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**Field scale
parameterisation
from TDR time series**

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Field scale effective hydraulic parameterisation obtained from TDR time series and inverse modelling

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Abstract

Due to the large heterogeneity in the hydraulic properties of natural soils, estimation of field scale effective hydraulic parameters is difficult. Past research revealed that data from accurate but small scale laboratory measurements could hardly ever be transferred to the field scale. In this study, we explore an alternative approach where hydraulic properties of a layered soil profile are directly estimated from hydraulic inverse modelling using a time series of in situ measured soil water contents obtained from time domain reflectometry. Simulations were conducted for natural boundary conditions and run for a one-year time period including both wet and dry soil conditions. For the time period used for inversion, the model is able to reproduce the general evolution of water content in the different soil layers reasonably well. However, distinct drying and wetting events could not be reproduced in detail which we explain by the complex natural processes that are not included in the rather simple model, e.g. an accurate site-specific representation of the evapotranspiration process and, potentially, preferential flow. The study emphasizes the importance of a correct representation of the various processes occurring in the soil-plant-atmosphere continuum. Still, we conclude that – for time periods where measured data for calibration are available – this simple estimation of effective hydraulic properties from in situ data is a good approach to obtain effective parameters for describing unsaturated water movement in field soils which are not dominated by complex processes like preferential flow.

1 Introduction

Soil hydraulic and transport properties are key parameters required for modelling water and solute movement in soils. The estimation of their effective parameterisation at the field scale remains a challenge for hydrology, however. Original concepts envisaged soil as an essentially uniform medium. In this context, properties could be determined by extracting small samples and by performing appropriate measurements on them.

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Initially, these aimed at the direct determination of the properties of interest (e.g., Topp and Miller, 1966; Klute, 1986). It turned out, however, that these methods yield rather inaccurate results (Flühler et al., 1976). This led to the development of inverse methods where a given parameterisation is adjusted such that modelled results are in optimal agreement with the corresponding measurement. Comprehensive reviews are provided e.g. by Hopmans and Šimůnek (1999) and Vrugt et al. (2008). Significant effort has been spent to improve the methods from the original One-Step Outflow (Parker et al., 1985), through Multi-Step Outflow (van Dam et al., 1994), all the way to evaporation experiments (e.g., Šimůnek et al., 1998; Schneider et al., 2006). As a result, the hydraulic properties of a soil sample can now be determined rather accurately and over a wide range of hydraulic states. The methods are very time consuming, however, hence expensive.

A more severe problem, whose implications were not realized immediately, arose with the insight that the subsurface is heterogeneous (Nielsen et al., 1973) and even worse that this heterogeneity is of a hierarchical nature (Gelhar, 1986; Cushman, 1990; Vogel and Roth, 2003). Indeed, a number of studies reported disagreement between hydraulic parameters determined by lab methods and parameters estimated with direct or inverse methods using field data (e.g., Dane and Hruska, 1983; Ritter et al., 2003; Wöhling et al., 2008). With this, the question of effective material properties emanated. While the issue has been discussed to great depths for the linear dynamics of groundwater flow (e.g., Dagan, 1986; Gelhar, 1986; Neuman and Di Friderico, 2003), corresponding studies on the effective properties for the highly non-linear regimes of soils have been anecdotal.

For the time being, until solid theoretical and experimental solutions are available, the inverse estimation of effective hydraulic parameters from in situ measured state variables is a pragmatic path to follow. Examples of readily available state variables are volumetric water content and matric potential which can be measured continuously by time domain reflectometry (TDR) and tensiometry, respectively. The advantage of using in situ data is that the sensors experience all processes affecting the measured

state variables in their natural environment, implicitly including interactions between different soil layers and across scales. This can hardly ever be achieved in lab measurements.

A number of inverse estimations of hydraulic parameters in field soils have been conducted using data from infiltration and drainage experiments in lysimeters (Dane and Hruska, 1983; Abbaspour et al., 1999; Sonnleitner et al., 2003; Mertens et al., 2006). In addition to state variables, these experiments also yield data on leachate volume which further constrain the model.

So far, only a few studies aimed at the inverse estimation of effective hydraulic parameters from state variables measured directly in natural soil profiles (Vereecken et al., 2008). Lehmann and Ackerer (1997) used pressure head data measured in one single soil layer together with precipitation and evapotranspiration measurements from a one year period to determine hydraulic parameters of a two-layer soil profile. Abbaspour et al. (2000) ran an irrigation and drainage experiment in a layered field soil and estimated the hydraulic parameters of the profile from transient data of water content and matric potential. Doing measurements in a rather complicated soil profile they found that a fairly correct representation of soil structure in the model is essential to infer a reasonable set of parameters from the inverse simulations. Jacques et al. (2002) estimated hydraulic and solute transport parameters of a layered field soil under natural rainfall conditions using time series of water content, electrical conductivity and pressure head. In their experiment, evapotranspiration was eliminated by a thin gravel layer placed on the bare soil surface. Ritter et al. (2003) conducted an inverse estimation of hydraulic parameters from a time series of measured water content from different depths of a temporarily irrigated, layered field soil on Tenerife. Their simulations suffered from ill-posedness of the inverse problem however which did not lead to a global solution. Ritter et al. (2003) referred this result to the large amount of hydraulic parameters to be estimated and suggested a need for more experimental data like pressure head and/or outflow data to additionally constrain the inversion. In a recent article, Wöhling et al. (2008) compared three different multiobjective optimisation al-

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gorithms for the estimation of hydraulic properties from pressure head data measured in a layered field soil on the Spydia site, New Zealand. Compared with forward simulations using hydraulic parameters derived from lab experiments all inverse models were more successful in estimating parameter sets which reproduced the measured field data. Differences in some of the parameters derived from the three optimisation algorithms were explained by the occurrence of local optimal solutions and the high dimensionality of the inverse problem combined with the applied multiple objectives.

Most of the previous studies either operated in a rather narrow range of hydraulic states with approximately constant water contents, hence in a quasi-linear regime, and under fairly wet conditions. Even though they were conducted in natural soils, boundary conditions were often controlled in some way, either by eliminating evapotranspiration or by applying artificial irrigation.

The objective of our study is to estimate the hydraulic parameters of a layered soil profile under completely natural and highly variable forcing. To this end, we explore the numerical inversion of a time series of in situ measured water contents over a time period of one year. The water content in the topsoil shows a rather intense temporal dynamics which is expected to stabilise the inversion on the one hand but also tends to invoke processes that are not incorporated sufficiently well in most models like, e.g., evolution of cracks under dry conditions, preferential flow or an accurate representation of evapotranspiration.

