Combined Transient Method for Determining Soil Hydraulic Properties in a Wide Pressure Head Range

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Simulation of water flow in unsaturated soils requires knowledge of the soil hydraulic properties. Two standard methods for the simultaneous determination of the water retention and hydraulic conductivity function in the laboratory are the multistep-outflow and the evaporation method. The multistep-outflow method provides information primarily in the pressure head range corresponding to relatively moist conditions, whereas the evaporation method has its highest information content in the medium to dry range. In the moisture ranges not covered by the experiments, an extrapolation of the soil hydraulic functions leads to very uncertain and possibly incorrect estimations of hydraulic properties. To obtain reliable estimates of soil hydraulic properties in a wider range of soil moisture contents, we combined both methods in a successive manner. The combined experiment starts with a multistep-outflow experiment, which is directly followed by an evaporation experiment. We tested this experimental design using synthetic data and laboratory measurements evaluated by inverse modeling. In the evaluation of the combined experiment, data points for the retention and conductivity functions were calculated from the evaporation experiment and included in the objective function for the inverse simulation of the multistep-outflow experiment. The combined evaluation led to greatly improved estimates of the hydraulic properties in a wide moisture range, circumvented the unreliable extrapolation beyond the pressure head ranges of the separate experiments, and significantly reduced the model error caused by such extrapolations.

Abbreviations: EVA, evaporation; FF, free form; MSO, multistep-outflow; MVGB, modified bimodal van Genuchten–Mualem; VGM, van Genuchten–Mualem; VGB, bimodal van Genuchten–Mualem; XMSO, extended multistep-outflow.

Transient water flow in unsaturated porous media is usually described by the Richards equation. For one-dimensional flow without sinks or sources, the Richards equation is written as

$$\frac{\partial \theta(h)}{\partial t} - \frac{\partial}{\partial z} [K(h) \frac{\partial h}{\partial z}]$$

where $\theta$ (dimensionless) is the volumetric water content, $h$ (cm) is the matric potential, $t$ (d) is the time, $z$ (cm) is the distance, positive upward, and $K$ (cm d$^{-1}$) is the hydraulic conductivity. To be able to solve the Richards equation, knowledge of the two soil hydraulic property functions is required, i.e., the soil water retention function $\theta(h)$ and the unsaturated hydraulic conductivity function $K(h)$.

Various standard methods exist for the determination of the water retention and hydraulic conductivity functions in the laboratory (Leij and van Genuchten, 1999; Dane and Topp, 2002). Transient flow experiments like multistep-inflow and -outflow experiments (van Dam et al., 1994; Durner et al., 1999; Hopmans et al., 2002) or evaporation experiments (Wind, 1968; Schindler, 1980; Wendroth et al., 1993; Minasny and Field, 2005) are frequently used for the simultaneous determination of both soil hydraulic functions.
Multistep-outflow (MSO) experiments yield reliable information on the hydraulic properties in the wet range but not near water saturation. Water is extracted from a soil column by applying a suction to a boundary, and outflow across this boundary and the pressure head inside the column are monitored. In theory, the soil hydraulic properties can be measured down to pressure heads of −1000 cm (van Dam et al., 1994). In practice, the pressure head range is limited to smaller suction values because at lower water contents samples may lose contact with the ceramic plate placed below the soil cores (van Dam et al., 1994; Hopmans et al., 2002). Eching et al. (1994) proposed to extend the measurement range of MSO experiments to the dry end by including steady-state retention points from pressure-plate data in the objective function; however, this does not provide direct additional information about the unsaturated hydraulic conductivity function. To yield reliable information about the saturated conductivity from an MSO experiment, we extended the MSO method by starting the experiment with a saturated soil column and an initial ponding on top of the soil column. This makes it possible to determine the saturated hydraulic conductivity, $K_s$ (cm d$^{-1}$), and the unsaturated soil hydraulic properties in one single experiment.

In evaporation (EVA) experiments, the soil water content of a soil column changes during evaporation across the top boundary while water flow across the lower boundary is prevented. These experiments provide reliable information on the soil hydraulic properties down to pressure heads smaller than −1000 cm. With improved tensiometers, which resist cavitation to much lower pressure heads than conventional tensiometers, the range can be extended to about −3000 cm (Schindler et al., 2010a). Due to small hydraulic gradients in the near-saturated water content range, EVA experiments do not provide conductivity data in the wet range (Peters and Durner, 2008b; Schelle et al., 2010). Wendroth et al. (1999) determined saturated and near-saturated hydraulic conductivities by a steady-state percolation method and subsequently analyzed the same soil samples with an EVA method at lower pressure heads.

The few studies comparing soil hydraulic properties obtained from MSO and EVA experiments have shown that both methods yield very similar results in the moisture range where both experiments provide information (Eching et al., 1994; Garnier et al., 1997; Schelle et al., 2010). This suggests applying both methods to get the best out of each method in a combined experiment. A two-stage laboratory method consisting of an MSO stage and an EVA stage has already been presented by Fujimaki and Inoue (2003). With their method, they were able to determine soil water retention across a wide pressure head range. Their method was limited, however, because only data from the evaporation part was used for the calculation of the $K(h)$ function, which implies that they had to interpolate between the data in the dry range and the saturated conductivity, which had to be determined in a separate experiment.

The objective of this study was to develop and analyze the combination of an extended multistep-outflow (XMSO) method with the EVA method of Schindler (1980) to simultaneously determine water retention and hydraulic conductivity functions across a wide range of pressure heads, including the saturated conductivity. In a study with synthetic data, the advantages of the combined method (XMSO-EVA) over the individual methods was evaluated using different parameterizations of the soil hydraulic properties. Subsequently, the method was tested with real data obtained from measurements on undisturbed columns of a sandy loam soil.

**MATERIALS AND METHODS**

**Combined Method: Principle of the Experimental Setup**

In the combined XMSO-EVA experiment, an initially saturated soil sample is subjected to a falling-head percolation experiment (X), followed by an MSO experiment where a stepwise increased suction is applied to the lower boundary, down to a pressure head of about −100 cm. After an equilibration phase, an EVA experiment follows, where water evaporates from the top of the sample while the bottom is sealed (Fig. 1).

As in a standard MSO experiment, a soil column of height $L$ (cm) is placed on a porous plate of height $L_p$ (cm). The water phase below the plate is connected to a pressure reservoir that allows the application of temporally changing pressure heads at the lower boundary, $h_{LB}(t)$ (cm). One or more tensiometers are installed inside the soil core to monitor the pressure heads inside the samples. An extension of the soil cylinder is set on top of the soil column to enable the ponding of water. The upper end is sealed to prevent evaporation, with the exception of a small access tube that allows the gas pressure to remain in equilibrium with the atmosphere.

