Inversion of time-lapse MRS for estimating unsaturated flow parameters by including hydraulic modelling in the forward calculation

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SUMMARY

The Combination of time-lapse MRS measurements with infiltration experiments has a great potential for estimating unsaturated flow parameters in situ. An inversion scheme is introduced that involves hydraulic modelling in the MRS forward calculation and approximates the measurements at all time steps of the experiment simultaneously. In this way, the hydraulic parameters characterizing the unsaturated zone can directly be estimated. The application of this scheme is shown with a synthetic time-lapse MRS data example, i.e., a simulated MRS monitoring of a virtual infiltration experiment.

Key words: Time-lapse MRS, time-lapse inversion, infiltration experiments

INTRODUCTION

Time-lapse MRS (TLMRS) is a reliable tool to visualize water infiltration into and (vertical) movement through the unsaturated zone in situ (Walsh et al., 2014). Herckenrath et al. (2012) have suggested a TLMRS inversion scheme for directly estimating aquifer parameters (specific yield and saturated hydraulic conductivity) based on the coupling of MRS and pumping test experiments. It is expected that combining artificial infiltration experiments with TLMRS-based monitoring can non-invasively provide important unsaturated subsurface flow parameters (e.g. after van Genuchten, 1980 and Mualem, 1976). Up to now, the direct estimation of water retention parameters by MRS in the unsaturated zone is only possible if the capillary fringe is resolved adequately and if it is in equilibrium (Costabel and Günther, 2014). This is, however, seldom the case in reality. In this work, an inversion approach for directly estimating flow parameters from TLMRS data is introduced that combines the MRS forward calculation (considering only the signal amplitudes, i.e., the time-dependent water content distributions) with unsaturated flow modeling. The approach is demonstrated with a synthetic data example. A real-life experiment is planned for autumn 2015.

HYDRAULIC MODELLING AND MRS FORWARD CALCULATION

For the demonstration in this work, an infiltration experiment considering 1D conditions is simulated. The modelling is realized using the Subsurface Flow Module of the commercially available software COMSOL Multiphysics®, which solves the Richards equation to calculate the vertical water movement through the unsaturated zone along the z-axis. The pressure head h is used as simulation variable, while the water content θ is related to h by the water retention function. The relationship between h, θ, and the hydraulic conductivities K_U (unsaturated) and K_S (saturated) is defined by the often-used van-Genuchten/Mualem model (e.g. Hinnell et al., 2010). The material parameters of the subsurface model represent a sandy soil (Fig. 1a). The depth of the water table z_{table} is determined at 10 m, which is the bottom boundary of the considered model and characterized by zero pressure. The gradually decreasing θ above z_{table} (capillary fringe) is controlled by the initial condition $h = -z + z_{table}$ up to the depth of 8 m. The initial condition for the depth range of 0 to 8 m is characterized by h = -2 m, a typical value representing the field capacity of a soil, i.e., the pressure head, at which residual water is kept in the pore space against the gravity force. The corresponding θ in the unsaturated zone for the given material before infiltration is 11% (Fig.1b). The boundary condition at the top of the model represents an artificial irrigation of 0.05 m/h for a time period of 10 h. Afterwards, the inlet is zero. The simulation was performed for 73 h. The resulting θ distributions of some chosen time steps in Fig.1b show the movement of the infiltration front into the subsurface.

The total amount of infiltrated water in the 1D simulation is given by 0.5 m. In reality, this amount would correspond to a total mass of 12.5 t of water if the irrigation takes place at an area of 5 by 5 m. This area would be large enough for a small circular MRS measurement loop with a diameter of 5 m, which is the chosen loop geometry for the MRS forward calculation. Only the initial signal amplitudes and no relaxation aspects are considered. The pulse moment vector ranges from 0.01 to 3 As. Figure 1c shows the simulated MRS curves for the θ distributions in Fig.1b. For the subsequent test of the TLMRS inversion scheme, these sounding curves were superposed with Gaussian-distributed noise. The noise level is defined according to Costabel and Günther (2014) and represents the fitting uncertainty of the initial amplitudes in practise. In Figure 1d, a real MRS signal measured with a 5-m loop at our test site (z_{table} at about 9 m) is shown. It exhibits a noise level of 0.42 nV. Based on this test measurement, the noise level for the realistic simulations were determined with 0.5 nV. A proof of concept is realized with an (unrealistically low) noise level of 0.1 nV.