2 Materials and methods

2.1 Site description and instrumentation

Experiments were conducted at the Grenzhof Test Site (49°25' N, 8°37' E) near Heidelberg, SW-Germany. The site is a former agricultural field which, since the beginning of the experiments in spring 2003, is covered with grass that is regularly cut to a height of a few centimeters. According to the USDA-Soil Taxonomy (Soil Survey Division Staff,

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1993) the overall soil texture can be classified as sandy loam (Fig. 1). The topmost 0.28 m consist of a humous plough horizon that is underlain by a rather homogeneous sandy loam. At 0.82 m, we found a sharp transition to a more dense sandy loam including aggregates of secondary minerals. Further down, the clay content of this horizon increases continuously. Below 1.44 m, there follows a transition to a thin layer of gravels within a loamy matrix. It is underlain by fluvial gravels embedded in a sandy matrix starting between 1.54 m and 1.65 m depth.

The site is equipped with an automatic weather station that continuously measures precipitation, air temperature and relative humidity, barometric pressure, wind speed and direction, and incoming and outgoing solar and far infrared radiation (Table 1). In addition, volumetric soil water content and soil temperature are recorded in three nearby profiles. Meteorological parameters and soil temperature are measured in 10-min intervals. TDR measurements of soil volumetric water content are recorded hourly.

Soil temperature probes are installed in a soil profile at depths of 0.12 m, 0.17 m, 0.265 m, 0.47 m, 0.67 m, 0.865 m and 1.64 m. Volumetric soil water content is measured with TDR using standard 3-rod probes (CS610, Campbell Scientific, Logan, UT; rod length: 0.3 m, rod diameter: 0.48 cm, rod spacing: 2.2 cm). They are installed in two adjacent soil profiles in 0.13 m, 0.72 m and 1.41 m depth (first profile) and 0.30 m, 0.63 m, 0.92 m and 1.16 m depth (second profile). Before installation, TDR probes were calibrated for water content estimation with measurements in water and air. Bulk dielectric permittivities ϵ_c [-] were derived from the measured L_a/L values using

$$\sqrt{\epsilon_c} = \frac{L_a}{L} \tag{1}$$

where L_a [m] is the apparent length of the TDR probe rods which varies with water content, and L [m] is the real rod length (Campbell Scientific Inc., 2004).

Volumetric water contents θ [-] were calculated using the CRIM (Complex Refractive Index Model) formula

$$\sqrt{\epsilon_c} = \theta \sqrt{\epsilon_w} + [1 - \phi] \sqrt{\epsilon_s} + [\phi - \theta] \sqrt{\epsilon_a} \tag{2}$$

$$\theta = \frac{\sqrt{\varepsilon_c} - \sqrt{\varepsilon_s} - \phi(1 - \sqrt{\varepsilon_s})}{\sqrt{\varepsilon_w} - 1} \quad (3)$$

where ε_s [-], ε_w [-], and ε_a [-] are the dielectric permittivities of the solid matrix, water and air, respectively, and ϕ [-] is porosity. The dielectric permittivity of water (ε_w) was temperature corrected according to Roth et al. (1990), and ε_s was set to an estimated constant value of 5. The porosity of each soil layer was determined gravimetrically from the dry weight of undisturbed volumetric soil samples taken during a profile excavation.

2.2 Hydraulic model

Simulations were run using the numerical model HYDRUS-1D (Šimůnek et al., 2005) in the forward mode accompanied by external routines for inversion which were programmed in MATLAB (The MathWorks, Inc., Natick, MA).

2.2.1 Governing equations

Slow vertical water movement in a one-dimensional, unsaturated rigid porous medium is described by the Richards equation (Jury et al., 1991)

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K \left(\frac{\partial h}{\partial z} - 1 \right) \right] - S, \quad (4)$$

where θ is the volumetric water content [-], h is the matric head [m], t is time [d], z is the spatial coordinate [m], K is the hydraulic conductivity function [m d^{-1}], and S is a sink term [$\text{m}^3 \text{m}^{-3} \text{d}^{-1}$].

The unsaturated hydraulic properties are parameterised by the Mualem-van Genuchten model (Mualem, 1976; van Genuchten, 1980):

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^{1-\frac{1}{n}}} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \quad (5)$$

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$$K(\Theta) = K_s \Theta' \left[1 - \left(1 - \Theta^{n/[n-1]} \right)^{1-1/n} \right]^2 \quad (6)$$

with

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (7)$$

where θ_r [-] and θ_s [-] are the residual and saturated water contents, respectively, α [m^{-1}] is the inverse of the air entry value, n [-] is a pore size distribution factor, K_s [m d^{-1}] is the hydraulic conductivity at saturation, Θ [-] is the effective saturation, and l [-] is a pore-connectivity factor.

Root water uptake is described by the model of Feddes et al. (1978) where the sink term S is defined as

$$S(h) = \beta(h) S_p \quad (8)$$

with $\beta(h)$ [-], a stress response function for root water uptake ($0 \leq \beta \leq 1$) and S_p [d^{-1}] the potential water uptake rate (Šimůnek et al., 2005).

2.2.2 Material model

The material model was set up employing the textural information of the soil profile shown in Fig. 1. The partitioning into different layers was adapted to the observed boundaries of soil horizons (Sect. 2.1) and the availability of TDR probes installed in the profile. We chose five uniform layers with a constant vertical discretisation of 0.01 m. The first layer represents the humous plough horizon. It is followed by the homogeneous sandy loam located between 0.28 m and 0.82 m. Soil layer 3 is modelled as two separate layers in order to account for the continuous increase in clay content with depth. In fact, this textural transition implies also a continuous alteration of the hydraulic properties which is not represented in our material model, however. For the

deeper section of the profile we simplified the model by adding the small layer of gravels with loamy matrix that occurs below 1.44 m depth to the fourth model layer. Additionally, we inserted a further layer at the lower end of the profile (1.55 m to 4.00 m) for representing the coarse grained gravels and sands below. This transition is expected to act as a capillary barrier which is assumed to be hydraulically relevant. Due to the high fraction of gravel and stones no further TDR probes could be installed below 1.44 m in the soil profile.

