ON THE SOLUTION OF SOME INVERSE PROBLEMS IN INFILTRATION

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Dedicated to Prof. J. Nečas on the occasion of his 70th birthday

Abstract. In this paper we discuss inverse problems in infiltration. We propose an efficient method for identification of model parameters, e.g., soil parameters for unsaturated porous media. Our concept is strongly based on the finite speed of propagation of the wetness front during the infiltration into a dry region. We determine the unknown parameters from the corresponding ODE system arising from the original porous media equation. We use the automatic differentiation implemented in the ODE solver LSODA. Several numerical experiments are included.

Keywords: porous media equation, inverse problems, Richard's equation

MSC 2000: 35R35, 49M15, 49N45

1. Introduction

We will consider

$$\partial_t u = \partial_x(\partial_x \beta(u) + K(x,u)) \tag{1}$$

in $x \in (0, L)$, $L > 0$, where $\beta(u)$ is an increasing function, and the convective term is generated by $K(x,u)$. The boundary conditions that we consider are either of Dirichlet type,

$$u(0,t) = 0, \qquad u(L,t) = C, \tag{2}$$

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or of mixed, Neumann-Dirichlet type,

$$-(\partial_x\beta(u)+K(x,u))_{x=0}=q(t), \qquad u(L,t)=0, \tag{3}$$

with the initial condition

$$u(x,0)=u_0(x). \tag{4}$$

If $\beta'(0)=0$ (or, more specially, $\int_0^\delta(\beta'(u)/u)\,\mathrm{d}u<+\infty$), then equation (1) represents a porous media type equation with convection. In that case, the support of the initial data $u_0(x)$ (i.e., the closure of the set of x for which $u_0(x)>0$) propagates with finite speed. Then the movement of the interface $x=s(t)$ (the boundary between the region where $u(x,t)>0$ and $u(x,t)=0$) is a very significant characteristic of the solution of (1). This phenomenon has been intensively studied in the last two decades, see [1], [2], [8], [9], [13]. A very important role in its analysis is played by the exact solution given by Barenblatt-Pattle for the special case when $\beta(u)=u^p$, $p>1$, and $K(x,u)=0$. If $u_0=\delta(x)$ (the Dirac measure) then this solution is given by the formula

$$u(x,t)=\begin{cases} t^{-1/(p+1)}(1-(x/s(t))^2)^{1/(p-1)}, & \text{for } |x|<s(t),\\ 0, & \text{for } |x|\geqslant s(t),\end{cases} \tag{5}$$

with the interface given by

$$s(t)=\sqrt{\frac{2p(p+1)}{p-1}}\,t^{1/(p+1)}.$$

This solution has a singularity at $x=s(t)$. More generally, the solution of the system (1), (4) and either (2) or (3) exists only in the variational sense,

$$\int_0^T\int_\Omega u\varphi_t\,\mathrm{d}x\,\mathrm{d}t-\int_\Omega u(x,0)\varphi(x,0)\,\mathrm{d}x+\int_0^T\int_\Omega(\partial_x\beta(u)+K(u))\partial_x\varphi\,\mathrm{d}x\,\mathrm{d}t=0$$

holds for all $\varphi\in C^1((0,L)\times(0,T))$ with $\varphi(x,T)=0$ (and $\varphi(0,t)=0$ if (2) is considered). If the initial profile $u_0(x)=0$ and the flux enters at $x=0$ only, the interface $s(t)$ appears and moves to the right. The mathematical models (1) can include the infiltration with gravitation in unsaturated porous media (see Section 4). Then $s(t)$ represents the wetness front which can be also measured, e.g., by γ-rays. As we shall see, there is a sharp wetness front and therefore the value $s(t)$ can be easily measured.

Our main aim is to restore the functions $\beta(u)$, $K(x,u)$ from additional measurements. The solution of (1) is uniquely determined by (4) and by either (2) or (3). If we have additional measurements, e.g., $u(x^*,t)=\psi(t)$, $q(t)$ (when (2) is considered), or combinations of these, then we have to restore the functions $\beta(u)$ and $K(x,u)$ so that the solution of (1) gives the same values as those obtained by the measurements. This is an inverse problem to (1)–(4) and it is well known to be ill-posed.

The classical way of solving inverse problems is very similar to the solution of optimal control problems. A cost functional is constructed that evaluates the distance between the measurements and the data obtained by solving the direct problem with some given $\beta_d(u)$ and $K_d(x,u)$, where d represents a set of approximation parameters. To improve β_d and K_d we must know the gradient of the cost functional with respect to d. For this purpose the adjoint problem to (1)–(4) is constructed. The numerical realization of this can be difficult and substantially depends on the precise solution of the direct problem of (1)–(4) for given β_d and $K_d(x,u)$.

In our concept we avoid the construction of the adjoint problem and use automatic differentiation to evaluate the gradient (and also the Hessian if desired) of the cost function, see [4]. Our approach to solving the inverse problem to (1)–(4) is based on the following arguments:

1. determining the governing ODE for the interface $s(t)$;
2. use of a fixed-domain transformation and reduction of the system (1)–(4) to a system of ODEs with parameters d;
3. use of an efficient solver (based on self-adaptive BDF methods) to solve the stiff system of differential equations, implementing automatic differentiation;
4. use of an optimization method (Newton-Raphson, Broyden, Levenberg-Marquardt) to determine the optimal (finite-dimensional) vector of parameter values.