The soil core is fully saturated from the bottom by applying a gradually increasing pressure head to the water phase at the lower boundary until a ponding height of about $h_p = 2$ cm is reached. Assigning the reference position of the vertical coordinate $z = 0$ cm to the bottom of the porous plate and taking it positive upward, this corresponds to a lower boundary condition of $h_{LB}(t = 0) = h_p + L + L_p$ (cm). The initial condition for the experiment is given by a hydrostatic pressure head distribution, $h(z = 0) = h_{LB}(t = 0) = z$. To initiate the XMSO experiment, the pressure head at the bottom is lowered to 0 cm. This induces a saturated percolation. Both flow rate and ponding head decrease exponentially, in accordance with the classic falling-head experiment (Kutilek and Nielsen, 1994), until the ponding height reaches zero. Then saturated percolation changes to drainage, which implies that the upper boundary condition changes from a pressure head condition to a no-flux condition. The soil sample is then drained further by...
a stepwise decrease in pressure head at the bottom (MSO). Cumulative outflow across the lower boundary, $Q(t)$ (cm), and pressure head inside the sample, $h(t)$ (cm), are monitored. The last pressure step (in this study, −100 cm) is maintained until hydrostatic equilibrium is reached (equilibration phase). Then the water outlet at the lower boundary is closed.

The soil column is removed from the porous plate, sealed at the bottom and placed on a scale. Whereas for the XMSO part of the experiment one tensiometer inside the soil sample is sufficient, for the EVA part two tensiometers at depths 0.25 and 0.75 L are necessary to calculate the hydraulic gradient. The EVA phase starts by removing the lid from the top of the sample to expose the soil to evaporation. Total mass and pressure heads at the two height levels in the soil column are monitored. The experiment continues until the measurement limit of the upper tensiometer is reached.

The soil core is weighed twice, first between the XMSO and the EVA phases and second at the end of the combined experiment. Then it is oven dried at 105°C for 24 h and weighed again to determine the final water content, and the mass balance is derived from all cumulative water losses during the experiment.

### Parameterization of Soil Hydraulic Properties

In this study, we used the unimodal (VGM) and bimodal (VGBMi) van Genuchten–Mualem models (van Genuchten, 1980; Durner, 1994), a modified van Genuchten–Mualem model with distinct air-entry pressure by Vogel et al. (2000), and the free-form (FF) algorithm of Iden and Durner (2007) to parameterize the water retention and hydraulic conductivity functions.

The unimodal and bimodal van Genuchten retention functions are defined as

$$
\theta(h) = \theta_s + (\theta_i - \theta_s)^{\frac{1}{n_i}} \left[1 + \left(\frac{\theta_i - \theta_s}{\theta_i - \theta_r}\right)^{n_i} h^2 \right]^{\frac{1}{n_i} - 1}
$$

where $\theta_s$ (dimensionless) and $\theta_i$ (dimensionless) are saturated and residual water contents; $\theta_i$ are the weighting factors for the $k$ contributing functions of the original van Genuchten (1980) type, constrained by $0 < \theta_i < 1$ and $\sum \theta_i = 1$; and $a_i$ (cm$^{-1}$) and $n_i$ (dimensionless) are shape parameters. For $k = 1$, Eq. [2] gives the unimodal retention curve of van Genuchten (1980) and, for $k = 2$, the bimodal retention function introduced by Durner (1994).

In the forward simulation for the generation of synthetic measurement data, we used the bimodal van Genuchten–Mualem model modified with an air-entry pressure $h_0$ (cm) (VGBMi) as proposed by Vogel et al. (2000). The advantage of the modified model over the ordinary unimodal or bimodal van Genuchten–Mualem model is the improved stability of the numerical solutions of the Richards equation for small values of the van Genuchten parameter $n$. The retention function of the VGBMi model is given as (Iden and Durner, 2007)

$$
\theta(h) = \begin{cases} 
\theta_s + (\theta_s - \theta_i)^{\frac{1}{n_i}} \left[1 + \left(\frac{\theta_i - \theta_s}{\theta_i - \theta_r}\right)^{n_i} h^2 \right]^{\frac{1}{n_i} - 1} & b < h \\
\theta_i & h \geq b
\end{cases}
$$

where the saturated water content, $\theta_s$, is replaced by the fictitious parameter $\theta_{0_m}$, which is defined by the condition $\theta(h_0) = \theta_s$, leading to

$$
\theta_s = \theta_i + (\theta_i - \theta_s)^{\frac{1}{n_i}} \left[1 + \left(\frac{\theta_i - \theta_s}{\theta_i - \theta_r}\right)^{n_i} b^2 \right]^{\frac{1}{n_i} - 1}
$$

To calculate the unsaturated hydraulic conductivity functions, the retention functions were coupled with Mualem’s capillary pore-bundle model (Mualem, 1976):

$$
K(S) = K_s \left( \frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\beta} \left( 1 - \frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\gamma}
$$

where $K_s$ (cm d$^{-1}$) is the saturated hydraulic conductivity, $S$ is effective saturation, given by $S(h) = (\theta(h) - \theta_r)/(\theta_s - \theta_r)$, and $\tau$ (dimensionless) is a shape parameter. For the VGM and VGBMi models, the conductivity functions were computed by the closed-form expressions given by van Genuchten (1980) for the unimodal case and by Priesack and Durner (2006) for the bimodal case. For the VGBMi model, the integral given by Eq. [5] was solved numerically using the trapezoidal rule.

In the FF algorithm, the retention and hydraulic conductivity curves are estimated without any coupling between them and without assigning a priori shapes to $\theta(h)$ and $K(h)$ except for monotony. By a multilevel routine, $r$ nodes are positioned at the pressure head axes $h_j = \log_{10}(-b)$, and the corresponding values at the ordinates, $b_j$ and $\log_{10}K_j$, are estimated by inverse modeling. Cubic Hermite spline interpolation between these nodal values yields the two soil hydraulic functions. The number of estimated parameters sums to $2r + 1$ with $r$ nodes in each function plus $K_s$ which is estimated as well. The FF approach has the advantage that no errors are caused by missing flexibility of the functions for the constitutive relationships. Because the free-form functions are based on interpolation, they can only be estimated in the pressure head range where experimental information is available. Outside this range, extrapolation is necessary. Because such extrapolations must be based on assumptions and are therefore prone to errors, we do not show extrapolations here but restrict ourselves to the estimated functions within the measurement range.

### Generation of Synthetic Data by Forward Simulation

To analyze the potential advantage of the combined method over the separate XMSO and EVA methods, synthetic data were generated by one-dimensional forward simulation with the HYDRUS-1D code (Šimůnek et al., 2008). The synthetic experiments were evaluated both separately and in combination. The parameterization of the soil hydraulic properties for the forward simulation was selected on the basis of a study by Durner (1991) and represents a typical loam formed from unsorted parent material, e.g., moraine detritus. Such soils are often not well described by the standard hydraulic functions, such as the van Genuchten function (Durner, 1994). The hydraulic properties were parameterized by the VGBMi model given by Eq. [3–5]. The parameter values for the VGBMi model used for the generation of the synthetic data are $\theta_i = 0.40$, $\theta_r = 0.04$, $a_1 = 0.130$ cm$^{-1}$, $n_1 = 1.60$, $a_{0} = 0.6$, $a_2 = 0.009$ cm$^{-1}$, $n_2 = 1.54$, $K_s = 20$ cm d$^{-1}$, $\tau = -1$, and $b_r = -2$ cm. The hydraulic properties for the generation of the synthetic data were deliberately parameterized by a model different from the VGM model, which was used for the parameter estimation. This procedure served the aim of illustrating how a fit to measurements representing a limited range of pressure heads can produce considerable errors in the extrapolated range of the identified properties (Peters and Durner, 2008a; Schelle et al., 2010).
The two successive experimental phases were simulated separately. This was necessary because the simulation domain in both experiments was different, i.e., in the XMSO part a porous plate was included whereas in the EVA part only the soil column was regarded. Geometries for the soil column (7.2 cm long) and the sensor positions inside the sample were adopted from those used in the real experiments. The simulation domains were discretized into adjoining elements of 0.05 cm length.