According to the information from the texture analysis we used standard parameters for sandy loam (Carsel and Parrish, 1988) provided in the HYDRUS-1D database as a first reasonable initial estimate for the Mualem-van Genuchten parameters of the upper four model layers. For each parameter, bounds were used to limit the inversion to a reasonable parameter range (Table 2). To investigate the uniqueness of the estimated parameters, inverse simulations were repeated using loam, silt loam and loam (Carsel and Parrish, 1988) as initial parameter guesses. In all runs, the standard values for the water content at saturation θ_s of each layer were replaced by the measured porosities which were assumed to be equal to θ_s . For the coarse grained sediments of model layer 5 we used hydraulic parameters of sand given by Carsel and Parrish (1988). Since no TDR measurements in this layer are available these initial values were kept constant during all simulation runs.

2.2.3 Initial and boundary conditions

Estimating the initial pressure head profile for a field soil under non-steady state conditions is difficult since the exact distribution of the soil moisture content over depth is not known. Hence, for a first guess, pressure heads for day 777 (the first day in the simulations, Fig. 2) were calculated from the inverse of Eq. 5, $h(\theta)$, for the water contents measured at the different TDR probes. These point values were then interpolated linearly for each model cell between the installed sensors. The pressure heads calculated for the upper- and lowermost TDR positions were extrapolated to the layer boundaries of model layer 1 and 4, respectively (Fig. 3). For the pressure head con-

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dition in model layer 5 we assumed hydrostatic equilibrium conditions for initialisation of the model. To allow an equilibration of the artificially set initial pressure heads we used a spin-up time of 45 days and started the inverse parameter estimation subsequently. The calculation of the initial pressure head distribution using the measured water contents was included in the update-loop of the inversion (see Sect. 2.2.4).

The lower boundary of the model was realised by a groundwater table ($h=0$) at 4 m depth, which is deep enough to prevent an influence of the capillary fringe on the measured water contents in the upper section of the profile. In reality, the water table is some 10 m below ground surface (Arbeitsgruppe Hydrogeologische Kartierung und Grundwasserbewirtschaftung Rhein-Neckar-Raum, 1999).

For the transient upper boundary condition we used daily sums of precipitation and daily average values of reference evapotranspiration (Fig. 2). Reference evapotranspiration j_0^{ET} [mm d^{-1}] as part of the upper boundary condition was calculated from daily average values of air temperature, relative humidity, wind speed and net radiation using the FAO Penman-Monteith equation (Allen et al., 1998)

$$j_0^{ET} = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T + 273} u_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34u_2)}, \quad (9)$$

where R_n is the net radiation at the crop surface [$\text{MJ m}^{-2} \text{d}^{-1}$], G is the soil heat flux density [$\text{MJ m}^{-2} \text{d}^{-1}$], T is the air temperature [$^{\circ}\text{C}$] and u_2 is the wind speed [m s^{-1}], both at 2 m height, e_s is the saturation vapour pressure [kPa], e_a is the actual vapour pressure [kPa], $e_s - e_a$ is the saturation vapour pressure deficit [kPa], Δ is the slope of the vapour pressure curve [$\text{kPa } ^{\circ}\text{C}^{-1}$], and γ is the psychrometric constant [$\text{kPa } ^{\circ}\text{C}^{-1}$]. Since, on a daily basis, the soil heat flux G can be assumed to be relatively small compared to R_n (Allen et al., 1998) it was neglected in our calculations of j_0^{ET} . The FAO Penman-Monteith equation yields a reference evapotranspiration assuming a “hypothetical crop with an assumed height of 0.12 m, with a surface resistance of 70 s m^{-1} and an albedo of 0.23, closely resembling the evaporation from an extensive surface of

green grass of uniform height, actively growing and adequately watered” (Allen et al., 1998).

Since the Grenzhof Test Site is covered with grass, in this study, reference evapotranspiration j_0^{ET} was initially assumed to be equal to potential evapotranspiration.

5 Following Campbell and Norman (1998) potential evaporation j_0^E can be calculated using $j_0^E = \tau j_0^{ET}$, and potential transpiration j_0^T is derived from $j_0^T = (1 - \tau) j_0^{ET}$. The fraction of incident radiation τ [-] which reaches the soil surface and is not intercepted by the canopy is derived from

$$\tau = \exp(-kL_t) \quad (10)$$

10 where k is the extinction coefficient [-] which was set to a constant value of 0.398 (Ritchie, 1972), and L_t [-] is the leaf area index. L_t was calculated according to Menzel (1997) who determined an empirical formulation for the leaf area index of grassland

$$L_t = -1.552 + 51.188h_g - 74.967h_g^2 \quad (11)$$

15 where h_g [m] is the height of the grass. Since we use the FAO Penman-Monteith reference evapotranspiration j_0^{ET} (Eq. 9), the height of the grass was set to a constant value of 0.12 m for calculating L_t , even if h_g at the Grenzhof Test Site was lower on average.

20 Root water uptake was simulated employing the model of Feddes et al. (1978). We used root water uptake parameters for grass according to Taylor and Ashcroft (1972), both as provided in HYDRUS-1D. For the rooting depth only a rough estimation from visual inspection of a soil profile was available. Grass roots were densely distributed within the top 0.08 m and decreasing rather sharply below. In the model this was realized by applying a homogeneous root distribution over the first eight centimeters and then decreasing it by a factor of two for each consecutive model cell of 0.01 m
25 thickness over the following 0.06 m. The impact of this parameter was explored by running simulations with various homogeneous rooting depths for the upper dense section and the same decrease in root distribution below.

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2.2.4 Inverse parameter estimation

Inverse estimation of the hydraulic parameters was conducted by choosing the objective function

$$OF(\mathbf{b}) = \sum_{i=1}^N [\theta_{\text{meas}}(t_i) - \theta_{\text{sim}}(t_i, \mathbf{b})]^2 \quad (12)$$

5 where θ_{meas} and θ_{sim} are measured and simulated volumetric water contents, respectively, N is the number of observations, and \mathbf{b} is the parameter vector. For the inversion we applied a trust-region solver. In contrast to standard optimisation algorithms such as Levenberg-Marquardt (Marquardt, 1963), trust-region methods do not operate on a single point in parameter space, but approximate the local neighbourhood, and minimize over this region. This increases the stability of the algorithm and makes it less susceptible of getting trapped in local minima. The algorithm we used is described in Coleman and Li (1996). An implementation is provided by the MATLAB optimisation toolbox, which uses preconditioned conjugate gradients (Hestenes and Stiefel, 1952) to solve the linear equation system for each step.

