorithm introduced in the area of unsaturated zone hydrology by Lambot *et al.* [2002] is very efficient for the complex topography of nonlinear objective functions containing many local minima and compares favorably with other existing global search algorithms [Huyer and Neumaier, 1999; Lambot *et al.*, 2002]. The GMCS-NMS algorithm used in this study is entirely programmed in MATLAB routines (version 5.3 [The MathWorks, 1999]) and directly linked to the SWAP model (Fortran executable). Details of the programming procedure can be obtained upon request.

### 2.2.3. Parameter Uncertainty

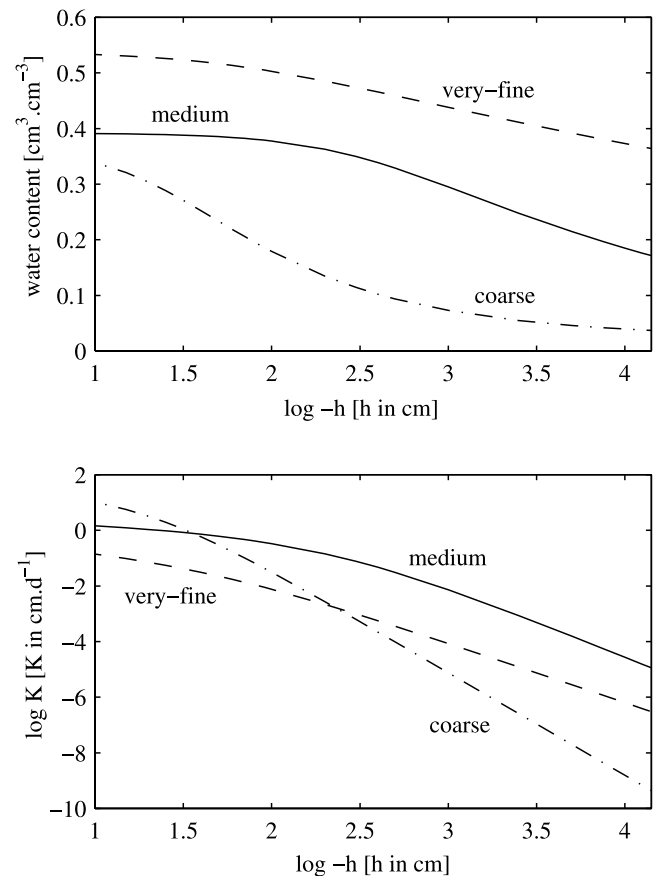
[10] Besides the optimized parameter values, it is also desirable to determine the precision of those estimates, i.e., the optimized parameter uncertainty. In this study, this was

derived by two different methods. The first is used exclusively when only RWUP are optimized and is based on Monte Carlo simulations. This method generates many optimized parameter sets from model fitting of data (in our case produced by the reference run) corrupted with measurement errors. Uncertainty of the optimized parameters in terms of standard deviations and confidence intervals is subsequently derived from the optimized parameter distributions obtained [Press *et al.*, 1992; e.g., Clausnitzer *et al.*, 1998]. As this first method requires quite high computing resources, we used a second method when the number of parameters was larger. This method approximated parameter confidence intervals using classical linear regression analysis, i.e., by assuming local linearity around the minimum of the OF. Uncertainty of the optimized parameters is derived from the parameter variance-covariance matrix  $\mathbf{C}$  [Kool and Parker, 1988] calculated as follows:

$$\mathbf{C} = \frac{\mathbf{e}^T \mathbf{e}}{n - p} \mathbf{H}^{-1} \quad (8)$$

where  $n$  is the number of observations,  $p$  is the number of parameters, and  $\mathbf{H}$  is the Hessian matrix whose elements are defined by

$$H_{ij} = \frac{\partial^2 OF(\mathbf{b})}{\partial b_i \partial b_j} \quad (9)$$



**Figure 2.** Water retention and hydraulic conductivity curves of the three differently textured soils.

Approximate individual confidence intervals of the estimated parameters are finally calculated as follows:

$$b_i - t_{1-\alpha/2}^{n-p} \sqrt{C_{j,j}} \leq b_i \leq b_i + t_{1-\alpha/2}^{n-p} \sqrt{C_{j,j}} \quad (10)$$

where  $C_{j,j}$  is the diagonal elements of the variance-covariance matrix,  $t_{1-\alpha/2}^{n-p}$  is the value of the Student distribution with  $(n - p)$  degrees of freedom, and  $(1 - \alpha)$  is the confidence level, i.e., in our case 0.95 for the 95% confidence interval.

#### 2.2.4. Parameter Sensitivity

[11] Assessment of parameter sensitivity prior to any model calibration is of paramount importance, as efforts must normally be concentrated on parameters to which the model simulation results are most sensitive [Beven, 2001]. In the present work, sensitivity coefficients are calculated for each day and each depth as follows:

$$\Omega_{ij} = b_j J_{i,j} \quad (11)$$

where  $\Omega_{i,j}$  is the  $ij$  elements of the sensitivity matrix  $\Omega$  (size  $n \times p$ ) and  $J$  is the Jacobian matrix (size  $n \times p$ ) whose elements  $J_{i,j}$  are defined as the partial derivatives  $\partial e_i / \partial b_j$  and obtained by forward difference approximation with  $\delta b_j = 0.01 b_j$ . Note that such an expression for the sensitivity coefficients allows a direct comparison between different parameters whatever the invoked units. We also calculated for each parameter a mean absolute space and time sensitivity coefficient defined as

$$\bar{\Omega}_j = \frac{1}{n} \sum_{i=1}^n |\Omega_{i,j}| \quad (12)$$

### 2.3. The Identification Strategy

#### 2.3.1. Sensitivity Analysis

[12] In a preliminary step we performed a thorough sensitivity analysis for all parameters governing the transport of water within the soil-plant-atmosphere system, i.e., RWUP ( $RD$ ,  $TRLD$ ,  $BRLD$ ), parameters of the water stress function ( $h_1$ ,  $h_2$ ,  $h_{3b}$ ,  $h_{3h}$ ,  $h_4$ ), parameters expressing the crop development ( $LAI$ ,  $K_c$ ) and hydraulic parameters ( $\theta_s$ ,  $\theta_r$ ,  $\alpha$ ,  $n$ ,  $K_{sat}$ ,  $\lambda$ ). For the three differently textured soils, mean absolute space and time sensitivity coefficients were calculated with equation (12) for a perturbation of 1% of the parameters with respect to the true parameters (i.e., the reference run). Further, as sensitivity coefficients represent quite abstract values, we generated the water content dynamics for each soil in four additional runs corresponding to the bounds of the RWUP space ( $RD = 50$  and  $150$  cm;  $BRLD = 0$  and  $1$ ).

#### 2.3.2. Optimization of RWUP Only

[13] Where only RWUP parameters are optimized (i.e., one or two parameters), we investigated first the uniqueness of the solution by visually checking the behavior (in one or two dimensions) of the objective function calculated with equation (7). The parameter space of the optimized parameters was divided into 100 discrete values while all the other parameters were fixed at their true values. Subsequently, we investigated instability with respect to measurement errors on soil water content data, to measurement errors on some

