Acta Math. Univ. Comenianae
Vol. LXX, 1(2001), pp. 1–13
Proceedings of Algoritmy 2000

ON THE SOLUTION OF SOME INVERSE PROBLEMS IN POROUS MEDIA FLOW

D. CONSTALES AND J. KAČUR

ABSTRACT. In this paper we discuss the numerical modelling of two inverse problems in porous media flow. In the first problem, we determine the soil parameters that occur in the retention and hydraulic permeability curves of the Van Genuchten ansatz for Richard's equation. In the second problem we determine the hydraulic permeability, longitudinal dispersivity and adsorption isotherms using the measurements in a single injection-extraction well.

1. INTRODUCTION

The flow in unsaturated porous media is governed by Richard's equation

$$\partial_t \theta = \operatorname{div}(k(\Psi) \operatorname{grad} \Phi) \tag{1}$$

where θ is a volumetric water content, Ψ is the matric potential (generated by the capillary pressure) and $\Phi = \psi + z$ is the total head including the gravitational potential z. The hydraulic permeability we denote by $k = k(\psi)$ and by u we denote the effective saturation, $u = \frac{\theta - \theta_r}{\theta_s - \theta_r}$ where θ_s is the volumetric water content at saturation and θ_r is the residual water content. Van Genuchten [**18**] derived an empirical relationship between u and ψ and between k and ψ (constitutive laws) in the form

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

where k_s is the saturated hydraulic conductivity

$$k_s = k_0 \frac{\rho_w g}{\mu}$$

with k_0 the intrinsic permeability (depending on the structure of the porous media only), ρ_w and μ are the density and dynamic viscosity of the water and g is the gravitational constant. The values k_s, α, $0 < m < 1$, $n = 1/(1-m)$ and θ_r, θ_s are soil parameters that have to be determined from additional measurements in infiltration. We assume that the porous medium is homogeneous. In this case

Received January 10, 2001.
2000 *Mathematics Subject Classification.* Primary 35R35, 49M15, 49N50.
Key words and phrases. Porous media equation, inverse problems, Richard's equation.
The authors gratefully acknowledge the financial support from the project BOF/GOA 12051 598 of Ghent University. The second author was also partially supported by GACR201/00/0557.

it is sufficient to consider a one-dimensional sample along which the infiltration proceeds.

By means of (2) we can rewrite Richard's equation in terms of u (in 1D) as follows

$$\partial_t u = \partial_x(\partial_x \beta(u) + K(u)) \tag{3}$$

in $x \in (0, L)$, $L > 0$, where

$$\beta'(u) = -\frac{k_s}{(\theta_s - \theta_r)\alpha} u^{1/2-1/m}(1 - u^{1/m})^m(1 - (1 - u^{1/m})^{-m})^2,$$

$K(u) = (\bar{e}/(\theta_s - \theta_r))k(u)$ and $\bar{e}$ is 0 for infiltration without gravitation, 1 for infiltration with gravitation and -1 for infiltration against gravitation. In 3 we have $\beta(s) = s^p \bar{g}(s)$ with $p = \frac{1}{2} + \frac{1}{m} + 1$ and $\bar{g}(0) \geq \delta > 0$, where $\bar{g}$ is a smooth function. The boundary conditions that we consider are either of Dirichlet type,

$$u(0, t) = 1 - \varepsilon, \qquad u(L, t) = 0, \tag{4}$$

or of mixed, Neumann-Dirichlet type,

$$-(\partial_x \beta(u) + K(u))_{x=0} = q(t), \qquad u(L, t) = 0, \tag{5}$$

with the initial condition

$$u(x, 0) = u_0(x). \tag{6}$$

If $\beta'(0) = 0$ (or, more precisely, $\int_0^\delta (\beta'(u)/u)\, du < +\infty$), then equation (3) 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 — see [**2, 11, 13**]. Then the movement of the interface $x = s(t)$ (the boundary between the regions where $u(x, t) > 0$ and where $u(x, t) = 0$) is a very significant characteristic of the solution of (3) and is fundamental to our numerical solution. The qualitative properties of the solution have been intensively studied in the last two decades — see [**1, 3, 10, 11, 13, 17**]. 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 $K(x, u) = 0$ — see [**2**]. We also use it for comparison with our numerical solution. The wetness front $x = s(t)$ is sharp and thus can be measured, e.g., by γ rays relatively precisely. In our numerical experiments we show that the information on the wetness front evolution is sufficient to restore the soil parameters.

