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CENTRIFUGATION SCENARIOS FOR DETERMINATION OF SOIL PARAMETERS

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Summary. Several centrifugation scenarios for the determination of soil parameters for saturated-unsaturated flow in porous media are discussed. Only global characteristics of the infiltration process in the sample are required. These characteristics can be the rotational momentum, the gravitational center, the mass of water in the sample, or the mass of expelled water measured at known time sections. These simple measurements can be used because of the application of an accurate and efficient numerical solution in the present paper. The mathematical model of infiltration is represented by Richards strongly nonlinear and degenerate equation expressed via the Van Genuchten-Mualem ansatz for the soil parameters in the unsaturated zone. The identification process is realized in an iterative way applying the Levenberg-Marquardt method.

1 INTRODUCTION

To predict the flow and solute transport in soils concerns the soil hydraulic properties in terms of soil parameters which are the input data in the governing mathematical model. This model is expressed in terms of saturation and pressure head via Richards equation, which is a nonlinear and degenerate parabolic equation with free boundaries between saturated and partially saturated zones, and between the dry zone and partially saturated zone. The soil retention and hydraulic permeability functions linking the saturation and pressure head are expressed using the Van Genuchten-Mualem ansatz by means of soil parameters. The measurement of capillary pressure curves with a centrifuge was initiated in [2]. With the development of more efficient numerical modeling this method became more popular in the last decades. A more detailed overview on this topic can be found in [4] (see also citations there). Recently, the method of centrifugation has been applied in [1] and [5] where the equilibrium analysis at a set of rotational speeds has been used for

the determination of soil parameters. In [5], the distribution of saturation in equilibria (linked with the correspondent rotational speeds) are measured via electrical signals from electrodes installed in the sample.
The presently used centrifugation scenarios are closely related with the available numerical models of the infiltration process during centrifugation. The solution of the mathematical model based on Richards equation has a sharp front at the interface between partially saturated and dry zones in the sample. Furthermore, the free boundary between the fully saturated and partially saturated front is difficult to identify (when they are expressed in terms of saturation). It is a difficult task for numerical approximations to supply accurate results as needed in the determination process of model parameters. Our main goal in this paper is to present a new approximation method which is accurate and efficient to supply us with the computation of global characteristics such as: rotational momentum of infiltrated water in the sample, gravitational center of the water, and the time evolution of input and output water in the sample. The considered measurements do not include pointwise saturation or head distributions over the sample. This makes the determination process more difficult since the sensitivity of global characteristics on soil parameters could be small, and moreover, the numerical error could shadow it. Therefore the numerical method should be accurate and efficient.
Here, we present a centrifugation scenario in which water infiltrates into an originally dry sample from a water chamber situated before the sample. In this scenario we have a fully saturated zone, a partially saturated zone and the dry zone of the sample. Following the water movement in this system gives us a complex map of the infiltration process and representative data of the global characteristics.
The presented mathematical model and its numerical realization can be applied in many different centrifugation scenarios. The accurate numerical approximation is based on the following attributes:

- application of the mathematical model for the evolution of the wetness front (interface between partially saturated and dry region), which we have developed in papers [1] and [3]
- application of moving grid points which significantly increase the numerical accuracy and effectiveness
- numerical modeling of the free boundary between saturated and partially saturated zone, based on global water mass balance
- expressing the Richards equation locally in terms of saturation and locally in pressure head depending on the distance to both free boundaries.

In Section 1 we introduce the mathematical model. In Section 2 we present the numerical method used, while numerical experiments are discussed in Section 3. There, in Experiment 1 we present the solution of the present centrifugation scenario. In Experiment 2 and 3 the soil parameters are restored from simulated global characteristics applying the well-known iteration process of the Levenberg-Marquardt (LM) method.