**Table 2.** Considered Levels of Uncertainty on the ‘‘Fixed’’ Parameters in Terms of Coefficients of Variation ( $CV = (\sigma/\mu)100$ )

| Level of Error | $\theta_s$ | $\alpha$ | $n$ | $K_{sat}$ | $K_c$ |
|----------------|------------|----------|-----|-----------|-------|
| 1              | 1.25       | 3.33     | 0.4 | 10        | 0.9   |
| 2              | 1.9        | 6.66     | 0.8 | 15        | 1.8   |
| 3              | 2.5        | 10       | 2   | 20        | 2.7   |
| 4              | 3.8        | 13.33    | 3.2 | 30        | 3.6   |
| 5              | 5.1        | 16.66    | 4.0 | 40        | 4.5   |

fixed parameters, and to both combined. For water contents, we chose five different levels of measurement errors (normally distributed with zero mean), i.e., 0.005, 0.01, 0.015, 0.02, and 0.025 in terms of standard deviation (SD), corresponding typically to TDR calibration equations of different quality. The 0.01 error level will be considered in the following as the most realistic, although many studies have found larger values (e.g.,  $\sim 0.015$  [Hupet and Vanclooster, 2002] and 0.02 [Vrugt et al., 2001a]). Subsequently, for each level of error and for the three soil types, we performed 250 Monte Carlo simulations optimizing with PEST (see section 2.2.2) separately  $RD$  and  $BRLD$  and both parameters simultaneously. This resulted in  $250 \times 3 \times 3 \times 5$  optimized parameter sets. After visually checking for normality of the distributions obtained, confidence intervals were constructed with the true distribution of the 250 parameters. Note that in our study we assumed that the confidence intervals were well approximated with quite a low number (i.e., 250) of Monte Carlo simulations. Therefore we checked the validity of this assumption for some cases by generating confidence intervals with 5000 Monte Carlo simulations. In all analyzed cases, confidence intervals derived with 250 and 5000 Monte Carlo simulations were very similar, validating our assumption of constructing confidence intervals with ‘‘only’’ 250 Monte Carlo simulations. When  $RD$  and  $BRLD$  were simultaneously optimized, the correlation coefficient between the two parameters was also determined. Next, instability analysis was performed considering measurement errors on some fixed parameters. Other system parameters such as soil hydraulic parameters and crop coefficients are intrinsically uncertain since the scale of the modeled soil-plant-atmosphere system is inevitably quite large, i.e., at least that of the pedon or the lysimeter (1 to a few cubic centimeters). In this study, we considered five different error levels on five ‘‘fixed’’ system parameters, i.e.,  $\theta_s$ ,  $\alpha$ ,  $n$ ,  $K_{sat}$ , and  $K_c$ . The error level expressed in terms of CV was specified considering the likely uncertainty resulting from the use of different methods for the determination of these ‘‘fixed’’ parameters (Table 2). Note that uncertainty levels reported for  $K_c$  were chosen quite arbitrarily although the selected values seem quite small and plausible for the case of a field experiment. For the measurement error on fixed parameters, the third level of error will be considered in the following as the most realistic. Again 250 Monte Carlo simulations were performed with error (normally distributed and with zero mean) added simultaneously to the five ‘‘fixed’’ parameters, considering first that the water content data are error-free. Subsequently, confidence intervals were derived from the obtained distribution of optimized RWUP. These confidence intervals represent in fact the range of variation of the optimized RWUP due to uncertainty on

some fixed parameters. Finally, Monte Carlo simulations were performed combining both corrupted soil water content data and “fixed” parameters corresponding to a practical case. To avoid too many simulations, we combined the second level of error for soil water content data, i.e., that considered as the most realistic ( $SD = 0.01$ ), with the five different levels of error for “fixed” parameters.

### 2.3.3. Optimization of RWUP Plus Additional Parameters

[14] We finally addressed the case where RWUP plus additional parameters are simultaneously optimized. Uniqueness was investigated by launching the inverse procedure on error-free data for the identification of a gradually increasing number of unknown parameters, systematically including  $RD$  or  $RD$  and  $BRLD$  and some additional normally “fixed” parameters among ( $\theta_s$ ,  $\alpha$ ,  $n$ ,  $K_{sat}$ ), and  $K_c$ . In a first step, the optimization was performed with PEST, i.e., with the Gauss-Marquardt-Levenberg (GML) algorithm. As suggested by, e.g., *Simunek and Van Genuchten* [1996], each optimization case was repeated with three different initial estimates of the unknown parameters to assess the uniqueness of the inverse problem. The different initial estimates were selected randomly at the bounds of the parameter space which was deliberately small for the normally “fixed” parameters (true value  $\pm 2$  SD for level of error 5 in Table 2) as if prior information about these parameters were available. For  $RD$  and  $BRLD$ , the initial estimates were chosen randomly between the bounds of the parameter space, namely, 50 or 150 cm for  $RD$  and 0 or 1 for  $BRLD$ . Note that we also used the GMCS-NMS [*Lambot et al.*, 2002] algorithm to make sure that any nonuniqueness problems encountered were not simply related to the use of the local optimization algorithm (GML). This strategy to tackle nonuniqueness problems was chosen rather than the traditional approach consisting of a visual inspection of two-dimensional (2-D) response surfaces of the OF, as this method is not totally reliable for multidimensional parameter space [*Simunek and Van Genuchten*, 1996]. Finally, we investigated instability problems by launching the inverse procedure as for the nonuniqueness analysis but with a noise of 0.01 added to soil water content data. For that case, we used only the GMCS-NMS algorithm and instability problems were derived from the width of the confidence intervals of the parameter estimates quantified with equations (8) and (10).

## 3. Results and Discussion

### 3.1. Sensitivity Analysis

[15] Results of the sensitivity analysis are presented in Table 3 in which mean absolute space and time sensitivity coefficients ( $\bar{\Omega}$ ) are shown for the three differently textured soils. In this table we also indicated the ranking of the sensitivity coefficients for all parameters with the values 1 and 16 assigned to parameters affecting the most and the least the soil water content dynamics. The results show that soil water content dynamics are much more sensitive (1–2 orders of magnitude) to some hydraulic parameters, i.e.,  $\theta_s$  and  $n$ , than to RWUP. Similar results were found by *Hupet et al.* [2002] for the RWU conceptualization proposed by *Hoogland et al.* [1981]. Yet soil water content dynamics in the study of *Hupet et al.* [2002] was completely insensitive

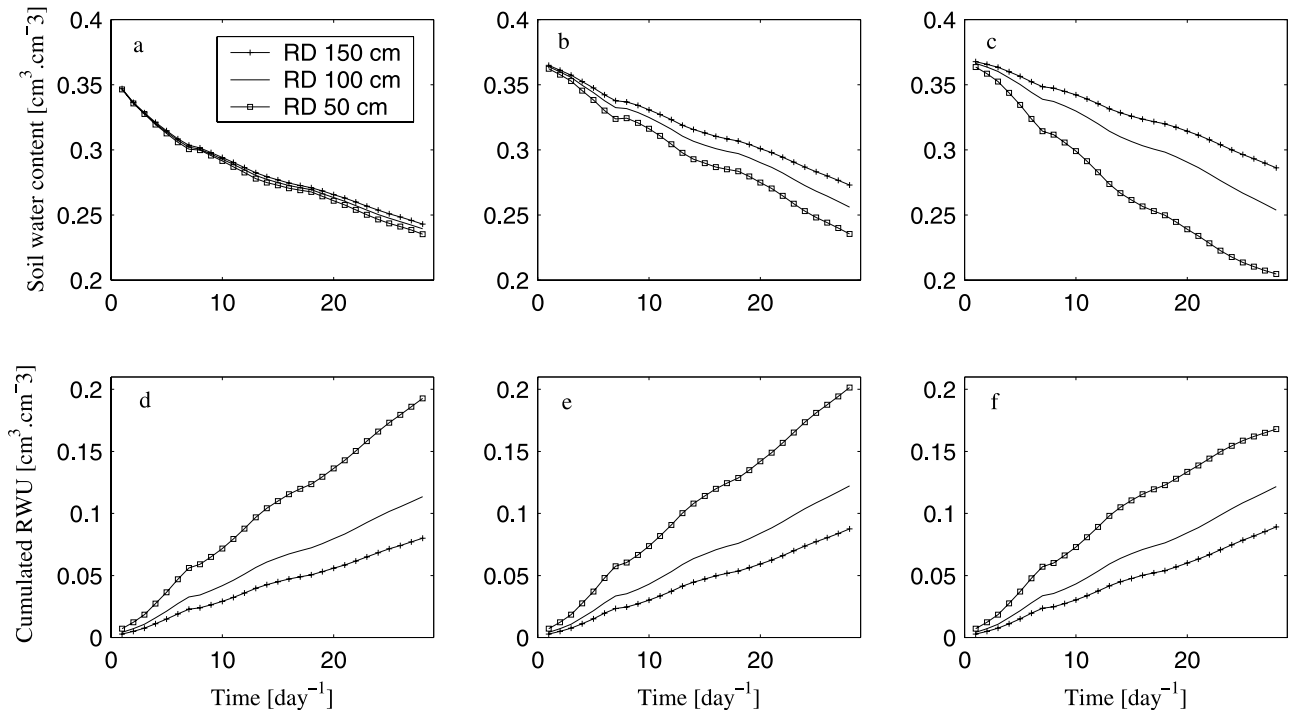
**Table 3.** Mean Absolute Space and Time Sensitivity Coefficients ( $\bar{\Omega}$ ) Calculated for the Different Textured Soils (Coarse, Medium-Fine, and Very Fine)<sup>a</sup>