In the second inverse problem we use a single injection-extraction well for restoring basic parameters in contaminant transport by underground water flow. We shall use the simplified mathematical model for the flow in unsaturated-saturated porous media which is based on the Dupuit-Forheimer approximation. In this concept the vertical component of the flow is neglected. We consider radial symmetric flow around a well with radius r_0. The well lies in an aquifer of height H. The flow in the unsaturated zone is governed by

$$S_1 \partial_t h = \frac{1}{r} \partial_r (rkh \partial_r h), \quad (0 \leq h < H), \tag{7}$$

where h is the height of the phreatic surface (assumed to coincide with the hydraulic head) and k is the hydraulic permeability.

In the saturated zone, the governing equation is

$$S_2\partial_t h = \frac{1}{r}\partial_r(rkH\partial_r h), \quad (H \le h), \tag{8}$$

where h is again the hydraulic head measured from the bottom of the aquifer.

Introduce the abbreviation $h_e = \min(h, H)$. The transport of the tracer (contaminant) with concentration C and source term F is modelled by

$$\partial_t(h_e C) = \frac{1}{r}\partial_r[rh_e(D_0 + \alpha_L|v|)\partial_r C] - \frac{1}{r}\partial_r(rh_e vC) + \frac{F}{\theta_0}h_e, \tag{9}$$

where α_L represents the longitudinal dispersion coefficient, D_0 is molecular diffusion,

$$v = -\frac{k}{\theta_0}\partial_r h \tag{10}$$

is the Darcy velocity of the water, and θ_0 is the porosity. The source term F represents the adsorption of the tracer. When the tracer is radioactive then F can represent also its decay. In the general case we have

$$F = -\kappa(\Psi(C) - W(t)) - \lambda C, \tag{11}$$

where λ is the decay constant, $\Psi(C)$ is the sorption isotherm, κ is the rate constant of the adsorption and $W(t)$ represents the amount of adsorbed tracer per unit mass of the porous medium. The adsorbed mass is governed by

$$\partial_t W(t) = \kappa(\Psi(C) - W(t)) - \lambda W(t). \tag{12}$$

If the sorption is irreversible we must consider $(\Psi(C) - W(t))_+$ instead of $(\Psi(C) - W(t))$ ($a_+ = 1/2(a + |a|)$). The most common adsorption isotherms are of Langmuir and Freundlich type

$$\Psi_L(s) = \frac{as}{1 + bs}, \quad \Psi_F(s) = as^b,$$

where a, b are model parameters — see [**12**].

The equations (7)–(12) are to be completed with initial and boundary conditions. In the injection regime, during the time interval $(0, T_1)$, we assume that $H \le h$ (i.e. the aquifer is saturated) for $r_0 \le r \le R$ and

$$\begin{aligned} h(r_0,t) = h_{in}, \quad h(R,t) &= h_R, \quad h(r,0) = h_0(r) \\ C(r_0,t) = C_0, \quad C(R,t) &= 0, \quad C(r,0) = 0 \\ W(0) &= W_0, \end{aligned} \tag{13}$$

in which h_{in}, C_0 can be time-dependent, e.g., piecewise constant or piecewise linear in subintervals of $(0, T_1)$. In the last subinterval we assume $C_0 \equiv 0$.

The extraction regime extends over the time interval (T_1, T_2). For $t \ge T_1$ we shall consider $h(r_0, t) = h_{ex} < H$, so that an unsaturated zone appears in

$r \in (0, s(t))$, and a saturated zone in $r \in (s(t), R)$. Then the following initial and boundary conditions will hold:

$$\begin{aligned} h(r_0,t) = h_{ex}, \quad h(R,t) &= h_R, \quad h(r,T_1) = h_{ex}(r) \\ C(r_0,t) = C_0, \quad C(R,t) &= 0, \quad C(r,T_1) = C_{ex} \\ W(T_1) &= W_{ex}, \end{aligned} \tag{14}$$

where H_{ex}, C_{ex}, W_{ex} are the values of corresponding solutions h, C, W of (7)–(12) at the time $t = T_1$. The free boundary $x = s(t)$ has to be determined from 'contact' conditions

$$h(s(t)^+, t) = h(s(t)^-, t), \quad \partial_r h(s(t)^+, t) = \partial_r h(s(t)^-, t), \tag{15}$$

which represent the continuity of the head and the flux at $x = s(t)$.

From additional measurements of $C(r_0, t)$ during the extraction period (T_1, T_2) we have to determine the model parameters $d = (k, \alpha_L, a, b)$.

