Four Decades of Progress in Monitoring and Modeling of Processes in the Soil-Plant-Atmosphere System: Applications and Challenges

Simultaneous estimation of soil hydraulic and root distribution parameters from lysimeter data by inverse modeling

Henrike Schelle\(^\text{a}\)*, Wolfgang Durner\(^\text{a}\), Sascha C. Iden\(^\text{a}\), Johann Fank\(^\text{b}\)

\(^\text{a}\)Institute of Geoecology, TU Braunschweig, Langer Kamp 19c, 38106 Braunschweig, Germany

\(^\text{b}\)Resources, Joanneum Research, Elisabethstraße 16 / 2, A-8010 Graz, Austria

Abstract

Weighable lysimeters are powerful measurement systems for identifying soil hydraulic processes and properties, because the boundary fluxes (precipitation, actual evapotranspiration, and seepage across the bottom) can be determined very precisely. However, root water uptake by plants and the soil water flux are interrelated. Thus, the simultaneous estimation of root water uptake parameters and soil hydraulic parameters from macroscopic state observations is a challenge. In this study we investigated the possibility of simultaneously estimating root water uptake and soil hydraulic parameters by inverse simulation of soil water flow in monolithic lysimeters under atmospheric boundary conditions. We used the Richards equation and a macroscopic root water uptake model to simulate the processes. The amount of information needed for the unique identification of parameters was analyzed and the magnitude of their uncertainties was investigated. To check the principal feasibility of our approach, we first examined synthetic data sets for different scenarios and instrumentation campaigns that differed in their information content and complexity of soil properties. The investigations of synthetic data showed that for homogeneous profiles, cumulative outflow and profile-averaged water content data contained enough system information to allow the simultaneous estimation of soil hydraulic properties and root-distribution parameters. In contrast, for soil profiles consisting of two layers, unique soil hydraulic parameters and the correct rooting depth could only be estimated if matric potential measurements from both layers were included in the objective function. To test the procedure with real data, soil hydraulic properties of the grass-reference lysimeter at Wagna (Austria) were estimated using actual measurements. Water dynamics in the lysimeter could be described well by an effective parameterization assuming a homogeneous soil profile. Furthermore, the system behavior under different boundary conditions could be predicted adequately with the estimated parameters.

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* Corresponding author. Tel.: +49-(0)531-391-5931; fax: +49-(0)531-391-5637.
E-mail address: h.schelle@tu-bs.de.
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1. Introduction

Modeling of water and solute transport in soil-plant-atmosphere systems is often done by numerical simulations, based on the Richards equation. To obtain reliable simulation results, exact knowledge of the soil hydraulic properties (SHPs) at the scale of interest is indispensable. This is problematic, because predictions of water and solute transport for hydrologic management decisions are generally needed at larger scales such as the field scale, whereas SHPs are usually determined in the laboratory on small soil cores. Due to spatial variability and high nonlinearity of SHPs, these were often found to be inadequate for describing water dynamics at larger spatial scales [e.g. 1, 2, 3]. An alternative is to use observations made at the scale of interest under known boundary conditions and to estimate system parameters by inverse modeling [4]. Thereby the system dynamics are simulated by an adequate model and the overall differences between observed data and corresponding simulation results are minimized by an optimization algorithm.

A precondition for inverse parameter estimation with numerical models is the exact knowledge of the initial and boundary conditions [5]. These cannot be accurately determined in the field and are therefore often incomplete and erroneous. This limitation can be overcome by using weighable lysimeters from which the boundary fluxes can be determined very precisely [6]. Particularly, if equipped with additional sensors for water content or matric potential, weighable lysimeters are promising tools for the inverse estimation of system parameters at a relatively large scale and under realistic boundary conditions.

Because soils are generally covered with vegetation, and water uptake by plant roots largely controls water and nutrient fluxes in soils [7], root water uptake has to be included in the simulation of the water dynamics. In the widely used macroscopic approach by Feddes et al. [8] root water uptake is included in the Richards equation as a depth- and pressure-head-dependent sink term. Thus, information about the effective spatial root distribution is needed. But as this is difficult and labor-intensive to measure, the information is seldom available. An alternative approach is to identify depth-dependent root water uptake parameters by inverse simulation [7].