| Parameter  | Medium-Fine                | Coarse                    | Very Fine                 |
|------------|----------------------------|---------------------------|---------------------------|
| $\theta_s$ | 0.364 (1)                  | 0.134 (2)                 | 0.48 (2)                  |
| $n$        | 0.149 (2)                  | 0.309 (1)                 | 0.75 (1)                  |
| $K_c$      | 0.038 (3)                  | 0.0315 (4)                | 0.029 (4)                 |
| $\alpha$   | 0.019 (4)                  | 0.051 (3)                 | 0.021 (5)                 |
| $RD$       | 0.01488 (5)                | 0.0308 (5)                | 0.0296 (3)                |
| $K_{sat}$  | $7.6 \times 10^{-3}$ (6)   | $2.3 \times 10^{-3}$ (11) | $2.8 \times 10^{-3}$ (10) |
| $LAI$      | $6.2 \times 10^{-3}$ (7)   | $8.1 \times 10^{-3}$ (7)  | $7.9 \times 10^{-3}$ (6)  |
| $TRLD$     | $2.7 \times 10^{-3}$ (8)   | $5.8 \times 10^{-3}$ (8)  | $5.5 \times 10^{-3}$ (7)  |
| $BRLD$     | $2.7 \times 10^{-3}$ (9)   | $5.8 \times 10^{-3}$ (9)  | $5.5 \times 10^{-3}$ (8)  |
| $h_{3l}$   | $8.5 \times 10^{-4}$ (10)  | $2.6 \times 10^{-4}$ (13) | $5.8 \times 10^{-4}$ (12) |
| $h_4$      | $7.4 \times 10^{-4}$ (11)  | $9.8 \times 10^{-4}$ (12) | $2.38 \times 10^{-3}$ (9) |
| $\lambda$  | $7.2 \times 10^{-4}$ (12)  | $3.9 \times 10^{-3}$ (10) | $1.2 \times 10^{-6}$ (14) |
| $\theta_r$ | $3.7 \times 10^{-4b}$ (13) | 0.0158 (6)                | $1.1 \times 10^{-3}$ (11) |
| $h_{3h}$   | $1.1 \times 10^{-4}$ (14)  | $1 \times 10^{-4}$ (14)   | $7.4 \times 10^{-5}$ (13) |
| $h_1$      | 0 (15)                     | 0 (15)                    | 0 (15)                    |
| $h_2$      | 0 (16)                     | 0 (16)                    | 0 (16)                    |

<sup>a</sup>Also indicated are the rankings of the sensitivity coefficients for all parameters with the values 1 and 16 assigned to parameters affecting the most and the least the soil water content dynamics.

<sup>b</sup>Values of the reference run were perturbed from 0 to 0.005.

to the rooting depth, showing clearly that the impact of RWUP on soil water content dynamics depends also on the model concept adopted. Similar results showing insensitivity of soil water content dynamics to RWUP, although this was not quantified in a classical sensitivity analysis, were also found by *Musters and Bouten* [2000]. Additionally, the results of our study show that the two parameters that influence the gradually drying soil profile the most are  $\theta_s$  and  $n$ , which are also the main governing parameters during evaporation experiments [see *Simunek et al.*, 1998]. Visual inspection of the space and time patterns of sensitivity coefficients (not shown here) shows that perturbing RWUP affects soil water dynamics over the whole soil profile, though generally this is more apparent close to the soil surface. It also shows that sensitivity coefficients of RWUP increase gradually as the experiment progresses, i.e., when the soil profile becomes drier. The relative sensitivity of the soil water content dynamics to moisture retention curve (MRC) parameters and RWUP may seem quite surprising for a dry period. The sensitivity of MRC parameters suggests that a small error in, e.g.,  $\theta_s$  will directly affect simulated soil water content even for the case where the temporal dynamics of soil water content are mainly driven by RWU and where vertical water fluxes are negligible. Note that in this case soil water content variation ( $\partial\theta/\partial t$ ) is much less sensitive to MRC parameters than soil water content itself, as noted by *Hupet et al.* [2002]. The relative insensitivity of soil water content to RWUP suggests that a small perturbation of RWUP results in almost all cases in a proportional modification of the sink term. This modifies indirectly vertical soil water fluxes, which compensate and mask in some way the perturbation effect of RWUP on soil moisture. To illustrate this “compensating effect,” we generated numerical runs for the loamy soil described in Table 1 and for the same soil with hypothetical saturated conductivities of  $100 \text{ cm d}^{-1}$  and  $0.01 \text{ cm d}^{-1}$  and with  $RD$  set to 50, 100, and 150 cm. Results presented in Figure 3 show the temporal dynamics of soil water content at 25 cm depth (Figures 3a, 3b, and 3c) and the accumulated RWU at



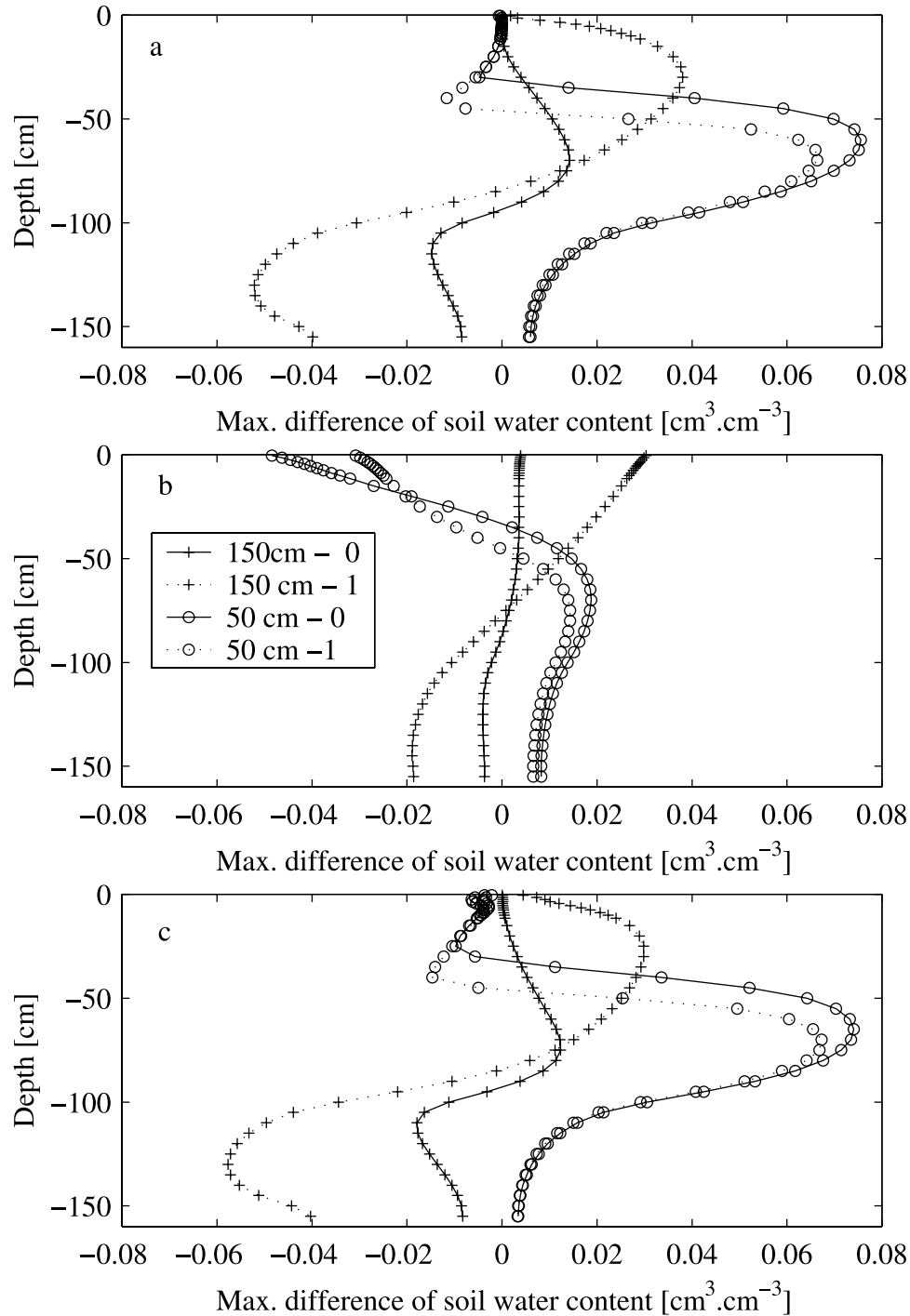
**Figure 3.** “Compensating” effect of the soil according to different conductivity characteristics. Figures 3a, 3b, and 3c show the temporal dynamics of soil water content at 25 cm depth for a medium-fine soil with a  $K_{sat}$  of 100, 5, and  $0.01 \text{ cm}\cdot\text{d}^{-1}$ , respectively. Figures 3d–3f show for the same depth and for the same three different  $K_{sat}$  cumulated root water uptake ( $\text{cm}^3 \text{ cm}^{-3}$ ).