2. Solution of the Direct Problem (3)–(6)

We sketch the idea of the solution method for the direct problem (3)–(6) with the initial condition $u_0 \equiv 0$. In this case the wetness front $x = s(t)$ moves from $x = 0$ and its movement is governed by (see [**6**])

$$\dot{s}(t) = -\lim_{x \to s(t)^-} \Big(\partial_x F(u) + \frac{K(u)}{u} \Big), \tag{16}$$

where $F(u) = \int_0^t (\beta'(u)/u)\, du$. This is the crucial point in constructing a very accurate solver. To make practical use of (16) we must to avoid the degeneracy of F since it can be so that $F'(0) = 0$. For this purpose we introduce the transformed dependent variable $v = F(u)$. Then we apply a fixed-domain transformation $y = \frac{x}{s(t)}$ in (3)–(5), (16). In our special case of β in (3) we easily verify that

$$\beta'(s) = s^p g(s), \quad p = \frac{1}{2} + \frac{1}{m} > 1, \quad g(s) \geq \delta > 0$$

where g is a smooth function. To remove the singularity in (16) it is sufficient to use the transformation $v = u^{p-1}$. Then we rewrite (3), (16) into the form

$$\begin{aligned} \partial_t v = \beta'(v^{1/(p-1)}) \partial_x^2 v + \frac{(\partial_x v)^2}{(p-1)v} (\beta''(v^{1/(p-1)}) v^{1/(p-1)} \\ + (2-p)\beta'(v^{1/(p-1)})) + K'(v^{1/(p-1)}) \partial_x v, \end{aligned} \tag{17}$$

$$\dot{s}(t) = -\frac{1}{p-1} \lim_{x \to s(t)^-} \frac{\beta'(v^{1/(p-1)})}{v} \partial_x v. \tag{18}$$

As a consequence of the used transformation we have that

$$\lim_{x \to s(t)^-} \frac{\beta'(v^{1/(p-1)})}{v} \equiv g(0) \neq 0.$$

Applying the fixed-domain transformation $y = x/s(t)$ and writing $w(y,t) = v(x,t)$, we obtain

$$\partial_t w = \frac{\beta'(w^{1/(p-1)})}{s^2(t)}\partial_y^2 w + \frac{(\partial_y w)^2}{(p-1)s^2(t)w}\Big(\beta''(w^{1/(p-1)})w^{1/(p-1)} + (2-p)\beta'(w^{1/(p-1)})\Big) + \frac{K'(w^{1/(p-1)}) + \dot{s}(t)y}{s(t)}\partial_y w \tag{19}$$

and

$$\dot{s}(t) = -\frac{p}{(p-1)s(t)}g(0)\partial_y w, \tag{20}$$

which can be substituted on the right-hand side of equation (19). The boundary conditions are transformed into

$$w(0,t) = (1-\varepsilon)^p - 1, w(1,t) = 0 \tag{21}$$

$$-\frac{\beta'(w^{1/(p-1)})w^{1/(p-1)}}{(p-1)ws(t)}\partial_y w - K(w^{\frac{1}{p-1}}) = q \quad \text{for } y = 0, w(1,t) = 0. \tag{22}$$

Next, we reduce (19)–(20) to a system of ODE, using the space discretization in $y \in (0,1)$ consisting of points $0 = y_0 < y_1 < \ldots < y_N = 1$. Denote by $C_i(t)$ the approximation to $w(y_i,t)$ (so that $C_N(t) = w(1,t) = w(s(t),t) = 0$ 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 $\partial_y w$ 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 (22) 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 $C_{-1} = C_1 - 2y_1(\partial_y w)_{y=0}$, where $(\partial_y w)_{y=0}$ is obtained from the Neumann condition.

The result of this discretization is a system of ODEs

$$\dot{X} = f(X, t; d), \tag{23}$$

where $X(t) = (X_0, X_1, \ldots, X_N, s(t))$ and d is a vector of approximate parameters of $\beta_d(u)$ and $K_d(u)$. The initial condition $X(0) = X_0$ 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 (23) reasonably small.

To solve (23) we use an efficient solver for stiff ODE, e.g. LSODA, which is based on time-adaptive BDF methods. Comparing our numerical solution with the analytical one by Barenblatt-Pattle for $\beta(s) = s^p$ and $u(x,0) = \delta(x)$ (the Dirac measure) the error in L_2 norm is smaller than 10^{-6} using only $N = 20$ nodal points.

Denote by $s^\star(t)$ the measured movement of the interface at discrete time instants $t = \{t_i\}_{i=1}^m$. Then in the inverse problem we want to find such a soil parameter

vector d, that the penalty functional

$$\mathcal{F}(X,d) \equiv \sum_{i=1}^{m}(s_d(t_i) - s_i^\star)^2 \tag{24}$$

reaches the minimum among all admissible vectors d. We can add to (24) an additional penalty term

$$\sum_{i=1}^{m}(Q_d(t_i) - Q_i^\star)^2$$

based on measurements of total infiltrated mass

$$Q_d(t) = \int_0^t q(z)\,dz,$$

where d is the model parameter vector and the $Q^\star(t_i)$ are the corresponding measured values.