The functions β_d and K_d are approximated in the form

$$\beta'_d(u) = u^{p-1}(1-u)^q(a_0 + a_1 u + a_2 u^2) \tag{6}$$

and

$$K_d(x,u) = A(x)k_d(u) \tag{7}$$

where A is a given function and $k_d(u)$ is approximated as

$$k_d(u) = u^{r_k}(c_0 + c_1 u), \tag{8}$$

with the parameter vector $d = (p, q, r_k, a_0, a_1, a_2, c_0, c_1)$.

Then we apply our method to the infiltration in unsaturated porous media where β_d and k_d have special, model-defined forms and the convection is caused by gravitation, or $A(x) = b_0 + b_1 x$ for some known constants b_0 and b_1 if it is caused by centrifugation. The function $\beta_d(u)$ is expressed in terms of the soil parameters arising in the constitutive laws (saturation versus pressure, hydraulic permeability versus pressure) as expressed in the Van Genuchten ansatz, see Section 4.

In Section 2 we present the method for numerical computation of the flow in unsaturated porous media using Richard's equation, i.e., the direct problem. In Section 3 we present the method for solving the inverse problem and in Section 4 we apply our methods to the restoration of soil parameters. In Section 5 we present some numerical experiments supporting the effectiveness of the method suggested.

2. Solution of the direct problem

The governing equation for the movement of the interface is (see [5])

$$\dot{s}(t) = -\lim_{x\to s(t)^-}\Big(\partial_x F(u) + \frac{K(x,u)}{u}\Big), \tag{9}$$

where $F(u) = \int_0^t (\beta'(u)/u)\,\mathrm{d}u$, under the assumption that the initial and boundary conditions guarantee the existence of a unique interface at $s(t) \in (0, L)$.

If a solution $u(x,t)$ of (1)–(4) is smooth in $(0, s(t)]$, we can justify (9) by L'Hospital's rule: starting from $\mathrm{d}u(s(t),t)/\,\mathrm{d}t = 0$ we get $\dot{s}(t) = -(u_t/u_x)_{x=s(t)^-}$, where we replace u_t by $\partial_x(\partial_x\beta(u) + K(x,u))$. Since both u and the flux $-(\partial_x\beta(u) + K(x,u))$ must vanish at $x = s(t)$, we apply L'Hospital's rule in reverse to obtain

$$\dot{s}(t) = -\lim_{x\to s(t)^-}\frac{\partial_x(\partial_x\beta(u) + K(x,u))}{\partial_x u} = -\lim_{x\to s(t)^-}\frac{\partial_x\beta(u) + K(x,u)}{u}, \tag{10}$$

from which (9) follows at once by the definition of F.

Now we solve the system (1)–(4). To avoid the degeneracy $F'(0) = 0$ at $x = s(t)$ we use the transformation $v = F(u)$. Actually, it is sufficient to use the simpler transformation $v = u^{p-1}$ when $\beta(u)$ can be written as $\beta(u) = u^p g(u)$ and $g(0) \neq 0$. Then the system (1)–(4) is transformed into

$$\begin{aligned}\partial_t v = \beta'(v^{1/(p-1)})\partial_x^2 v + \frac{(\partial_x v)^2}{(p-1)v}(\beta'(v^{1/(p-1)})v^{1/(p-1)} + (2-p)\beta'(v^{1/(p-1)}))\\ + K_u(x, v^{1/(p-1)})\partial_x v + (p-1)v^{1-1/(p-1)}K_x(x, v^{1/(p-1)}),\end{aligned} \tag{11}$$

and (9) into

$$\dot{s}(t) = -\frac{1}{p-1}\lim_{x\to s(t)^-}\frac{\beta'(v^{1/(p-1)})}{v}\partial_x v = -\frac{p}{p-1}g(0)\lim_{x\to s(t)^-}\partial_x v. \tag{12}$$

Now we use a fixed-domain transformation $y = x/s(t)$ and for $\bar{v}(y,t) = v(x,t)$ we obtain

$$
\begin{aligned}
\partial_t \bar{v} = {} & \frac{\beta'(\bar{v}^{1/(p-1)})}{s^2(t)} \partial_y^2 \bar{v} \\
& + \frac{(\partial_y \bar{v})^2}{(p-1)s^2(t)\bar{v}} (\beta'(\bar{v}^{1/(p-1)})\bar{v}^{1/(p-1)} + (2-p)\beta'(\bar{v}^{1/(p-1)})) \\
& + \frac{K_u(s(t)y, \bar{v}^{1/(p-1)}) + \dot{s}(t)y}{s(t)} \partial_y \bar{v} + (p-1)\bar{v}^{1-1/(p-1)} K_x(s(t)y, \bar{v}^{1/(p-1)})
\end{aligned}
\tag{13}
$$

and

$$
\dot{s}(t) = -\frac{p}{(p-1)s(t)} g(0) \lim_{x \to s(t)^-} \partial_y \bar{v}, \tag{14}
$$

which can be substituted on the right-hand side of equation (13).