the same depth (Figures 3d, 3e, and 3f). We notice that for the most conductive loamy soil, the perturbation of the  $RD$  does not have a significant effect on the soil water content dynamics at 25 cm depth (Figure 3a) in contrast to accumulated RWU (Figure 3d). Hence vertical water fluxes are able to mask RWU differences in the soil moisture observations. For the other two loamy soils (Figures 3b and 3c), the “compensating effect” is less marked and the impact of the different  $RD$  on the soil water content dynamics is more pronounced as the soil becomes less conductive. Hence the “compensating effect” of the soil plays a certain role in the insensitivity of the soil water content dynamics to RWUP, but this insensitivity is soil specific. In particular, for the coarse and the very fine textured soils, values of the unsaturated conductivity are smaller than those of the medium-fine (for  $h < -100 \text{ cm}$ ), preventing therefore that vertical unsaturated flow overshadows the root water uptake “signal.”

[16] We also generated four additional runs for each soil, selecting  $RD$  and  $BRLD$  at the bounds of the parameter space ( $RD = 50$  and  $150$ ;  $BRLD = 0$  and  $1$ ). Figure 4 shows for the whole soil profile the maximum difference in terms of soil water content between the reference run ( $RD = 100$  and  $BRLD = 0.5$ ) and these other four runs. Note that maximum differences between the reference run and the other four runs were systematically encountered at the end of the 28-day simulation period. For the loamy soil (Figure 4b), maximum differences are very small (maximum  $0.02 \text{ cm}^3 \text{ cm}^{-3}$ ) except for the first 20 cm, and the order of magnitude of this maximum difference corresponds to the standard deviation of a “poor” quality calibration curve of a soil water measurement device. Furthermore, we

note that for the two runs with  $RD$  equal to 50 cm, the shape of the root length density distribution has virtually no effect on the magnitude of the maximum difference. Coarse and the very fine textured soil behave quite similarly, with larger maximum differences ranging between  $-0.06$  and  $0.07 \text{ cm}^3 \text{ cm}^{-3}$ . Again, in this case, the two simulation runs with  $RD$  equal to 50 cm are very similar whatever the shape of the root length density distribution. We also note that nearly all the depths are informative. The largest values of the maximum difference are observed at various depths for the selected cases. This may seem in contradiction to the results obtained in the sensitivity analysis where information content was generally larger close to the soil surface. This may be explained by the fact that during the sensitivity analysis, in contrast to the additional runs, small perturbations were induced in the close vicinity of the true parameters. We further looked at the impact of the four different runs on the accumulated actual transpiration fluxes, as this kind of information might be additionally used for the inverse procedure. Results of Table 4 suggest that for medium-fine textured soil, RWUP have no significant impact on the accumulated transpiration, which is obviously consistent with the small impact of RWUP on soil water content dynamics. For the two other soils, the impact is much larger and particularly well pronounced when the  $RD$  is reduced. To conclude, we can state that the results of this sensitivity analysis are clearly not favorable for the identification of RWUP parameters from soil water content observations alone. Soil water content dynamics are relatively insensitive to RWUP, i.e., to  $RD$  and  $BRLD$ , at least compared to other parameters of the system. This suggests implicitly that small errors on the time series of soil





**Figure 4.** Maximum difference between soil water content of the reference run and that of the other four simulations run for the bounds of the parameter space. Figures 4a, 4b, and 4c are given for the coarse, medium-fine, and very fine textured soils, respectively.

water content will have quite a large effect on the uncertainty associated with optimized RWUP. Furthermore, small errors on some parameters for which soil water content dynamics are much more sensitive may well result in very different RWUP estimates.

### 3.2. RWU Parameters

[17] Results obtained for the uniqueness analysis are illustrated in Figure 5 for coarse textured soil. The response

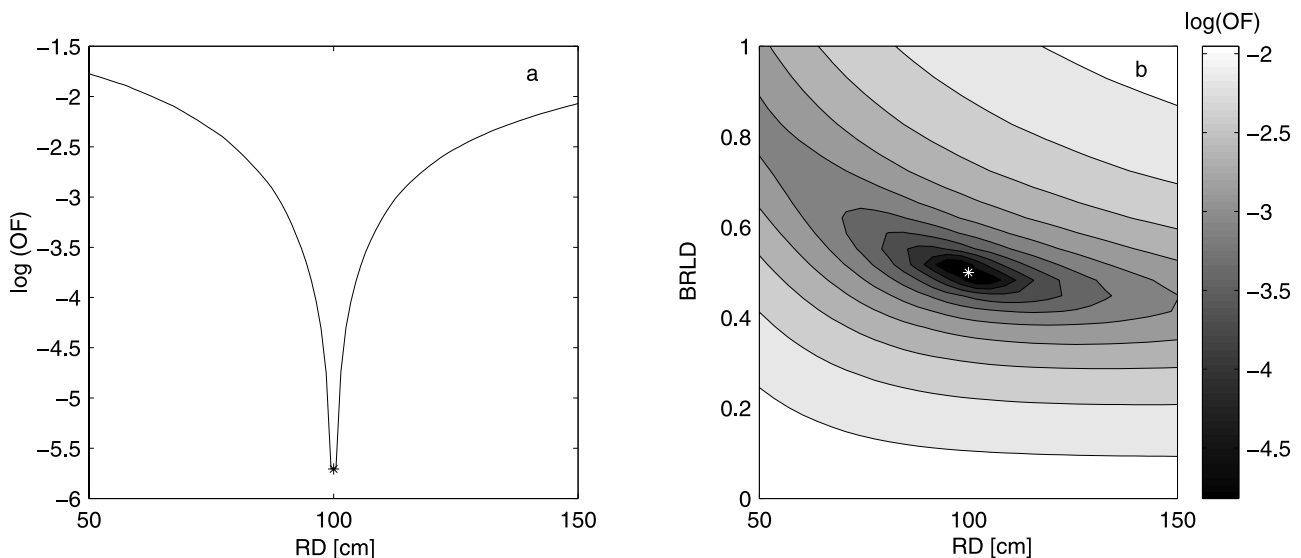
of the logarithm of OF is presented in Figures 5a and 5b for two different cases, i.e., for the optimization of  $RD$  alone and  $RD$  and  $BRLD$  simultaneously, respectively. In each figure, we can see a well-defined global minimum corresponding to the true parameter values ( $RD = 100$  cm and  $BRLD = 0.5$ ). Note that these results were obtained from error-free soil water content data for a coarse textured soil but that similar results were obtained from corrupted soil water content data and for the two other textured soils.