To increase the sensitivity of the solution on the soil parameters in d, we have to make the solution very dynamical. We can do this by switching the boundary conditions and using centrifugation. Then, instead of the usual gravitation potential we can create an modified potential with

$$z = \frac{\omega^2(x+l)^2}{2g},$$

which we substitute into (1). Here, l is the distance between the top of the sample and the center of the centrifuge. In this case we have (see (3))

$$K(u) = \frac{k_s\omega^2(x+l)}{g(\theta_s - \theta_r)}u^{1/2}(1-(1-u^{1/m})^m)^2.$$

Changing the rotational speed of the centrifuge, we can change the evolution of the saturation in the sample very effectively. Moreover, the propagation of infiltration can be significantly influenced also in low-permeability materials. This makes the method efficient, precise and cheap.

3. Solution of Direct Problem (7)–(12)

We briefly describe the solution of the flow and transport equations under the extraction regime of the well. There is an unsaturated zone in $(r_0, s(t))$ around the well and saturated zone for $r \in (s(t), R)$. In that case the equation (7) holds in the unsaturated zone and (8) in the saturated zone. The unknown interface $x = s(t)$ has to be determined from (14) which is coupled with (7) and (8). This free boundary problem we treat similarly as in previous section, using a fixed domain transformation. In $(r_0, s(t))$ we use $y = (R-r)/(R-s(t))$. We denote by

$$h_1(y,t) = h(r,t) - H \quad \text{for} \quad r \in (0, s(t),$$
$$h_2(y,t) = h(r,t) - H \quad \text{for} \quad r \in (s(t), R).$$

Then we obtain

$$S_1\partial_t h_1 = \frac{k}{(s(t)-r_0)^2}\Big\{\partial_y[(h_1+H)\partial_y h_1] + \frac{s(t)-r_0}{r_0+y(s(t)-r_0)}(h_1+H)\partial_y h_1\Big\} + \frac{S_1}{s(t)-r_0}\dot{s}(t)y\partial_y h_1, \tag{25}$$

$$S_2\partial_t h_2 = \frac{kH}{(R-s(t))^2}\Big[\partial_y^2 h_2 - \frac{R-s(t)}{R-y(R-s(t)}\partial_y h_2\Big] - \frac{S_2\dot{s}}{R-s(t)}y\partial_y h_2 \tag{26}$$

for $y \in (0,1)$, with the boundary conditions

$$\begin{aligned} &h_1(0,t) = h_{ex} - H, \quad h_1(1,t) = 0, \\ &h_2(0,t) = h_R - H, \quad h_2(1,t) = 0. \end{aligned} \tag{27}$$

The point $y = 1$ corresponds to the interface $x = s(t)$. The 'contact' condition (16) can be expressed in the form

$$\frac{1}{s(t)-r_0}\partial_y h_1 = -\frac{1}{R-s(t)}\partial_y h_2 \quad \text{for } x = s(t). \tag{28}$$

In this case we do not have a governing equation for $\dot{s}(t)$. We shall determine $\dot{s}(t)$ (and consequently s by integration) by forcing $s(t)$ to satisfy (28). We use the relaxation

$$\varepsilon\dot{s}(t) = \frac{1}{s(t)-r_0}\partial_y h_1 + \frac{1}{R-s(t)}\partial_y h_2 \quad \text{for } y = 1. \tag{29}$$

If $\varepsilon \to 0^+$, we expect that (28) will be satisfied. Now we substitute for $\dot{s}(t)$ in (25), (26) from (29). We use a similar space discretization as in Section 2. Then we obtain an ODE system

$$\dot{Z}(t) = f_1(Z,d), \tag{30}$$

where d represents the model parameters $(S_1, S_2, k, \alpha, a, b, \kappa)$ and $Z = (Z_1, Z_2, s)$ represents an approximation of h_1, h_2 in the nodal points $\{y_i\}_{i=1}^m$ and s is from (29). Similarly we transform and approximate the concentration $C = (C_1, C_2)$ in the corresponding nodal points $\{y_i\}_{i=1}^m$ in both the saturated and the unsaturated zone. Then we obtain an ODE system

$$\dot{V} = f_2(V,s,F,d), \tag{31}$$

where $V = (V_1, V_2)$ are the approximations of C_1, C_2 in the nodal points $\{y_i\}_{i=1}^m$. We note that in the unsaturated zone $h_e = h$, which is time-dependent and thus

$$\partial_t(h_e C) = h\partial_t C + C\partial_t h,$$

where $\partial_t h$ can be eliminated from (7). In the saturated zone $h_e = H$ and therefore $\partial_t(h_e C) = H\partial_t C$.