The simulation domain for the XMSO experiment consisted of a soil column and a porous plate at the bottom (0.7 cm long). The hydraulic properties of the porous plate were defined in such a way that the plate did not release water during the simulated experiment. The saturated conductivity of the plate, \( K_{s\text{-plate}} \), was set to 1 cm d\(^{-1}\). The initial condition was given by a hydrostatic pressure head distribution with a pressure head of 10 cm at the lower boundary (ponding of 2.1 cm). At the upper boundary, we applied an atmospheric boundary condition allowing for surface ponding. This boundary condition uses a so-called surface reservoir condition (Šimůnek et al., 2008) as long as water is ponding at the surface (percolation phase) and switches to a no-flux condition when ponding terminates (drainage phase). The pressure head at the lower boundary was decreased in seven steps (10, 20, −10, −30, −50, −80, and −100 cm) during a total of 4 d. The cumulative outflow across the lower boundary and the pressure head at the 1.8-cm depth in the soil column provided synthetic data.

In the EVA experiment, the simulation domain consisted of the soil column only. Two simulations were performed, one for the individual EVA experiment, which started nearly saturated with \( h_{\text{LB}}(t = 0) = 0 \) cm, and one for the second part of the combined XMSO-EVA experiment, where the simulation started with \( h_{\text{LB}}(t = 0) = −100 \) cm. The initial condition for both simulations was given by hydrostatic equilibrium with the respective lower boundary pressure heads. No flux was set at the lower boundary and an atmospheric boundary condition with a potential evaporation rate \( q_{\text{eva}} = 0.25 \) cm d\(^{-1}\) was applied at the upper boundary. This rate corresponds to the average potential evaporation rate in our laboratory. When the pressure head at the upper boundary of the drying soil reached a value of \( −10^5 \) cm, the boundary condition was changed automatically to a first-type boundary condition, i.e., \( h_{\text{UB}} = −10^5 \) cm (Šimůnek et al., 2008). Pressure heads at 1.8 and 5.4 cm below the top and cumulative evaporation across the upper boundary were used as synthetic data.

All computer-generated data were perturbed with normally distributed noise with zero expectation and a standard deviation reflecting the measurement accuracies in our laboratory setup. Values for the standard deviations (SD) of the measurement error of the devices used in the XMSO and EVA experiments were \( \text{SD}_h = 0.01 \) cm for the cumulative outflow of the XMSO experiment, \( \text{SD}_{\text{Qeva}} = 0.1 \) g (corresponding to 0.0014 cm for a soil column with 69.4 cm\(^2\) surface area) for the cumulative evaporation (EVA experiment), and \( \text{SD}_h = 0.5 \) cm for the pressure head measurements of both experiments.

### Experiments on Real Soils

Three undisturbed sandy loam samples (67% sand, 29% silt, and 4% clay) were investigated by the combined method as described above. Soil samples (Ls1, Ls2, and Ls3) were taken in autumn 2009 from the subsoil (35–45 cm) of a Luvisol at a field site close to the city of Braunschweig, Germany. The field was cultivated with rapeseed (Brassica napus L) as a catch crop. Bulk densities and porosities of the soil samples are given in Table 1. Soil cores were 9.4 cm in diameter and 7.2 cm in height. Experiments were performed at 21 ± 1°C in an air-conditioned laboratory.

Each soil sample was placed on a 0.7-cm-thick porous plate that was covered by a fine-pored diaphragm. We used coarse porous plates with relatively high conductivities, therefore it was necessary to cover them with water-permeable but air-impermeable diaphragms to prevent air entry when lowering the pressure head during the XMSO experiments. Saturated conductivities of the porous plates with the diaphragms, \( K_{s\text{-plate}} \), were determined separately; the values are given in Table 1. For the XMSO phase, one tensiometer was inserted horizontally into each sample at 1.8 cm below the top. The saturated samples were equilibrated with an initial soil water pressure head of 10 cm at the bottom of the porous plates, which led to a ponding height of 2.1 cm at the top of the soil cores. Pressure head steps applied during the XMSO phase were 10, 0, −10, −20, −30, −40, −60, −80, and −100 cm. The last pressure step was maintained for 24 h to approach hydrostatic equilibrium. Because water flow had almost ceased and pressure head readings were constant after this time period, hydrostatic equilibrium was almost achieved at the end of the MSO phase. Afterward, the water outlets at the lower boundaries were closed and the tensiometers were removed.

For the EVA phase, which followed after equilibration, the soil columns were turned upside down for a moment to remove the porous plates and diaphragms, turned back to their original orientation, sealed at the bottom, and placed on a scale. The samples were left untouched and sealed for at least 24 h again to attain hydrostatic equilibrium in the soil columns. Two tensiometers were installed in each soil column at the 1.8- and 5.4-cm heights. To achieve measurements at matric potentials as low as possible, we used improved tensiometers with boiling retardation (T5x, UMS, Munich, Germany), which resist cavitation to much lower pressure heads than conventional tensiometers. To start the evaporation phase, the surfaces of the samples were uncovered. The experiments continued until the measurement limits of the upper tensiometers were reached. We measured pressure heads down to −2900 cm.

Water contents at the different stages of the combined experiment were determined from the mass balance as described above. Water contents at the end of ponding in the first phase of the XMSO experiment were used as \( \theta_s \). The end of ponding can be identified unambiguously from the data because the tensiometer readings pass \( b = 0 \) cm when ponding ceases. This is the case because at that point in time the pressure head at both upper and lower boundaries is zero and the pressure head distribution is always linear during saturated flow.