**Table 4.** Differences (in Millimeters) Between Accumulated Actual Transpiration Fluxes of the Reference Run and of the Four Other Runs

|           | $RD = 150 \text{ cm},$<br>$BRLD = 1$ | $RD = 150 \text{ cm},$<br>$BRLD = 0$ | $RD = 50 \text{ cm},$<br>$BRLD = 1$ | $RD = 50 \text{ cm},$<br>$BRLD = 0$ |
|-----------|--------------------------------------|--------------------------------------|-------------------------------------|-------------------------------------|
| Coarse    | 8.76                                 | 1.35                                 | -32.2                               | -44.8                               |
| Medium    | 2.18                                 | 0.56                                 | -4.8                                | -10.1                               |
| Very fine | 12.32                                | 2.56                                 | -28.5                               | -39.5                               |

Results of the stability analysis generated with the five levels of error on soil water content “measurements” are presented in Table 5 for the medium and coarse textured soil. Means and individual parameter confidence intervals at 95% (CI) are presented separately for the optimization of  $RD$ ,  $BRLD$ , and both simultaneously. For the  $RD$  we observe that the range of the confidence intervals are quite small ( $6.5 < CI < 32 \text{ cm}$ ) and that the ranges increase as the magnitude of the “measurement” error increases. Confidence intervals for  $BRLD$  are much larger, with values covering a large proportion of the predefined parameter space already when considering the second level of error. This means that small errors in soil water content measurements have a very large effect on the stability of optimized  $BRLD$ . Note that the difference in stability of identifying  $RD$  and  $BRLD$  is a direct consequence of the difference of sensitivity for these two parameters (see Table 3). When  $RD$  and  $BRLD$  are optimized simultaneously, results are markedly worse. Indeed, for the second error level, the confidence interval of  $BRLD$  (0.08–0.92) is almost the same as the size of the initial parameter space (0–1), meaning that uncertainty on  $BRLD$  generated by the parameter estimation method is virtually equivalent to the original uncertainty. Given these results, Monte Carlo simulations for the next three error levels were not run. Note that optimizing both parameters simultaneously substantially increases the confidence intervals as compared to the case when the parameters are optimized separately.

Indeed, the parameters  $RD$  and  $BRLD$  are strongly negatively correlated (see correlation coefficients in Table 5) meaning that a small increase of  $RD$  can be compensated by a small decrease of  $BRLD$  and can lead to very similar soil water content dynamics. The high correlation between  $RD$  and  $BRLD$  is clearly not optimal in terms of parameter estimation, as it could substantially contribute to the nonuniqueness of the problem. For coarse textured soil (see Table 5), the generated confidence intervals are much smaller. For the optimization of  $RD$  or  $BRLD$  alone, the confidence intervals are acceptable for all considered error levels with maximum values of 9.8 cm and 0.26, respectively, for level 5. The smaller confidence interval for the coarse soil is obviously a direct consequence of the higher sensitivity of the soil water content dynamics to RWUP. For the simultaneous optimization of both RWUP, confidence intervals hardly increase while the correlation between the two estimated parameters is also smaller ( $-0.66 < r < -0.6$ ). Results for very fine textured soil are very similar to those obtained for coarse soil and are therefore not presented here. This similar behavior can probably be explained by the fact that although less sensitive to RWUP, the range of soil water content “measurements” for very fine textured soil is about  $0.2 \text{ cm}^3 \text{ cm}^{-3}$  larger than for coarse textured soil, giving less weight to the added noise (similar in terms of standard deviation for the two soils). Before constructing the aforementioned confidence intervals, we checked for normality of the parameter distribution by visual inspection of the histogram. In the vast majority of cases, distributions of the 250 optimized parameters were close to normal. Furthermore, we also compared true confidence intervals produced by Monte Carlo simulations and those calculated with equation (10). In the few cases investigated, the confidence intervals were very similar (not presented), thus validating the local-linearity assumption for constructing confidence intervals. At this stage of the analysis, we can state that measurement errors have a markedly different impact on the stability of the optimized RWUP for different



**Figure 5.** Uniqueness illustrated for the estimation of (a)  $RD$  alone and (b)  $RD$  and  $BRLD$  together. The true minimum is indicated with a marker.

**Table 5.** Impact of Measurement Errors in Soil Water Content on the Optimized RWUP for the Medium-Fine and Coarse Textured Soils<sup>a</sup>

| Level of Error (SD)               | One Parameter |                 |                     |           | Two Parameters Simultaneously |            |                     |           | r <sup>c</sup> |
|-----------------------------------|---------------|-----------------|---------------------|-----------|-------------------------------|------------|---------------------|-----------|----------------|
|                                   | Rooting Depth |                 | Root Length Density |           | Rooting Depth                 |            | Root Length Density |           |                |
|                                   | Mean          | CI <sup>b</sup> | Mean                | CI        | Mean                          | CI         | Mean                | CI        |                |
| <i>Medium-Fine Textured Soils</i> |               |                 |                     |           |                               |            |                     |           |                |
| 0.005                             | 99.89         | 96.6–103.1      | 0.498               | 0.35–0.64 | 99.6                          | 87.7–111.4 | 0.52                | 0.24–0.86 | –0.86          |
| 0.01                              | 100.04        | 93.5–106.6      | 0.509               | 0.19–0.83 | 99.5                          | 79–119.9   | 0.505               | 0.08–0.92 | –0.90          |
| 0.015                             | 99.98         | 89.8–110.1      | 0.517               | 0.15–0.88 | ...                           | ...        | ...                 | ...       | ...            |
| 0.02                              | 100.05        | 87.4–112.6      | 0.5305              | 0.1–0.97  | ...                           | ...        | ...                 | ...       | ...            |
| 0.025                             | 99.61         | 83.5–115.6      | 0.541               | 0.03–1.03 | ...                           | ...        | ...                 | ...       | ...            |
| <i>Coarse-Textured Soils</i>      |               |                 |                     |           |                               |            |                     |           |                |
| 0.005                             | 100.95        | 100–101.8       | 0.521               | 0.49–0.55 | 100.97                        | 99.4–102.4 | 0.5                 | 0.45–0.55 | –0.63          |
| 0.01                              | 100.98        | 99.2–102.7      | 0.517               | 0.46–0.57 | 100.89                        | 98.3–103.3 | 0.5                 | 0.42–0.58 | –0.66          |
| 0.015                             | 101.08        | 98.4–103.7      | 0.519               | 0.42–0.61 | 101.02                        | 97.1–104.9 | 0.505               | 0.39–0.61 | –0.60          |
| 0.02                              | 100.83        | 97.1–104.4      | 0.529               | 0.41–0.65 | 100.82                        | 95.5–106.1 | 0.508               | 0.36–0.65 | –0.65          |
| 0.025                             | 101.02        | 96.1–105.9      | 0.517               | 0.38–0.64 | 100.95                        | 95.2–106.6 | 0.512               | 0.31–0.7  | –0.60          |

<sup>a</sup>Rooting depth and root length density values are expressed in cm and cm cm<sup>-3</sup> respectively.

<sup>b</sup>Bounds of the 95% confidence interval.

