Inverse modelling techniques for determining hydraulic properties of coarse-textured porous media by transient outflow methods

G. Nützmann, M. Thiele, S. Maciejewski & K. Joswig

A series of multi-step outflow experiments was carried out to identify the unsaturated hydraulic properties of two homogeneous coarse-textured porous media (glass beads and sand). Because of the measured sharp fronts of water content decrease during these experiments the hydraulic functions are assumed to be represented by the complete van Genuchten–Mualem closed-form expressions with variable coefficients $\alpha, \eta, m$ and $v_r$. The values of $v_s$ and $K_s$ were measured directly. A sensitivity analysis with respect to $\alpha, \eta$, and $m$ shows that conditions of local identifiability are satisfied if measurements of water content at some inner points inside the column are considered. The inverse modelling technique consists of two steps: first, computation of objective function values based on water content data responses to obtain initial parameter estimations, and second, a more detailed parameter determination using a Levenberg–Marquardt scheme. In both steps a numerical model incorporating the hydraulic functions is utilized to simulate theoretical pressure head and water content distributions along the column. For both porous media unique solutions of the inverse problem could be obtained, and afterwards, the corresponding hydraulic functions were verified from additional drainage experiments.

Keywords: porous media, hydraulic properties, unsaturated flow, parameter identification.

1 INTRODUCTION

With increasing demands on groundwater resources the need for an accurate prediction of the subsurface flow and chemical species transport under different hydro-geological, climatic and ecological conditions have greatly accentuated the need to understand these processes and to evaluate effects of management practices and remediation techniques. Several computer codes based on numerical models have been used, but with these powerful tools comes the need for the ability of accurate determination of required model parameters. In some cases, only groundwater flow is of interest, and the saturated hydraulic conductivity, $K_s$, must be determined. However, the processes of flow and transport in the vadose zone are essential because most groundwater contaminant sources originate in this zone. Model calibration in the unsaturated zone may be particularly difficult due to problems in formulating the constitutive relations for this special type of two-phase flow, namely the water retention curve and the unsaturated hydraulic conductivity.

There are some laboratory and field methods to determine the relationships between the pressure head $h$, the water content $\theta$, and the hydraulic conductivity $K$. Traditionally, direct steady-state methods for the determination of these highly non-linear functions exist, but recently, transient experimental methods coupled with inverse modelling techniques have become more attractive. This parameter identification technique involves the numerical solution of the water flow equation for unsaturated/saturated porous media, subject to the imposed initial and boundary conditions. The constitutive relations, the so-called hydraulic properties are assumed to be described by analytical functions characterized by a limited number of parameters. During an experiment some auxiliary variables are...
measured, e.g., cumulative outflow, pressure head, water content, or infiltration. Then, the a priori unknown parameters are determined by minimizing the objective function containing the deviations between observed and predicted quantities.

The use of laboratory outflow experiments for estimation of unsaturated hydraulic properties is advantageous because it is flexible in initial and boundary conditions and not very time-consuming. One-step outflow experiments (OS), where an initial saturated soil column is drained by a one-step pressure change at the lower boundary, were used in conjunction with inverse modelling techniques first by Parker et al. and Kool et al. If only cumulative water outflow is measured there, the inverse problem could be ill-posed and lead to a non-unique solution. Finally, it appears that either equilibrium data are needed, or measurements of pressure head at one point inside the soil column can improve the performance of the OS-method. However, OS methods on large columns can produce dynamic capillary pressure–saturated relationships depending on the lower boundary value changes. The reasons for that and a theoretical model of such relationships were discussed by Hassanizadeh.

These considerations stimulated the investigation of the multi-step outflow method (MS), which uses small pressure steps to induce drainage of the soil column. Superiority of the MS to the OS-method on small columns was reported in Van Dam et al. They showed that the MS experiments with only cumulative outflow data contain sufficient information for the unique determination of the soil hydraulic functions, using initial estimates derived from the outflow experiment itself. Eching and Hopmans found that the inverse solution technique is greatly improved when cumulative outflow data are supplemented with simultaneously measured pressure head data from some position inside the column during the MS-experiment.