In this study we tested if it is possible to simultaneously identify soil hydraulic and rooting depth parameters by inverse simulation of observations from monolithic lysimeters covered with vegetation and operated under natural atmospheric boundary conditions. This work is based on the paper by Schelle et al. [9], but goes beyond it in specifically examining the possibility to estimate more than one rooting depth parameter. To investigate the feasibility of the approach, we work with synthetic data, generated by forward simulation. Thereby the information content of the synthetic measurements and the complexity of the soil profiles were systematically varied. Boundary conditions determined at the grass-reference lysimeter at the agricultural test field in Wagna (Austria) were used for the water flow scenarios.

2. Material and Methods

2.1. Forward simulations to generate synthetic data

One-dimensional forward simulations of transient water regimes were performed to generate synthetic data which we needed to test our hypotheses. At the upper boundary, realistic atmospheric boundary conditions were applied, based on measurements from the grass-reference lysimeter at the agricultural test site in Wagna, Austria (operated by the Institute of Water, Energy and Sustainability of the Joanneum Research Forschungsgesellschaft m.b.H.). The water dynamics were calculated for the period of one year,
using daily values of precipitation, evaporation and transpiration determined from 1 Jan to 31 Dec 2008. In advance, warm-up simulations covering a period of 12 months were carried out to obtain reasonable initial conditions. We performed simulations in free-draining lysimeters and suction controlled lysimeters (as the one in Wagna), respectively. At the lower boundary, a seepage face condition was used for the free-draining lysimeter, and a time-dependent Dirichlet condition for the suction-controlled lysimeter. Adequate time-dependent pressure head values to parameterize the latter were obtained from a previous simulation of a deeper soil profile. Details are given by Schelle et al. [9]. Synthetic measurement data were sampled in a way as obtained in reality from the grass-reference lysimeter in Wagna, where lysimeter weight and cumulative outflow are monitored with high temporal resolution. We used daily values of cumulative outflow across the lower boundary and water contents averaged over the entire profile, in practice obtained from lysimeter weights.

Three inverse scenario types with increasing information content were calculated: (A) a free drainage lysimeter with seepage face condition at the lower boundary, (B) a suction lysimeter with controlled variable pressure head at the lower boundary, and (C) a suction lysimeter as (B), but additionally equipped with tensiometers at 10 and 50 cm depth to observe matric head data, that are included in the objective function. Scenario (A) provides less information than the other two, because there is no additional pressure head information given by the lower boundary condition. The synthetic measurement data were perturbed with a normally distributed measurement error with zero mean and standard deviation $\sigma$. We used $\sigma_\theta = 1.1 \times 10^{-4}$ for the profile averaged water content, $\sigma_q = 0.01$ cm for cumulative outflow, and $\sigma_h = 1.0$ cm for matric head. The precisions reflect the data quality obtained at the lysimeter in Wagna [6].

2.2. Numerical model

One-dimensional variably saturated water flow including root-water uptake was simulated with the Richards equation:

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

(1)

where $\theta(h)$ is the water retention curve, i.e., volumetric water content $\theta [-]$ dependent on matric head $h$ [cm], $t$ [d] is time, $z$ [cm] is the vertical space coordinate, defined as positive upwards with $z = 0$ cm at the bottom of the simulation domain, $K(h)$ [cm d$^{-1}$] is the unsaturated hydraulic conductivity function, and $S(z,h)$ [d$^{-1}$] is the depth and pressure-head dependent sink term describing the macroscopic water uptake by plant roots. The Hydrus-1D software code [10] was used to numerically solve this equation. In the forward simulations, the soil hydraulic properties were parameterized by the van Genuchten-Mualem (VGM) model [11], using parameter values for a loam soil: $\theta_r = 0$, $\theta_s = 0.3382$, $a = 0.0111$ cm$^{-1}$, $n = 1.4737$, $K_s = 12.04$ cm d$^{-1}$ and $\tau = 0.5$ [9].

In the inverse simulations, we used two different parameterizations for the hydraulic properties. On one hand, we applied the VGM model, which intrinsically means that we used an error-free function of the constitutive relationships in the identification. Since this is in reality never known a priory, we additionally used the free-form (FF) approach by Iden and Durner [12]. In this approach, values of $\theta(h)$ and $\log_{10}[K(h)]$ are locally estimated at $r$ nodes positioned on the log pressure head axis. Continuous functions are then derived by cubic Hermite spline interpolation between these nodal values. As in this manner, $\theta(h)$ and $K(h)$ curves do not have any a priori shape, except for monotony, and both functions are estimated independently from each other, the free-form approach provides a maximal flexibility. This is
on one hand a much more rigorous test for the identifiability of hydraulic functions, which really reflects the information content of the measurements in different moisture regions. On the other hand, it avoids a parameterization error of the SHPs due to the flexibility of the functions and thus any interference with estimates of other parameters, such as rooting depth. Furthermore, it leads to an improved resolution of the estimation uncertainties which can vary significantly in different pressure head ranges [13].