15 An overview of the workflow of the inversion procedure is shown in Fig. 4. Inverse estimation of hydraulic parameters was initially done by optimisation of the parameter vector $\mathbf{b}=(\theta_r, \alpha, n, K_s)$. Parameter estimation was conducted for model layers 1 to 4. This leads to a 16-dimensional optimisation problem. To reduce the probability of ill-posedness of the inverse problem, the water content at saturation θ_s was assumed to be equal to the measured porosities and hence was not inverted. Also the pore connectivity factor l was set to a constant value of 0.5 as suggested by Mualem (1976).

20 The inverse simulations were done by using HYDRUS-1D in the forward mode as a module of the parameter optimisation which was implemented in MATLAB. The first inversion run was conducted using the initial guesses for the hydraulic parameters of each layer and the previously calculated initial pressure head profile. After each inversion step, the optimised Mualem-van Genuchten parameters were updated in the

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forward model. Additionally, the initial pressure head profile was recalculated and updated in the forward model using the measured water contents from the different TDR probes together with the optimised parameters from the actual inversion step.

For minimisation of the objective function we used daily average values of measured water contents from one of the soil profiles (see Sect. 2.1) of the TDR probes installed at 0.63 m, 0.92 m and 1.16 m depth (Fig. 2). Data from the TDR probe at 0.30 m was neglected since this probe is located very close to the first layer boundary and measured water contents are expected to be a mixture of water contents in the first and in the second layer. For the estimation of hydraulic parameters of the uppermost layer we used water contents measured in the adjacent soil profile at 0.13 m depth assuming textural homogeneity over this short distance of 2.8 m.

3 Results and discussion

3.1 Measured data

We used measurements from the time interval ranging from 15 February 2006 to end of January 2007 (Fig. 2). The data set contains volumetric soil water contents and atmospheric boundary conditions (reference evapotranspiration and precipitation) covering almost 12 consecutive months including a wide range in soil water contents with high values in winter and low soil water contents during summer. The meteorological data of the first 45 days were used for model spin-up to allow distortions caused by the calculated initial pressure head distribution to equilibrate. Data from April 2006 to January 2007 were employed for inverse parameter estimation.

The most significant changes in volumetric soil water content can be observed at the uppermost TDR probe which shows a very high variation particularly during the summer months. In contrast, the deeper TDR probes experience a comparably moderate decrease in water contents during summer. In total, a number of 1228 daily average water content values were available for the parameter estimation. As expected, ref-

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erence evapotranspiration shows very low values during winter and high values during summer. The precipitation data shown in Fig. 2 represent the random incoming fluxes across the soil-atmosphere interface. In August 2006 the rain gauge was clogged for several days. To account in the model for the lack in incoming fluxes the amount of water (25 mm) which was removed from the clogged funnel of the device was distributed uniformly over the measured precipitation values of the time period between 23 August 2006 and 30 August 2006 where the TDR probe at 0.13 m depth showed a significant increase in soil water content.

3.2 Inverse simulations

Inverse simulations were conducted for different model setups. In a first run the parameters θ_r , α , n and K_s were estimated for the first four model layers using the precipitation and reference evapotranspiration values shown in Fig. 2 as upper boundary conditions. Initial parameters for sandy loam (Carsel and Parrish, 1988) were applied according to the information from the texture analysis for calculation of the initial pressure head profile and as initial parameter guess for the inversion. The rooting depth was set to 0.08 m as it was observed during the profile excavation. Evapotranspiration was prescribed as given in Sect. 2.2.3. To investigate the influence of rooting depth, the simulation was repeated using a rooting depth of 0.12 m. Measured and simulated volumetric water contents resulting from the inverse simulations are compared in Fig. 5. Focusing here on the uppermost TDR probe, measured water contents in both runs clearly cannot be reproduced adequately by the inverse model. During March and April, when evapotranspiration increases (Fig. 2), simulated water contents already show a significant decrease while the measured data still remain at the high winter values. Moreover, the model is not able to reach the very low water contents measured during dry periods in summer. To assess the dependence of the inversion result on both the rooting depth and the initial set of hydraulic parameters the simulations for both rooting depths were repeated using loam, silt loam and silt (Carsel and Parrish, 1988) as initial parameter guesses. At the position of the uppermost TDR probe all

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simulations led to water content evolutions which were similar to those described for the sandy loam examples above (results of other materials not shown here) and did not qualitatively improve the result of the inversion.

Since we trust the rainfall measurements from the weather station and surface run-on on the flat site can be neglected, we suspect the reason for the poor inversion results in the reference evapotranspiration. On average, the grass at the test site is shorter than the 0.12 m underlying the FAO Penman-Monteith equation. Hence, evapotranspiration may be expected to be less than calculated. The difference between reference evapotranspiration and evapotranspiration from a crop surface with specific properties being different from the reference surface is incorporated into a crop factor κ [-] such that $j_C^{ET} = \kappa j_0^{ET}$ (Allen et al., 1998). The application of the crop factor still assumes standard conditions. Hence, influences of soil water availability, which are accounted for in the root water uptake function of HYDRUS-1D, are not considered when using j_C^{ET} . In our simple approach, we presume that the general shape of the calculated reference evapotranspiration curve is correct, and that j_0^{ET} can be scaled with a constant value for κ . This is a highly simplified model since κ may be expected to vary in time. This may be due to changes in the height of the canopy, reduced evaporation caused by a very dry soil surface, or different development stages of the crop to name some.

In a next simulation we used κ as an additional parameter in the objective function of the inversion. All other parameters were treated as in the previous runs leading to the parameter vector $\mathbf{b} = \{\theta_r, \alpha, n, K_s, \kappa\}$. Simulations were again conducted using four different rooting depths: 0.08 m, 0.10 m, 0.15 m, and 0.20 m in combination with literature values for sandy loam, loam, silt loam and silt (Carsel and Parrish, 1988) for model initialisation. This leads to 16 different model realisations.

The simulated volumetric water contents resulting from all 16 runs in comparison with the measured data at each TDR probe are shown in Fig. 6. The goodness of fit of every simulation was evaluated by calculating the root mean square error (RMSE) of all measured and simulated water contents which ranged between 0.013 and 0.038 in the different runs. For better distinction between simulations with low and high RMSE

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values runs with an RMSE of 0.013 are shown with red lines, runs leading to larger RMSE values are displayed in grey.