### Data Evaluation and Parameter Estimation

To be able to compare the results of the separate experiments with those of the combined method, we evaluated the XMSO and EVA experi-

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**Table 1. Measured bulk densities (\( \rho \)), porosities (\( \phi \)), and saturated water contents (\( \theta_s \)) of the real soil samples (Ls1, Ls2, and Ls3), and saturated hydraulic conductivities of the porous plates topped by fine-pored diaphragms (\( K_{s\text{-plate}} \)).**

<table>
<thead>
<tr>
<th>Soil</th>
<th>( \rho )</th>
<th>( \phi )</th>
<th>( \theta_s )</th>
<th>( K_{s\text{-plate}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ls1</td>
<td>1.672</td>
<td>0.369</td>
<td>0.336</td>
<td>7.37</td>
</tr>
<tr>
<td>Ls2</td>
<td>1.699</td>
<td>0.359</td>
<td>0.332</td>
<td>3.02</td>
</tr>
<tr>
<td>Ls3</td>
<td>1.733</td>
<td>0.346</td>
<td>0.313</td>
<td>3.84</td>
</tr>
</tbody>
</table>
ments individually and in a combined form. In the evaluation of the synthetic data, we used the VGM model for the parameterization of the soil hydraulic properties although we knew that the model was not able to perfectly describe the synthetically observed data, which were generated using a more complex model, i.e., the MVMbi model given by Eq. [3–5]. This mimics a typical and realistic measurement situation because small deviations from the assumed parametric model are very common, and the shape of the hydraulic functions outside the experimental measurement range is obtained by extrapolation. Additionally, we applied the FF approach to achieve an optimal flexibility in the shape of the soil hydraulic properties. For the evaluation of the experiments on the real soil samples, the VGM, VGMbi, and FF parameterizations were used. In all cases, all parameters of the soil hydraulic functions except for \( \theta_s \) were estimated.

Estimation of the optimal parameter vector \( \hat{p} \) for the soil hydraulic properties was achieved by minimization of the objective function

\[
\Phi(p) = \sum_{j=1}^{n_j} \sum_{i=1}^{n_j} w_{ij} [r_j(p)]^2
\]

where \( r_{ij} \) are the residuals, i.e., the differences between measured and corresponding simulated system responses, \( p \) is the vector of estimated parameters, \( n_j \) is the number of data groups in the objective function, \( n_j \) is the number of data points within each data group, and \( w_{ij} \) are the weighting factors for the data points. The weighting factors are discussed below for the different cases. Parameter optimization by minimization of Eq. [6] was done by the globally convergent optimization algorithm SCE-UA (Duan et al., 1992) for the VGM and VGMbi models. In case of the free-form estimation for numbers of nodes \( r = 1 \) to 4, we used the modified version of the SCE-UA described in Iden and Durner (2007). To reduce calculation time for \( r > 4 \), we applied the evolutionary scheme CMA-ES by Hansen (2006). The CMA-ES algorithm yields equally accurate solutions with a smaller number of function evaluations than the SCE-UA.

### Extended Multistep-Outflow Experiment

The XMSO experiments were evaluated by inverse modeling. The HYDRUS-1D code was used to numerically solve the Richards equation (Eq. [1]) using the appropriate initial and boundary conditions described above. The porous plate was included in the simulation domain and its saturated conductivity was set to its experimentally determined value. Because the effective conductivity of the composite system can be determined accurately from the outflow data, the saturated conductivity of the soil column can be estimated by inverse modeling. The data types in the objective function were cumulative outflow, \( Q(t) \), and pressure head inside the soil sample at 1.8 cm from the top, \( h(t) \). The weights in the objective function defined by Eq. [6] were set reciprocal to the variance of the measurement error of the data points, \( \sigma_y^2 \). Values of the standard deviation \( \sigma_y \) were set according to the accuracy of the measurement devices, i.e., \( \text{SD}_Q = 0.01 \text{ cm} \) for the pressure transducer connected to the burette for the cumulative outflow and \( \text{SD}_h = 0.5 \text{ cm} \) for the tensiometers used for the pressure head measurements.

### Evaporation Experiment

The EVA experiments were evaluated according to Peters and Durner (2008b). Data points for the retention function were calculated by pairing the average pressure head and column-averaged water content data. Average pressure heads at each time were calculated as the arithmetic mean of the measured pressure heads at the two height levels. Water contents were derived from the total mass of the soil column at each time and the determined water content at the end of the EVA experiment. Hydraulic conductivity data were calculated by inversion of the Buckingham–Darcy law:

\[
k(h) = \frac{q}{\nabla H}
\]

where \( q = q_{eva}/2 \text{ (cm d}^{-1} \text{)} \) is the flux density across the center plane of the soil column. It is assumed to be half of the evaporation flux density derived from the change in total mass for each time interval. The hydraulic gradient \( \nabla H = \Delta h/\Delta z + 1 \text{ (dimensionless)} \) was calculated from the difference between the two pressure head measurements in the soil column, \( \Delta h \text{ (cm)} \), averaged across each time interval, and the spatial distance between the measurement levels of the two tensiometers, \( \Delta z \text{ (cm)} \). Despite the manifold linearization assumptions involved in the evaluation of this simplified EVA method, the resulting data pairs for the retention and conductivity curves are in excellent agreement with the true hydraulic functions as shown by Peters and Durner (2008b).

Parametric models for the retention and related conductivity curves were fitted to the obtained data points by minimizing the objective function (Eq. [6]). The two data groups in the objective function were the water retention data, \( \theta(h) \), and the common logarithms of the hydraulic conductivity data, \( \log_{10} K(h) \). The standard deviations of the computed \( \theta(h) \) and \( \log_{10} K(h) \) values were calculated by Gaussian error propagation from the accuracy of the measuring devices, which were \( \text{SD}_Q = 0.1 \text{ g for the scale and SD}_h = 0.5 \text{ cm for the tensiometers. All water content data have the same standard deviation because their error depends only on the measurement accuracy of the scale. Data points of the conductivity curve have different uncertainties because these are dependent on the magnitude of the hydraulic gradient and the flux density. The standard error for \( \theta(h) \) and the average, minimum, and maximum standard deviations for \( \log_{10} K(h) \) are given in Table 2.}

The weights in the objective function were set proportional to the reciprocal of the variance of the measurement error. The different number of data points in each group (the number of water contents is, in most cases, higher than the number of conductivities) was additionally accounted for by normalization to bring the contribution of the data groups into line with each other. The weights were therefore calculated as

\[
w_{ij} = \frac{1}{\sigma_y^2 n_j}
\]

<table>
<thead>
<tr>
<th>Statistic</th>
<th>( \theta(h) )</th>
<th>( \log_{10} K(h) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>SD</td>
<td>( S^* )</td>
<td>( S )</td>
</tr>
<tr>
<td>Mean error</td>
<td>( 2.83 \times 10^{-4} )</td>
<td>0.108</td>
</tr>
<tr>
<td>Minimum error</td>
<td>0.068</td>
<td>0.110</td>
</tr>
<tr>
<td>Maximum error</td>
<td>0.331</td>
<td>1.064</td>
</tr>
</tbody>
</table>
Because the error of the conductivity data is heteroskedastic, each conductivity data point had a different weight in the objective function, whereas all water contents had the same weights.

**Combined Experiment**

In the evaluation of the combined experiment, the retention and hydraulic conductivity data calculated from the EVA part were included in the objective function for the inverse simulation of the XMSO part. This approach is a simplified alternative to a joint inversion of both experimental parts using numerical solutions of the Richards equation. The main advantages are that it is easy to implement and that it circumvents the necessity to solve Richards’ equation numerically for the evaporation phase. The problems associated with the latter aspect are a considerably higher computational burden to solve the inverse problem and numerical problems that can occur for coarse materials and at low soil water contents. In particular, the physical and numerical treatment of the topsoil and the upper boundary condition during the late evaporation phase are issues that are still under scientific investigation (Hopmans et al., 2002; Shokri et al., 2009). As a consequence, we decided to apply a simpler evaluation method to enable a widespread use in scientific and applied practice.