When F represents the adsorption governed by (11), we add to the ODE systems (30), (31) also a system

$$\dot{W} = \kappa(\Psi(V) - W) - \lambda W + y\frac{\dot{s}}{s}\partial_y W, \quad W(0) = W_0, \tag{32}$$

which represents a transformation of (12) in the variable y. The same nodal points have been used in the unsaturated and the saturated zone. Finally, our complete ODE system is in the form

$$\dot{X} = f(X, F, d), \quad X(0) = X_0 \quad \text{with} \quad X^T = (Z^T, V^T, W^T). \tag{33}$$

This system we then solve using the LSODA package.

Similar systems are obtained when we inject into the unsaturated zone. Then, a saturated zone occurs in $(r_0, s(t))$ and an unsaturated zone in $(s(t), R)$. When we repeat the injection-extraction regime switches, several interfaces can appear. In that case the resulting system is more complicated. This situation has been discussed in [**7**].

The inverse problem consists in determining the model vector d so as to fit the measurements (during the extraction regime), for the penalty functional

$$\mathcal{F}(X, d) = \mu \sum_{i=1}^{N} (V_{0,d}(t_i) - C_i^*)^2 + \nu \sum_{i-1}^{N} (Q_d(t_i) - Q_i^*)^2, \tag{34}$$

to attain its minimum over all admissible vectors d. Here, $Q_d(t)$ represents the total amount of injected or extracted water, where

$$Q_d(t) = -k \int_0^t 2\pi r_0 h_d \partial_r h_d|_{r=r_0} \, dt$$

and $V_{0,d}(t)$ is the first component of V_d which approximates $C(r_0, t)$ in $t \in (T_1, T_2)$. The vector $X^T(t) \equiv (Z^T(t), V^T(t), W^T(t))$ is governed by (33).

4. Solution of Inverse Problems

We solve the inverse problems, introduced in Sections 2 and 3, using Newton-Raphson, Broyden, or Levenberg-Marquardt methods. The details of the minimization methods can be found, e.g., in [**15**]. Applying the Newton-Raphson method in minimization of penalty functional we need $\nabla_d \mathcal{F}(X, d)$ and $\nabla_d^2 \mathcal{F}(X, d)$ (Hessian). Consequently we need $\nabla_d X_d$ and $\nabla_d^2 X_d$. These we can obtain using the concept of automatic differentiation implemented into LSODA (cf. [**5**]). In the output of this solver we obtain, additionally to $X_d(t)$, also $\nabla_d X_d(t)$ and $\nabla_d^2 X(t)$ for $t \in (0, T)$. Then the minimization procedure is as follows. Let d_k is known and let X_{d_k} be the corresponding solution of (33). Then the improved vector d_{k+1} is obtained as the solution of the linear system

$$\nabla_d^2 \mathcal{F}(X, d)(d_{k+1} - d_k) = -\nabla_d \mathcal{F}(X_k, d_k).$$

If the Hessian is not a positive definite matrix, we use a steepest descent step instead. It is well known the slow convergence of steepest descent method. If the vector d contains only a few components then also Levenberg-Marquardt method is suitable since the penalty functional is quadratic. In that case $\nabla_d X_d$ is constructed numerically. By means of approximate values $\nabla_{d_k} X_k$ and $\nabla_{d_{k-1}} X_{k-1}$ an

approximation of the Hessian is constructed. Also in Broyden method an approximation of Hessian is constructed (on each iteration step) by means of $\nabla_{d_k} X_k$ and $\nabla_{d_{k-1}} X_{k-1}$ — see [**15**]

5. Some Numerical Experiments

5.1. Infiltration

Let us consider sand soil with the model vector $d = (k_s, m, \alpha)$ where

$$k_s = 2.4 \times 10^{-7}\text{m/s}, \quad m = 0.644, \quad \alpha = -1.89\text{m}^{-1}.$$

The length of the sample is 10cm. This sample will be subjected to the following infiltration procedure:

- during the first 30 minutes there is infiltration into the dry region from the saturated boundary $x = 0$ under gravitation;
- for the next two hours the top $x = 0$ is sealed (zero flux) and centrifugation is used with $\omega = 5\text{t/s}$ with $l = 0.1\text{m}$;
- again, the Dirichlet boundary condition $u(0, t) = 0.995$ is used and infiltration with gravitation proceeds for one hour;
- finally, centrifugation with $\omega = 5\text{t/s}$ is used for one hour with sealed boundary $x = 0$.