2 MATHEMATICAL MODEL

We consider a one dimensional dry sample in the form of a tube which starts at the distance $r = r_0$ from the center of the centrifuge and ends at the distance $r = r_0 + L$. At position $r \in (r_0 - \ell_0, r_0)$ of the centrifuge a water chamber is placed. The saturated flow in porous media under centrifugation is modeled by Darcy's equation and for unsaturated flow by Richards equation,

$$\begin{aligned} K_s\, \partial_r \left[\left(\partial_r h - \tfrac{\omega^2}{g} r \right) \right] &= 0, \quad \text{in saturated region } h \geq 0, \\ \partial_t \theta = K_s\, \partial_r \left(k(\theta) \partial_r h - \tfrac{\omega^2}{g} r \right), &\quad \text{in unsaturated region } h < 0, \end{aligned} \tag{1}$$

where h is the piesometric head, θ is saturation of the porous media, ω is the angular speed of rotation (in radians per second), K_s is the saturated hydraulic conductivity, g is the gravitational constant and function $k(\theta)$ is the hydraulic conductivity in the unsaturated region (see, e.g. [5, 1]). Denote by $u = \frac{\theta - \theta_r}{\theta_s - \theta_r}$ the effective saturation where θ_s is the volumetric water content at saturation and θ_r is the residual volumetric water content. We have $u \in (0, 1)$, since $\theta \in (\theta_r, \theta_s)$. The soil hydraulic properties are represented by empirical expressions (see [Van Genuchten])

$$u = \frac{1}{(1 + (\gamma h)^n)^m}, \quad h \in (-\infty, 0), \quad k(u) = u^{1/2} \left[1 - \left(1 - u^{1/m} \right)^m \right]^2 \tag{2}$$

where $m = 1 - 1/n, n > 1$ and $\gamma = -(2^{1/m} - 1)^{1-m}/h_b$ are empirical soil parameters with h_b the bubbling pressure. Hence, the flow in the unsaturated region can be rewritten in the form

$$\partial_t u = \partial_r \left(D(u) \partial_r u - \frac{\omega^2}{g} k(u) r \right), \tag{3}$$

where

$$D(u) = -\frac{K_s}{(n-1)\gamma(\theta_s - \theta_r)} u^{1/2 - 1/m} (1 - u^{1/m})^{-m} [1 - (1 - u^{1/m})^m]^2. \tag{4}$$

Equation (3) is strongly nonlinear and degenerate. We note that $D(0) = 0$, $D(1) = \infty$. As a consequence of these facts the propagation of the wetness front into the dry region will proceed with finite speed (i.e. there appears an interface or free boundary). The first equation in (1) can be integrated and we obtain

$$h(r) = \frac{\omega^2}{2g} r^2 + C_1 r + C_2.$$

The integration constants can be determined from boundary conditions. In the process of centrifugation the water from the reservoir is pushed to the dry region of the sample and creates saturated and unsaturated subregions in the sample. Denote by $s_1(t) \in (0, L)$ the free boundary which separates the saturated and unsaturated regions in the sample. We also denote by $s_2(t)$ the free boundary ($s_1(t) < s_2(t) \in (s_1, L)$) separating the partially saturated zone from the dry zone. We can easily determine

$$h(r_0, t) = \frac{\omega^2}{2g}\ell(2r_0 - \ell), \quad h(s_1(t)), t) = 0,$$

since the piesometric head at r_0 is equal to the pressure of water from the reservoir ($(r_0 - \ell(t), r_0)$) and the piesometric head on the interface $r_0 + s_1(t)$ is zero.
Then, for $r \in (r_0, r_0 + s_1(t))$ we have

$$h(r_0 + y) = \frac{\omega^2}{2g}[y^2 - y(\frac{1}{s_1}\ell(2r_0 - \ell) + s_1) + \ell(2r_0 - \ell)], \tag{5}$$

with the flux

$$q(t) = K_s \frac{\omega^2}{2g}\, \frac{1}{s_1(t)}[2r_0 s_1(t) + s_1(t)^2 + \ell(t)(2r_0 - \ell(t))], \tag{6}$$

