Parameter estimation for unsaturated flow models using sensitivity analysis
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Abstract

The results of several multi-step outflow experiments on a 150-cm column were analyzed to identify the unsaturated hydraulic properties of a coarse-textured sandy soil. The hydraulic functions are assumed to be represented by the complete van Genuchten - Mualem closed-form expressions with variable coefficients $a$, $n$, and $m$. A sensitivity analysis with respect to these parameters shows, that conditions of local identifiability are satisfied if exclusively measurements of water content in some inner points of the column are considered. For this porous medium unique results of the identification problem could be obtained, and afterwards, the corresponding hydraulic functions have been verified with respect to additional drainage experiments.

1 Introduction

Model calibration in the unsaturated zone may be particularly difficult due to problems in formulating the constitutive relations for this special kind of two-phase flow, namely the water retention curve and the unsaturated hydraulic conductivity. There are some transient experimental methods
coupled with inverse modelling techniques to determine the relationships between the pressure head $h$, the water content $\theta$, and the hydraulic conductivity $K$. It was found that the $\theta(h)$-relationship may be not 'static' if boundary conditions were changed rapidly and flow process is extremely large, Vachaud et al.\textsuperscript{5}. Secondly, these experiments commonly were carried out on small in-situ soil samples and the optimized soil hydraulic functions do not necessarily represent in-situ soil behaviour.

The objective of the present study was to estimate unsaturated hydraulic properties of an artificial packed, homogeneous coarse-textured sandy soil with inverse modelling of multistep-outflow experiments (MSO), and to extend the theoretical analysis of Toorman et al.\textsuperscript{4} and the results of Van Dam et al.\textsuperscript{6} on larger soil columns. Conditions of identifiability were investigated using the concept of sensitivity analysis to get a well-posed inverse problem formulation with an unique solution. There was special interest in the comparison of parameter sensitivity of water content in comparison with pressure head data measured inside of the column.

2 Methods

Multistep outflow experiments were carried out in a column with a length of 150 cm as described in Nützmann et al.\textsuperscript{3}. During the experiments the cumulative volumetric outflow was stored. Microtensiometers and TDR (time domain reflectory) - probes were used to measure the pressure head and the volumetric water content at different positions in the column. The governing equation for transient saturated-unsaturated water flow in a vertical soil column without sinks and sources is given by the Richards-equation, and their solution was obtained by a Galerkin finite-element code. As shown by van Genuchten and Nielsen\textsuperscript{7} the water retention relation

$$\Theta(h) = \frac{(\theta - \theta_r)}{(\theta_s - \theta_r)} = \frac{1}{1 + (\alpha h)^n}^{m},$$  (1)

with the relative water saturation $\Theta$ ($0 \leq \Theta \leq 1$), the saturated water content
\( \theta_s \), the residual water content \( \theta \), and the parameters \( \alpha, m, \) and \( n \) 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\(^2\).

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

\[
O(a) = w\left[ Q^* - Q(a) \right]^T \left[ Q^* - Q(a) \right] + (1 - w) \cdot v \left\{ \sum_i \left[ \theta_i^* - \theta_i(a) \right]^T \left[ \theta_i^* - \theta_i(a) \right] \right\}
\]

where \( a = (\alpha, n, m)^T \) is the vector of the unknown parameters, \( Q^* \) and \( Q(a) \) are the vectors of measured and calculated outflows, \( \theta_i^* \) and \( \theta_i(a) \) stands for the vectors of measured and predicted water contents (or the measured and predicted pressure head vectors), \( i \) is the number of measurement positions inside of the column. The factor \( w, 0 \leq w \leq 1 \), allows to weight between the outflow and the potential quantities in the objective function. The weight \( v \) accounts for the different measurement scales of outflow volumes and water contents or pressure heads respectively.