The sink term accounting for root water uptake is defined as [8]

\[ S(z, h) = \gamma(h)S_p(z)T_p \]  

where \( \gamma(h) \) is the dimensionless water stress reduction function of Feddes et al. [8] accounting for reduction of root water uptake due to insufficient aeration under very moist conditions and due to water stress under dry conditions. It was parameterized with values for grass vegetation [14]. The grass vegetation of the grass reference lysimeter is cut regularly to keep it at a constant height of 12 cm. Therefore we assumed the normalized potential root water uptake distribution \( S_p(z) \) to be constant with time. It is given by

\[ S_p(z) = \frac{S_p^*(z)}{\int_0^L S_p^*(z) \, dz} \]  

The potential root water uptake distribution \( S_p^*(z) \) (dimensionless) was considered as a piecewise linear function of depth as proposed by Hoffman and van Genuchten [15]

\[ S_p^*(z) = \begin{cases} 
1 & \text{for } z > L - r_1 \\
\frac{z - [L - (r_1 + r_2)]}{r_2} & \text{for } L - r_1 \geq z \geq L - (r_1 + r_2) \\
0 & \text{for } z < L - (r_1 + r_2) 
\end{cases} \]  

where \( L \) [cm] is length of soil profile, i.e. 90 cm, and the two rooting depth parameters \( r_1 \) and \( r_2 \) [cm] are defined as shown in Fig. 1. In the forward simulations they were set to \( r_1 = 10 \) cm and \( r_2 = 20 \) cm.

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Fig. 1. Overview of the three soil profiles used in the inverse simulations; green lines/patches: relative root water uptake distribution as defined by the two rooting depth parameters \( r_1 \) and \( r_2 \) and equation (4); black squares illustrate the suction cups at the lower boundaries for the application of pressure heads; matric potential sensors are shown in the appropriate measurement depths.
2.3. Inverse modeling scenarios

For each of the three data cases A, B, C, we investigated by inverse simulations whether we can simultaneously estimate the SHP with one rooting depth parameter (A1, B1, C1), or with two rooting depth parameters (A2, B2, C2). As indicated in section 2.2., in each case we parameterized the SHPs by (i) the van Genuchten-Mualem and (ii) the free-form model. Altogether this leads to 12 inverse scenarios with different information content in the data and greatly varying degrees of freedom in the inverse analysis (Tab. 1). In case of the FF model, saturated water content was fixed whereas for the VGM model all parameters were estimated [9]. We used the sum of weighted least squares as objective function, which was minimized by the shuffled complex evolution algorithm (SCE-UA) [16]. The residuals were weighted by the reciprocal of the variance of the measurement error of each data type, i.e., 10,000 cm$^{-2}$ for cumulative outflow, 8.1×10$^7$ for profile averaged water content, and 1.0 cm$^{-2}$ for matric head, respectively.

The root mean square error (RMSE) was calculated for each data type in the objective function to quantify the goodness-of-fit. For the quantification of the uncertainty of the estimated parameters, the parameter covariance matrix (Cov) was calculated by the first-order-second-moment method [13]. Since in this method linearity of the underlying model is assumed, the resulting parameter uncertainty is only approximate [13]. From this 95% confidence intervals were calculated as described by Durner and Iden [13]. To examine the correlation between the two estimated rooting depth parameters in cases A2, B2, and C2, correlation coefficients were calculated from the parameter covariance matrix and the standard errors $\sigma$ of the estimated parameters:

$$\rho(r_1, r_2) = \frac{\text{Cov}(r_1, r_2)}{\sigma(r_1)\sigma(r_2)}$$ (5)

3. Results and Discussion

The measurements used in the inverse analysis are shown in Fig. 2 for scenario A with a seepage-face lower boundary condition (left) and for scenario C with a variable-pressure-head lower boundary condition (right). Measurements from scenario B are not shown, because they are a subset of C (no pressure head data). The figure depicts, from top to bottom, cumulative outflow across the lower boundary, profile averaged water contents, and matric heads at 10 and 50 cm depth. We note that the free drainage lysimeter A shows more rugged outflow dynamics, and distinctly higher mean water contents, which reflects that the missing deep drainage keeps the lysimeter much wetter than its counterpart, where a suction is applied that mimics the typical field condition. The water content changes, however, are of comparable magnitude.