To study the reason for this behaviour the mathematics of inverse problems has to be considered. Carrera and Neu- man defined criteria of identifiability and uniqueness according to which inverse problems are well-posed for determining the aquifer parameters of groundwater flow. Russo et al. and Toorman et al. analyzed conditions of well-posedness by evaluating the response surfaces of an inverse problem to estimate the unsaturated hydraulic properties. As shown by Mous, the non-uniqueness of the estimates is not due to a bad choice of the optimization algorithm, but is merely a consequence of the structure of the model and the design of the experiment. Based on a rank-analysis of the Hessian matrix conditions of local identifiability could be proved, and the number of identifiable parameters related to the experiment was calculated. Zurmühle investigated parameter identifiability and uniqueness on OS- and MS-experiments with respect to sensitivity coefficients, and showed that only the MS-method can produce uncorrelated and thus linear independent parameters.

One-step and multi-step experiments commonly were carried out on small in-situ soil samples. Eching and Hopmans pointed out that the optimized soil hydraulic functions as determined from soil cores do not necessarily represent in-situ soil behaviour. This may be due to the heterogeneity of undisturbed soil cores and their small sizes, see also Kool and Parker.

The results reported here are part of more comprehensive experiments for determining hydrodynamic dispersion coefficients in unsaturated porous media. The objective of the present study was to estimate unsaturated hydraulic properties of homogeneous, artificially packed coarse-textured porous media with inverse modelling of MS-experiments on large columns. There was special interest in the applicability of the complete van Genuchten–Mualem hydraulic functions for describing high unsaturated water fluxes and sharp fronts of water content decrease, which are typical for poorly graded porous media. Conditions of identifiability were investigated using the concept of sensitivity analysis. We extended the theoretical analysis of Toorman et al. and the results of Eching and Hopmans and Van Dam et al. to large soil columns. The experiments carried out revealed a much larger parameter sensitivity of water content in comparison with pressure head data inside the column.

2 METHODS

2.1 Experimental set-up

Outflow experiments were carried out for glass beads and sand with particle sizes ranging from 0.25 to 0.63 mm. Results of the particle-size analyses are given in Table 1. The general layout of the experimental set-up is depicted in Fig. 1.

The porous media were air-dried, sieved and packed to a uniform bulk density \( \rho_b = 1.68 \text{ g/cm}^3 \) for glass beads, \( \rho_b = 1.69 \text{ g/cm}^3 \) for sand. The particle mass densities were determined as \( \rho_s = 2.522 \text{ g/cm}^3 \) (glass) and \( \rho_s = 2.502 \text{ g/cm}^3 \) (sand). The columns are made of Plexiglas with a length of 100 cm for glass beads and 150 cm for sand, and a diameter of 206 mm. Air entry to any part of the column was through the surface of both porous media because the upper end of the column was open. Initially for all MSO experiments the columns were saturated, with the piezometric level at the top of the column (\( x = L \)). This was done stepwise from bottom to top with the help of reservoir 1, each time waiting for equilibrium to be reached. The base

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Table 1. Particle size distribution of investigated porous media

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of the columns were connected to a variable piezometric surface which is controlled by reservoir 2. Fig. 2 shows time distributions of these piezometric levels at lower boundaries in both experiments. Starting an MSO experiment, the water flowing out of reservoir 2 was collected in a vessel, which was connected to an electronic balance. During the experiments the signal of the balance was recorded by a PC and the volumetric outflow as well as the cumulative volumetric outflow were stored.

The measurement accuracy of the electronic balance is approximately ± 0.05 g. About seven identical experiments were conducted with each column. Average values and standard deviations of cumulative outflows were calculated transforming the weighted outflows to an equivalent outflow height by dividing the corresponding volumes by the column cross-sectional area. Thus, the mean cumulative outflow at the end of the glass-bead experiments was \( \bar{Q}_{\text{glass}} = 16.74 \text{ cm} \) with a standard deviation of \( \sigma_{\text{glass}} = 0.37 \text{ cm} \), for the sand experiments we found \( \bar{Q}_{\text{sand}} = 31.61 \text{ cm} \) with \( \sigma_{\text{sand}} = 0.226 \text{ cm} \).

Microtensiometers (P1 – P3) with a 3-cm-long ceramic cup and TDR (time domain reflectory) probes (T1 – T3) were used to measure the pressure head and the volumetric water content at different positions in the column. Their locations in both column experiments are given in Table 2. Each tensiometer was calibrated independently across the entire pressure range before and after each experiment using linear regression. The accuracy of the pressure head reading is approximately ± 0.1 cm of water, and that of water content is ± 2 vol% or ± 0.02.