<sup>c</sup>Correlation coefficient.

soil types. For medium textured soil, even if all 14 other parameters are known, the small noise added to the soil water content data will produce large uncertainties that preclude simultaneous inverse modeling of *RD* and *BRLD*. In contrast, solutions are much more stable with respect to soil water content measurement errors for the other two soils.

[18] The effect of “measurement” errors on some “fixed” parameters of the modeled system is presented in Tables 6a and 6b for medium-fine and coarse textured soils, respectively. For medium-fine textured soil, the confidence interval of the optimized *RD* parameters increases with the increase of the magnitude of the error. For the fifth error level, the confidence interval is as large as the predefined parameter space (50–150). For the third error level, considered the most realistic, uncertainty in the optimized *RD* parameter ranges from 65 to 138 cm. This is of the same order of magnitude of uncertainties associated with “expert” judgment. The results are even worse for *BRLD*. Indeed, at the third level of error, the uncertainty corresponds to the size of the original parameter space (0–1). These results suggest that irrespective of the optimization algorithm used, the inversion will lead to completely different estimates of *BRLD* parameter values if small errors on some other system parameters are explicitly accounted for. Such a large instability arises directly from the relative insensitivity of the *BRLD* parameter compared to other parameters (see Table 3). Given the results at the third level of error, Monte Carlo simulations were not generated for the fourth and fifth error levels. The impact of error in “fixed” parameters was not investigated for the simultaneous optimization of both parameters. Indeed, previous results showed for medium-fine textured soil that the simultaneous optimization is not feasible due to instability problems with respect to errors in soil water content “measurements.” For coarse textured soil, results (see Table 6b) are substantially different. Indeed, for *RD* and *BRLD* parameters optimized separately, confidence intervals produced at the third error level seem acceptable, with ranges of 18 cm and 0.38, respectively. We suspect that the

difference of sensitivity for the different parameters (both *RWUP* and “fixed”) explains this success. For the simultaneous optimization of *RD* and *BRLD*, however, the results are very poor in that the estimated confidence intervals are very large at the third error level. A high correlation between the two optimized parameters ( $-0.96 < r < -0.9$ ) exists in this case. Consequently, these results suggest that simultaneous optimization of *RD* and *BRLD* parameters, while fixing other parameters of the system at measured values, is not recommended. Small perturbations on fixed parameters will lead to completely different *RD* and *BRLD* parameter estimates. Results for very fine soil (not shown) are very similar although the estimated confidence intervals are generally a little larger. In conclusion, the effect of instability arising from measurement errors on some “fixed” parameters is soil specific. For medium-fine textured soil, only the optimization of the *RD* parameter tolerates some uncertainty on the “fixed parameters.” For the other two soils, separate optimization of *RD* or *BRLD* seems feasible, although its performance deteriorates for *BRLD* at the fourth and fifth error level. Within this context, one can speculate whether the third error level for “fixed” parameters chosen as the most realistic one in this study is underestimated. Indeed, for field experiments where soil layering is generally more the rule than the exception, it is really difficult (if not impossible) to obtain at the considered scale (1 to a few cubic decimeters) such accurate parameter estimates.

[19] The combined effect of errors on some “fixed” parameters of the modeled system and on soil water content data (SD = 0.01) is presented in Tables 7a and 7b for medium and coarse textured soils, respectively. Note that this corresponds to a realistic case, i.e., a field or a laboratory experiment, for which errors are encountered at all levels. Results for very fine textured soil are very similar to coarse textured soil and are therefore not presented here. Results are quite similar to those obtained in the previous step, but increased confidence intervals are found. Nonetheless, they are slightly smaller than if we had simply added the confidence intervals produced in the two previous

**Table 6a.** Impact of Measurement Errors in Some “Fixed” Parameters on the Optimized RWUP for the Medium-Fine Textured Soils<sup>a</sup>

| Level of Error | Rooting Depth |                 | Root Length Density |             |
|----------------|---------------|-----------------|---------------------|-------------|
|                | Mean          | CI <sup>b</sup> | Mean                | CI          |
| 1              | 100.24        | 89.5–110.9      | 0.498               | 0.35–0.64   |
| 2              | 98.63         | 77.1–120.1      | 0.56                | 0.13–0.99   |
| 3              | 101.64        | 65.2–138        | 0.492               | 0.002–0.982 |
| 4              | 101.05        | 59–143          | ...                 | ...         |
| 5              | 101.5         | 54–149          | ...                 | ...         |

<sup>a</sup>Rooting depth and root length density values are expressed in cm and cm cm<sup>-3</sup>, respectively.

<sup>b</sup>Bounds of the 95% confidence interval.

steps. For medium-fine textured soil, we observe that at the third error level the estimated confidence intervals are quite large (60.5–136.4), illustrating the limitations of the inverse procedure for the identification of the *RD* parameter. The same reasoning holds for the identification of the *BRLD* parameter for coarse textured soil, as the confidence interval ranges between 0.23 and 0.76 (compared to the original 0–1). Only the inverse modeling of the *RD* parameter for very fine and coarse textured soil seems robust to both errors in soil water contents and on the other fixed parameters of the system. Note that these results are consistent with the study of *Musters and Bouten* [1999], who assessed the spatial variability of rooting depths of an Austrian pine stand on a sandy soil by inverse modeling and using soil water content data. In their study, more than one third of the optimized rooting depths were outside the physically reasonable range (i.e., 0.5–3 m). As stated by *Musters and Bouten* [1999] and confirmed by our results, this can be explained by errors in the other fixed parameters of the system (e.g., soil hydraulic properties). On the other hand, our results question the study of *Vrugt et al.* [2001a, 2001b], who optimized up to nine parameters related to the maximum RWU while fixing four other parameters of the system at measured values (i.e.,  $\theta_s$ ,  $\theta_r$ ,  $\alpha$ , and  $K_c$ ). Even though the RWUP obtained were well correlated with root observations and soil water dynamics were quite well reproduced, our results suggest that there is a great chance that slightly perturbing some of the fixed parameters would have led to quite different estimated RWUP. Nevertheless, it is worth noting that in the study of *Vrugt et al.* [2001a] two hydraulic parameters are simultaneously optimized with the

RWUP and that the parameters fixed at “measured” values ( $\theta_s$ ,  $\theta_r$ ,  $\alpha$ ,  $K_c$ ) are not exactly similar to those of our study, which could explain the different results that were obtained.

### 3.3. RWUP and Additional Parameters

[20] Results of the uniqueness analysis are presented in Tables 8a, 8b, and 8c. Note that only six different combinations of parameters are reported here, though all the 29 possible combinations were tested. Table 8a shows that for medium textured soil the GML algorithm reaches the true minimum when the number of parameters is less than or equal to four. Indeed, the three different runs launched with different initial estimates (GML<sub>1</sub>- GML<sub>2</sub>- GML<sub>3</sub>) all led to exactly the same true minimum. For the case where five different parameters are optimized, identification of the true minimum is no longer guaranteed and depends strongly on the initial values. Generally, only one of the three runs was successful in finding the true minimum. When all six parameters are optimized, the optimization algorithm was not able to find the correct minimum irrespective of the initial estimate. Results obtained with the GMCS-NMS algorithm are markedly different. This algorithm succeeds in retrieving the true minimum for all tested combinations of parameters even when the number of optimized parameters is large (i.e., five or six). For this optimization algorithm, only one run was launched for each combination of parameters, as the global search procedure uses the bounds of the parameter space instead of specified initial estimates. Similar results are obtained for coarse textured soil (Tables 8b and 8c) for the optimization of only *RD* or *RD* and *BRLD* together. Again, the success of the GML algorithm is limited to four parameters, or sometimes five depending on the chosen initial estimates. Furthermore, for a larger number of parameters (six or seven), this algorithm is not able to find the true minimum, which seems quite logical as such a demanding exercise is clearly beyond the capabilities of a local search optimization algorithm. In contrast, the GMCS-NMS algorithm is powerful enough to retrieve the correct minimum for all the tested combinations of parameters, and even for the cases where six and seven parameters are simultaneously optimized. These results were systematically obtained with a number of optimization runs smaller than 2500. Similar good results were also obtained for very fine textured soil (not presented). Therefore the results of this uniqueness analysis show that the chosen optimization algorithm strongly conditions the success of the optimization when the number of parameters