The corresponding matches from the inverse simulations are also shown, exemplarily for cases A1 and C1, i.e., using the VGM functions and simultaneously estimating $r_1$. For scenario A, only matric heads from the inverse simulation are shown, because in that scenario no measured matric head data were involved. Below each plot, residuals between measured data and predictions are depicted. They basically display the measurement error, because the fits to the synthetic observations are excellent, reflecting the fact that there is no systematic model error. All fits yield a very good description of the measurements. This is quantified by the RMSE values, which are close to the stochastic “measurement errors” added to the measurement values (Tab. 1).

Figures 3 and 4 depict the estimated SHPs and rooting depth parameters. In Fig. 3, the identified VGM functions are shown together with the true functions and 95% confidence intervals. These are so small that
Fig. 2: Cumulative outflow, profile averaged water content, and matric head data at 10 and 50 cm depth, generated in the forward simulations; left: with a free drainage lower boundary condition (scenario A), and right: with a variable pressure head condition at the lower boundary (scenario C); synthetic data points, fitted values obtained from scenarios A1 and C1 with one estimated rooting depth parameter and using the van Genuchten-Mualem model, and corresponding residuals (small plots). For scenario A only the model-predicted matric heads based on the best-fit parameters are shown.

...they are hidden by the lines and therefore not visible. The true and estimated rooting depth parameters ($r_1$ in case of scenarios (1) and $r_1$ and $r_2$ in case of scenarios (2)) with standard deviation are depicted as bar charts with error bars; the respective parameter values are listed in Tab. 1. In scenario A, information about pressure heads in the lysimeter system is only indirectly provided by the initial condition. This suffices to accurately identify SHPs in the moisture range reached during the simulation, i.e., from near saturation down to a pressure head of $\log_{10}|h|$ (cm) = 2.45 (Fig. 3-A). Beyond this value, we see a marked difference between true and identified retention functions. It is remarkable that this deviation between the
functions is not reflected in the uncertainty bands of the wrongly estimated SHP. This points to an interesting feature of low-parameterized functions. If the information content in a certain region of the moisture curve is high, it leads to a well-posed inverse problem and small parameter uncertainties. This leads to a small uncertainty of the whole function, which strongly underestimates the true uncertainty in a region where information content is small. We will come back to this when we discuss the fits with the free-form approach. Furthermore, the estimated conductivity functions deviate from the truth in different directions, depending on whether one or two rooting depth parameters have been estimated. This indicates an interference of rooting-depth and SHPs estimation, which is particularly clear in this scenario. A with low information content in the data. Still, it was possible to quite accurately estimate one rooting depth parameter together with the SHPs. But if both \(r_1\) and \(r_2\) are estimated, they cannot be identified at all. This is much better in scenarios B and C. In both cases, the SHPs are estimated correctly over the whole moisture range, and also the rooting depth parameters are estimated accurately (Fig. 3-B and 3-C, Tab. 1). These findings lead to the conclusion that for the given atmospheric boundary conditions, the observations contain sufficient information to correctly identify the hydraulic and rooting depth parameters. However, this is only valid if the model for the SHPs and the process model are free of error, which is an over-optimistic assumption for natural soils.

Fig. 3. True and estimated retention (top) and hydraulic conductivity functions (middle) for scenarios A, B, and C. Inverse modeling was performed using the van Genuchten-Mualem parameterization and simultaneously estimating one (blue) or two (red) rooting depth parameters. Shaded areas, visualizing the 95% confidence bands of the estimated functions, are so small that they are hidden by the lines. The simultaneously estimated rooting depth parameters \(r_1\) and \(r_2\) and their standard errors are given on a normalized scale as bar plots with error bars in corresponding colors (bottom) together.
Table 1. Root mean square errors (RMSE) for the cumulative outflow ($Q$), the profile averaged water content ($\theta$), and the pressure head in the lysimeter ($h$); optimized rooting depth parameters $r_1$ and $r_2$ and their standard errors ($\sigma_1$ and $\sigma_2$) for all scenarios, and the correlation coefficient $\rho(r_1,r_2)$ giving the correlation between the two rooting depth parameters; VGM denotes inversions using the van Genuchten-Mualem model; FF denotes inversions using the free-form approach; $r$ is the number of interpolation nodes for the respective FF parameterization.