Statistical estimates for the saturated water content \( \bar{v}_s \) and for the residual water content \( \bar{v}_r \) can be given based on measurement values before starting and after finishing the outflow experiments, respectively. Averaging over all three TDR-probe locations, a mean value of \( \bar{\theta}_s = 0.342 \) with a standard deviation of \( \sigma_{\bar{\theta}_s} = 0.0055 \) was determined for the glass-bead column, and a value of \( \bar{\theta}_s = 0.318 \) with \( \sigma_{\bar{\theta}_s} = 0.0035 \) for the sand column. At location T2, e.g., the mean residual water content was \( \bar{\theta}_r = 0.084 \) for the glass-beads and \( \bar{\theta}_r = 0.063 \) for the sand, with standard deviations of 0.0028 and 0.0017, respectively. Consequently, errors are of comparable relative magnitude for outflow and water content measurements.

A series of classical Darcian experiments was carried out

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**Fig. 1.** Scheme of the outflow experiments.

**Fig. 2.** Time distributions of lower boundary values during MSO experiments.

**Table 2.** Local positions of measurement devices (distances in cm from the column bottom, for probe location, see Fig. 1)

<table>
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<th>Tensiometers</th>
<th>TDR-probes</th>
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<tr>
<td>Column length [cm]</td>
<td>P1</td>
</tr>
<tr>
<td>Fine sand</td>
<td>150</td>
</tr>
<tr>
<td>Glass beads</td>
<td>100</td>
</tr>
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</table>
Before and after the outflow experiments in order to control possible changes in the pore size structure and effects of compaction due to transient water flow through the column. As a result, the saturated hydraulic conductivities of the porous materials were determined to be \( K_c = 4.764 \text{ cm/min} \) for the glass beads and, \( K_c = 3.738 \text{ cm/min} \) for the sand.

The porosity of both materials was calculated from bulk and particle mass densities (see above) as \( \epsilon = 0.347 \) for glass beads and \( \epsilon = 0.52 \) for sand. Measuring the saturated volumetric water content at the beginning of each experimental series, after packing the column, values of \( \theta_w = 0.348 \) for the glass beads and \( \theta_w = 0.314 \) for the sand were found. A very good coincidence of both estimations can be noticed.

Both the saturated hydraulic conductivity and the saturated water content were kept constant during parameter estimation. This is based on results from Van Dam et al., who recommended that the parameters \( \theta_w, \theta_s \) and \( K_c \) be determined independently, and to optimize the remaining parameters \( a, n \) and \( m \), if the hydraulic functions are to be used in simulations with both saturated and dry conditions. Following the investigations of van Genuchten and Nielsen, Eching and Hopmans, and Zurnmüll we considered \( \theta_w \) to be an empirical parameter that should be fitted to the data.

### 2.2 Mathematical model

The governing equation for transient saturated–unsaturated water flow in a vertical soil column without sinks and sources is given by the Richards equation:

\[
\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial x} \left[ K(\theta) \left( \frac{\partial h}{\partial x} + 1 \right) \right] = 0,
\]

where \( \theta \) is the volumetric water content, \( h \) is the pressure head, \( K \) is the hydraulic conductivity, \( x \) is the vertical distance taking on positive values upwards, and \( t \) is the time. The appropriate initial and boundary conditions for the one-step and multi-step outflow experiments are:

\[
h = L - x, \quad t = 0, \quad 0 \leq x \leq L
\]

\[
-h_{gw}(t) = 0, \quad t > 0, \quad x = L
\]

\[
h = h_{gw}(t), \quad t > 0, \quad x = 0
\]

where \( x = 0 \) is the bottom of the column, \( x = L \) is the top of the soil, and \( h_{gw} \) is the actual groundwater level in the column which is kept constant for OS experiments, and which is a stepwise function of time for MS experiments (see Fig. 2).

The solution of eqn (1) and Eq. (2) was obtained from a Galerkin finite-element code, and the cumulative outflow \( Q(t) \) is then calculated as:

\[
Q(t) = A \int_0^t \left[ \theta(x, 0) - \theta(x, t) \right] \, dx,
\]

using spline interpolation, and where \( A \) is the cross-sectional area of the column.

As shown by van Genuchten and Nielsen, the water retention relation

\[
\Theta(h) = \frac{(\theta - \theta_w)}{(\theta_s - \theta_w)} = \left[ 1 + (a/h)^n \right]^{-m}.
\]

with the effective water saturation \( \Theta(0 \leq \Theta \leq 1) \), the saturated water content \( \theta_s \), the residual water content \( \theta_r \), and the parameters, \( a, m, n \) has great flexibility in describing retention data from various soils. At the same time, it has a simple inverse function and permits the derivation of closed-form analytical expressions for \( K(\Theta) \) when combined with the predictive theory of Mualem.