where $\ell(t), s_1(t)$ have to be determined. Since the flux of water along $(r_0, r_0 + s_1(t))$ is constant, it follows

$$\dot{\ell}(t) = -q(t) := f_1(\ell, s_1), \tag{7}$$

where q is from (6). Now, we construct the model for $\dot{s}_1(t)$. Again from mass balance reasons we deduce that the flux $q(t)$ is used to increase the water content in the saturated and unsaturated subregions. The crucial point is to obtain the flux $q_{int}(t)$ entering the unsaturated subregion $x \in (r_0 + s_1(t), r_0 + s_2(t))$. We note that $u(s_2(t), t) = 0,\ \forall t$ and $u(s_1(t), t) = 1$. Then u in the unsaturated region is governed by (1) with $(s_1(t), s_2(t))$ the moving domain of the solution (we shift the original domain by r_0). We transform it to a fixed domain using the transformation $y = \frac{x - s_1(t)}{s_2(t) - s_1(t)}$. We denote by $\bar{u}(z, t) := u(x, t)$ and for simplicity we keep the notation u instead of $\bar{u}$. Then,

$$\partial_t u(y, t) = \frac{K_s}{ss(t)^2}\partial_y \left(D(u)\partial_y u - ss(t)k(u)\frac{\omega^2}{g}\left(r_0 + s_1(t) + y\, ss(t)\right)\right) \tag{8}$$

$$+ \left(\dot{s}_1(t)(1 - y) + \dot{s}_2(t)y\right)\frac{1}{ss(t)}\partial_y u$$

where $ss(t) := s_2(t) - s_1(t)$, with boundary and initial conditions

$$u(0, t) = 1, \quad u(1, t) = 0; \quad u(y, 0) := u_0(y).$$

To model the interface $s_2(t)$ we follow [1] (see also [3]) where problems similar to (8) have been studied. For this purpose we have to compute

$$\lim_{z \to 0} \frac{D(z)}{z^p} = m^2, \quad \text{where } p = 1/2 + 1/m.$$

Then the model for the evolution of $s_2(t)$ reads as follows

$$\dot{s_2}(t) = -\frac{K_s m^2}{p(\theta_s - \theta_r)\gamma(n-1)} \, \frac{1}{ss(t)} \partial_y u(1,t)^p, \text{ where } p = 1/2 + 1/m. \tag{9}$$

Now, the solution of (8), (9) defines a flux $q_{int}(t)$. Finally, we close our system with the mass balance condition $q(t) = \dot{s_1}(t) + q_{int}(t)$ from which we have

$$\dot{s_1}(t) = q(t) - q_{int}(t) \tag{10}$$

where q is from (6) and $q_{int}(t)$ is the flux of the solution at $y = 0$ of the model (8),(9) with the initial and the boundary conditions as above. Now, the final system (7)-(10) can be solved by approximating it with a corresponding ODE system, using a space discretization (MOL method).

3 NUMERICAL METHOD

The 1D mathematical model results in a coupled system of PDE and ODE (7)-(10). We apply now space discretization, and solve the resulting ODE system (MOL method). Let

$$0 = y_0 < y_1 < \ldots < y_i < \ldots < y_N = 1; \ \alpha_0 = 0, \ \alpha_i := y_i - y_{i-1}, \ i = 1, \ldots, N.$$

be the grid points in the fixed domain $y \in (0,1)$. This corresponds to the moving grid points $x_i(t) = s_1(t) + y_i\, ss(t)$ in the sample. We integrate (8) over $I_i := (y_i - \alpha_i/2, y_i + \alpha_{i+1}/2)$, $\forall i = 1, ..., N-1$ and denote by $u_i(t) \approx u(y_i, t)$, $\forall i = 1, \ldots, N-1$. We approximate $\partial_t u(y,t) \approx \dot{u}_i(t)$ in the interval I_i, and also

$$\partial_y u|_{y=y_{i+1/2}} \approx \frac{u_{i+1}(t) - u_i(t)}{\alpha_{i+1}} =: \partial^+ u_i, \quad \text{where } y_{i+1/2} := y_i + \alpha_{i+1}/2.$$