The corresponding time evolution of the effective saturation u is graphed in Figs. 1 to 3. We present the iteration process of restoration of $d = (k_s, m, \alpha)$ in Table 1. We start with the initial approximation $d_0 = (3.10^{-7}, 0.6, -2.5)$. The effectiveness of the used iteration process (Newton-Raphson) is measured by the RMS values

$$\text{RMS} = \left(\frac{1}{m} \sum_{i=1}^{m} (s_k(t_i) - s_i^*)^2 \right)^{1/2}.$$

The measurements $s^*(t)$ we have generated from the solution of the direct problem (i.e. $s_d(t)$) with the vector d, and were then perturbed with artificial noise (normally distributed with standard deviation 0.1).

5.2. Injection/extraction well

We consider a numerical experiment with the following data:

1. well radius $r_0 = 0.2\text{m}$, domain radius $R = 10\text{m}$;
2. porosity $\theta_0 = 0.2$, hydraulic conductivity $k = 10^{-5}\text{m/s}$, storativities $S_1 = 0.05$, $S_2 = 1$;
3. saturation head $H = 20\text{m}$, injection head $h_{\text{in}} = 25\text{m}$, extraction head $h_{\text{ex}} = 12\text{m}$, boundary head value $h_R = 20.1\text{m}$;
4. molecular diffusion $D_0 = 10^{-8}\text{m}^2\text{/s}$, dispersivity $\alpha_L = 0.2\text{m}$.

The injection regime lasts for 200000s; during the first 100000s a contaminant is injected at concentration 1 (a conventional value), and during the next 100000s no contaminant is injected. Then the extraction regime lasts for 750000s, during which the contaminant concentration in the extracted water is measured every

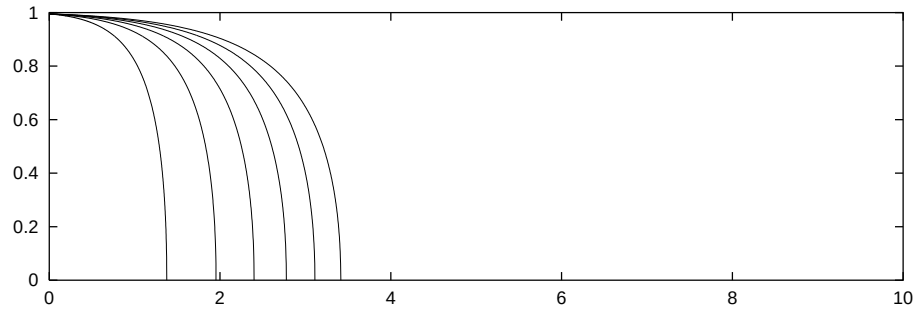

Figure 1. Saturation distribution along sand sample (of 10 cm lenghth) under gravitation, after 600, 1200, . . . , 3600 seconds.

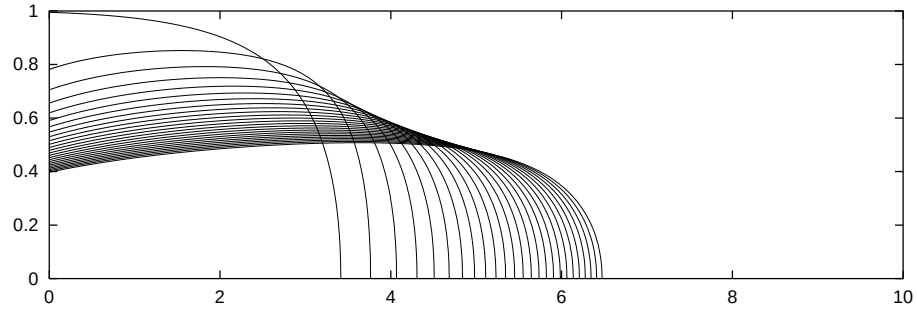

Figure 2. Subsequent saturation distribution in the sealed centrifugation, after 0, 600, 1200, . . . , 14400 seconds.