This model can be written in the form

\[
K_i(\Theta) = \Theta \sqrt{\left[ \frac{f(\Theta)}{f(1)} \right]^2},
\]

where \( K_i(\Theta) \) is the relative hydraulic conductivity, \( K/K_r \), or

\[
K_r(\Theta) = \sqrt{\left[ I_q(p, q) \right]^2},
\]

which is the general expression for variable \( m \) and \( n \). Here, \( I_q(p, q) \) is the incomplete beta function with \( q = \Theta(1)^m, p = m + 1/n \). \( q \) is \( 1 - 1/n \). A simple expression of unsaturated hydraulic conductivity results from eqn (6), if the parameter of the water retention relation (4) is connected to \( m \).

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\[
K_r(\Theta) = \Theta \sqrt{\left[ 1 - \left( 1 - \Theta(1)^m \right)^{1/2} \right]^2},
\]

\[
m = 1 - 1/n, \quad 0 < m \leq 1.
\]

Both models (6) and (7) have been tested to describe our data from MSO experiments.

### 2.3 Optimization procedure

Differences between observed flow responses and numerically predicted values were minimized to obtain estimates of the hydraulic function parameters of interest using the following objective functions:

\[
O_1(a) = w \left[ Q' - Q(a) \right]^T \left[ Q' - Q(a) \right] + (1 - w) \sum_i \left\{ \frac{\theta_i - \theta(a)}{\theta_i - \theta(a)} \right\}
\]

\[
(8a)
\]

and

\[
O_2(a) = w \left[ Q' - Q(a) \right]^T \left[ Q' - Q(a) \right] + (1 - w) \sum_i \left\{ \frac{h_i - h(a)}{h_i - h(a)} \right\}
\]

\[
(8b)
\]

where \( a = (\alpha, n, m, \theta_r)^T \) is the vector of the unknown parameters, \( Q' \) and \( Q(a) \) are the vectors of measured and
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calculated outflows, \( \theta^2 \) and \( \theta(a) \) are the vectors of measured and predicted water contents, and \( \mathbf{h} \) and \( \mathbf{h}(a) \) are the measured and predicted pressure head vectors. Measurement errors were assumed to be uncorrelated and to have constant variances, \( P \) is the number of measurement locations inside the soil column (Table 2). All measured quantities (water outflow, pressure head, water content) were sampled simultaneously every 2, 4, or 6 s, depending on the duration of the actual experiment. Thus, the original length of vectors \( \mathbf{Q} \), \( \theta^2 \), and \( \mathbf{h} \) is from 2000 to more than 7000 elements. To calculate Eq. (8) they were reduced to 90...135 values with a non-equidistant distribution vs. time adjusting to the dynamic behaviour of the observed outflow process.

The factor \( w \), \( 0 \leq w \leq 1 \), allows to weight between outflow and potential quantities in the objective function: if \( w = 0 \), only water contents or pressure heads affect estimation, if \( w = 1 \), only the outflow data control the parameter optimisation procedure. According to Kool et al.\(^{2} \) the weight \( v \) accounts for the different measurement scales of outflow volumes and water contents or pressure heads. It was defined as

\[
v_1 = P \left( \sum_{k=1}^{M} Q' (t_k) \right)^2 \left( \sum_{i=1}^{p} \sum_{j=1}^{n} \theta_i^j(t_k) \right)^2,
\]

and

\[
v_2 = P \left( \sum_{k=1}^{M} Q' (t_k) \right)^2 \left( \sum_{i=1}^{p} \sum_{j=1}^{n} h_i^j(t_k) \right)^2.
\]

where the \( \theta_i^j(t_k), h_i^j(t_k) \) and \( Q' (t_k) \) are the discrete measurements at \( t_k, k = 1, \ldots, M \).