Similarly we approximate $\partial_y u|_{y=y_{i-1/2}}$ and denote it by $\partial^- u_i$. We also denote $u_{i+1/2} := (u_{i+1} + u_i)/2$ and $k_{i+1/2} := k(u_{i+1/2})$ (similarly for $i - 1/2$). Then, the ODE approximation of (8) at point $y = y_i$ reads as

$$\dot{u}_i = \frac{2K_s}{\theta_s - \theta_r} \, \frac{1}{ss^2} [D_{i+1/2}\partial^+ u_i - D_{i-1/2}\partial^- u_i + (\dot{s}_1(1-y_i) + \dot{s}_2 y_i) \left. \frac{d\mathcal{L}(z; y_i)}{dz} \right|_{z=z_i} -$$

$$\frac{\omega^2 ss}{2g}(k_{i+1/2}(r_0 + s_1 + y_{i+1/2}ss) - k_{i-1/2}(r_0 + s_1 + y_{i-1/2}ss))], \quad i = 1, ..., N-1, \tag{11}$$

$$\dot{\ell}(t) = f_1(\ell, s_1) \tag{12}$$

$$\dot{s_1}(t) = f_1(\ell, s_1) - f_2(s_1, s_2, u_1, u_2) \tag{13}$$

$$\dot{s_2}(t) = f_3(s_1, s_2, u_{N-2}, u_{N-1}) \tag{14}$$

where $\mathcal{L}(z; y_i)$ is the Lagrange polynomial of the second order crossing the points $(y_{i-1}, u_{i-1}(t))$, $(y_i, u_i(t))$, $(y_{i+1}, u_{i+1}(t))$, and f_3 is given by

$$f_3(s_1, s_2, u_{N-2}, u_{N-1}) = -\frac{K_s m^2}{p(\theta_s - \theta_r)\gamma(n-1)} \; \frac{1}{ss(t)} \; \left[\frac{d\mathcal{L}_-(z; y_N)}{dz}|_{z=1}\right]^p,$$

where $p = 1/2 + 1/m$ and $\mathcal{L}_-(z; y_N)$ is the Lagrange polynomial crossing the points $(y_{N-2}, u_{N-2}(t))$, $(y_{N-1}, u_{N-1}(t))$, $(1, 0)$. The function f_2 represents the numerical approximation of the flux q_{int} and reads as

$$f_2(s_1, s_2, u_1, u_2) = \frac{K_s}{ss(\theta_s - \theta_r)} \left(\left.\frac{d\mathcal{L}_+(z; y_0)}{dz}\right|_{z=0} - \frac{\omega^2}{2g} s_1 \right)$$

where $\mathcal{L}_+(z; y_0)$ is the Lagrange polynomial crossing the points $(0, 0)$, (y_1, h_1), (y_2, h_2), with $h_i = -\frac{1}{\gamma}[-1 + u_i^{-1/m}]^{1/n}$, $i = 1, 2$. We note that the flux at $y = 0$ must be expressed in terms of head (instead of saturation) since at $y = 0$ we have $u_0 = 1$, $h_0 = 0$ and $D(1) = +\infty$. We replace $\dot{s_1}$, $\dot{s_2}$ in (11) by $f_1 - f_2$ and f_3, respectively, and obtain an ODE system