Next, we introduce a space discretisation in the variable $y \in [0,1]$ consisting of points $0 = y_0 < y_1 < \ldots < y_N = 1$ and denote by $C_i(t)$ the approximation to $\bar{v}(y_i, t)$ (so that $C_N(t) = \bar{v}(1,t) = v(s(t),t) = 0$ identically). Let $p_2(y; C, y_i)$ be the second-order Lagrange polynomial interpolating the points (y_{i-1}, C_{i-1}), (y_i, C_i) and (y_{i+1}, C_{i+1}), then we approximate $\partial_y \bar{v}$ at the point y_i by $\partial_y p_2(y; C, y_i)$ and $\partial_y^2 \bar{v}$ by $\partial_y^2 p_2(y; C, y_i)$. If the Neumann-type boundary condition in (3) is considered, then $C_0(t)$ is variable in time, and we obtain the differential equation for it by introducing a fictive point at $y_{-1} = -y_1$ with value $C_{-1} = C_1 - 2y_1(\partial_y \bar{v})_{y=0}$, where $(\partial_y \bar{v})_{y=0}$ is obtained from the Neumann condition.

The result of this discretisation is a system of ODEs

$$
\dot{C} = f(C, t; d), \tag{15}
$$

where $C(t) = (C_0, C_1, \ldots, C_N, s(t))$ and d is a vector of approximate parameters of $\beta_d(u)$ and $K_d(x,u)$. The initial condition $C(0) = C_0$ is obtained from the known initial profile u_0. The choice of a nonuniform partition (y_i), with a higher density of points near $y = 0$ and $y = 1$, yields very good approximations of the solution even for relatively low numbers of nodal points, thereby keeping the size of the system (15) reasonably small.

3. Solution of the inverse problem

Together with the boundary conditions (2) or (3), we assume that some additional measurements are available, e.g. $\hat{u}_{i,j} \approx u(x_j, t_i)$ at the fixed points x_j and time instants t_i, $1 \leqslant i \leqslant k$. Another important source of information on the model data is obtained from measurements of the interface movement, $\hat{s}_i \approx s(t_i)$. Moreover, when the Dirichlet condition (2) is considered, the total flux

$$\hat{Q}_i \approx \int_0^{t_i} q(t)\,\mathrm{d}t$$

can also be measured.

The corresponding cost functional is of the form

$$\mathcal{F}(C; d) = \lambda \sum_{i=1}^{k} (Q(t_i; d) - \hat{Q}_i)^2 + \mu \sum_{i=1}^{k} (s(t_i; d) - \hat{s})^2 + \nu \sum_{j=1}^{h} \sum_{i=1}^{k} (u(x_j, t_i; d) - \hat{u}_{i,j})^2.$$

The expressions $u(x, t; d)$ and $s(t; d)$ are expressed in terms of $C(t; d)$, which are governed by (15). The solution of the inverse problem leads to a minimization problem: find the optimal parameters d^* such that

$$\mathcal{F}(C^*; d^*) = \min_{d \in U_d} \mathcal{F}(C; d), \tag{16}$$

where U_d is the set of admissible parameters. The numerical approach to solving the problem (16) relies on one of the existing optimization methods: steepest descent, Broyden search, Newton-Raphson, or, in view of the special form of the cost functional as a weighted sum of squares of discrepancies, the Levenberg-Marquardt method. All of these methods are iterative, and they all require knowledge of the gradient of the cost functional with respect to the parameters; the Levenberg-Marquardt method also requires knowledge of the gradients of all $Q(t_i; d)$, $s(t_i; d)$ and $u(x_j, t_i; d)$ with respect to the parameters. To obtain such gradients, we use automatic differentiation implemented in the LSODA ODE solver (see [11]).

4. Determination of soil parameters

The unsaturated flow in porous media is modelled by the Richards equation

$$\partial_t \theta = \operatorname{div}(k(\psi)\operatorname{grad}(\psi + z)), \tag{17}$$

where θ is the volumetric water content, ψ is the matric potential (capillary pressure), z is the gravitational potential, and $k(\psi)$ is the hydraulic conductivity.

We denote by $u = (\theta - \theta_r)/(\theta_s - \theta_r)$ the effective saturation, where θ_s is the volumetric water content at saturation and θ_r the irreducible water content. The constitutive laws for the Van Genuchten ansatz then read

$$u = \frac{1}{(1+\alpha\psi)^n)^m}, \qquad k(\psi(u)) = k_s u^{1/2}(1-(1-u^{1/m})^m)^2,$$

where k_s is the saturated hydraulic conductivity. The parameters k_s, α, m, $n = 1/(1-m)$ and θ_r, θ_s are soil parameters that have to be determined.

Expressing (17) in terms of u we obtain

$$\partial_t u = \operatorname{div}(D(u)\operatorname{grad} u) + \partial_z K(u), \tag{18}$$

where $K(u) = (\bar{e}/(\theta_s - \theta_r))k(u)$, $D(u) = -k_s/((\theta_s - \theta_r)\alpha))u^{1/2-1/m}(1-u^{1/m})^m(1-(1-u^{1/m})^{-m})^2$, and $\bar{e}$ is 0 for infiltration without gravitation, 1 for infiltration with gravitation and -1 for infiltration against gravitation.

Now (18) is in the form of (1), where $\beta(u) = \int_0^u D(w)\,\mathrm{d}w$ and $0 < m < 1$, $\alpha < 0$, $1 > \theta_s > \theta_r \geqslant 0$, k_s are the soil parameters that constitute the parameter vector d. In fact, θ_s and θ_r can be determined using direct methods, so we shall take them as known. Then it remains to determine k_s, m and α. We easily obtain that $\beta_d(z) = z^p g(z)$ with $g(0) \neq 0$ and $p = 1/2 + 1/m + 1$, so that (18) does represent a porous media type equation. Moreover, we obtain that $D(1) = +\infty$, so that an additional degeneracy occurs at the saturation level. Therefore (17) can only be applied when $u \in (0,1)$. As a consequence we consider the Dirichlet boundary condition at $x = 0$ in the form $u(0,t) = 1 - \varepsilon$, where $\varepsilon > 0$ is small, representing saturation at $x = 0$.