The actual conditions of parameter identifiability were investigated using the concept of sensitivity analysis, see, e.g., Refs. 2,9,19 though due to the non-linearity of the model it may be very difficult to prove it globally identifiable in a mathematical sense, in most practical situations, it is easy to show its local identifiability (or least-squares identifiability).\(^{10} \) A necessary condition for a local minimum is that the Jacobian matrix \( \mathbf{X} \) of partial derivatives of a calculated model output \( f_{k} \), e.g. of the cumulative water outflow \( f_{2} = Q(t, a) \), \( k = 1, \ldots, M \), with respect to the parameters \( a = (a_l), l = 1, \ldots, N \), be full of rank,\(^{10} \) or the rows of this matrix, the so-called sensitivity coefficients \( x_{i} = \partial f_{i} / \partial a \) be linearly independent. The time-dependent sensitivity coefficients of the parameter identification problem considered here can be calculated from eqn (8a) as

\[
x_{i} = x_{i}(t, a) = -w \frac{\partial Q(t, a)}{\partial a} - (1 - w)v_1 \sum_{i=1}^{p} \frac{\partial \theta_i^j(t, a)}{\partial a},
\]

where \( v_1 = 1 \) and \( v_2 = 0 \), are due to the change of the weighting factor \( w \) and all other parameters. As the \( v \)-values for coarse-textured soils

were produced in the same range as the variations of parameters themselves. This may be very helpful for controlling the optimization procedure.\(^{3} \) To compare relative values of sensitivity coefficients with respect to the different parameters to be optimized one must consider their normalized values as

\[
x_{i}^n = x_{i} \frac{1}{a} k = 1, \ldots, M.
\]

Besides, the matrix (8) must be available in the optimization routine, thus, the sensitivity coefficients (10) are calculated without any additional effort. The computation of the Jacobian matrix was carried out numerically for each parameter using a central difference scheme. The optimization procedure applied here is the method of Levenberg–Marquardt (see Press et al.\(^{16} \) ); the computations were run on an IBM RS/6000 work station.

3 RESULTS AND DISCUSSION

3.1 Glass beads (\( \theta \)-measurements)

Several multi-step outflow experiments were carried out in a 100 cm glass-bead column measuring the cumulative outflow and the water content (no measurements of pressure heads). Computations of sensitivity coefficients with respect to the parameters \( a, n, \theta, m \), and \( w \) were done investigating the influence of the weighting factor \( w \) in eqns (10) and (12). Fig. 3 shows these sensitivity coefficients calculated from eqn (12) as functions of time and varying factor \( w \).

It becomes obvious that for all parameters the highest sensitivities were calculated for \( w = 0 \) (only water content and no outflow values to be considered in the objective function), for \( w = 0.5 \) and \( w = 1 \) the sensitivity values were much lower. At those moments, when the outflow boundary condition is changed the sensitivity curves are responding to this change immediately, although, at the beginning of the outflow process, only for \( w = 1 \) and \( w = 0.5 \), see Fig. 3. This is because of the reaction of the different auxiliary variables: the cumulative outflow is directly produced by drainage from the very beginning, but the water content at the lowest position in the soil column (Table 2) remains saturated as long as the piezometric surface is higher than this location. The large alteration steps of the sensitivity curves, especially for \( w = 0 \), are due to the changing outflow boundary condition. Further away from these alteration moments sensitivities become nearly constant again indicating a steady-state or equilibrium situation attained in the unsaturated soil column.

Note that the sensitivities of \( n, \theta, m \), and \( n \) are ten times lower than for the parameter \( a \), which partly corresponds to results of Zurmühl.\(^{25} \) The figures show that the sensitivity coefficients of \( a, n \), and \( m \) are uncorrelated and linear independent. There are only small correlations between \( a \) and \( m \), and no correlations between \( n \) and \( m \), nor between \( \theta \) and all other parameters. As the \( n \)-values for coarse-textured soils
are very large, variations in $n$ are generally insensitive relative to changes in $\alpha$. This has been the case for the glass bead column, where $n$ was identified larger than 10, see also Fig. 4.

Thus, these parameters appear to be identifiable from MS-experiments using water content measurements exclusively, or, combined with outflow measurements. For cumulative outflows, however, the sensitivities seem to be too small, leading to numerical difficulties when solving the inverse problem.

To examine the uniqueness of the inverse problem response surfaces of the different parameter combinations were calculated. In this study, the concept of response surfaces was used to find good initial estimates for the three parameters $\alpha$, $n$ and $m$ as starting values for the Levenberg–Marquardt algorithm. These surfaces were computed from eqn (8), varying the parameters $n$ and $m$ while keeping $\alpha$ at different constant values. In Fig. 4 the $(m,n)$-response surfaces are depicted for the objective function (8a) with $w = 0$ for the MS-boundary condition case, $\alpha$ is varying from 0.0412 cm$^{-1}$ to 0.05265 cm$^{-1}$. In these computations the variations of $n$ and $m$ were $\Delta n = \Delta m = 0.1$, $\theta_1$ was fixed at 0.047.