The number of data groups in the objective function (Eq. [6]) for the combined experiment was \( m = 4 \), i.e., (i) pressure head at the predefined observation depth, \( h(t) \), and (ii) cumulative water flow across the lower boundary, \( Q(t) \), during XMSO, and (iii) water retention, \( \theta(h) \), and (iv) common logarithm of the hydraulic conductivity data, \( \log_{10} K(h) \), obtained from EVA. Due to the different number of data points within these four groups, the weighting scheme given by Eq. [8] was used in the objective function.

**Model Evaluation Criteria and Uncertainty Calculation**

The characteristics of an optimal model performance are a good match to the observed data (goodness-of-fit), a sufficient identifiability of the estimated model parameters, and a minimum number of model parameters. As a measure of the goodness-of-fit, we calculated the root mean square error (RMSE) for each data group contained in the objective function.

In the FF parameterization, the optimal number of nodes \( r \) that determines the number of degrees of freedom must be selected. It was inferred from the heuristic test variable \( P^* \) discussed by Iden and Durner (2007), which aggregates information on (i) the goodness-of-fit indicated by the minimum value of the objective function, (ii) the identifiability of the model parameters, quantified by the collinearity index \( \gamma \) of Brun et al. (2001), and (iii) the number of estimated model parameters \( 2r + 1 \).

The first-order-second-moment (FOSM) method as described in Durner et al. (2008) was used to quantify the uncertainties of the estimated soil hydraulic parameters and functions. The resulting uncertainties are approximate because the method assumes linearity of the underlying model. The sensitivity matrix \( S \) was computed at the optimum parameter vector by a central difference approximation using a 1% relative perturbation in both directions. The approximate parameter covariance matrix was computed as (Seber and Wild, 1989)

\[
\Sigma_p = \sum_{j=1}^{n_p} \left( \frac{\partial s_j}{\partial \hat{p}} \right) \left( \frac{\partial s_j}{\partial \hat{p}} \right)^T \left( S \right)^{-1} \left( S \right)^{-1}
\]

where \( n_p \) is the number of estimated model parameters, \( \hat{p} \) is the optimum parameter vector, \( S \) is the weighted sensitivity matrix obtained from multiplying the entries of \( S \) with the square roots of the weights in the objective function, and all other variables have been defined above.

Approximate confidence intervals for the parameters were calculated from the entries at the main diagonal of the parameter covariance matrix and the appropriate value of Student’s \( t \)-distribution reflecting the number of degrees of freedom and the confidence level. Approximate confidence intervals of the estimated soil hydraulic functions were computed by the FOSM method using the sensitivity matrix of the soil hydraulic functions and the entries of the parameter covariance matrix (Draper and Smith, 1998). The uncertainty intervals for the XMSO model predictions were computed by first calculating the variance of the model prediction caused by the uncertainty and cross-correlation of the model parameters contained in the parameter covariance matrix (FOSM) and then adding the variances of the measurement error. Approximate 95% confidence intervals were then calculated from the square root of the overall variance for each simulated model response and the appropriate value of Student’s \( t \)-distribution given the chosen confidence level.

**RESULTS AND DISCUSSION**

**Synthetic Data**

**Van Genuchten–Mualem Parameterization**

The results of the VGM parameterization for the synthetic data are shown in Fig. 2. Confidence intervals were calculated as described above but are not shown in the figures because they are so small that they would scarcely be visible, with the exception of the uncertainties of the conductivity function near saturation obtained from the EVA experiment. The first row (Fig. 2a, 2b, and 2c) shows the results from the XMSO experiment alone, the second row (Fig. 2d and 2e) those from the EVA experiment alone, and the third row (Fig. 2f, 2g, and 2h) those from the combined XMSO-EVA experiment. The left column (Fig. 2a and 2f) shows the synthetically generated and fitted data from the XMSO phase, i.e., cumulative outflow and pressure head at 1.8 cm below the top. The middle and right columns (Fig. 2b, 2c, 2d, 2e, 2g, and 2h) show the true retention and hydraulic conductivity curves used in the forward simulations to create the synthetic data, the estimated functions, and the data points obtained from the simplified EVA method. Because the fits matched the synthetically generated data closely, we depicted the corresponding residuals for the different data types (Fig. 3, black) to give an even better impression of the quality of the fits.

The inverse simulation of the XMSO phase alone yielded a good match of the synthetic outflow and pressure head data (Fig. 2a). A small systematic misfit is only visible from closer examination of the residuals (Fig. 3a and 3c, black). Figure 2b shows that the true retention curve was reproduced well in the moist range, but in the dry range beyond \( h = -100 \) cm, where the function was extrapolated, the error was considerable. The true hydraulic conductivity function was matched quite well in the intermediate pressure head range but not near saturation and not beyond the measurement range in the dry region (Fig. 2c). Although the experimental data were reproduced well, the estimated soil hydraulic functions showed a considerable systematic deviation. This
obvious model error could not be recognized by a mismatch to the observed data because no experimental data were available in the dry range. Note that the statistical uncertainties of the identified functions were so small that they would be hardly visible and thus would neither give a hint about the actual uncertainty of the functions in the dry range nor even contain the true functions.

The evaluation of the EVA experiment led to data points for water retention and hydraulic conductivity that agree very well with the true functions (Fig. 2d and 2e). This indicates that the linearization assumptions that are made in the evaluation lead to unbiased estimates of the soil hydraulic functions. The experiment yielded reliable information in the pressure head range from near saturation down to about −1000 cm for the retention curve and from about −100 to −1000 cm pressure head for the conductivity curve. In the dry range, the conductivity data tend to scatter moderately as a result of the perturbation of the synthetic measurement data with noise. This is because the relative measurement error in the evaporation rate is increased at the small evaporation fluxes when the sample gets drier (Fig. 1). Fitting the data points with the van Genuchten–Mualem functions resulted in a good match to the true functions except for slight systematic deviations. This becomes more obvious in the residual plots (Fig. 3e and 3g, black). It is important to recognize, however, that the conductivity function in the moist range was determined only by coupling the Mualem integral to the estimated van Genuchten retention function and is therefore not supported by any experimental information on $K_s(h)$. In particular, the true $K_s$ value could not be estimated correctly (Table 3). The very large confidence interval of the parameter $K_s$ (Table 3) confirms that there is basically no information content with respect to the saturated conductivity.

