HYDRAULIC PARAMETER ESTIMATION IN HETEROGENEOUS POROUS MEDIA

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Abstract

To make the estimation of hydraulic parameter functions from heterogeneous soil samples possible, a parallel inverse model for two- and threedimensional simulations was developed. The model was used to study the possibility to get unique and correct parameter estimations from multistep-outflow experiments with heterogeneous soil samples of known structure. While a numerical experiment provided promising results, laboratory experiments were complicated by perturbations caused during the construction of the sample.

1. INTRODUCTION

The determination of hydraulic parameter functions is crucial for the modeling of multiphase flow in porous media. Classical multistep-outflow experiments are a standard method for the determination of hydraulic properties for unsaturated flow (e.g. [1, 3, 4]). As the estimation of hydraulic parameters from this type of experiment is usually done by one-dimensional inverse modeling and as the internal structure is not known, it is up to now necessary to assume that the sample is homogeneous, which is not true for most natural porous media.

In the last years measurement techniques like x-ray tomography, geoelectrics and georadar have been developed, which allow the non-destructive determination of the spatial structure of a sample. If by application of one of these methods the structure of a sample is known, it can be possible to estimate the hydraulic property functions of the basic materials of a soil with multistep-outflow experiments and an optimization procedure which takes the structure explicitly into account. To test this approach a code for parameter optimization in 2D and 3D structured material was developed. Numerical and laboratory experiments have been conducted and the estimated hydraulic parameters for homogeneous and heterogeneous samples are compared. The main questions are:

- Is the information provided by a MSO-type experiment sufficient to get a reliable estimation of the parameters?
- Are the estimated values unique?

2. MODEL DESCRIPTION

The water transport in the porous medium was simulated with Richards' equation

$$\frac{\partial \left(S_{l}\phi\right)}{\partial t} = \nabla \cdot \left[K(S_{l})\nabla \left(p_{l} + \rho_{l}gz\right)\right],\tag{1}$$

where S_l is the saturation of the liquid phase, ϕ the porosity, t time, $K(S_l)$ the hydraulic conductivity, p_l the pressure of the liquid phase, ρ_l the density of the liquid phase, g gravity and z the vertical coordinate. Richards' equation is derived from multiphase flow equations by assuming that the mobility of the gas phase is high enough to keep the gas phase always at atmospheric pressure.

The Levenberg-Marquardt iteration scheme [2] in combination with a forward solver was used to solve the optimization problem. The sensitivity matrix was derived by external numerical differentiation, where each parameter in turn was disturbed by a small fraction, the response of the model was calculated and the deviation divided by the perturbation. Thus the assembling of a sensitivity matrix for the estimation of n parameters requires (n + 1) runs of the forward model. Singular value decomposition was used to calculate the correction which makes it possible to treat under-determined systems as well.

As stability and robustness are the primary goal for a forward solver in an inverse modeling approach, a cell-centered finite volume scheme is used for the space discretization with harmonic averaging of the absolute permeabilities and full-upwinding for the relative permeabilities. An implicit Euler scheme was used for the time discretization. The non-linear equations resulting from discretization of equation 1 are linearized by an incomplete Newton-method with line-search. The linear equations are solved with an algebraic multi-grid solver. For the time solver the time step is adapted automatically. As the measured structure of a soil sample is normally complex and therefore the generation of an optimal unstructured grid is hard to realize, the faster computation on a structured grid outweighs the gain by using an unstructured grid. The model therefore was optimized for structured rectangular grids. Two- and threedimensional simulations are possible. An object-oriented approach was used and the simulation is realized in C++.

To speed up the calculations the computation of the sensitivity matrix was parallelized using MPI. If $p \ge (n+1)$ parallel nodes are available for the estimation of n parameters the computation time for one iteration of the Levenberg-Marquardt algorithm is essentially independent of the number of estimated parameters.

3. EXPERIMENTS

3.1. Numerical Tests. A typical MSO experiment was simulated with the forward model. The usual experimental setup is shown in figure 1a. The soil sample is placed on a ceramic plate. A computer controlled increasing suction pressure is applied below the plate and the outflow as well as the capillary pressure at a tensiometer are measured in small time intervals. A radially symmetric structure composed of a coarse and a fine sand was used in the simulation (figure 1b). A continuous connection for both materials to the upper boundary was ensured to ensure the applicability of Richards' equation. Table 1 shows the van Genuchten-parameters used for the two materials. The simulation was conducted in two dimensions using radial coordinates. No-flux boundary conditions were used at the sides and at the top, the prescribed capillary pressure was used at the bottom.

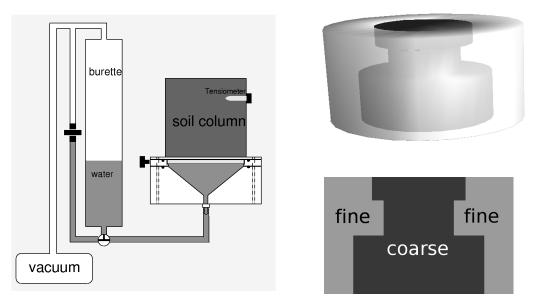


FIGURE 1. a) Typical experimental setup of a MSO simulation (left). b) Simulated structure in volume rendering and cross section (right).

The ceramic plate was included in the simulation as its permeability of 18 cm/h influences the information content of the measured data. After the simulation an random error of one percent was added to the data. Then the data was fitted with the inverse model. Additional knowledge about the sequence of the permeabilities of the two materials are necessary to ensure uniqueness of the parameters. If this is incorporated in the inversion process there is a perfect agreement between "measured" and simulated data (figure 2). All parameters are recovered with sufficient precision (table 1). Distinct deviations are found only in the saturated conductivities K. This can be explained by the limiting effect of the ceramic plate on the outflow velocity.