5. Numerical experiments

In the numerical experiments we demonstrate the effectiveness of the present method. The numerical method has been validated using the Brenblatt-Pattle analytical solution. The differences cannot be distinguished in a graph. To illustrate the solution of inverse problems, we present four numerical experiments.

To make the parameters that should be restored more influent on the measurements, we need to make the solution more dynamic. This can be achieved by changing the initial conditions and the gravitational forces. Using centrifugation, we can also obtain artificial gravitational forces: in that case the term corresponding to $K(u)$ in equation (18) is of the form

$$K(x,u) = k(u)\frac{\omega^2}{g(\theta_s - \theta_r)}(x_0 + x),$$

where ω is the angular speed of rotation and x_0 is the distance from the centrifuge center to the top of the sample under consideration.

First we let the sample be infiltrated from the top boundary (with or without gravitation, depending on whether it is in a horizontal or vertical position). Next, we insulate this boundary and use centrifugation. Then we use again infiltration without centrifugation. Correspondingly, we have to change the boundary conditions in the model: Dirichlet for the infiltration phases, Neumann for the insulated centrifugation. As is clear from the graphs in Figs. 1, 4, 6, the profile of u undergoes considerable changes and consequently the measurements become more sensitive to the parameters that we wish to restore.

In all experiments we use measurements of the wetness front $s(t)$ and of the total amount of water taken up, $Q(t) = (\theta_s - \theta_r) \int_0^t q(s)\,\mathrm{d}s$, both of which can be easily measured externally.

As many experiments show the measurement of head pressure (and consequently of saturation) at many different points of the sample does not give much more information than measurements at a single point. The way of amplifying the changes in the saturation profile is far more effective.

Most methods of restoration of soil parameters are based on Richard's equation in terms of pressure, see [3], [6], [12]. To use the phenomenon of finite propagation of the wetness front, we use (18), which is expressed in terms of saturation. The lack of variety in boundary conditions we effectively compensate by using centrifugation.

5.1. First experiment: restoration of Van Genuchten parameters. In this first example we consider infiltration modelled by the Van Genuchten ansatz (1) and (18). We use parameters corresponding to a sand soil: $k_s = 2.4 \times 10^{-5}\,\mathrm{cm}\,/\,\mathrm{s}$, $\alpha = -0.0189\,\mathrm{cm}^{-1}$, $m = 0.644$, $\theta_r - \theta_s = 1$.

The measurements proceed with horizontal infiltration under Dirichlet BC during three hours, then we use centrifugation with $x_0 = 1\,\mathrm{cm}$ and $\omega = 9.9\,\mathrm{s}^{-1}$ during three more hours, and finally three hours of horizontal Dirichlet BC infiltration.

The corresponding saturation profiles $u(x,t)$ are pictured in Fig. 1. In Fig. 2 we have graphed the corresponding $s(t)$ and $Q(t)$.

The measurements are taken every minute. Then, using the measurements we attempt to restore the soil parameters from initial values $k_s = 1 \times 10^{-5}$, $\alpha = -0.21$, $m = 0.81$ and $\theta_s - \theta_r = 0.8$.

The effectiveness of the restoration procedure is demonstrated in Table 2 that lists the approximation parameters and the root-mean-square error

$$\mathrm{RMS} = \sqrt{\frac{\sum_{j=1}^{k} (s(t_j) - \hat{s}(t_j))^2 + (Q(t_j) - \hat{Q}(t_j))^2}{2k}}.$$

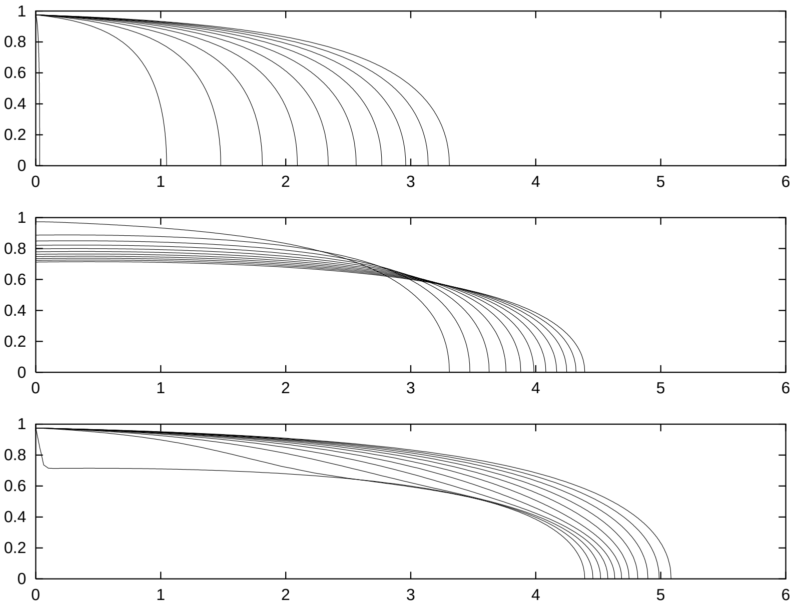

Figure 1. Effective saturation (u) profiles vs. distance x in cm, for the sand soil under consideration, every 18 minutes, for (topmost) the initial horizontal wetting, (middle) centrifugation with insulated end, (bottom) the final horizontal wetting.