Since the different simulations do not result in a common water content evolution it is first obvious that our model is not able to find a global minimum in the parameter space. We attribute this to the high-dimensionality of the problem and the occurrence of local minima as has already been observed in similar modelling studies, e.g. by Ritter et al. (2003) and Wöhling et al. (2008). However, seven out of 16 runs lead to an RMSE between measured and simulated water contents of 0.013 and nearly equal temporal developments of water contents at the different TDR probes. Focusing only on these simulations (Fig. 6), the inclusion of κ in the objective function improves the results of the inverse simulations significantly and now leads to reasonable fits between measured and simulated data. Particularly, the water contents at the position of the uppermost TDR probe are reproduced much better than in the simulations without κ .

The success of the inversion leading to low differences between measured and simulated water contents predominantly depends on the choice of the parameter set taken for initialising the model. Low RMSE values result from simulations using sandy loam and loam as initial parameter set whereas silt and silt loam lead to higher deviations between measured and simulated data. The estimated hydraulic parameters and values of κ of the runs leading to an RMSE of 0.013 are listed in Table 2. All these inverse simulations give reasonable parameter sets for the soil under investigation. Even so, the inferred parameter sets are not equal if different initial parameter guesses are used. This is primarily true for the inverse of the air entry value, α , which, especially for soil layer 2 and 3, in most simulations is enhanced by a factor of about two if sandy loam is taken as initial parameter guess compared to the loamy case. However, even though the inverse model is not robust with regard to the resulting Mualem-van Genuchten parameters, the calculated cumulative fluxes across the upper boundary and through the root zone of the model (Fig. 7) are very robust throughout all these simulations. This makes us confident that the calculated fluxes are reasonable. In contrast to the Mualem-van Genuchten parameters, rooting depth has almost no influence on the sim-

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ulated water content evolutions in the fine grained soil at our site. This is manifest in the nearly equal Mualem-van Genuchten parameters calculated for different rooting depths if the same initial parameter guess is used. This is in accordance to modelling results conducted by Hupet et al. (2002) who found that soil water content has a low sensitivity concerning root water uptake parameters compared to soil hydraulic properties.

The value of κ resulting from the inverse simulations leading to an RMSE of 0.013 is quite similar in all runs and ranges between 0.59 and 0.62 meaning that the calculated reference evapotranspiration using the FAO Penman-Monteith formula is reduced by the model by more than one third. This also shows the strong influence of κ on the absolute fluxes entering the root zone of the soil profile. Additionally, for the time period of our simulations, about 3/4 of the water entering the root zone of the model is immediately removed by transpiration within the uppermost few centimeters of the profile and only a small amount of water is transferred to deeper sections of the soil. During summer, water is even taken from greater depths to be available for evapotranspiration. This observation stresses the need for a correct representation of the processes occurring in soil-plant-atmosphere continuum in this kind of model study.

Taking a closer look at the residuals between measured and simulated water contents (Fig. 8), one can still observe significant differences between measured and simulated data. Most prominently, end of May and beginning of August, after longer, very dry periods and a following period of longer and continuous rainfall (cf. Fig. 2), the simulated water contents at 0.13 m depth rise much earlier than do the measured data. We presume that this discrepancy results from our simple representation of the crop factor which, in fact, should be a function of time. During these time periods modelled evapotranspiration is less than actual evapotranspiration. For the deeper layers of our model, simulated changes in volumetric water contents are generally more damped than in the measurements (Fig. 6), meaning that simulated water contents react slower to variations of near-surface water contents than they do in reality. The most significant difference between measured and simulated water contents occurs in August 2006 at the TDR probes at 0.63 m and 0.92 m depth. During this time the grass at the site had

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grown significantly higher and should also have resulted in a higher transpiration rate. At the same depths, single wetting events, e.g. at the beginning and end of October, occur later in the simulations than they do in the measurements which may again be an indication for a stronger coupling of the deeper soil sections to the processes in the uppermost layers or, potentially, be a sign for preferential flow.

3.3 Discussion of overall results

We explain the observed deviations between measured and modelled water contents by the rather complicated reality which is not represented in our comparably simple 1-dimensional model. The model is by nature unable to reproduce three-dimensional phenomena like horizontal run-off on layer boundaries and it also has no provisions for preferential flow. Furthermore, the vegetation model is still fairly simple and neglects the influence of changes in crop height as well as temporal variations in the ratio between evaporation and transpiration. Finally, soil hydraulic parameters are presumed to be static, but may not be so.

While all the approximations used for setting up the model originate from an intuitive assessment, eventual justification emanates from a successful representation of all the available data. The decision if the model is “successful” may depend on the questions to be addressed: Since the observed water contents are fitted reasonably well and calculated fluxes are robust with respect to the obtained range of in Mualem-van Genuchten parameters, the estimated average water flow is expected to be correct for the analysed time period. For practical issues this could, for instance, be applied for estimating groundwater recharge. Also for large-scale hydrologic models the parameters may be applicable to describe average water movement in this specific soil compartment.

Finally, we comment that constant hydraulic parameters are a basic assumption of our model. Whether this is a valid one remains to be demonstrated with additional data.

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4 Summary and conclusions

We estimated the hydraulic properties of a layered field soil from numerical inversion of a time series of in situ measured volumetric soil water contents. The model was driven by the transient fluxes across the soil-atmosphere-interface which were measured by an automatic weather station located next to the instrumented soil profile. The inverse estimation of hydraulic parameters, while based on a rather simple process model results in quite a reasonable agreement between measured and simulated data. This, together with the rather wide range of hydraulic states covered by the data and the reasonable values of the estimated parameters makes us confident that the obtained parameters are useful for large scale applications for the time period of the inverse parameter estimation.

One important observation revealed by our simulations is the importance of the fluxes passing the soil-vegetation-atmosphere continuum. Here, rather accurate values of the time-dependent evapotranspiration fluxes are necessary to better represent the upper boundary of the model which drives the simulation.

Besides of being very cost effective, the method circumvents two crucial issues: (i) extraction of undisturbed soil samples and (ii) estimating field-scale properties from those determined in the lab. Similarly comprehensive data sets are recorded in many transient field experiments by many monitoring stations, hence the method is broadly applicable. Furthermore, it is broadly applicable since the required data are gathered by many monitoring stations. If this is not the case, installation of sensors is quick, and cheap if manual reading is chosen which suffices for many situations. The method has clear limitations as was illustrated by the postulated preferential flow. This is more in the model formulation, however, and not so much in the actual method. While further studies will have to substantiate the claim, we see the prospect of abandoning lab experiments entirely as far as field-scale understanding and prediction is the goal.