$$\dot{w} = F(t, w), \quad w = [u_1, ..., u_{N-1}, \ell, s_1, s_2],$$

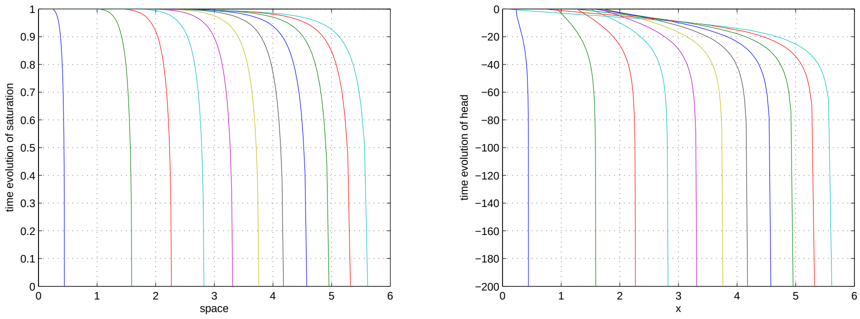
which canbe solved by an ODE solver for stiff systems. This system must be completed by the initial state $w(0) = [u_1(0), ..., u_{N-1}(0), \ell(0), s_1(0), s_2(0)]$.

Above model is valid up to a time T_1, which is characterized by $\ell(T_1) = 0$. For $t > T_1$, the model must be changed, because of a change in boundary condition at $y = 0$ which for $T > T_1$ will be free of flux. In this case, the solution vector w changes in such a way that component $s_1(t)$ is replaced by a new unknown, namely $u_0(t)$. This mathematical model can be used up to the time $t = T_2$, which is defined by the interface arriving at the right edge, $s_2(T_2) = L$.

A more accurate approximation of (13) is linked with the global mass balance argument of infiltrated water. The numerical approximation of Richards equation will increase if we express Richards equation in terms of both pressure head and saturation which are related in (2). In the grid points where saturation is close to 1, we use the head variable and where the saturation is close to zero, we use the saturation variable. In this way we increase the approximation of the flux in and near the free boundaries. To increase the approximation of interface s_1, instead of (13), we consider the mass balance equation

$$(\theta_s - \theta_r)\ell(t) + s_1(t) - r_0 + \sum_{i=0}^{N-1} c_i u_i = \ell(0); \tag{15}$$

where $c_i = (\alpha(i+1) - \alpha(i))/2, \quad i = 1, ..., N-1; c_0 = \alpha(0)/2;\; u_0 = 1$ (integration by the trapezoidal rule). Now, the approximation consists of $N+1$ ODE (SR and (12), (14)) and the algebraic equation (15). In this way we replace ODE (13) (with low approximation



(a) Saturation (b) Head

Figure 1: Evolution of saturation and head, $t \in (0, 1672)$, Exp. 1.

$time$.10s	$M.10^{-6}$	G	Mw	Gs	Mws
0	0.7880	0.2112	0.1595	1.0388	2.0613
17	0.8180	0.7675	0.5815	1.1578	2.0612
102	0.9188	2.0255	1.5343	1.9419	2.0613
167	0.9959	2.7248	2.0609	2.7231	2.0615

Table 1: Rotational momentum, Gravitational center, Water amount

accuracy of f_2) by (15) representing the global mass balance condition. This system can be written in the form

$$M(t, z)\dot{z}(t) = f(t, z) \tag{16}$$

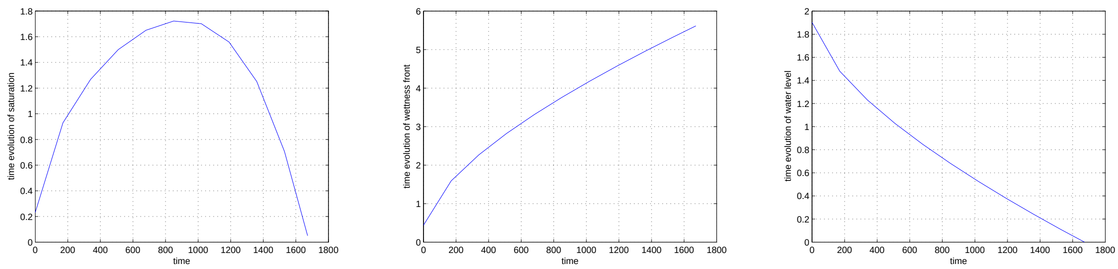
where $z = [h_1, ..., h_{i0}, u_{i0+1}, ..., u_{N-1}, s_1, s_2, \ell]$. During the time period $t \in (T_1, T_2)$ the system is regular and at time $t = T_2$ it needs to be modified, since the right boundary could be sealed and s_2 will be replaced by u_N. Another possibility is to let this boundary free and collect the expelled water.