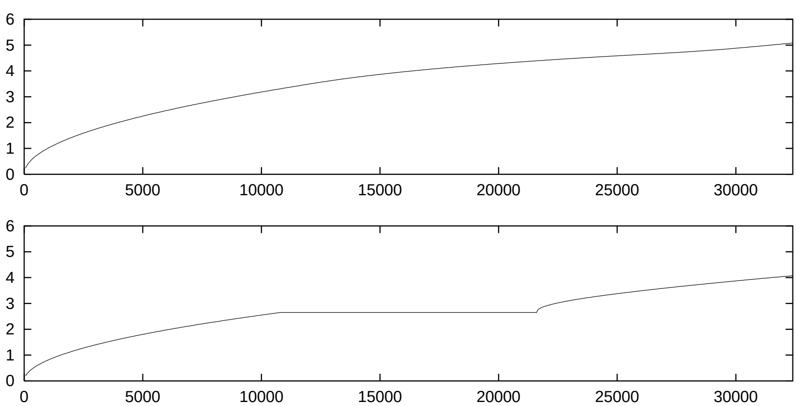

Figure 2. The corresponding evolution of (top) the interface position s in cm, (bottom) the total flux input Q, vs. time in seconds.

Note that the parameter $\theta_s - \theta_r$ is estimated with high accuracy even at relatively high values of the RMS; k_s and m are only estimated accurately for lower values of the RMS, and α is the hardest parameter to estimate accurately.

a_0	$p-2$	c_0	r_k-1	$-q$	RMS
8.0000e-01	7.0000e-01	1.2000e-02	3.8000e+00	1.2000e+00	2.9138e-01
7.8434e-01	7.0097e-01	1.2000e-02	3.8000e+00	1.1432e+00	1.1027e-01
7.7523e-01	7.0299e-01	1.2000e-02	3.7999e+00	1.1167e+00	4.0311e-02
7.6945e-01	7.0924e-01	1.2000e-02	3.7998e+00	1.1133e+00	3.3001e-02
7.5500e-01	7.3364e-01	1.2001e-02	3.7994e+00	1.1232e+00	2.5606e-02
7.2597e-01	7.8811e-01	1.2003e-02	3.7987e+00	1.1443e+00	1.0337e-02
7.2412e-01	8.2640e-01	1.2002e-02	3.7995e+00	1.1467e+00	4.6279e-03
7.3394e-01	8.3622e-01	1.2000e-02	3.8006e+00	1.1405e+00	4.3234e-03
7.5376e-01	8.4980e-01	1.1996e-02	3.8025e+00	1.1281e+00	3.9159e-03
7.9898e-01	8.7947e-01	1.1988e-02	3.8068e+00	1.1007e+00	3.8218e-03
8.2867e-01	8.9829e-01	1.1982e-02	3.8097e+00	1.0846e+00	2.6261e-03
8.6933e-01	9.2384e-01	1.1975e-02	3.8138e+00	1.0627e+00	2.2350e-03
8.9376e-01	9.3843e-01	1.1970e-02	3.8163e+00	1.0504e+00	1.4756e-03
9.2607e-01	9.5765e-01	1.1964e-02	3.8196e+00	1.0343e+00	1.2281e-03
9.4434e-01	9.6807e-01	1.1961e-02	3.8215e+00	1.0256e+00	7.4465e-04
9.6561e-01	9.8043e-01	1.1957e-02	3.8237e+00	1.0156e+00	5.3584e-04
9.8753e-01	9.9296e-01	1.1952e-02	3.8260e+00	1.0055e+00	3.8151e-04
9.9860e-01	9.9914e-01	1.1950e-02	3.8271e+00	1.0006e+00	9.2744e-05
1.0003e+00	1.0001e+00	1.1949e-02	3.8271e+00	9.9988e-01	7.5091e-06
1.0004e+00	1.0001e+00	1.1943e-02	3.8257e+00	9.9983e-01	6.7487e-06
1.0004e+00	1.0001e+00	1.1906e-02	3.8163e+00	9.9983e-01	6.4136e-06
1.0005e+00	1.0002e+00	1.1650e-02	3.7550e+00	9.9980e-01	5.6724e-06
1.0005e+00	1.0002e+00	1.0778e-02	3.5761e+00	9.9978e-01	2.8881e-06
1.0004e+00	1.0002e+00	1.0444e-02	3.5222e+00	9.9981e-01	2.7643e-06
1.0002e+00	1.0001e+00	1.0171e-02	3.5039e+00	9.9992e-01	8.2565e-07

Table 1. Restoration steps in the recovery of three of the altenartive ansatz parameters from Van Genuchten horizontal infiltration measurements of the sand soil under consideration.

5.2. Second experiment: approximation of horizontal infiltration under the Van Genuchten model by the alternative ansatz. Now we consider the alternate ansatz expressed by the equations (6), (7) and (8). We restore the parameter vector d using measurements of $s(t)$ and $Q(t)$ corresponding to the Van Genuchten model with no gravitation and with a Dirichlet BC corresponding to three hours of horizontal infiltration. In this case, the gravitational/centrifuge term $K_d(x,u)$ is zero, and therefore we set $q = a_1 = a_2 = b_0 = b_1 = c_1 = 0$ in the parameter vector. In addition to p and a_0 we must also restore $\theta_s - \theta_r$, the coefficient appearing in $Q(t)$.