Based on this study, we propose that for a site where continuous measurements of soil water content and meteorological data are available and the soil is not subject

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to preferential flow, inverse estimation of effective hydraulic parameters from in situ measurements is a good alternative to traditional lab methods.

Acknowledgements. We thank Eckart Boxheimer for access to his field, Michael Sommer, ZALF Müncheberg for textural analysis of soil samples, and Carolin Ulbrich and Angelika Gassama for measuring porosity. Gabriele Schenk implemented the calculation of confidence intervals in our MATLAB code. Financial support was provided by the Deutsche Forschungsgemeinschaft (DFG): project RO 1080/8-1,2.

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Table 1. Configuration of weather station: sensors used for this study.

value	sensor
air temperature/rel. humidity	MP100A Temperature and Relative Humidity Probe ^a
wind speed/direction	05103 Wind Monitor ^b
radiation	CNR 1 Net Radiometer ^c
precipitation	52202 Tipping Bucket Raingauge ^b
volumetric soil water content	TDR100 Time domain reflectometer ^d SDMX50 Multiplexer ^d TDR probe CS610 ^d
soil temperature	107 Temperature Probe ^d AM16/32 Relay Multiplexer ^d

^a Rotronic AG, Switzerland; ^b R. M. Young, Traverse City, MI; ^c Kipp & Zonen, Delft, The Netherlands; ^d Campbell Scientific, Logan, UT.

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Table 2. Example set for initial hydraulic parameters (here sandy loam for layer 1...4 and sand for layer 5 – Carsel and Parrish, 1988) and parameter bounds used in model layers 1...4 for the inversion. The pore connectivity factor l was set to 0.5 for each layer. Mualem-van Genuchten parameters of model layer 5 were kept constant throughout the inversion.

	θ_r [-]	θ_s [-]	α [m ⁻¹]	n [-]	K_s [md ⁻¹]
<i>initial</i>					
layer 1	0.065 [0...0.08]	0.39 [-]			
layer 2	0.065 [0...0.09]	0.40 [-]	7.50 [0.2...50]	1.89 [1.1...4.0]	1.061 [10 ⁻³ ...10 ³]
layer 3	0.065 [0...0.10]	0.36 [-]	(layers 1...4)	(layers 1...4)	(layers 1...4)
layer 4	0.065 [0...0.10]	0.36 [-]			
layer 5	0.045	0.43	14.50	2.68	7.128

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Table 3. Effective hydraulic parameters and crop coefficients inferred from simulations with RMSE = 0.013. Values in brackets indicate 95% confidence intervals.

	θ_r [-]	α [m ⁻¹]	n [-]	K_s [md ⁻¹]		θ_r [-]	α [m ⁻¹]	n [-]	K_s [md ⁻¹]
<i>IC: sandy loam; rooting depth: 0.08 m</i>					<i>IC: loam; rooting depth: 0.10 m</i>				
layer 1	0.02 (0.009)	4.57 (0.37)	1.65 (0.03)	4.88 (2.92)	layer 1	0.03 (0.006)	3.53 (0.28)	1.61 (0.03)	2.81 (1.54)
layer 2	0.07 (0.01)	11.72 (1.23)	1.74 (0.06)	0.60 (0.07)	layer 2	0.07 (0.008)	5.71 (0.43)	1.97 (0.02)	0.30 (0.05)
layer 3	0.08 (0.03)	6.57 (1.84)	1.38 (0.06)	0.11 (0.05)	layer 3	0.07 (0.02)	3.58 (0.56)	1.54 (0.03)	0.03 (0.006)
layer 4	0.08 (0.02)	3.74 (0.70)	1.28 (0.03)	0.31 (0.15)	layer 4	0.07 (0.03)	2.46 (0.45)	1.35 (0.03)	0.73 (1.46)
κ : 0.61 (0.01), RMSE: 0.013					κ : 0.61 (0.01), RMSE: 0.013				
<i>IC: sandy loam; rooting depth: 0.10 m</i>					<i>IC: loam; rooting depth: 0.15 m</i>				
layer 1	0.02 (0.007)	4.82 (0.33)	1.61 (0.007)	2.02 (0.65)	layer 1	0.02 (0.008)	3.44 (0.32)	1.62 (0.04)	2.18 (1.12)
layer 2	0.07 (0.008)	10.95 (1.13)	1.80 (0.01)	0.47 (0.09)	layer 2	0.06 (0.009)	6.50 (0.63)	1.83 (0.06)	0.46 (0.09)
layer 3	0.09 (0.01)	7.43 (1.47)	1.43 (0.01)	0.09 (0.02)	layer 3	0.07 (0.02)	4.41 (0.72)	1.49 (0.04)	0.04 (0.009)
layer 4	0.10 (0.03)	2.87 (0.52)	1.36 (0.02)	0.37 (0.34)	layer 4	0.07 (0.03)	1.97 (0.24)	1.44 (0.04)	0.41 (0.21)
κ : 0.61 (0.02), RMSE: 0.013					κ : 0.60 (0.01), RMSE: 0.013				
<i>IC: sandy loam; rooting depth: 0.15 m</i>					<i>IC: loam; rooting depth: 0.20 m</i>				
layer 1	0.03 (0.01)	4.09 (0.31)	1.83 (0.08)	1.92 (0.81)	layer 1	0.02 (0.006)	3.56 (0.31)	1.52 (0.03)	1.31 (0.32)
layer 2	0.06 (0.009)	11.89 (1.77)	1.79 (0.07)	0.43 (0.11)	layer 2	0.05 (0.008)	5.72 (0.47)	1.78 (0.02)	0.65 (0.12)
layer 3	0.10 (0.04)	3.92 (1.15)	1.48 (0.04)	0.10 (0.04)	layer 3	0.07 (0.01)	3.61 (0.47)	1.53 (0.02)	0.03 (0.007)
layer 4	0.10 (0.09)	2.66 (1.36)	1.39 (0.02)	0.41 (0.34)	layer 4	0.09 (0.01)	2.92 (0.33)	1.36 (0.02)	0.25 (0.08)
κ : 0.59 (0.01), RMSE: 0.013					κ : 0.62 (0.01), RMSE: 0.013				
<i>IC: sandy loam; rooting depth: 0.20 m</i>									
layer 1	0.04 (0.02)	5.11 (0.51)	1.62 (0.02)	5.00 (4.01)					
layer 2	0.06 (0.008)	11.22 (0.94)	1.75 (0.02)	0.59 (0.08)					
layer 3	0.09 (0.02)	6.33 (1.49)	1.44 (0.02)	0.09 (0.02)					
layer 4	0.10 (0.04)	2.74 (0.76)	1.38 (0.02)	0.32 (0.20)					
κ : 0.59 (0.01), RMSE: 0.013									