4 NUMERICAL EXPERIMENTS

In the numerical experiments we will use $r_0 = 30$ $L = 10, \omega = 20$, $K_s = 2.4\,10^{-5}$, $\theta_r = 0.02$, $\theta_s = 0.4$ $\gamma = -0.0189$ and $n = 2.81$. The space discretization for $T \in (0, T_1)$ is not equidistant. We shall consider $N = 40$ grid points with the following geometrical distribution: the first space interval is $d_1 = 1/20$ and then $d_{i+1} = qd_i$ with $q < 1$. In the numerical approximation of the infiltration during the time interval $t \in (T_1, T_2)$ a uniform space discretization with $N = 40$ will be used.

Experiment 1 In this experiment we show the time evolution of the saturation and the head in 10 equidistant time sections for $t \in (0, T_1)$, see Fig. 1(a) and 1(b). For the same time sections we draw s_1, s_2, ℓ in Fig. 2.

The rotational momentum M (rotational kinetic energy of the infiltrated water mass in the sample), gravitational center G and water mass Mw of the sample $(r_0+s_1(t), r_0+s_2(t))$



(a) Saturation front (b) Wetness front (c) Water level

Figure 2: Evolution of saturation front, wetness front and water level, Exp. 1.

iteration	$-100.\gamma$	n	$K_s\,10^5$	RMS
0	1.2	2.	1.6	$1.5014\,10^5$
4	1.0071	2.1956	1.7213	$9.7204\,10^3$
8	1.8651	2.8258	2.3910	20.572
12	1.8862	2.8094	2.4000	$9.4134\,10^{-2}$
16	1.8863	2.8090	2.3997	$1.5563\,10^{-2}$
18	1.8864	2.8097	2.3996	$2.8347\,10^{-3}$

Table 2: LM -iterations for determination of γ, n, K_s

are computed from (at time t)

$$M = \frac{\omega^2 L}{2g} \int_0^1 (r_0 + Lz)^2 u(t,z)\, dz,$$

$$Mw = L \int_0^1 u(t,z)dz; \quad G = L \int_0^1 yu(t,z)dz/M_w,$$

which we evaluate numerically using the trapezoidal rule. Here M_s, G_s, Mw_s will represent M, G, Mw for the entire system where water is present, i.e., in $r \in (r_0 - \ell(t), r_0 + s_2(t))$, which means that Mw_s should be a constant.

The values for the global characteristics M, G, Mw for this experiments at the corresponding time sections are included in Table 1. From this table we can see that the water mass is conserved up to 3-4 digits. The entire computation takes 6 seconds on a normal desktop PC.

In Fig. 1(b) we have drawn only the non-positive part of the head in the sample, i.e., only in the region $(s_1(t), s_2(t))$. In the region $(0, s_1(t))$ the head is positive and a convex parabola as given in formula (5).