CLASSICAL SMOOTH INVERSION

A smooth initial value inversion (IVI) was individually applied to the simulated MRS curves for the several time steps. Four example results are depicted in Fig.2. Except for early times, where the contrast in θ is still large enough to be resolved (Fig.2b), the smoothness constraint of the inversion leads to a smearing of θ along z. As a consequence, the resulting θ distributions fail to provide useful insights into the actual infiltration process.

MRS TIME-LAPSE INVERSION

As an alternative to the individual inversion for every time step, all time-dependent information can be included simultaneously if a reliable flow model is involved that describes the temporal variations of the θ distribution realistically. A similar principle was already applied for the inversion of time-lapse geoelectric data (e.g. Hinnell et al., 2010). Figure 3 shows an adaptation for MRS as a block diagram. After finishing the infiltration experiment and acquiring the MRS (and ideally some additional hydraulic) data at certain time steps t_n, an unsaturated flow model must be chosen at first. Along with the chosen flow model, the fitting parameters are defined, e.g., as in this work, the van-Genuchten/Mualem parameters n, α, θ_R, θ_S, and K_S. The corresponding starting values and inversion boundaries must be determined next. In principle, it is also possible to include additional fitting parameters describing the geometry of the model, e.g., layer thicknesses. The hydraulic modelling is started and the resulting θ distributions at t_n are used for an MRS forward calculation. The modelled and the measured MRS data are compared to each other by means of an objective function that has to be minimized iteratively, while the parameters to be fitted are updated in every iteration step. If a minimum can be reached, i.e., if the modelled and the measured data coincide after the inversion process has converged, the chosen flow model and the resulting parameters estimates can be considered to be reliable. In the case that the process does not converge the chosen model must be considered to be falsified.

To demonstrate the effectiveness of this inversion scheme, it was applied using the synthetic MRS data of the simulated infiltration experiment introduced above (Fig.2). Figure 4 shows the results for both noise levels. In both cases, the hydraulic parameters are estimated within reliable uncertainties (Table 1).

DISCUSSION AND OUTLOOK

By combining MRS time-lapse measurements with infiltration experiments, hydraulic parameters characterizing the unsaturated zone can be estimated directly if an inversion scheme is applied that involves hydraulic modelling. In this way, the plausibility of flow models can effectively be tested for the area of investigation and the parameter estimates can be used for predicting, for instance, groundwater recharge or solute transport scenarios. A real-life experiment to demonstrate this application is planned for autumn 2015.

However, when applying the introduced time-lapse inversion, the choice of the flow model is a very crucial aspect. The inversion scheme might estimate reliable parameters for the chosen flow model, but in case that the real flow conditions differ from the chosen model, this kind of inversion hardly provides indications for choosing a plausible alternative (e.g. preferential flow). So, it is always recommended to use the time-lapse inversion if additional a priori information is at hand that allows at least a pre-selection of eligible models.

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Table 1. Hydraulic model parameters, their starting values, inversion boundaries, and estimations provided by MRS time-lapse inversion for synthetic data sets with different noise levels

van Genuchten/Mualem-Parameter	K_S [cm/h]	θ_S [-]	θ_R [-]	n [-]	α [1/cm]
Model	100.0	0.40	0.05	2.0	0.030
Dataset with 0.1 nV noise	107.7 +/- 10.0	0.40 +/- 0.00	0.05 +/- 0.01	2.0 +/- 0.1	0.032 +/- 0.002
Dataset with 0.5 nV noise	207.1 +/- 29.3	0.42 +/- 0.02	0.06 +/- 0.02	1.9 +/- 0.1	0.047 +/- 0.016
Dataset with 1.0 nV noise	114.4 +/- 108.3	0.38 +/- 0.05	0.06 +/- 0.06	2.1 +/- 0.7	0.031 +/- 0.025
Starting model	11.00	0.30	0.15	1.40	0.002
Inversion boundaries	10.0 -> 500.0	0.20 -> 0.50	0.01 -> 0.20	1.3 -> 2.5	0.005 -> 0.05