The restoration procedure is presented in Table 3. The time evolutions of $s(t)$ and $Q(t)$, both for the target (Van Genuchten) and for the approximation (new ansatz) data are plotted in Fig. 3. It is clear that these quantities are very nearly lines in a log-log plot; furthermore, the slope of both lines must be the same, since the ratio of $s(t)$ to $Q(t)$ must be bounded both from above and below. This explains why at most three parameters can be restored from such measurements; to extract more information, we shall have to make these graphs more complex by introducing gravitation, centrifugation or a switch in the boundary conditions.

$\theta_s - \theta_r$	k_s	$-\alpha$	m	RMS
8.0000e-01	1.0000e-05	2.1000e-02	8.1000e-01	1.3394e+00
8.1169e-01	1.1461e-05	1.7970e-02	5.8451e-01	9.8017e-01
8.8827e-01	1.4360e-05	1.3448e-02	6.8067e-01	2.7058e-01
9.8981e-01	1.5508e-05	1.2377e-02	6.7447e-01	2.4146e-02
1.0044e+00	1.5555e-05	1.2342e-02	6.7389e-01	1.7440e-03
1.0051e+00	1.5560e-05	1.2348e-02	6.7556e-01	1.5631e-03
1.0057e+00	1.5588e-05	1.2376e-02	6.7862e-01	1.5114e-03
1.0057e+00	1.5802e-05	1.2546e-02	6.7864e-01	1.4619e-03
1.0045e+00	1.7340e-05	1.3766e-02	6.7104e-01	1.3579e-03
1.0036e+00	1.8646e-05	1.4788e-02	6.6527e-01	1.0457e-03
1.0030e+00	1.9469e-05	1.5427e-02	6.6183e-01	7.9637e-04
1.0021e+00	2.0716e-05	1.6394e-02	6.5655e-01	7.0535e-04
1.0016e+00	2.1501e-05	1.6996e-02	6.5347e-01	4.5146e-04
1.0010e+00	2.2488e-05	1.7753e-02	6.4962e-01	3.5826e-04
1.0003e+00	2.3442e-05	1.8479e-02	6.4603e-01	2.5938e-04
1.0001e+00	2.3842e-05	1.8781e-02	6.4461e-01	4.2965e-05
1.0000e+00	2.3993e-05	1.8895e-02	6.4403e-01	8.5061e-06
1.0000e+00	2.4001e-05	1.8901e-02	6.4400e-01	1.2506e-06
1.0000e-00	2.4001e-05	1.8901e-02	6.4400e-01	1.1367e-07

Table 2. Restoration steps in the recovery of the four Van Genuchten parameters of the sand soil under consideration.

5.3. Third experiment: restoration of the alternative ansatz model. To prove that the alternative ansatz can be used to restore more than the three parameters in the previous experiment, if gravitation, centrifugation and boundary condition switching is allowed, we consider nonphysical parameter values $a_0 = 1$, $p = 3$, $c_0 = 0.01$, $r_k = 4.5$, $q = -1$ and compute the corresponding $s(t)$ and $Q(t)$ for the time interval $t \in (0, 2)$, where

1. during the first unit of time, the sample is subjected to Dirichlet BC horizontal wetting;
2. during the second unit of time, it is insulated (Neumann condition), and subjected to a gravitational force $b_0 = -0.4$.

Next, we restore the five parameters starting with $a_0 = 0.8$, $p = 2.7$, $c_0 = 0.012$, $r_k = 4.8$ and $q = -1.2$.

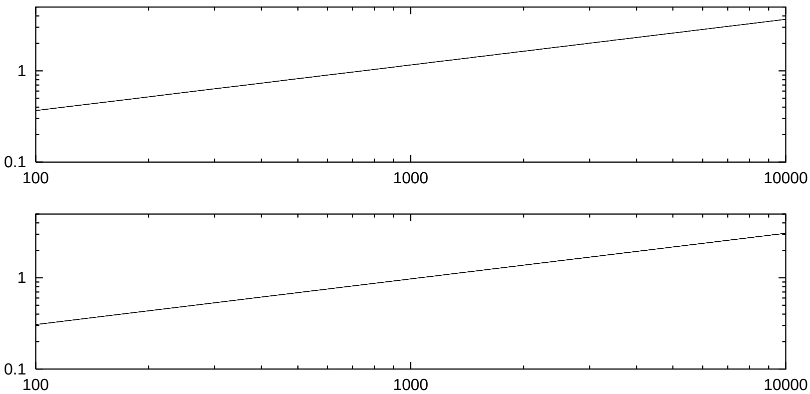

Figure 3. Comparison of the Van Genuchten model for the sand soil under consideration, and its three-parameter optimal match for a non-gravitational experiment, in log-log graphs vs. time in seconds: (top) s in cm; (bottom) Q.