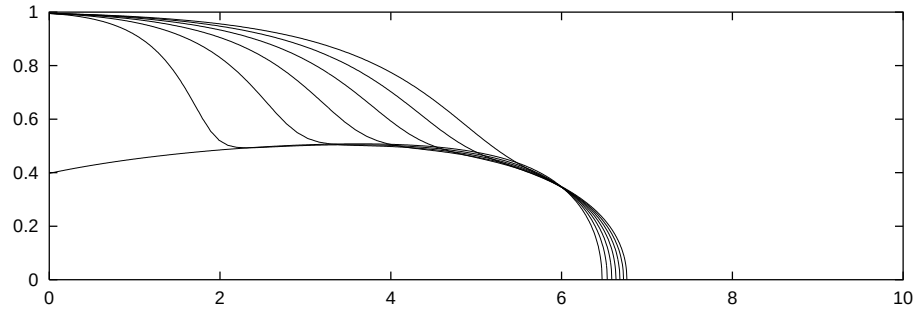

Figure 3. Subsequently saturation distributioin under gravitation, after 0, 600, 1200, . . . , 3600 seconds.

2000s. The simulations are carried out using $N = 120$ discretization intervals. The corresponding solutions are graphed in Fig. 4.

In this inverse problem, we recover the values of α_L, k and S_2 using the same model to generate the measurements and to match them, but starting from the perturbed initial values $\alpha_L = 0.4$m, $k = 3 \times 10^{-6}$m/s and $S_2 = 0.1$.

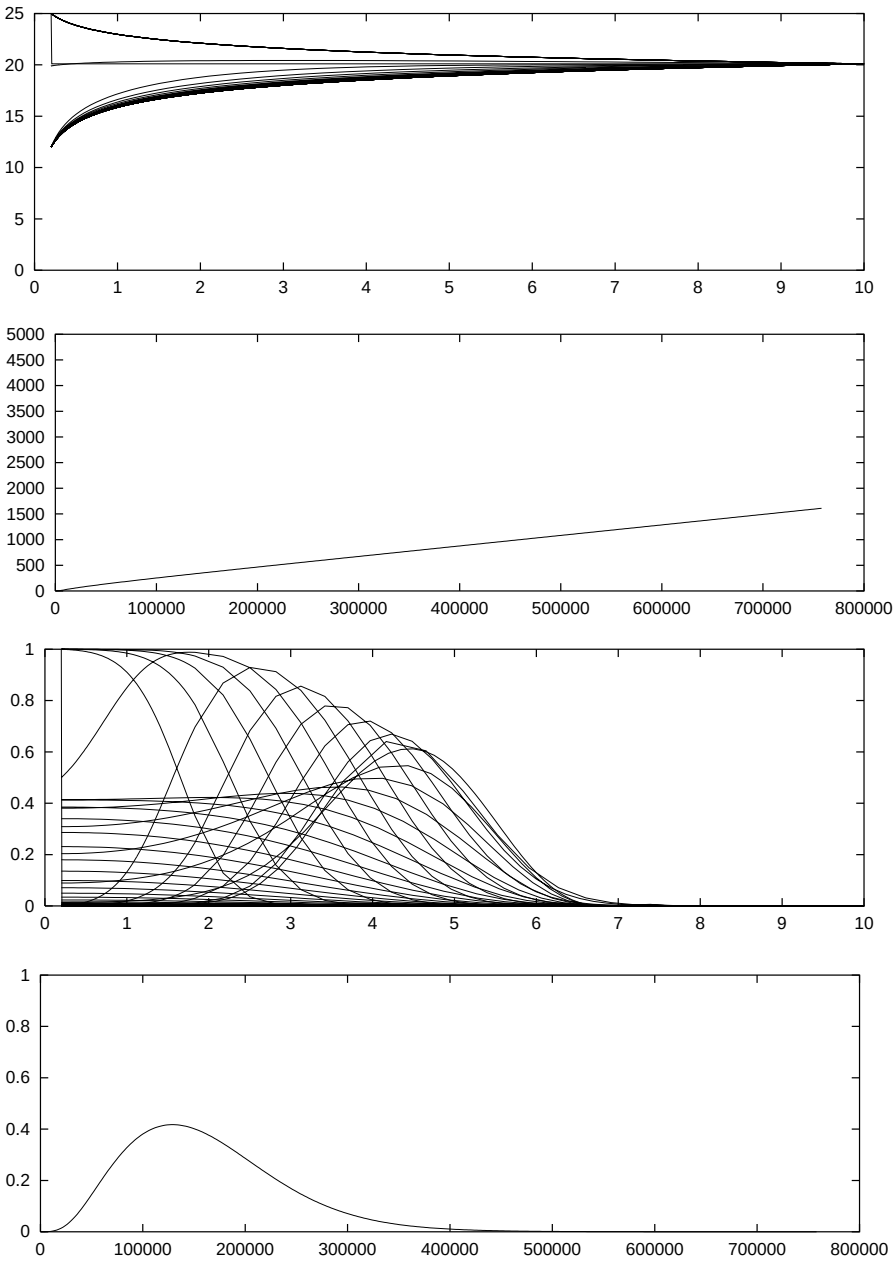

Figure 4. Simulation results of the direct problem in injection/extraction: (from top to bottom) successive profiles of hydraulic head (m) vs. radial coordinate (m); total amount of water extracted vs. time (s) during the extraction regime; successive profiles of contaminant concentration vs. radial coordinate (m); contaminant concentration at $r = r_0$ vs. time (s) during the extraction regime.