A clear minimum can be seen to exist for each of the chosen $\alpha$-values (Fig. 4). The valley of local minimum, which has an ellipsoidal form, is moving with growing $\alpha$ from the upper left corner, Fig. 4(a), to the lower right, Fig. 4(d). For smaller $\alpha$-values this valley seems to be parallel to the $m$-axis, paralleling the $n$-axis for further growing $\alpha$. Thus, for smaller values of $\alpha$ the contour plots reveal great sensitivity to $n$, and for larger values of $\alpha$ a major sensitivity to $m$. All surfaces in Fig. 4 show sensitivity to $\alpha$, $n$ and $m$. This means that for describing the hydraulic properties of the glass-bead porous medium it is necessary to use the general eqn (4) and (6) with a variable parameter $m$. Fig. 4 also shows that the localization of a minimum with respect to the parameters $n$ and $m$ is dependent on the level $\alpha$. Minimal values ($\alpha_{\text{opt}}$, $n_{\text{opt}}$, $m_{\text{opt}}$) were chosen according to those plots to start from in three-parameter searches with the help of the Levenberg–Marquardt technique. The obtained optimal parameters are $\alpha_{\text{opt}} = 0.045$ cm$^{-1}$, $n_{\text{opt}} = 10.715$, and $m_{\text{opt}} = 8.096$ with $x_{\text{opt}} = 1.08595$. Both the simulated distributions of water content and the curve of cumulative outflow are very close to the measured values. Note that the sharp profiles of water content during the outflow process could be simulated in strict agreement with the observed ones as depicted in Fig. 5.

To check the goodness-of-fit and to validate the model additional MS-outflow experiments with glass beads have been conducted and afterwards simulated with the above given optimized hydraulic functions.

Fig. 3. Comparison of sensitivity coefficients using water contents and different weights ($w = 0, 0.5, 1$) for glass bead MS-simulation: (a) $\alpha$-, (b) $n$-, (c) $\theta_1$- and (d) $m$-row of the Jacobian matrix.
3.2 Sand (θ- and h-measurements)

Multi-step experimental and modelling methods as discussed above were also used to determine the hydraulic functions (4) and (6) of the sandy porous material. In addition to the first experiment, pressure heads were measured in three locations inside the column (see Table 2). As in Toorman et al.19 and Eching and Hopmans, the influence of pressure head measurements to improve identifiability was investigated by considering the rows of the Jacobian. These sensitivity coefficients are shown as functions of time in Fig. 6 for some values of the weighting factor w.

Analogously calculated sensitivity coefficients based on eqn (10) for water contents show a behaviour similar to that of glass beads, the highest absolute value was reached for \( w = 0 \), but the \( \theta_r \), \( n \) - and \( m \)-sensitivities were still lower by one order of magnitude. Compared with previous results for \( w = 0 \) the sensitivity functions remain constant over longer time periods, and the alteration steps, if outflow boundary conditions are changed, were steeper and faster than those from glass bead simulations. The sensitivity coefficients based on pressure head responses as depicted in Fig. 6 differ totally from that behaviour. They are in general smaller by one or two orders of magnitude, and the smallest absolute values are found in the case of \( w = 0 \). The ratio between maximal sensitivity values of \( h \)-based and \( \theta \)-based sensitivity coefficients is 0.03 with respect to \( \alpha \), and 0.045 with respect to \( m \). This means that the sensitivities concerning outflow data are greater than those based on pressure heads, just the opposite of the case of \( \theta \)-based sensitivity coefficients. Referring to identifiability there are no correlations between \( \alpha \) and \( n \), whereas between \( \alpha \) and \( m \) some correlations seem to exist though not linear ones in general. Due to the small sensitivities, especially for \( w = 0 \) and \( w = 0.5 \), it is not advantageous using pressure head measurements for parameter estimation if water content data are available.