The results from the evaluation of the combined XMSO-EVA experiment are shown in Fig. 2f to 2h. Figure 2f and the corresponding residual plot (Fig. 3d, black) show that the pressure head data of the XMSO part were well matched, whereas the observed cumulative outflow data were not (Fig. 2f and 3b). This is most significant at the beginning of the XMSO experiment and in the pressure head range −20 to −60 cm [corresponding to $\log_{10}(-h\ [cm]) = 1.3–1.8$]. The systematic deviation is reflected in a mismatch of the retention function (Fig. 2g) between $\log_{10}(-b\ [cm]) = 0.8$ and 2. The EVA
data in both soil hydraulic functions were matched well. Note that the data points from the EVA phase differ slightly from those of the EVA experiment alone. The single EVA experiment started near saturation, whereas the EVA phase in the combined method started at \( h = -100 \) cm because the moist range was covered by the XMSO phase. Summarizing these findings, the mismatch of the XMSO data indicates that the VGM model is unable to describe the true soil hydraulic functions. It is an advantage of the combined XMSO-EVA experiment that the wider measurement range leads not only to a greater overall reliability of the identified hydraulic functions but helps furthermore to recognize potential model errors that would probably not be noticed using the XMSO or EVA method alone.

**Free-Form Parameterization**

The results of the FF parameterization for the XMSO and combined XMSO-EVA experiments are shown in Fig. 4a to 4c and 4d to 4f, respectively; corresponding residuals are depicted in Fig. 3 (gray). Based on the test variable \( P^* \), the optimal values of numbers of nodes were calculated as \( r = 4 \) for the XMSO part alone and \( r = 8 \) for the combined XMSO-EVA experiment.

The inverse simulation of the XMSO experiment using the FF approach yielded an excellent agreement between fitted and synthetically generated cumulative outflow and pressure head data (Fig. 4a). The absence of any model error is confirmed by the time series of the residuals (Fig. 3a and 3c, gray), which simply represent the measurement noise that was added to the synthetic data, and by the RMSE values (Table 4), which are not bigger than the standard deviations of the measurement error of the respective data types that are listed above. Accordingly, the true soil hydraulic functions used in the forward simulation were perfectly matched in the range where the experiment provided information, i.e., saturation down to a pressure head of \(-100 \) cm (Fig. 4b and 4c). The true \( K_s \) value was estimated very accurately as well (Table 5).

![Fig. 3](image-url)  
Residuals for the fits of the (a,b) cumulative outflow (\( Q \)) and (c,d) pressure heads (\( h \)) for the extended multistep-outflow (XMSO) experiments and (e,f) retention (\( \theta \)) and (g,h) conductivity (\( K \)) for the evaporation (EVA) experiments from the separate XMSO and EVA experiments (left) and from the combined XMSO-EVA experiment (right) for the synthetic soil using the van Genuchten–Mualem (VGM) and free-form (FF) parameterizations.

### Table 3. Optimized (Opt.) values of the residual water content (\( \theta_r \)), shape parameters \( a, n \), and \( \tau \), and saturated conductivity (\( K_s \)) and 95% confidence intervals for the van Genuchten–Mualem (VGM) parameterization from the extended multistep-outflow (XMSO), evaporation (EVA), and combined (XMSO-EVA) experiments for real soils (Ls1, Ls2, and Ls3) and synthetic soils (S* for EVA experiment; S for XMSO and XMSO-EVA experiments).

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Parameter</th>
<th>S/S*</th>
<th>2.5%</th>
<th>97.5%</th>
<th>2.5%</th>
<th>97.5%</th>
<th>2.5%</th>
<th>97.5%</th>
<th>2.5%</th>
<th>97.5%</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSO</td>
<td>( \theta_r )</td>
<td>0.170</td>
<td>0.175</td>
<td>0.179</td>
<td>0.042</td>
<td>0.045</td>
<td>0.048</td>
<td>0.003</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td></td>
<td>( a ), cm(^{-1} )</td>
<td>0.0665</td>
<td>0.0676</td>
<td>0.0688</td>
<td>0.0166</td>
<td>0.0169</td>
<td>0.0172</td>
<td>0.0103</td>
<td>0.0105</td>
<td>0.0107</td>
</tr>
<tr>
<td></td>
<td>( n )</td>
<td>1.54</td>
<td>1.56</td>
<td>1.58</td>
<td>1.70</td>
<td>1.71</td>
<td>1.72</td>
<td>1.79</td>
<td>1.81</td>
<td>1.84</td>
</tr>
<tr>
<td></td>
<td>( K_s ), cm d(^{-1} )</td>
<td>20.2</td>
<td>20.6</td>
<td>21.0</td>
<td>180.0</td>
<td>181.2</td>
<td>182.3</td>
<td>53.1</td>
<td>53.4</td>
<td>53.8</td>
</tr>
<tr>
<td></td>
<td>( \tau )</td>
<td>-2.09</td>
<td>-2.00†</td>
<td>-1.91</td>
<td>-0.19</td>
<td>-0.17</td>
<td>-0.16</td>
<td>-2.03</td>
<td>-1.82</td>
<td>-1.61</td>
</tr>
<tr>
<td>EVA</td>
<td>( \theta_r )</td>
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<td>0.000†</td>
<td>0.006</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.012</td>
<td>0.012</td>
<td>0.012</td>
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<tr>
<td></td>
<td>( a ), cm(^{-1} )</td>
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<td>0.0496</td>
<td>0.0523</td>
<td>0.0280</td>
<td>0.0316</td>
<td>0.0357</td>
<td>0.0200</td>
<td>0.0217</td>
<td>0.0236</td>
</tr>
<tr>
<td></td>
<td>( n )</td>
<td>1.30</td>
<td>1.31</td>
<td>1.32</td>
<td>1.35</td>
<td>1.36</td>
<td>1.37</td>
<td>1.43</td>
<td>1.44</td>
<td>1.45</td>
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<tr>
<td></td>
<td>( K_s ), cm d(^{-1} )</td>
<td>2.82</td>
<td>43.2</td>
<td>661.8</td>
<td>53.8</td>
<td>84.6</td>
<td>133.2</td>
<td>74.3</td>
<td>116.7</td>
<td>183.2</td>
</tr>
<tr>
<td></td>
<td>( \tau )</td>
<td>-4.89</td>
<td>-4.62</td>
<td>-1.66</td>
<td>-0.31</td>
<td>-0.95</td>
<td>-0.59</td>
<td>-0.27</td>
<td>0.72</td>
<td>1.15</td>
</tr>
<tr>
<td>EVA-XMSO</td>
<td>( \theta_r )</td>
<td>-0.003</td>
<td>0.000†</td>
<td>0.003</td>
<td>0.029</td>
<td>0.031</td>
<td>0.032</td>
<td>0.067</td>
<td>0.069</td>
<td>0.072</td>
</tr>
<tr>
<td></td>
<td>( a ), cm(^{-1} )</td>
<td>0.0318</td>
<td>0.0325</td>
<td>0.0332</td>
<td>0.0248</td>
<td>0.0252</td>
<td>0.0256</td>
<td>0.0158</td>
<td>0.0160</td>
<td>0.0163</td>
</tr>
<tr>
<td></td>
<td>( n )</td>
<td>1.35</td>
<td>1.36</td>
<td>1.37</td>
<td>1.44</td>
<td>1.45</td>
<td>1.45</td>
<td>1.72</td>
<td>1.75</td>
<td>1.77</td>
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<td>( K_s ), cm d(^{-1} )</td>
<td>20.6</td>
<td>21.8</td>
<td>23.1</td>
<td>180.5</td>
<td>183.4</td>
<td>186.4</td>
<td>52.9</td>
<td>53.6</td>
<td>54.4</td>
</tr>
<tr>
<td></td>
<td>( \tau )</td>
<td>-1.63</td>
<td>-1.41</td>
<td>-1.20</td>
<td>0.03</td>
<td>0.04</td>
<td>0.06</td>
<td>0.23</td>
<td>0.34</td>
<td>0.45</td>
</tr>
</tbody>
</table>