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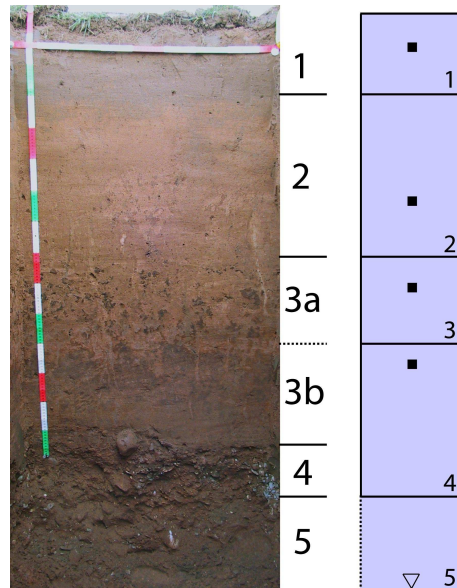


Fig. 1. Soil profile from the Grenzhof Test Site (left). The different colours on the scale indicate intervals of 0.1 m. 1: humous plough horizon; 2: sandy loam; 3a: dense sandy loam, aggregates of secondary minerals; 3b: dense sandy loam; 4: gravel, loamy matrix; 5: gravel, sandy matrix; right: model layers used for the numerical simulations and positions of TDR probes (black squares).

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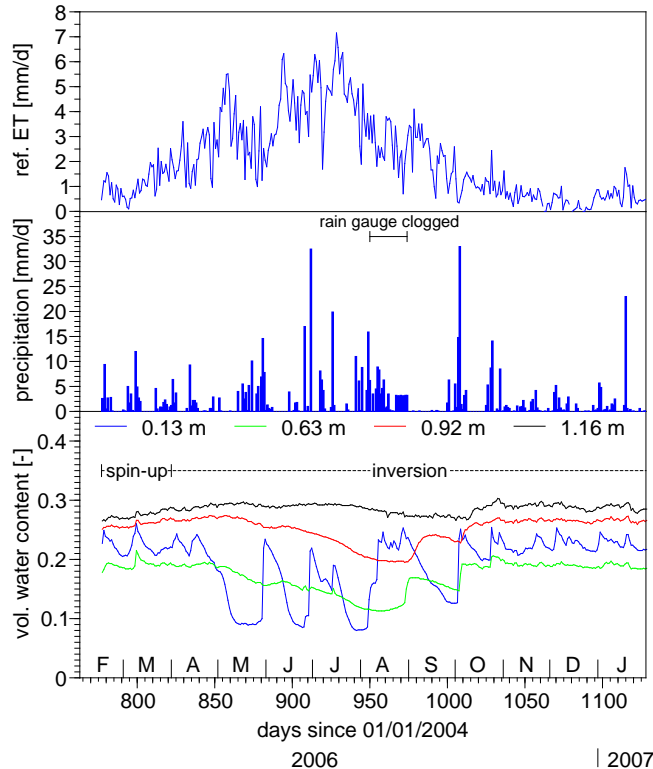


Fig. 2. Daily average values of reference evapotranspiration, daily sums of precipitation and daily average values of volumetric soil water content measured at the Grenzhof Test Site between February 2006 and January 2007. Meteorological data from the first 1.5 months (February to March 2006) were used for model spin-up, data starting from April 2006 was taken for inverse parameter estimation.

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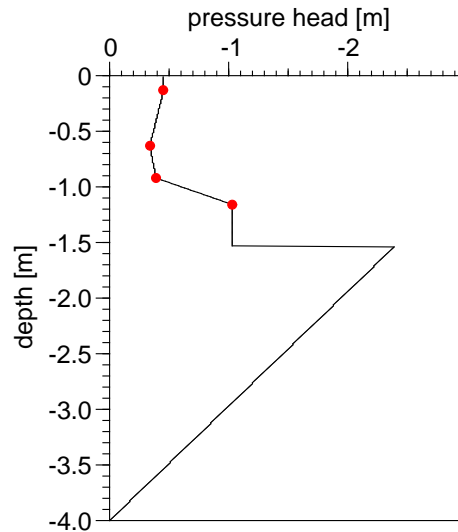


Fig. 3. Initial pressure head condition exemplified for sandy loam considered as initial parameter set for the inverse simulations. Red dots indicate positions of TDR probes.

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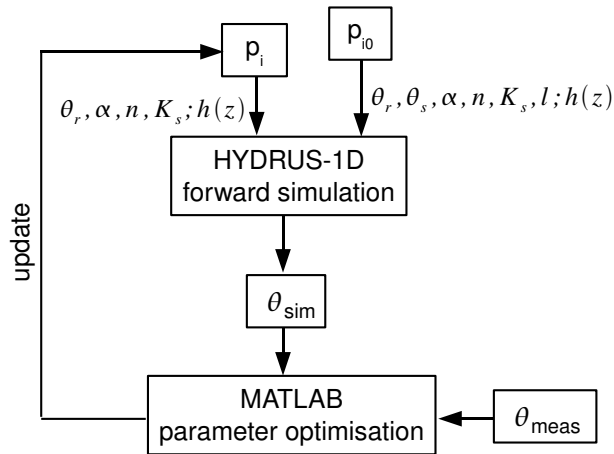


Fig. 4. Workflow of the inverse modelling. The initial parameters p_{i0} for model layers 1...4 were taken from the HYDRUS-1D database (Cassel and Parrish, 1988). In addition to the Mualem-van Genuchten parameters θ_r, α, n and K_s the initial pressure head profile $h(z)$ was updated subsequently for every single inversion step.