Experiment 2 In this experiment we shall simulate the determination of soil parameters γ, n, K_s using the global characteristics obtained by the following centrifugation scenario: infiltration into the dry sample along the time $t \in (0, T_2)$. The measurement data is generated by the solution of the direct problem (with given standard γ, n, K_s) and next

it	$-100.\gamma$	n	$K_s\,10^5$	RMS
0	1.3	2.	1.8	$1.2638\,10^5$
2	1.5676	2.7798	2.2608	94.329
4	1.7988	2.7715	2.3889	0.666
6	1.7638	2.7560	2.3804	0.216
8	1.7638	2.7560	2.2007	0.216

Table 3: LM -iterations for determination of γ, n, K_s, 5% noise.

it	$-100.\gamma$	n	$K_s\,10^5$	RMS
0	1.3	2.	1.8	$1.2638\,10^5$
2	1.3233	2.3180	2.3000	$1.2129\,10^3$
4	1.4005	2.4951	2.3364	1.1389
6	1.4003	2.4954	2.3367	1.1090
8	1.4174	2.5126	2.3379	1.1081
10	1.4711	2.5636	2.3411	1.0150

Table 4: LM -iterations for determination of γ, n, K_s, 10% noise.

we retain only the computed characteristics and forget the soil parameters. Finally, in an iteration process using the LM method the soil parameters are determened.
The global characteristics data are collected at time sections $t = 0;\ 360;\ 720;\ 1080;\ T1$, where for $t = T_1$ the water chamber is empty. We denote $data_1 = [\ell, M, G,\ M_s, G_s, T_1]$. Then, centrifugation prolongs up to the time when the water front reaches the right boundary of the sample (for $t = T_2$). At the same time sections (starting from $t = T_1$) we collect the $data_2 = [M, G, T_2]$. Then the measurements are $data = [data_1, data_2]$. In Table 2 we present the iterations of the LM method to determine γ, n, K_s. RMS_i represents $||res_i||^2$ where $res_i = data_i - data$. Here $data_i$ are obtained by the numerical solution in the i-th iteration step. In Table 2 row $i = 0$ contains the starting values for γ, n, K_s.

Experiment 3 In this experiment we use as measurements of global characteristics $data_1 = [\ell, M_s, T_1]$ collected in time sections $t = 100; 200; ...; 1100; 1200$ of $(0, T_1)$ and $data_2 = [M_s, T_2]$ collected in the same time sections during the time interval (T_1, T_2). Next,

it	$-100.\gamma$	n	$K_s\,10^5$	RMS
0	1.3	2.	1.8	$1.2629\,10^5$
2	1.5712	2.1365	1.6149	$2.4881\,10^1$
4	1.7086	2.7309	2.3748	4.2321
6	1.7100	2.7289	2.3726	2.8643
10	1.8469	2.7290	2.3728	2.8571

Table 5: LM -iterations for determination of γ, n, K_s, 10% noise, s_2 measured.

$data = [data1; data2]$ is perturbed with 5% and 10% of noise. For this, every component $data(i)$ is replaced by $data(i)(1 + q\,(rand - 0.5))$ for $q = 0.1, 0.2$ (for $5\%, 10\%$), respectively, here $rand$ is a random number in $(0, 1)$. The determination of the soil parameters by LM iterations is presented in Table 3 and 4. If we include in the measured data also the time evolution of the wettness front s_2, then we obtain the LM iterations (for 10% of noise) in Table 5. The results show the significant influence of knowing s_2 in determination procedure. As we can see from Fig. 1, the position of s_2 could be successfuly measured, e.g., by gama rays, since the saturation front is very sharp, especially at higher ω.

Remark As we can see from these experiments the chosen global characteristics in Experiment 2 are sufficient for determining soil parameters. We can increase the reliability of the determination of γ, n, K_s by extending the vector of measured characteristics. For example, we can collect output water (when the wetness front reaches the right boundary) in a chambre and extend the global characteristics with the measurements of expelled water. Also, we can continue with the injection of additional water into the injection chamber and repeat the collection of global characteristics. In this way it is possible to create a sufficiently long vector of measured global characteristics. Another possibility is to drop the gravitational center measurements (or the rotational momentum) from the collection of global characteristics (instead of using both of them). Measuring the indicated global characteristics is technically cheap.

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