**Table 6b.** Impact of Measurement Errors in Some “Fixed” Parameters on the Optimized RWUP for the Coarse Textured Soils<sup>a</sup>

| Level of Error | One Parameter |                 |                     |           | Two Parameters Simultaneously |            |                     |           |                |
|----------------|---------------|-----------------|---------------------|-----------|-------------------------------|------------|---------------------|-----------|----------------|
|                | Rooting Depth |                 | Root Length Density |           | Rooting Depth                 |            | Root Length Density |           | r <sup>c</sup> |
|                | Mean          | CI <sup>b</sup> | Mean                | CI        | Mean                          | CI         | mean                | CI        |                |
| 1              | 100.17        | 96.9–103.4      | 0.50                | 0.42–0.57 | 101.7                         | 82.3–121.1 | 0.495               | 0.2–0.79  | –0.91          |
| 2              | 100.10        | 93.8–106.4      | 0.50                | 0.37–0.63 | 106.1                         | 73.3–138.8 | 0.462               | 0.08–0.85 | –0.96          |
| 3              | 100.44        | 91.3–109.6      | 0.51                | 0.32–0.70 | 107.5                         | 66.6–148.3 | 0.498               | 0.03–0.97 | –0.90          |
| 4              | 101.22        | 83.3–119.1      | 0.51                | 0.2–0.82  | ...                           | ...        | ...                 | ...       | ...            |
| 5              | 101.17        | 78.9–123.4      | 0.51                | 0.14–0.88 | ...                           | ...        | ...                 | ...       | ...            |

<sup>a</sup>Rooting depth and root length density values are expressed in cm and cm cm<sup>-3</sup>, respectively.

<sup>b</sup>Bounds of the 95% confidence interval.

<sup>c</sup>Correlation coefficient.

**Table 7a.** Impact of Measurement Errors in Soil Water Content Data (Level of Error 2, SD = 0.01) and in Some Fixed Parameters on the Optimized RWUP for the Medium-Fine Textured Soils<sup>a</sup>

| Level of Error | Rooting Depth |                 |
|----------------|---------------|-----------------|
|                | Mean          | CI <sup>b</sup> |
| 1              | 99.37         | 86.32–112.4     |
| 2              | 101.21        | 75.21–127.32    |
| 3              | 98.33         | 60.54–136.54    |
| 4              | 103.47        | 55.85–151.11    |
| 5              | 102.34        | 47.01–157.02    |

<sup>a</sup>Rooting depth expressed in cm and cm cm<sup>-3</sup>.<sup>b</sup>Bounds of the 95% confidence interval.

increases. In such a context, the use of a powerful global search algorithm such as GMCS-NMS allows finding of the global minimum and simultaneous optimization of RWUP and up to five additional parameters. Note that such results may seem contradictory to the results obtained in the study of *Hupet et al.* [2002]. Nevertheless, the conclusions of this latter study concerning nonuniqueness problems were only derived from visual inspection of scatterplots, which is probably not totally robust. Note additionally that in the study of *Hupet et al.* [2002] the RWUP of interest (*A* and *B*) were different from those considered in this study, which might also partially explain the different results that are obtained.

[21] Results of the instability analysis are presented in the rightmost columns of Tables 8a, 8b, and 8c, in terms of confidence intervals calculated with equation (10) after the optimization run was finished. For medium-fine textured soil, the confidence intervals increase progressively with the number of optimized parameters. This is a logical consequence of the increasing degree of freedom caused by an increasing number of “free” parameters. By increasing the number of parameters, correlations between parameters may be activated, leading to a widening of the individual confidence intervals. The width of the confidence interval produced for the case when only *RD* is optimized, i.e., 12.9 cm, is very similar to the value of the true confidence interval presented in Table 5 for the second error level. For the case where all six parameters are simultaneously optimized, the range of the confidence interval estimated for *RD* is much larger, i.e., 44 cm, implying that the solution is unstable. We also tested the adopted methodology by

**Table 7b.** Impact of Measurement Errors in Soil Water Content Data (Level of Error 2, SD = 0.01) and in Some Fixed Parameters on the Optimized RWUP for the Very Fine Textured Soils<sup>a</sup>

| Level of Error | Rooting Depth |                 | Root Length Density |           |
|----------------|---------------|-----------------|---------------------|-----------|
|                | Mean          | CI <sup>b</sup> | Mean                | CI        |
| 1              | 100.16        | 95.8–104.5      | 0.503               | 0.39–0.61 |
| 2              | 100.07        | 92.91–107.22    | 0.503               | 0.34–0.66 |
| 3              | 100.02        | 89.88–110.15    | 0.510               | 0.28–0.71 |
| 4              | 100.75        | 84.6–116.88     | 0.516               | 0.19–0.83 |
| 5              | 100.33        | 77.16–123.57    | 0.507               | 0.11–0.88 |

<sup>a</sup>Rooting depth and root length density values are expressed in cm and cm cm<sup>-3</sup>, respectively.<sup>b</sup>Bounds of the 95% confidence interval.**Table 8a.** Results of the Uniqueness and Instability Analysis for the Case Where *RD* is Optimized With Additional Parameters for the Medium-Fine Textured Soil

| Nb Parameter | Parameters  | GML              |                  |                  |      | CI for <i>RD</i> , cm |
|--------------|---|------------------|------------------|------------------|------|-----------------------|
|              |   | GML <sub>1</sub> | GML <sub>2</sub> | GML <sub>3</sub> | GMCS |                       |
| 1            | <i>RD</i>   | U <sup>a</sup>   | U                | U                | U    | 12.9                  |
| 2            | <i>RD-n</i>   | U                | U                | U                | U    | 14.16                 |
| 3            | <i>RD-n-K<sub>c</sub></i>                                 | U                | U                | U                | U    | 26.54                 |
| 4            | <i>RD-n-K<sub>sat</sub>-α</i>                             | U                | U                | U                | U    | 42.85                 |
| 5            | <i>RD-θ<sub>s</sub>-n-K<sub>c</sub>-α</i>                 | U                | NU <sup>b</sup>  | NU               | U    | 47.05                 |
| 6            | <i>RD-θ<sub>s</sub>-n-K<sub>sat</sub>-α-K<sub>c</sub></i> | NU               | NU               | NU               | U    | 44–58–73              |

<sup>a</sup>Unique.<sup>b</sup>Nonunique.

slightly increasing the error added to the soil water content data for the most difficult case (optimization of *RD* plus five additional parameters). Two additional errors were considered, i.e., 0.015 and 0.02, in terms of standard deviation. For these cases, the range of the confidence intervals increase up to 58 and 73 cm, respectively. Such high values mean that the solution is highly unstable. For coarse textured soil, the results are completely different. Indeed, Table 8b shows, for the case where *RD* is optimized with additional parameters, that the ranges of the confidence intervals are very small ( $3.74 < CI < 4.82$ ) and only increase slightly with the increasing number of parameters. This is obviously the result of a highly stable solution, due to the higher sensitivity of soil water dynamics to RWUP for the coarse textured soil and to weaker correlations between RWUP and the additional optimized parameters. In addition, the range of the confidence intervals produced at the larger error level are only slightly larger with values of 6.25 and 8.1 cm for the 0.015 and 0.02 error levels, respectively. For the case where both *RD* and *BRLD* and additional parameters are optimized, the range of the confidence intervals still remain small, with values for *RD* ranging between 4.57 and 6.6 cm and for *BRLD* between 0.14 and 0.196. Such small values mean that the solution (*RD* and *BRLD*) is stable and that it is appropriate to use the inverse procedure. These results are consistent with the study of *Vrugt et al.* [2001a], who estimated RWUP of an almond tree on a sandy soil by inverse modeling using soil water content data. The confidence intervals obtained in their study for RWUP are similar to the values presented in Table 8c. By increasing the error in the soil water content data, the performance deteriorates only slightly. The range of the confidence interval reaches maximum values of 12.5 cm for *RD* and 0.34 for *BRLD* for the 0.02 error level. We do not present in Tables 8a–8c the confidence intervals of the other optimized parameters (i.e., the soil hydraulic parameters) as we are mainly interested in the optimization of RWUP. Nevertheless, some of the obtained confidence intervals, especially those of *K<sub>sat</sub>*, are very large. More detailed information for *K<sub>sat</sub>* should be obtained by alternative techniques for an accurate prediction of soil water movement during periods when *K<sub>sat</sub>* plays an important role (e.g., infiltration-redistribution events). In this framework we could suggest using a rewetting event during or at the end of the drying period which could help to improve the estimation of the simultaneously optimized hydraulic parameters. Nevertheless, the use of such a rewetting event