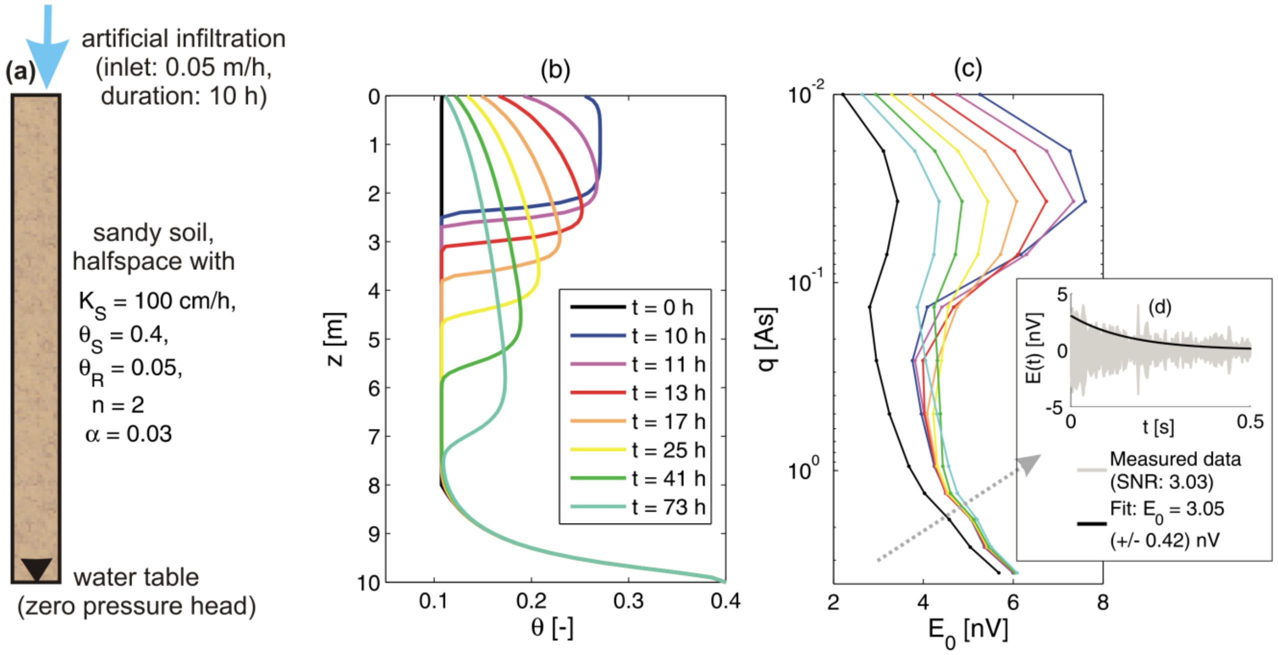

Figure 1. (a) Subsurface model for the underlying virtual infiltration experiment, its domain properties and boundary conditions, (b) time-dependent water content distribution being the result of the hydraulic modelling, (c) results of the MRS forward modelling for each time step (noise-free), and (d) real MRS data example using a 5-m diameter loop over an aquifer at a depth of about 9 m.