<table>
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<tr>
<th>Scenario</th>
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<th>$r$</th>
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<th>RMSE$_\theta$</th>
<th>RMSE$_h$</th>
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<th>$\sigma_1$</th>
<th>$r_2$</th>
<th>$\sigma_2$</th>
<th>$\rho(r_1,r_2)$</th>
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<td>-</td>
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A much stricter test of the identifiability and accuracy of the estimated SHPs is obtained by using the FF parameterization. Contrary to the VGM model, this approach does not assume the same model as was used for the generation of the data, and therefore reflects the information content of the experimental data more accurately. The SHPs obtained with the FF method are depicted in Fig.4. They are shown only in the range of measured data because identification outside the experimentally covered moisture range is not possible and the shape in that range would merely influence the model predictions.

For scenario A (Fig. 4-A), the SHPs can be estimated with the FF approach in the range where information is given. However, missing information in the dry range hinders the correct estimation of the rooting depth parameters. For scenario B, the higher information content of the suction lysimeter data in the medium to dry range, as compared to the gravity drainage lysimeter (scenario A), leads to hydraulic functions that match the true functions excellently in the medium moisture range (Fig. 4-B). But the measured data provide no information on the SHPs near saturation. This is reflected in the widening of the uncertainty bands of the FF functions. As we fixed $\theta_s$ in the FF simulations, in the retention curves, no uncertainties are visible at saturation. Only for scenario C, the identified hydraulic functions match the true functions perfectly down to $\log_{10}|h|$ (cm) = 3.9, i.e., to the wilting point of the grass vegetation. Also, the estimated functions are no longer affected by the interference with the simultaneous estimation of rooting depth parameters. This reflects the gain of information by matric head data in the objective function.

Contrary to the use of the VGM model for the inverse identification, the stricter test using the FF algorithm reveals that the rooting depth can only be estimated correctly, if pressure head data are used in the objective function. This does even work if both $r_1$ and $r_2$ are estimated. However, again the two parameters show a strong negative correlation (Tab. 1). The estimation uncertainty of the rooting depth parameters show that they can be identified more accurately (corresponding to smaller standard deviation), if only one of the two parameters is estimated, and also, if the VGM model is used to parameterize the SHPs (Tab. 1).
4. Summary and Conclusions

Lysimeter systems with adequate instrumentation are excellent tools to study water dynamics in the soil-plant-atmosphere continuum and to transfer the inverse modeling expertise of the vadose zone community from the laboratory to the field scale. In our study, we examined the possibility to simultaneously determine SHPs and rooting depth parameters by inverse modeling of variably-saturated water flow with root water uptake in lysimeter systems, operated under transient atmospheric boundary conditions. A prerequisite for our study was that boundary fluxes, i.e., flow across the lower boundary, precipitation, and actual evapotranspiration are accurately known.

Using synthetic measurement data, we showed that cumulative outflow and profile-averaged water content data in the objective function provided sufficient information for a unique estimation of SHPs in homogeneous soils. However, the accurate estimation of rooting depth parameters strongly depended on the information content of the measurements. If the same model of the SHPs was used in the inversion as was used for the generation of the data, i.e. the VGM model, one rooting depth parameter could be estimated correctly, and even two in case of the suction controlled lysimeters. These provide information into drier ranges, where the water dynamics become more sensitive with respect to the root distribution. In natural field soils, the general shape of hydraulic functions across the full moisture range, including textural and structural components, is generally unknown a priori and rarely (if ever) matched without noticeable error by a low-parameterized model. In this common situation, rooting depth can only be
estimated accurately, if information on pressure heads inside the lysimeter is given (scenario C). Furthermore, additional information from pressure head measurements leads to a marked increase in the precision of the estimated parameters.

These findings suggest that the inverse problem of identifying SHPs and rooting depth parameters is better posed for suction lysimeters than for free draining lysimeters. Also, instrumentation with pressure head sensors is recommended to significantly improve parameter identifiability, as already suggested by Hupet et al. [7] and Schelle et al. [9]. We are aware that our systematic study is based on highly idealized virtual systems, where a multitude of processes that occur in real systems are neglected, such as hysteresis and temporal changes in hydraulic properties, among many others. In that sense, our study is set as a best case, meant to investigate the possibilities and limits of parameter identification under optimal conditions. In real lysimeters, the neglected processes may exacerbate the accurate parameter estimation.

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