$\theta_s - \theta_r$	a_0	p	RMS
1.0000e+00	1.0000e-04	1.0000e+00	1.8131e+00
2.0531e+00	2.8369e-04	1.1997e-01	5.9186e-01
1.3517e+00	5.0225e-04	1.0708e-01	2.8624e-01
1.4953e+00	5.7994e-04	1.0567e-01	8.6950e-03
1.4849e+00	5.8366e-04	1.0557e-01	4.8758e-05
1.4849e+00	5.8368e-04	1.0557e-01	2.6575e-06

Table 3. Restoration steps in the recovery of three of the altenartive ansatz parameters from Van Genuchten horizontal infiltration measurements of the sand soil under consideration.

The restoration procedure is presented in Table 1, the corresponding profiles of u in Fig. 4 and the time evolutions of s and Q in Fig. 5.

We remark that the accurate estimation of the parameters c_0 and r_k occurs only at very low levels of the RMS.

5.4. Fourth experiment: approximation of Van Genuchten measurements by the alternative ansatz. The choice of an alternative ansatz is not obvious, since the convergence of the numerical method must be guaranteed through the absence of undesired phenomena such as degeneration of the parabolicity of the equations. Furthermore, there may well be several local minima to the cost functional, for which the less sensitive parameters may differ over several orders of magnitude.

To illustrate this, we approximate using our alternative ansatz (6), (7), (8) the Van Genuchten simulated minutely measurements of s and Q on a sample of the chosen sand soil, subjected to the following sequence of operations:

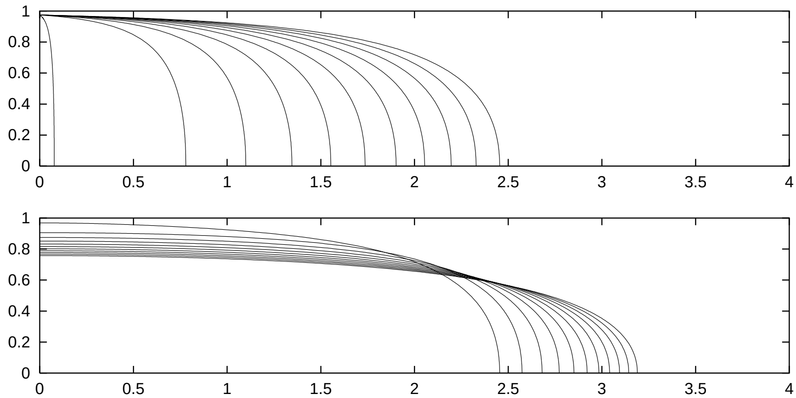

Figure 4. Effective saturation (u) profiles vs. distance x, for the example parameters under consideration, every 0.1 time units, for (topmost) the initial horizontal wetting, (bottom) gravitation.

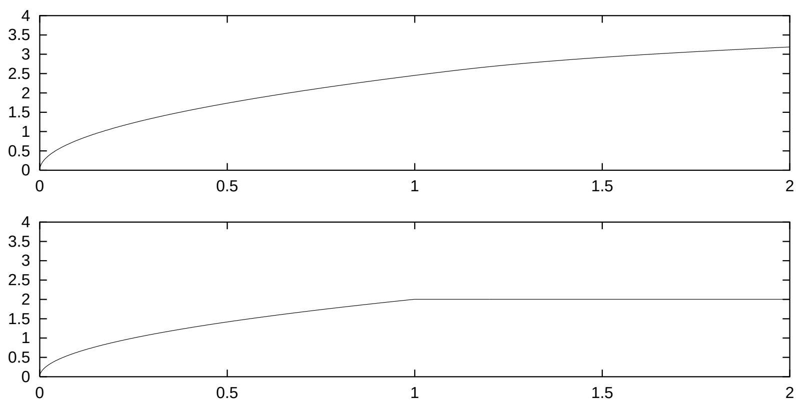

Figure 5. The corresponding evolution of (top) the interface position s, (bottom) the total flux input Q, vs. time.

1. vertical, downward infiltration with a Dirichlet boundary condition during three hours;
2. centrifugation with the top sealed and at 1 cm distance from the center, and $\omega = 31\,\mathrm{s}^{-1}$ during three hours;
3. again vertical downward infiltration during three hours.

Three local minima for the cost functional are listed in Table 4. The target van Genuchten profiles and time evolutions are presented in Figs. 6 and 7; the time evolution of the corresponding quantities for the third and best of the three local minima listed, are very close to that ones in Figures 6 and 7. (They are hard to distinguish visually.)

$\theta_s - \theta_r$	a_0	c_0	$p-2$	$r_k - 1$	$-q$	RMS
1.0628e+00	3.2367e-04	1.0668e-07	8.4871e-01	2.7794e+00	6.6819e-01	1.8664e-02
1.0130e+00	1.7303e-04	1.1124e-05	8.3336e-01	1.9504e+00	9.9405e-01	1.0077e-02
1.0344e+00	1.2815e-04	6.3313e-05	5.6220e-01	7.3279e+00	1.1274e+00	9.6668e-03

Table 4. Three distinct local minima for the approximation by the alternative ansatz of Van Genuchten measurements.