**Fig. 4.** Response surfaces for the glass bead medium (\( w = 0 \)), the minima were estimated to: (a) \( \mathbf{O}_{\text{min}} = 1.1757 \) with \( \alpha = 0.0412 \text{ cm}^{-1} \), \( n = 8.6 \), \( \theta_r; m = 11.0 \); (b) \( \mathbf{O}_{\text{min}} = 1.08597 \) with \( \alpha = 0.045 - 1 \), \( n = 10.7 \), \( m = 8.1 \); (c) \( \mathbf{O}_{\text{min}} = 1.08732 \) with \( \alpha = 0.0488 \text{ cm}^{-1} \), \( n = 11.4 \), \( m = 8.1 \); (d) \( \mathbf{O}_{\text{min}} = 1.09312 \) with \( \alpha = 0.05265 \text{ cm}^{-1} \), \( n = 12.4 \), \( m = 2.1 \).
A further comparison of the $\theta_r$-rows in Fig. 3(c) and Fig. 6(c) reveals that this parameter is very insensitive to water content or pressure head data ($w = 0$), but has much higher sensitivities with respect to outflow data ($w = 1$). This is due to calculating the hydraulic mass balance via eqn (3) substituting $\Theta$ with eqn (4). As is evident from Fig. 6, relative values of $\theta_r$-sensitivities are larger than those for $n$ and $m$, which is not the case for sensitivity functions based on $\theta$-data for both the glass beads and the fine sand. As a consequence, there is some justification for neglecting $\theta_r$ in automatic parameter estimation procedures when using the weight factor $w = 0$.

Calculations of response surfaces were done using eqn (8) and a weighting factor $w = 0$ to find initial estimates for the optimization procedure. A contour plot of the $n$–$m$-parameter response surface is given in Fig. 7. The minimum of the objective function was found at the level of $\alpha = 0.035 \text{ cm}^{-1}$ with $O_{\min} = 0.5679$, and the attached parameters are $n_{\min} = 22.5$ and $m_{\min} = 1.5$. Using them as initial values the optimized parameters were computed to be $\alpha_{\text{opt}} = 0.03492 \text{ cm}^{-1}$, $n_{\text{opt}} = 22.52$, and $m_{\text{opt}} = 1.511$ with a value of $O_{\text{opt}} = 0.5647$. Small variations of $\alpha$ lead to drastically differing $n$-values while $m$ remains nearly constant. On the one hand, this can be explained by the small sensitivity of $m$ and the partial correlation between $\alpha$ and $m$ (Fig. 6). On the other hand, this finding is also caused by the use of a coarse-textured soil, because for these media the $n$-values are very large and, consequently, variations in $n$ are insensitive to the other parameters. Nevertheless, inverse modelling of MS-outflow experiments for the sand on the base of parameter functions (4) and (6) proved possible.

To check the usefulness of the reduced parameter function (7) response surfaces based on eqn (8) were calculated...
in the $\alpha$–$n$-plane for the MS-outflow experiment, the results are shown in Fig. 8.

Here, a minimum of the objective function was found with $O_{\text{min}} = 0.58379$, and the attached parameters are $\alpha_{\text{min}} = 0.0355 \, \text{cm}^{-1}$ and $n_{\text{min}} = 22$. They are very close to the values that were computed based on the more complex model, see above. The $\alpha$–$n$ response surface has a valley almost parallel to the $n$-axis. This is not caused by a correlation between the two parameters, but results from the low sensitivity with respect to $n$ compared with $\alpha$. Zurmühl\textsuperscript{25} found such long-stretched valleys only in the case of one-step experiments, he improved this situation by switching to multi-step methods. The contour plot in Fig. 8 thus indicates a smaller parameter sensitivity than that in Fig. 7. For the glass-bead medium the simplified model occurred to be not appropriate yielding a much larger minimum of the objective function than for the more complex model.

Gribb\textsuperscript{4} also found long valleys in the response surfaces for the $\alpha$–$n$ plane parallel to the $n$-axis using MS-methods, but clear minima could not be detected. This is because of the specific insensitivity to $n$ indicated by the lack of curvatures in that direction originating most probably from the use of objective functions based on flow rate and pressure head responses. Thus, for the porous materials discussed here parameter identifiability proved to be much better when only water content measurements are taken into account.

In Fig. 9 both measured and calculated water content and pressure head distributions of an additional multi-step outflow experiment are compared for validation purposes, based on numerical simulation with the optimized parameters $\alpha_{\text{opt}} = 0.03492 \, \text{cm}^{-1}$, $n_{\text{opt}} = 22.52$, and $m_{\text{opt}} = 1.511$. A close agreement between measured and calculated values can be noticed again.