**Table 8b.** Results for the Coarse Textured Soil for the Estimation of Only *RD*

| Nb Parameter | Parameters   | GML <sub>1</sub> | GML <sub>2</sub> | GML <sub>3</sub> | GMCS | CI for RD, cm   |
|--------------|--|------------------|------------------|------------------|------|-----------------|
| 1            | RD   | U <sup>a</sup>   | U                | U                | U    | 3.74            |
| 2            | RD- <i>n</i>   | U                | U                | U                | U    | 3.67            |
| 3            | RD- <i>n</i> - <i>K<sub>c</sub></i>  | U                | U                | U                | U    | 4.12            |
| 4            | RD- <i>n</i> - <i>K<sub>sat</sub></i> - $\alpha$                                     | U                | U                | U                | U    | 4.36            |
| 5            | RD- $\alpha$ - <i>n</i> - <i>K<sub>sat</sub></i> - <i>K<sub>c</sub></i>              | NU <sup>b</sup>  | NU               | U                | U    | 4.5             |
| 6            | RD- $\theta_s$ - <i>n</i> - <i>K<sub>sat</sub></i> - $\alpha$ - <i>K<sub>c</sub></i> | NU               | NU               | NU               | U    | 4.82 -6.25 -8.1 |

<sup>a</sup>Unique.<sup>b</sup>Nonunique.

at the end of the drying period will inevitably require us to consider hysteresis issues. Consequently, there is a risk of making the inverse problem more complex and the optimized parameters more uncertain. The results obtained for very fine textured soil are not presented, as they are very similar to those obtained for coarse textured soil, with the confidence intervals broadening only a little.

#### 4. Conclusions

[22] In this paper we have tested the feasibility of the inverse modeling approach to derive root water uptake parameters (RWUP) with only soil water content data. This was performed with numerical experiments for three different textured soils and for a long dry period during which crop growth was considered negligible. The sensitivity analysis showed that soil water content dynamics are relatively insensitive to the RWUP though the sensitivity is higher for very fine and coarse textured soils. The insensitivity of soil water dynamics to RWUP for medium-fine textured soil compared to the other two textured soils can be explained by a “compensating effect,” i.e., by vertical unsaturated water flows overshadowing in some way the root water uptake “signal.” Visual inspection of response surfaces (in one and two dimensions) showed that the solution is unique when only *RD*, *BRLD*, or both are optimized. The instability analysis showed, for medium textured soils, that the inverse modeling approach is only feasible for estimating *RD*, although the estimated confidence interval is very large (60.5–136.4 cm). For coarse and very fine textured soil, the optimization of *RD* is robust to both errors in soil water contents and in the other “fixed” parameters of the system. These results suggest that the inversion of soil water content data for RWUP identification is ill-posed except for the estimation of *RD* for coarse and

very fine textured soil. These results are consistent with the study of *Hupet et al.* [2002] and *Musters and Bouten* [1999]. Finally, the well-posedness of the inversion was studied for the case where RWUP are simultaneously optimized with additional system parameters. For the three differently textured soils, the solution is unique if a powerful global optimization algorithm is used. For coarse and very fine textured soils, the solution is quite stable, which allows the simultaneous identification of *RD* and *BRLD*. These results clarify some of the conclusions presented by *Hupet et al.* [2002] concerning the unfeasibility of the simultaneous estimation of RWUP with additional soil hydraulic parameters.

[23] In conclusion, our study showed that the inverse modeling approach to estimate RWUP is feasible subject to two cautionary notes. First, the texture of the soil strongly influences the success of the inversion. Coarse and very fine textured soils are much more suitable for the identification of RWUP than medium-fine soils. Indeed, for these soils the “compensating effect” of vertical unsaturated water flows overshadowing the RWU is only slightly marked because the unsaturated conductivity of these soils decreases rapidly beyond a certain suction range. Second, the success depends on the choice of the parameters to optimize. Indeed, this study showed that the estimation of RWUP by fixing all the other parameters of the system is unreliable.

[24] We further recommend studying the impact of the sampling frequency (both temporal and spatial) of soil water content data on the results of the inverse procedure. Indeed, the sampling strategy adopted in this study was very intensive in both time and space, which is hard to implement in real experiments. Similar studies should also be tested for more pessimistic error levels both for soil water content measurements and for fixed parameters. Indeed, some presented results are probably dependent on the

**Table 8c.** Results for the Coarse Textured Soil for the Estimation of Only *RD* and Both *RD* and *BRLD* With Additional Parameters

| Nb Parameter | Parameters  | GML <sub>1</sub> | GML <sub>2</sub> | GML <sub>3</sub> | GMCS | CI for RD (cm)-BRLD, cm cm <sup>-3</sup> |
|--------------|---|------------------|------------------|------------------|------|--|
| 2            | RD-BRLD   | U <sup>a</sup>   | U                | U                | U    | 4.57–0.14                                |
| 3            | RD-BRLD- <i>n</i>   | U                | U                | U                | U    | 6.02–0.165                               |
| 4            | RD-BRLD- <i>n</i> - <i>K<sub>c</sub></i>  | U                | U                | U                | U    | 5.32–0.164                               |
| 5            | RD-BRLD- <i>n</i> - <i>K<sub>sat</sub></i> - $\alpha$                                     | NU <sup>b</sup>  | U                | NU               | U    | 5.2–0.21                                 |
| 6            | RD-BRLD- $\alpha$ - <i>n</i> - <i>K<sub>sat</sub></i> - <i>K<sub>c</sub></i>              | NU               | NU               | NU               | U    | 5.24–0.1845                              |
| 7            | RD-BRLD- $\theta_s$ - <i>n</i> - <i>K<sub>sat</sub></i> - $\alpha$ - <i>K<sub>c</sub></i> | NU               | NU               | NU               | U    | 6.66–0.196<br>9.4–0.254<br>12.5–0.34     |

<sup>a</sup>Unique.<sup>b</sup>Nonunique.

selection of the error levels, which remains in some way subjective. In addition, we recommend investigating the possibility of incorporating additional information such as measured transpiration fluxes or the time derivative of the soil water content in the inverse problem. Indeed, this study showed that the RWU parameterization has a pronounced impact on the transpiration fluxes for some soils and the study of Hupet *et al.* [2002] suggested that the use of the time derivative of soil water content could be valuable. The use of periods including a rewetting event during or at the end of the monotonic drying period should also be tested, as the use of shorter periods (e.g., a week) for which the assumption of no root growth is certainly more representative of real cases, i.e., field or laboratory experiments. We also recommend extending the methodology adopted in this paper to multidimensional (2-D and 3-D) root water uptake parameterizations. Indeed, such parameterizations raise additional problems, as they contain many more RWUP and the domain over which the soil water dynamics is simulated is larger, which necessitates dealing with the lateral spatial variability of the soil hydraulic properties. We finally suggest, before applying the inverse approach for real cases, studying the feasibility of the inverse estimation of RWUP for multilayered soils.

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