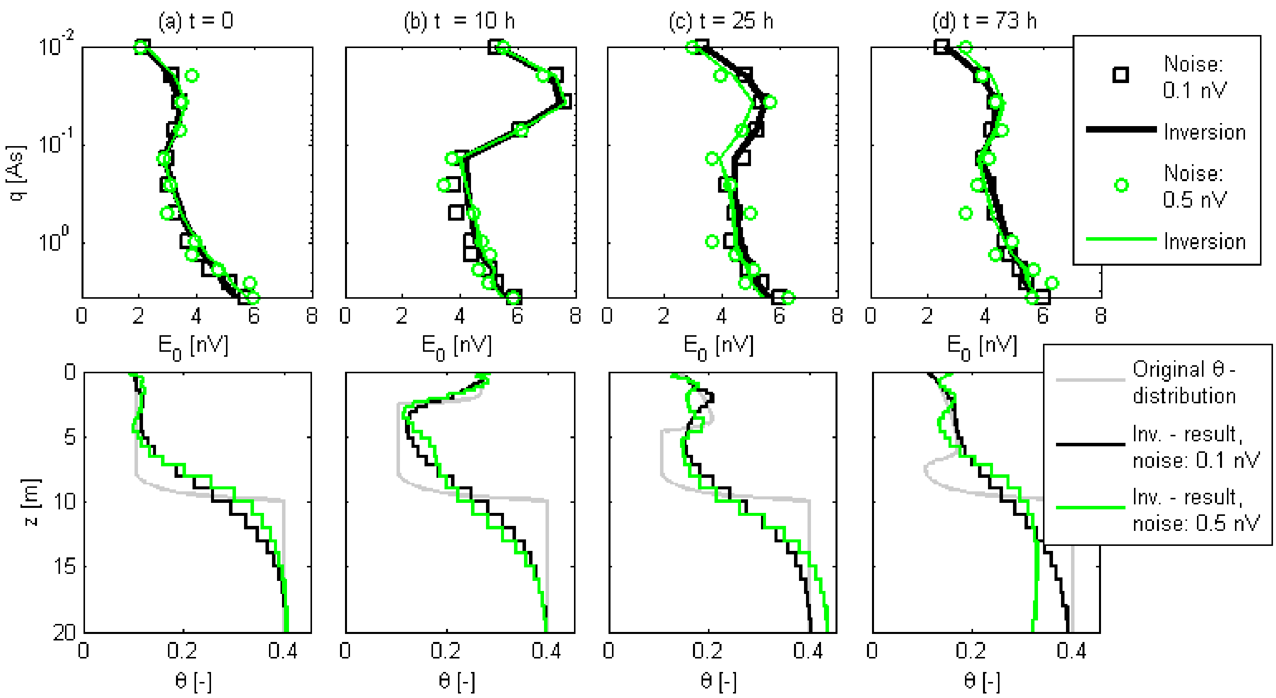

Figure 2. Smooth initial value inversion (IVI) results of the synthetic MRS data (two different noise levels) for certain time steps, top: initial amplitudes and approximations, bottom: inverted water content distributions compared to original model (see Figure 1b), (a) before infiltration, (b) immediately after finishing infiltration, i.e., 10 h, (c) 25 h, and (d) 73 h after beginning of infiltration.