† Parameter touches permissible range limit.
Table 4. Root mean square error values for the cumulative outflow ($Q$) and pressure head inside the sample ($h$) for the extended multistep-outflow (XMSO) experiment and retention data ($\theta(h)$) and logarithms of the hydraulic conductivity data [log$_{10}$ $K(h)$] for the evaporation (EVA) experiment obtained from the XMSO, EVA, and combined (XMSO-EVA) experiments using the van Genuchten–Mualem (VGM) and free-form (FF) parameterization for real soils (Ls1, Ls2, and Ls3) and synthetic soils (S* for EVA experiment; S for XMSO and XMSO-EVA experiments); $r$ is the number of interpolation nodes for the FF parameterizations.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Experiment</th>
<th>Model</th>
<th>RMSE($Q$) [cm]</th>
<th>RMSE($h$) [cm]</th>
<th>RMSE($\theta(h)$)</th>
<th>RMSE[log$<em>{10}$ $K(h)$] [log$</em>{10}$(cm d$^{-1}$)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>S/S*</td>
<td>XMSO</td>
<td>VGM</td>
<td>0.024</td>
<td>0.730</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>EVA</td>
<td>VGM</td>
<td>–</td>
<td>–</td>
<td>6.92 x 10$^{-3}$</td>
<td>0.121</td>
</tr>
<tr>
<td></td>
<td>XMSO-EVA</td>
<td>VGM</td>
<td>0.085</td>
<td>0.667</td>
<td>1.14 x 10$^{-3}$</td>
<td>0.189</td>
</tr>
<tr>
<td></td>
<td>XMSO</td>
<td>FF, $r=4$</td>
<td>0.010</td>
<td>0.485</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>XMSO-EVA</td>
<td>FF, $r=8$</td>
<td>0.010</td>
<td>0.486</td>
<td>2.73 x 10$^{-4}$</td>
<td>0.110</td>
</tr>
<tr>
<td>Ls1</td>
<td>XMSO</td>
<td>VGM</td>
<td>0.023</td>
<td>1.151</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>EVA</td>
<td>VGM</td>
<td>–</td>
<td>–</td>
<td>3.20 x 10$^{-4}$</td>
<td>0.030</td>
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<tr>
<td></td>
<td>XMSO-EVA</td>
<td>VGM</td>
<td>0.042</td>
<td>1.770</td>
<td>8.86 x 10$^{-4}$</td>
<td>0.200</td>
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<tr>
<td></td>
<td>XMSO</td>
<td>FF, $r=3$</td>
<td>0.020</td>
<td>0.746</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>XMSO-EVA</td>
<td>FF, $r=9$</td>
<td>0.021</td>
<td>0.837</td>
<td>2.35 x 10$^{-4}$</td>
<td>0.028</td>
</tr>
<tr>
<td>Ls2</td>
<td>XMSO</td>
<td>VGM</td>
<td>0.042</td>
<td>1.227</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>EVA</td>
<td>VGM</td>
<td>–</td>
<td>–</td>
<td>2.72 x 10$^{-4}$</td>
<td>0.034</td>
</tr>
<tr>
<td></td>
<td>XMSO-EVA</td>
<td>VGM</td>
<td>0.075</td>
<td>1.907</td>
<td>1.64 x 10$^{-3}$</td>
<td>0.098</td>
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<tr>
<td></td>
<td>XMSO</td>
<td>FF, $r=8$</td>
<td>0.014</td>
<td>0.751</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>XMSO-EVA</td>
<td>FF, $r=9$</td>
<td>0.029</td>
<td>0.871</td>
<td>4.88 x 10$^{-4}$</td>
<td>0.094</td>
</tr>
<tr>
<td>Ls3</td>
<td>XMSO</td>
<td>VGM</td>
<td>0.031</td>
<td>1.134</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>EVA</td>
<td>VGM</td>
<td>–</td>
<td>–</td>
<td>5.51 x 10$^{-4}$</td>
<td>0.069</td>
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<tr>
<td></td>
<td>XMSO-EVA</td>
<td>VGM</td>
<td>0.060</td>
<td>1.884</td>
<td>1.36 x 10$^{-3}$</td>
<td>0.179</td>
</tr>
<tr>
<td></td>
<td>XMSO</td>
<td>FF, $r=6$</td>
<td>0.019</td>
<td>0.629</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>XMSO-EVA</td>
<td>FF, $r=8$</td>
<td>0.025</td>
<td>0.991</td>
<td>1.56 x 10$^{-4}$</td>
<td>0.067</td>
</tr>
</tbody>
</table>
Because the FF parameters are defined locally, the additional consideration of the data from the evaporation experiment in the combined evaluation did not negatively affect the XMSO fit. This was in contrast to the parametric approach, which was discussed above. Thus, the soil hydraulic property functions estimated from the combined experiment by the FF approach yielded an excellent overall description of the XMSO data and the EVA data (Fig. 4d–4f). The residuals (Fig. 3b, 3d, 3f, and 3h, gray) and the RMSE values (Table 4) indicate no systematic deviations from the observed data. Figures 4e and 4f visualize that furthermore the true function was perfectly matched by the estimated FF function, i.e., the information content of the combined experiment was sufficient for a correct identification of the underlying functions across the whole experimental range.

Real Soils

The results of the three parallel soil samples that were investigated experimentally by the combined XMSO-EVA experiment were very similar. Hence, we show the results graphically only for one sample (Ls1) in detail. As for the synthetic experiments, we evaluated the experimental phases individually and in combination to emphasize the different results that are obtained when the model of the hydraulic properties is inadequate. The results for the VGM and FF parameterizations are shown in Fig. 5 and 6; bimodal functions are not shown because the VGMbi model yielded only slightly better fits than the VGM model. Soil hydraulic parameters, their confidence intervals, and RMSE values for all three samples are given in Tables 3 and 4. Figure 5 shows the data points that were used in the inverse simulation, i.e., cumulative outflow and pressure head data for the XMSO experimental part (left) and retention curve and hydraulic conductivity curve data from the EVA part (middle and right). The results for the individual XMSO and EVA experiments and for the combined XMSO-EVA experiment using the VGM parameterization are depicted in the upper row (Fig. 5a–5c), those from the FF parameterization in the lower row (Fig. 5d–5f). The corresponding residuals are shown in Fig. 6.

### Table 5. Optimized (Opt.) saturated conductivities ($K_s$) and their 95% confidence intervals for the free-form parameterization from the extended multistep-outflow (XMSO) and combined XMSO–evaporation (EVA) experiments for real (Ls1, Ls2, and Ls3) and synthetic soils (S).