4 SUMMARY AND CONCLUSIONS

In this paper methods for determining the parameters $\alpha$, $n$, and $m$ of the hydraulic functions described by eqns (4), (6) and (7) of two isotropic, homogeneous porous materials, glass beads and sand, from multi-step outflow experiments via indirect parameter estimation procedures have been investigated. Large columns with artificially packed materials were used in order to avoid heterogeneity effects of natural layered soils. Water outflow from the columns was controlled by stepwise head reduction corresponding to decreases of the piezometric surface observed in natural drainage systems with unsaturated/saturated flow. Analysis of sensitivity coefficients and response surfaces of appropriately defined objective functions allowed a
systematic assessment of identifiability for different parameter combinations and different weights between measured data of cumulative outflow, pressure head and water content. The coarse estimates thus obtained have been additionally used as starting points for automatic inverse parameter identification with a Levenberg–Marquardt scheme.

In contrast with earlier one-step outflow experiments conducted by the authors least-squares identifiability was in principal detected for both porous media if using MSO

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**Fig. 8.** Contour plot of objective function values based on water content data responses in the $\alpha$–$\eta$ parameter space for the fine-sand column experiment using model (7).

**Fig. 9.** Comparison of observed and simulated water content (left) and pressure head (right) distributions for the sand using MS-method at $x = 35$ cm (T1), $x = 65$ cm (T2), and $x = 125$ cm (T3).
methods and, if utilising the more general functions with the additional independent parameter \( m \) for describing hydraulic properties of coarse-textured porous media. Based on the identified parameters of these functions steep decreases of water content distributions during the outflow process (Figs 5, and 9) could be simulated in close agreement with measurements. Differences between observed and predicted cumulative outflows of water and pressure head distributions were small.

The utility of parameter estimation methods using one-step or multi-step outflow data has been studied in detail in the literature.\(^{19,21,22,3,4,25}\) It has been found that the outflow data from MS-experiments contrary to those from OS-experiments contain sufficient information for a unique estimation of the soil hydraulic functions. Additional pressure head measurements at some inner point of the column greatly improve parameter identifiability in both experimental methods. In the present study, however, highest parameter sensitivities were observed if only water content data are used in the objective function. They were considerably smaller when taking into account outflow and/or pressure head data. This result differs from previous investigations\(^{19,1}\) which may be explained by our findings, that for coarse-textured porous media water content expressed the dynamics of water desorption in a more sensitive manner related to the parameters \( \alpha, n, \) and \( m \) than outflow or pressure head. During MSO experiments strong changes for both water content and pressure head were observed (Fig. 9). The extent of these changes is comparable, but not their distribution over time. While the water content decreases in a very short time step, the pressure head decreases more slowly in dependence on the piezometric level. This behaviour is reflected by the sensitivity coefficients only in the case of water content data, compare Fig. 3 and Fig. 6 for \( w = 0 \). Consequently, a larger sensitivity of water content compared with pressure head can be stated.

As described by Toorman et al.\(^{19}\) and Van Dam et al.\(^{22}\) automatic inverse modelling can be improved if good initial estimates of the parameters are available from simulation studies with synthetic data or from the outflow experiment itself. In the present study, response surfaces were analysed to get initial values of the parameters \( \alpha, n, m \). Convergence of the Levenberg–Marquardt estimator could not be reached in all cases, and some experimentation with starting values became necessary. Based on the analysis of Mous\(^{10}\) conditions of local parameter identifiability were investigated by examination of the normalized sensitivity coefficients and by testing their linear independence.

In our study, beside from utilisation of different kinds of measured physical quantities, identifiability has benefited from measurements in more than one inner point (two to three) of the column. It was additionally improved by the drastic alterations in water content data resulting in strong non-linearities (jumps) of the sensitivity coefficient distributions (Fig. 3).

Comparing different parameter sensitivities we found that they were much smaller with respect to \( n \) and \( m \) than with respect to \( \alpha \). Because the \( n \)-values for coarse-textured porous media are very large, variations in \( n \) are generally insensitive to changes in \( \alpha \). This has also been the case for the glass bead column where \( n \) was identified to be larger than 10.

For both porous media MSO experiments allow to estimate static, unique hydraulic functions which could be described by eqns (4) and (6). Results of Vachaud et al.\(^{20}\) Stauffer,\(^{18}\) and Nützmann et al.\(^{13}\) point at the dependence of capillary pressure–saturation relationships on the rate of flow due to dynamic effects. The concept of dynamic capillary curves, considering furthermore effects as grain size distributions, wettability, microscale and macroscale heterogeneities, see Hassanizadeh,\(^{5}\) should be of future interest for studying water flow through large soil columns as used in the present study.

In addition, work is under way to estimate the hydraulic parameters of the used materials with inverse modelling of evaporation experiments in small columns. Besides the problems of ill-posedness and identifiability, scale effects are to be expected.

REFERENCES