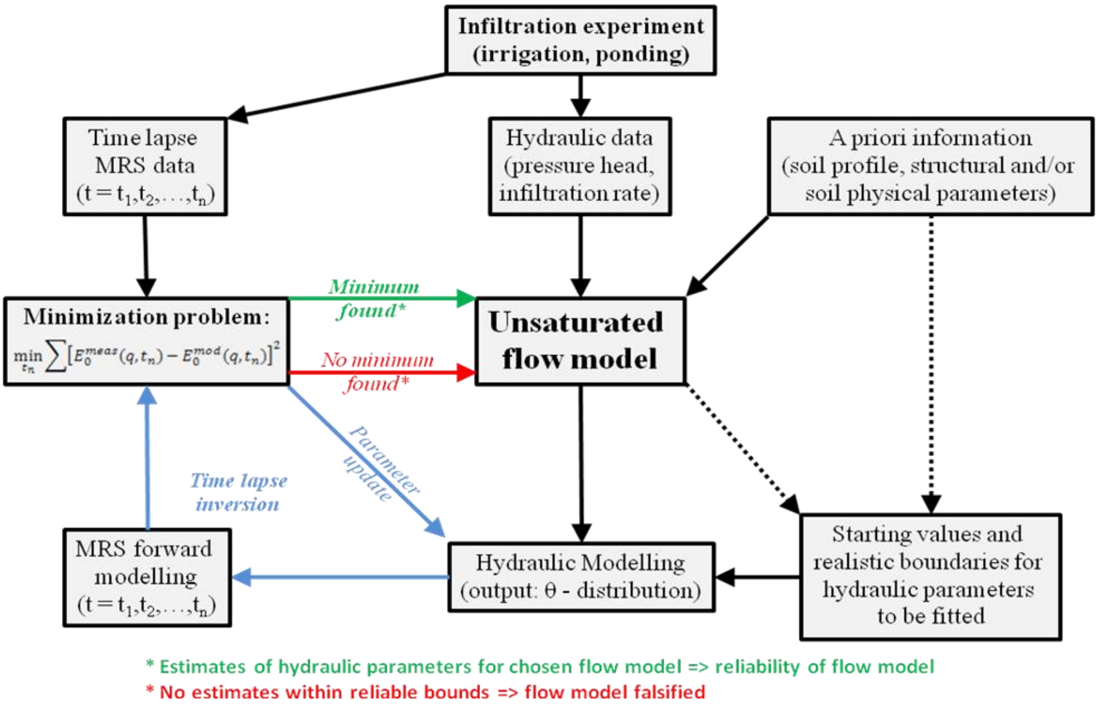

Figure 3. Block diagram showing how to apply the MRS time-lapse inversion for estimating hydraulic subsurface parameters.

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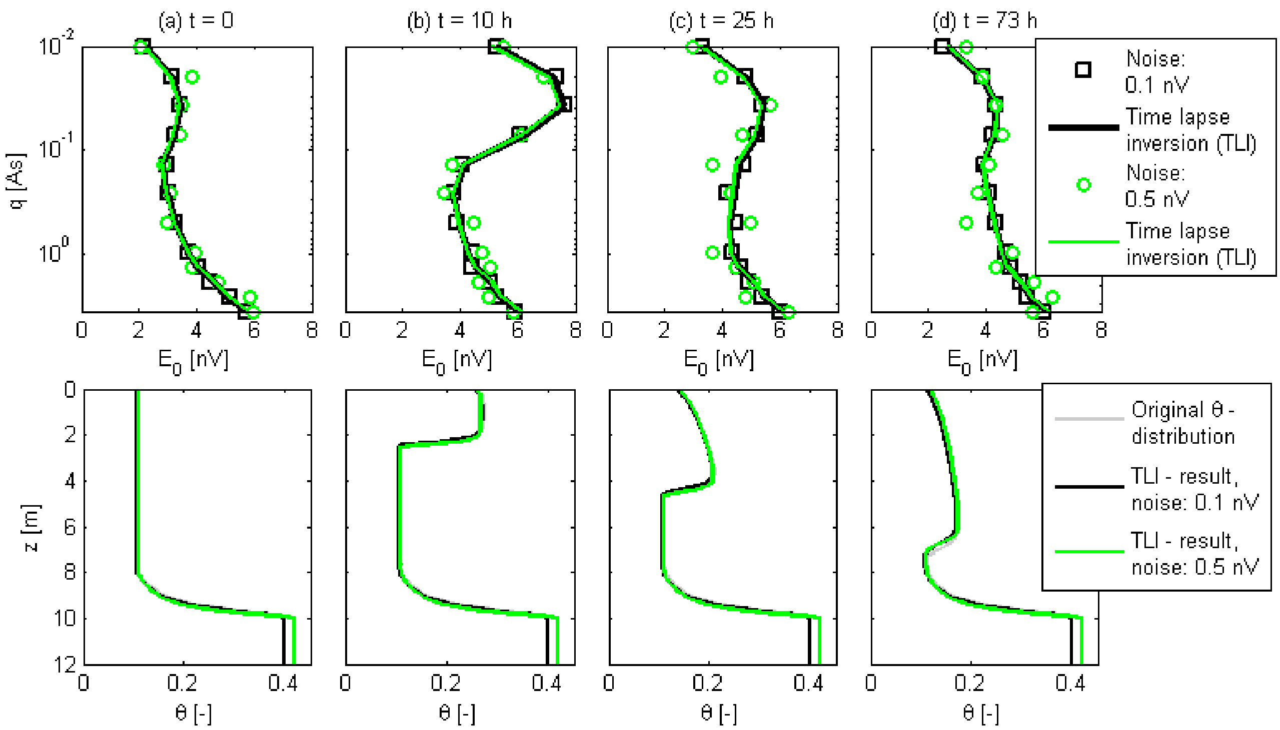

Figure 4. Time-lapse inversion (TLI) results of the synthetic MRS data (two different noise levels) for certain time steps, top: initial amplitudes and approximations, bottom: inverted water content distributions compared to original model (see Figure 1b), (a) before infiltration, (b) immediately after finishing infiltration, i.e., 10 h, (c) 25 h, and (d) 73 h after beginning of infiltration.