$k_s \times 10^5$	m	α	RMS
3.000000	0.600000	-0.025000	0.05782216
3.182745	0.618725	-0.025843	0.01877586
3.276472	0.599218	-0.025343	0.01215379
2.969023	0.609280	-0.022863	0.01096101
2.804175	0.620033	-0.021874	0.01050500
2.686874	0.626353	-0.020997	0.01028553
2.501224	0.637531	-0.019692	0.01013705
2.461581	0.640548	-0.019387	0.01002683
2.300516	0.651175	-0.018219	0.01006465
2.295148	0.652031	-0.018166	0.00989848
2.262489	0.654401	-0.017924	0.00995786
2.262520	0.654422	-0.017923	0.00994728

Table 1. Subsequent parameter values and RMS errors for the inverse problem in infiltration.

The successive iteration results of the Levenberg-Marquardt method are listed in Table 2. It is clear that α_L is the easiest of the three quantities to restore, followed by k, and then by S_2. In the absence of noise, the parameters are recovered exactly (up to perturbation induced by the precision limitations of the integration algorithm).

α_L	k	S_2	RMS error
0.400000	3.00000e-06	0.100000	0.04706172
0.171601	4.10545e-06	0.104566	0.01982622
0.155226	5.68765e-06	0.108296	0.00707935
0.167471	6.75390e-06	0.102463	0.00397516
0.190440	8.39317e-06	0.079443	0.00222197
0.197762	9.68133e-06	0.055072	0.00036735
0.199809	9.96590e-06	0.051009	0.00005947
0.200021	9.99143e-06	0.050495	0.00003558
0.199989	9.99523e-06	0.050218	0.00001009
0.200024	9.99755e-06	0.050059	0.00000886
0.200027	1.00010e-05	0.049992	0.00000401
0.200005	1.00002e-05	0.050029	0.00000202
0.199996	9.99913e-06	0.050043	0.00000158

Table 2. Successive steps of the solution of the injection/extraction inverse problem.

References

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

2. Barenblatt G. I., *On a class of exact solutions of the plane one-dimensional problem of unsteady filtration into a porous medium*, Prikl. Mat. Meh. **17** (1953), 739–742 (in russian).

3. Caffarelli L. A. and Friedman A., *Regularity of the free boundary for the one-dimensional flow of gas in a porous medium*, Amer. J. Math. **101**(6) (1979), 1193–1218.

4. Chen J., Hopmans J. W. and Grisnier M. E., *Parameter estimation of two-fluid capillary pressure – saturation and permeability functions*, Advances in Water Resources **22**(5) (1999), 479–493.

5. Constales D., *Automatic differentiation in LSODA*, in preparation.

6. Constales D. and Kačur J., *Inverse problems in porous media flow*, submitted to Computational Geosciences.

7. _____, *Parameter identification by a single injection-extraction well*, to appear.

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

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

10. Gilding B. H., *Flow and Transport in Porous Media*, World Scientific, Singapore, 1992.

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

12. Knabner P., *Finite-element-approximation of solute transport in porous media with general adsorption processes*, Flow and transport in porous media, Ed. Xiao Shutie, World Scientific, Singapore – New Jersey – London – Hong Kong, 1992.

13. Olejnik O. A., Kalašnikov A. S. and Jui-Lin Ch., *Cauchy problems and boundary-value problems for equations of type of infiltration*, Izv. AN SSSR Ser. Mat. **5** (1958), 667–704 (in russian).

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

15. Polak E., *Optimization*, Applied Mathematical Sciences **124**, Springer-Verlag, New York, Inc., 1997.

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

17. van Duijn C. J. and Peletier L. A., *Nonstationary filtration in partially saturated porous media*, Arch. Rational Mech. Anal. **78**(2) (1982), 173–198.

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

D. Constales, Department of Mathematical Analysis, Ghent University, Galglaan 2, B-9000 Gent, Belgium, *e-mail*: `dcons@world.std.com`

J. Kačur, Faculty of Mathematics, Physics and Informatics, Comenius University, Mlynská dolina 84248 Bratislava, Slovakia, *e-mail*: `kacur@fmph.uniba.sk`