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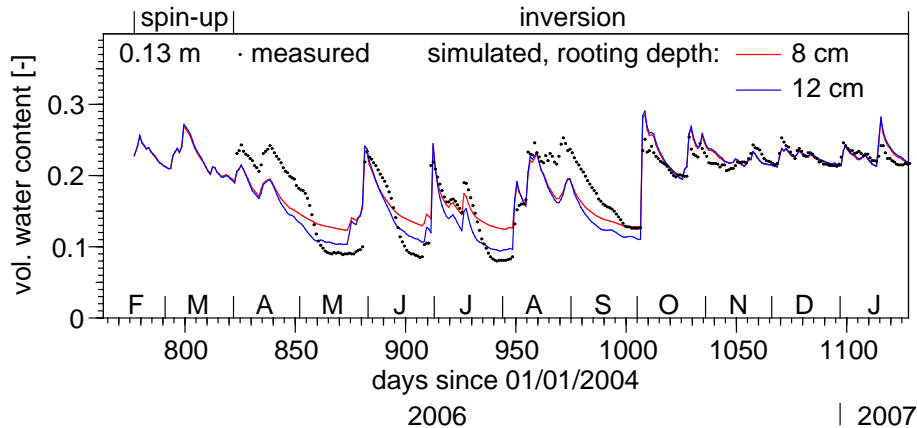


Fig. 5. Results of inverse simulations for the temporal water content evolution at 0.13 m depth using measured precipitation and calculated reference evapotranspiration (j_0^{ET}) data to represent upper boundary fluxes. Results calculated for two different rooting depths are compared to the measured water contents. During summer (high j_0^{ET}) the model is not able to reproduce the evolution of the measured data (only shown for time interval used for inverse parameter estimation).

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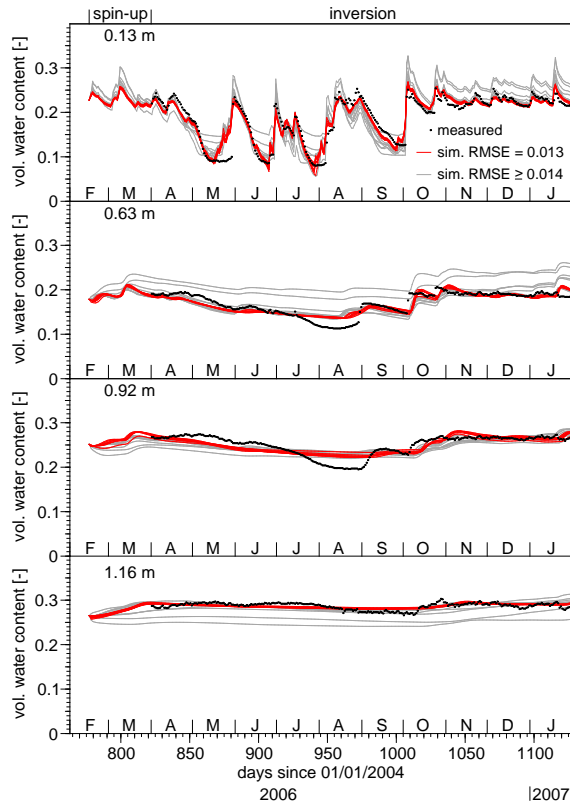


Fig. 6. Results of the inverse simulations using different initial parameter sets (sandy loam, silt, silt loam, loam – Carsel and Parrish, 1988) and various rooting depths (0.08 m, 0.10 m, 0.15 m, 0.20 m); black dots: measured water contents (daily average values, only shown for time interval used for inversion); red lines: simulated water contents, $RMSE = 0.013$ ($n=7$); grey lines: simulated water contents, $RMSE \geq 0.014$ ($n=9$).

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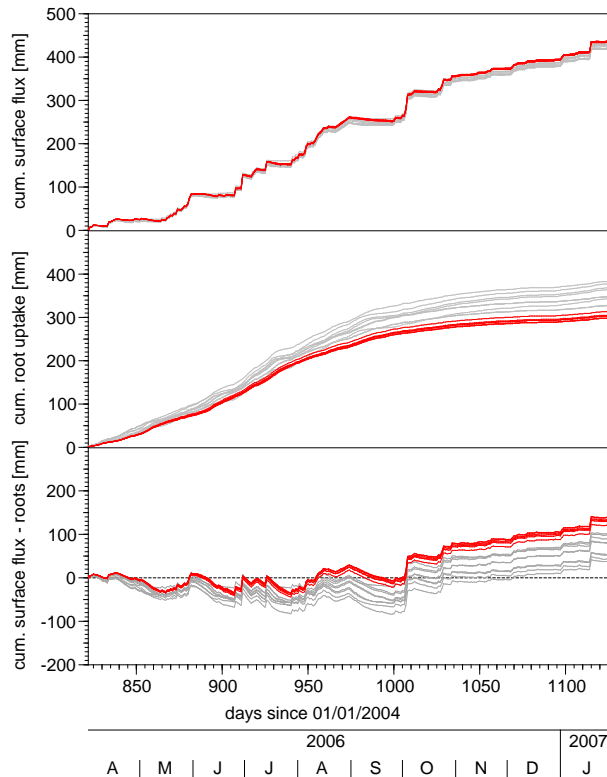


Fig. 7. Cumulative fluxes calculated for the time period of inversion, top: surface flux (precipitation minus evaporation from the soil surface), middle: root water uptake, bottom: water flux passing the root zone; red: $RMSE = 0.013$; grey: $RMSE \geq 0.014$. Considering only the simulations with $RMSE$ of 0.013, during the time period under investigation approximately 3/4 of the water infiltrating the soil profile is removed by root water uptake.

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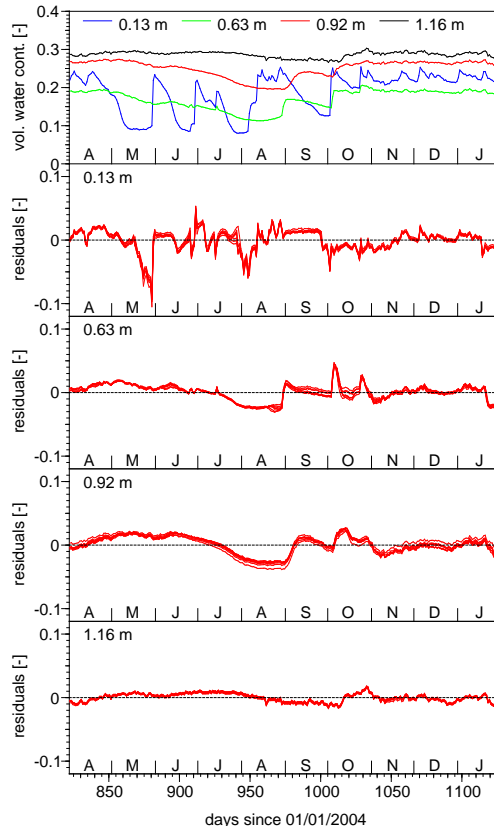


Fig. 8. Residual water contents (measurement-simulation) at the different TDR probes calculated for runs with RMSE between measured and simulated water contents of 0.013. For comparison, measured water contents are displayed in the topmost frame of the figure.

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