A necessary condition for \( O(a) \) having a local minimum is that the Jacobian matrix of partial derivatives of any calculated model output with respect to the parameters be full of rank, Mous\(^1\), or that the rows of this matrix, the so-called sensitivity coefficients, be linear independent. The sensitivity coefficients of the parameter identification problem considered here can be calculated from (2) for the \( a_i, i=1,...,N \) as

\[
X_1(t_k,a) = -w \frac{\partial Q(t_k,a)}{\partial a_1} - (1 - w) v^{1/2} \sum_i \frac{\partial f_i(t_k,a)}{\partial a_1}, \quad k = 1,...,M,
\]

where \( f_i(t_k,a) \) are model outputs of water content or pressure head. The computation of the Jacobian matrix was carried out numerically for each parameter using a central difference scheme.
3 Results

Computations of sensitivity coefficients with respect to the parameters $\alpha$, $n$, and $m$ were done for the MSO experimental data investigating the influence of the weighting factor $w$. For a better comparison of these values one must consider the normalized form of (3). Figure 1 shows normalized coefficients for $\alpha$ with $f_i = \theta_i$, in Fig. 2 these coefficients are depicted using $f_i = h_i$.

As shown in Fig. 1, the highest absolute sensitivities were calculated if 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.

Figure 1. Normalized $\alpha$-sensitivity coefficients for MSO using outflows and water contents in eq. (3), $\diamondsuit w = 0., \bullet w = 0.5, \triangle w = 1.$
Figure 2. Normalized $\alpha$-sensitivity coefficients for MSO using outflows and pressure heads in eq. (3), $\blacklozenge w = 0.$, $\bullet w = 0.5$, $\ast w = 1.$

The alteration steps of the sensitivity curves, especially for $w = 0$, are due to the changing outflow boundary condition. Note that the sensitivities of $n$ and $m$ (not shown here) are ten times lower than for the parameter $\alpha$, which determines the position of the $\theta(h)$ - function with respect to the $h$-axis. Thus, the value of $\alpha$ controls the pressure head $h^*$ when decreasing of water content with increasing pressure heads begins. The finding that sensitivity of $n$ is much lower than $\alpha$ is typically for a coarse-textured porous medium.

Comparison of different sensitivity curves show, that the coefficients of $\alpha$ and $n$ are uncorrelated and linear independent. There are only small correlations between $\alpha$ and $m$, and no correlations between $n$ and $m$. Thus, these parameters appear to be identifiable from MS-experiments using water content measurements exclusively, or, combined with outflow measurements.

The sensitivity coefficients based on pressure head responses differ totally from that behaviour as shown in Figure 2. 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 θ-based sensitivity coefficients is 0.03 with respect to α, and 0.045 with respect to n. This means that the sensitivities concerning outflow data are greater than those based on pressure heads; just in opposite to the case of θ-based sensitivity coefficients. Referring to identifiability there are no correlations between α and n, whereas between α 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.

To examine the uniqueness of the inverse problem response surfaces of the different parameter combinations were calculated, Toorman et al. The concept of response surfaces was used to find good initial estimates for the three parameters α, n, and m as starting values for the Levenberg-Marquardt algorithm. The minimum of the objective function was found with O_{min} = 0.5647, and the attached parameters are α_{min} = 0.03492 1/cm, n_{min} = 22.52, and m_{min} = 1.511. Small variations of α lead to clear different n-values while m remains nearly constant. This can be explained by the small sensitivities of m and n related to the large α-sensitivity.

Comparing measured and calculated quantities of multi-step outflow experiments based on numerical simulations with the optimized parameters in this way, close agreement can be noticed, Nützmann et al. For example, Figure 3a and 3b show outflows and pressure heads simulated with the optimized parameters in comparison with independently measured values of one MSO experiment.

4 Conclusions

In this paper methods for determining the parameters α, n, and m of the hydraulic functions of a homogeneous coarse-textured porous material from multi-step outflow experiments via indirect parameter estimation procedures have been investigated. Analysis of sensitivity coefficients and response
Figure 3a. Comparison of measured and simulated cumulative outflows

Figure 3b. Comparison of measured and simulated pressure heads
surfaces of appropriately defined objective functions allowed a systematic assessment of identifiability regarding data from different observations. In spite of the fact that sensitivities with respect to $n$ and $m$ were much smaller than with respect to $\alpha$, it proved possible to obtain optimal estimates of these parameters by considering water content data only for the coarse-textured medium used in this analysis. Knowledge of parameter sensitivities could be improve the inverse modeling and may lead to an unique estimation of the unsaturated hydraulic characteristics.

References