3.2. Laboratory Experiments. To test the positive findings of the numerical test in a real world setup, laboratory experiments have been conducted. MSO-experiments have been performed with one homogeneous column each of the fine and the coarse sand and a heterogeneous column with the same structure already used in the numerical experiment. The samples have been saturated in an exsiccator to avoid air entraption and ensure

Parameter	coarse		fine	
	fitted	exact	fitted	exact
$\alpha [\mathrm{m}^{-1}]$	8.2	8.0	2.1	2.1
n $[-]$	6.3	6.2	4.5	4.5
K [cm/h]	200.	120.	23.	20.
$\theta_s - \theta_r \ [-]$	0.30	0.30	0.31	0.30

TABLE 1. Numerical experiment: parameters used for the forward simulation (exact) and estimated from the simulated experiment (fitted).

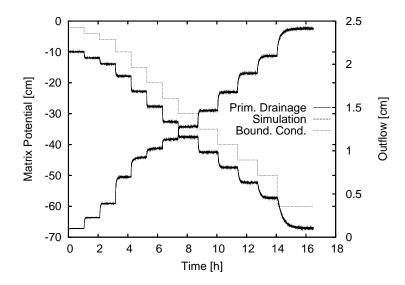


FIGURE 2. Boundary conditions and result of numerical experiment ("measured") and inverse modeling ("Simulation").

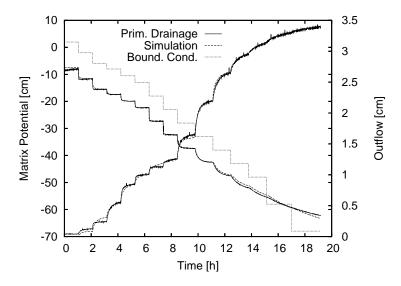


FIGURE 3. Boundary conditions, mesured data from the laboratory experiment and best fit.

full saturation of the sample. Brooks-Corey parameters λ and air entry values h_e , the hydraulic conductivities K and the available water content $\phi - \theta_r$ were estimated. While the agreement between measured and simulated outflow curves and tensiometer values was good for the homogeneous samples (not shown), it was not satisfying for the heterogeneous sample (figure 3).

Consequently the correlation between the parameters estimated for both materials from the homogeneous and the heterogeneous experiments is not too good. The resulting hydraulic functions are shown in figure 4. While the capillary pressure saturation curve and the hydraulic conductivity curve for the fine sand match reasonably well, there is no

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Parameter	coarse		fine	
	het.fit	hom.fit	het.fit	hom.fit
λ [-]	5.6	2.2	4.6	3.3
h_e [m]	0.11	0.11	0.39	0.35
K [cm/h]	330.	1.3	16.	11.
$\phi - \theta_r$ [-]	0.34	0.47	0.36	0.34

TABLE 2. Parameters estimated from the experiments with homogeneous coarse and fine sand columns and the heterogeneous sample

correspondence for the coarse sand. A forward simulation of the heterogeneous experiment with the parameters obtained from the homogeneous experiments (figure 5a) shows a slower outflow during the drainage of the coarse sand and an outflow curve which is shifted in time during the drainage of the fine sand. This seems to be a consequence of disturbances caused during the construction of the sample. Air gaps in the coarse sand reduce the permeability and cause the rounded outflow during the drainage of the coarse sand. A higher compaction of the fine sand leads to a higher air entry value and the time shift. This can be highlighted by a simulation where the parameters of the homogeneous experiments have been used but the air entry value of the fine sand was fitted (figure 5b), which results in a much better agreement for the drainage phase of the fine sand.

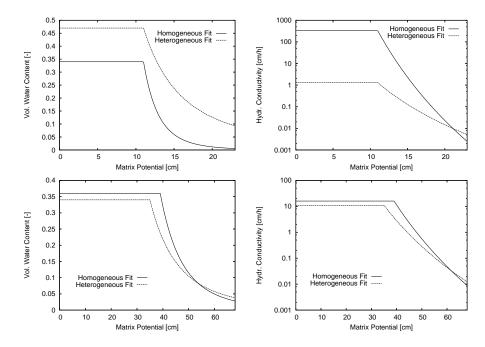


FIGURE 4. Comparison of capillary pressure/saturation curve for the coarse sand (upper left) and the fine sand (lower left) and the hydraulic conductivity curve for the coarse sand (upper right) and the fine sand (lower right) estimated from homogeneous and heterogeneous experiments.

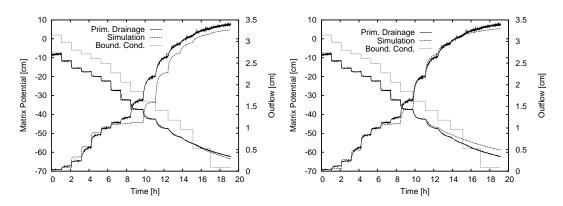


FIGURE 5. a) Forward simulation with parameters estimated from homogeneous simulations (left). b) Forward simulation with parameters from homogeneous simulations and fitted air entry value for the fine sand (right).

4. CONCLUSION

A parallel numerical model for parameter estimation from experiments with heterogeneous soil samples with known structure was developed. The numerical test was quite promising. A classical MSO-experiment seems to provide enough information the make parameter estimation for heterogeneous material with known structure possible. To ensure uniqueness additional knowledge about the sequence of the hydraulic permeabilites is necessary. The test of the parameter estimation approach with laboratory data was hampered by disturbances in the constructed soil sample. This problem might be less important in natural soil samples, where the structure is known from e.g. X-ray tomography. After parallelization of the forward solver the model will be applied to such, naturally more complex samples.

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