<table>
<thead>
<tr>
<th>Experiment</th>
<th>2.5% Opt.</th>
<th>97.5% Opt.</th>
<th>2.5% Opt.</th>
<th>97.5% Opt.</th>
<th>2.5% Opt.</th>
<th>97.5% Opt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>XMSO</td>
<td>19.8</td>
<td>20.0</td>
<td>20.2</td>
<td>176.3</td>
<td>177.4</td>
<td>178.5</td>
</tr>
<tr>
<td>EVA-XMSO</td>
<td>19.7</td>
<td>19.9</td>
<td>20.1</td>
<td>174.7</td>
<td>176.4</td>
<td>178.2</td>
</tr>
</tbody>
</table>

Fig. 5. Simulation results from the extended multistep-outflow (XMSO), evaporation (EVA), and combined (XMSO-EVA) experiments for a real soil sample (Ls1) using the van Genuchten–Mualem (VGM) and the free-form (FF) parameterizations: (a,d) measured and fitted values for cumulative outflow (increasing) and pressure head (decreasing) at 1.8 cm below the top (XMSO); estimated (b,e) retention and (c,f) hydraulic conductivity functions and data points from the EVA experimental part.
Van Genuchten–Mualem Parameterization

As for the synthetic data, the fitted model predictions based on the VGM parameterization described the experimental data from the XMSO phase alone quite well and slightly better than that obtained from the estimation using the combined XMSO-EVA data set (Fig. 5a, 6a, and 6b), where considerable systematic deviations with respect to the cumulative outflow are visible (Fig. 6b, black). The VGM model likewise was able to fit the EVA data alone very well. In the combined evaluation, the fit of the EVA retention curve remained very good but for the conductivity data, the residuals (Fig. 6h, black) and the RMSE values (Table 4) indicated a significantly worse fit. It appears that, similarly to the synthetic data case, the VGM parameterization was able to describe the single experimental parts satisfactorily but could not describe the entire data set of both experimental parts together.

The resulting soil water retention curves (Fig. 5b) and, even more, the hydraulic conductivity curves (Fig. 5c) obtained from the three evaluation approaches (EVA, XMSO, and XMSO-EVA) differ considerably. The differences are most pronounced in the regions beyond the respective measurement range. This result demonstrates the importance of using the hydraulic properties only in the pressure head range in which they were measured and to be very cautious in trusting extrapolations.

Free-Form Parameterization

Based on the test variable $P^*$, the optimal number of nodes for the FF parameterization for the soil sample Ls1 was $r = 3$ for the XMSO fit and $r = 9$ for the combined XMSO-EVA fit. Data of both the XMSO and the XMSO-EVA experiments were in general well matched by the FF fits. In particular, the EVA data were matched virtually error free (Fig. 6f and 6h, gray); however, systematic errors in matching the observed cumulative outflow and the observed pressure heads were evident for the XMSO part. Deviations between the observed and fitted pressure head data occurred at times of pressure head changes at the lower boundary (Fig. 5d and 6d, gray), where the observed tensiometer data reacted faster than could be described by the model. Deviations between the observed and fitted outflow data were caused by ongoing outflow at times when the observed and simulated pressure heads indicated hydrostatic equilibrium. This denotes that the assumption of local equilibrium between pressure head and water content is violated, which is usually referred to as “dynamic effects” (Schultze et al., 1999; Wildenschild et al., 2001). The discrepancies between observations and fitted model responses are not the result of parameterization error in the soil hydraulic properties and cannot be eliminated as long as a flow model assuming local hydraulic equilibrium like the Richards equation is applied. Besides these inevitable misfits caused by dynamic effects, the model describes the data in an excellent manner. This allows us to conclude that the estimated hydraulic properties are representative of the investigated soil samples.

In accordance with the equally good fit of the XMSO data by both versions (XMSO alone and XMSO-EVA combined), the soil hydraulic properties of both fits agree perfectly at saturation and toward the pressure range where the XMSO is continued by EVA (Fig. 5e and 5f). The estimated $K_s$ values are basically equal (Table 5).

**CONCLUSIONS**

We showed by analyses of synthetic and real experimental data that the successive combination of the XMSO and EVA experiments leads to much more reliable estimates of the soil hydraulic properties across a wide pressure head range than can be obtained by either of the two experiments alone. The saturated percolation phase (X) gives very accurate estimates of the saturated conductivity, which cannot be estimated reliably by traditional MSO experiments. The XMSO phase yields the information on both functions for the wet range, and the EVA phase contributes the information for the medium to dry range. The transition between the different experimental phases can be done experimentally in a straightforward manner, and the agreement of hydraulic functions in the overlapping range of the XMSO and EVA methods was found to be good in a previous
study (Schelle et al., 2010). These are preconditions for the successful combination of the two experiments.

The combined evaluation was based on an inverse simulation of the XMSO experiment using the Richards equation and including data from the simplified EVA method in the objective function. The weighting of data in the objective function was set in a manner that ensured that the contribution of the different data groups to the final objective function value would be equal if no model error was involved. The chosen approach is a simplified alternative to a joint inversion of both experimental parts using numerical solutions of the Richards equation for XMSO and EVA. Such a joint inversion should be accomplished in future research to verify the ability to describe the data of both experiments using current process knowledge.

Parameter estimation for a synthetic data set using a slightly wrong model for the soil hydraulic properties (VGM) yielded acceptable fits for the individual experiments but showed considerable deviations in the evaluation of the combined experiment. This shows that model errors could not be recognized by using only one of the presented experimental methods alone, which increases the risk of erroneous extrapolations. For the combined XMSO-EVA method, this risk is significantly reduced. Parameter estimation with the FF parameterization yielded results without systematic errors in the ranges in which information was available from the respective experimental phases.

In this study, the combined approach yielded accurate and reliable hydraulic properties from saturation down to pressure heads of −2000 cm. Extrapolation of the hydraulic functions into the experimentally unexplored dry range is extremely error prone because different models are available that will lead to markedly differing shapes in the extrapolated range. Without additional measurements in the dry region, model errors can neither be detected nor avoided. Currently, there is a lack of simple and quick methods to reliably obtain soil hydraulic functions in the dry range beyond the pressure head range measurable with tensiometers. Possibilities to extend the experimental range are the inclusion of advanced matric potential sensors in the evaporation method, such as MPS1 sensors (Decagon Devices, 2009), polymer tensiometers (van der Ploeg et al., 2010), or embedded heat dissipation sensors (Scanlon et al., 2002). Furthermore, the use of the air-entry value of the tensiometer cup in the evaporation method as an additional measurement point has been proposed (Schindler et al., 2010b).

Testing the combined method with three soil columns of an undisturbed sandy loam soil confirmed the expectations from the analysis of the synthetic data but it showed additionally that dynamic effects occurred in water flow during XMSO, which make a perfect fit to the observed data impossible. A thorough analysis of these effects and of the role they play in hydraulic parameter identification from dynamic flow experiments is beyond the scope of the present study but has to be considered in future research.

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