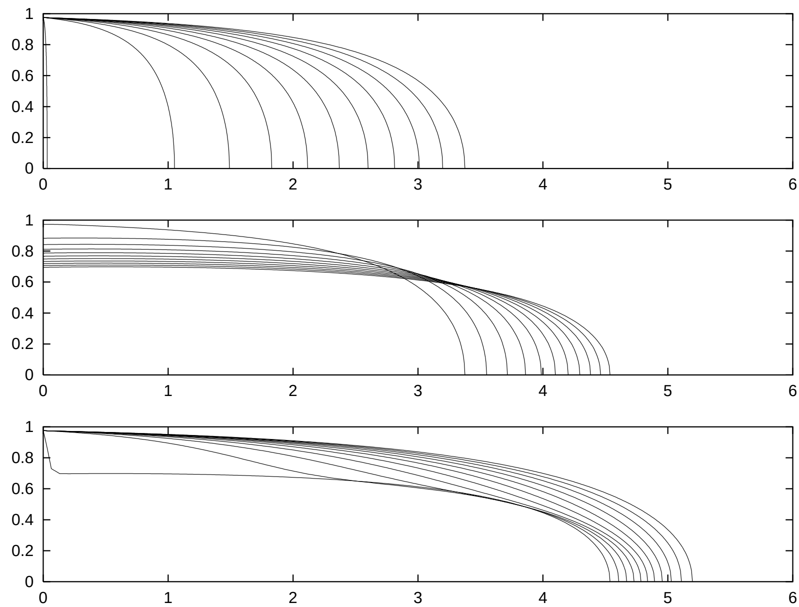

Figure 6. Effective saturation (u) profiles vs. distance x in cm, for the sand soil under consideration, every 18 minutes, for (topmost) the initial horizontal wetting, (middle) centrifugation with an insulated end, (bottom) the final horizontal wetting.

Note that the value of c_0 for the third local minimum is almost 600 times larger than that for the first local minimum listed. This is a consequence of the difficulty in determining c_0 and r_k from measurements in s and Q, as noted in the previous subsection. An important advantage of the Van Genuchten ansatz is that it offers an integrated model for β and K with fewer parameters, yet retaining the physical characteristics of infiltration processes.

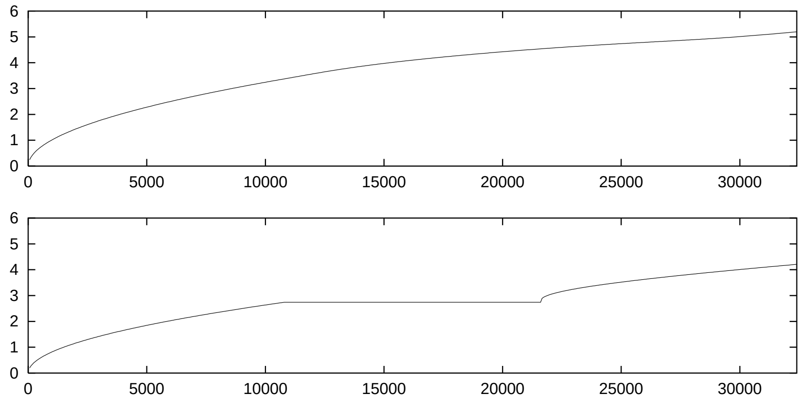

Figure 7. The corresponding evolution of (top) the interface position s in cm, (bottom) the total flux input Q, vs. time in seconds. These are the target evolutions for the matching using the new form of β and K.

References

[1] *D. G. Aronson*: Regularity properties of flows through porous media: The interface. Arch. Rational Mech. Anal. *37* (1970), 1–10.

[2] *L. A. Caffarelli, A. Friedman*: Regularity of the free boundary for the one-dimensional flow of gas in a porous medium. Amer. J. Math. *101* (1979), 1193–1218.

[3] *J. Chen, J. W. Hopmans, M. E. Grisnier*: Parameter estimation of two-fluid capillary pressure-saturation and permeability functions. Advances in Water Resources *22* (1999), 479–493.

[4] *D. Constales*: Automatic differentiation in LSODA. In preparation.

[5] *D. Constales, J. Kačur*: Inverse problems in porous media flow. Submitted to Computational Geosciences.

[6] *S. O. Eching, J. W. Hopmans*: Optimization of hydraulic functions from transient outflow and soil water data. Soil Sci. Soc. Am. J. *57* (1993), 1167–1175.

[7] *S. O. Eching, J. W. Hopmans, O. Wendroth*: Unsaturated hydraulic conductivity from transient multistep outflow and soil water pressure. Soil Sci. Soc. Am. J. *58* (1994), 687–695.

[8] *B. H. Gilding*: Flow and Transport in Porous Media. World Scientific, Singapore, 1992.

[9] *A. S. Kalašnikov*: Formation of singularities in solutions of the equation of nonstationary filtration. Ž. Vyčisl. Mat. i Mat. Fiz. *7* (1967), 440–444.

[10] *O. A. Olejnik, A. S. Kalašnikov, Chzhou Jui-Lin*: Cauchy problems and boundary-value problems for equations of type of infiltration. Izv. AN SSSR Ser. Mat. *5* (1958), 667–704. (In Russian.)

[11] *L. R. Petzold*: Automatic selection of methods for solving stiff and nonstiff systems of ordinary differential equations. SIAM J. Sci. Stat. Comput. *4* (1983), 136–148.

[12] *D. Russo, E. Bresler, U. Shani, J. C. Parker*: Analysis of infiltration events in relation to determining soil hydraulic properties by inverse problem methodology. Water Resources Research *27* (1991), 1361–1373.

[13] *C. J. van Duijn, L. A. Peletier*: Nonstationary filtration in partially saturated porous media. Arch. Rational Mech. Anal. *78* (1982), 173–198.

[14] *M. Th. van Genuchten*: A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. *44* (1980), 892–898.

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