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Generalisation of the Solution of the Inverse Richards' Problem

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In inverse problems defined by models that include partial differential equations, a part of the boundary conditions are unknown and are to be estimated from experimental measurements. We have shown in a previous contribution that the solution of the inverse Richards' problem can allow estimating percolation rates at the bottom of landfills through the use of measurements at the surface only. This can be a useful complement of the information furnished by the vadose measurement system, pointing to the possible presence of biases of in-situ equipment, and making it possible to use inexpensive mobile equipment to carry out surface measurements.

In this article, we consider a generalisation which makes it possible to consider the presence of unknown non-linear parameters, such as the effective hydraulic conductivity and the root uptake coefficients. This is accomplished using the method of separation of variables in the resulting estimation problem. Thanks to the linearity of the model, all these conditions can be expressed as linear functions of the unknown lower boundary condition. Otherwise, the relevant non-linear parameters are to be estimated from the data as well.

Obviously, the correlation between the linear parameters contained in the unknown lower boundary conditions and the non-linear parameters can reduce the reliability of the monitoring procedure and hence the necessity of limiting the number of the latter.

1. Introduction

The correct evaluation of water and solutes flow in the unsaturated zone is of fundamental importance in traditional applications of groundwater hydrology, soil physics and agronomy, such as storm water management, soil irrigation and drainage, or soil-water redistribution. More recently, the need to predict the transport of contaminants (De Rademaeker et al., 2014) and toxic chemicals in the unsaturated and saturated zones with a high degree of accuracy has given rise to a renewed interest in this subject, since dissolved contaminants may migrate through the unsaturated zone, reach the saturated zone, and contaminate the groundwater.

The combination of the fundamental theory developed by Buckingham (Buckingham, 1907) with Darcy's law on the flow of a fluid through a porous medium provides the Richards' equation (Richards, 1931), which, in its simplest formulation, is a time dependent one-dimensional partial differential equation.

However, the presence of highly non-linear parameters (such as diffusivity and hydraulic conductivity) and of a random forcing term (the erratic time distribution of precipitation in the area), makes analytical solutions capable of describing saturated and unsaturated infiltration difficult and generally based on linear or quasi linear approximations. Numerical schemes are suitable for the solutions of direct problems, i.e. the determination of water concentration and flux (or equivalently of the total head) when both the forcing term and the boundary conditions, as well as the physical-chemical parameters, are perfectly known. However, they may become clumsy or outright infeasible if inverse problems are considered, i.e. if parts of the boundary conditions (and possibly physical-chemical parameters) are unknown and are to be estimated from experimental measurements. In other words, whenever the required information is not accessible to direct measurement, but has to be estimated using mathematical models that relate the sought after variables to the actually measured quantities.

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This is for instance the case in landfills. Although there are many remediation technologies, and many others, some very promising, are constantly in development, the excavation and landfilling is still a widely used solution, although much less sustainable (Vocciante et al., 2016). In this context, the possibility to estimate the percolation rates in landfills at a fixed depth using reliable surface data (Solisio et al., 2012) can usefully complement the information provided by the vadose measurement system (Hix, 1998), possibly point to the presence of biases in it, and even help to contain the already high environmental impacts in the event of accidental leaks.

Several methods have been proposed for the analytical solution of Richards' equation (Ghotbi et al., 2011) – for a soil application, (Asgari et al., 2011) for a generalised case. In a previous contribution (Vocciante et al., 2015b), we have employed the solution obtained by Yuan and Lu (2005) for the development of an inverse algorithm capable of identifying the boundary conditions at the lower end of the domain from measurements at the surface, based on the general procedure showed in (Vocciante et al., 2015a). Using a piecewise constant temporal function for the unknown boundary condition in Yuan and Lu's model makes it possible to express the analytical solution of Richards' one-dimensional equation as a linear function of a finite number of variables. These latter, corresponding to the unknown coefficients of the piecewise constant function, can be estimated using statistical regression algorithms to reconstruct the unknown boundary condition without need for regularization techniques (Vocciante et al., 2015b).

In the present paper, we consider a generalisation that allows to consider the presence of unknown non-linear parameters, such as the effective hydraulic conductivity and the root uptake coefficients. This is accomplished using the method of separation of variables (Golub and Pereyra 1973) in the resulting estimation problem (Reverberi et al., 2013).

2. Theoretical model

The classical treatment of water flow in an unsaturated medium is provided by the Richards' equation (Richards, 1931), a general partial differential equation proposed on the basis of the studies carried out by Buckingham (Buckingham, 1907) and describing water flow in unsaturated, non-swelling soils, with soil water content θ as the only dependent variable.

$$\frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial z}\left[K\left(\frac{\partial \psi}{\partial z}+1\right)\right] \tag{1}$$

In this equation K is the hydraulic conductivity (which is in general a function of water content θ), and the total head h is given by the sum of the heights of the capillaries ψ and geometric z altitude. Thus, the overall model of water percolation within the porous medium consists in the superposition of pore-scale transport and gravity-maintained flow. Adopting the concept of differential water capacity, defined as the derivative of the soil water retention curve $C(\psi) = \partial\theta/\partial\psi$ makes it possible to eliminate either θ or ψ from the mixed formulation (1), without the necessity of employing constitutive relations for describing the interdependence of the two variables. If ψ is chosen as the independent variable, the so-called ψ-formulation of Richards' equation is obtained

$$C(\psi)\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right] \tag{2}$$

Eq(2) defines the infiltration problem provided a suitable initial condition (3) and two boundary conditions (4)-(5):

$$\psi(z,0) = \psi_0(z) \tag{3}$$

$$\psi(0,t) = \psi_b \tag{4}$$

$$\left[K(\psi)\left(\frac{\partial \psi}{\partial z}+1\right)\right]_{z=L} = -q_t(t) \tag{5}$$

where the forcing term q_t is the external time-dependent surface flow (precipitation rate). In direct problems the value of $z = 0$ coincides with the location of the water table, and consequently the saturation condition implies $\psi_b = 0$. Unfortunately this is not the case in inverse problems, in which the origin of the z coordinate typically coincides with a specific location (for instance the depth of a landfill) where the saturation condition is not satisfied and the corresponding value of ψ_b has to be estimated from the measurements available.

Using the Kirchhoff transformation (Gardner, 1958) allows solving the problem (2)-(5) using the method of characteristics in the Laplace domain. The inverse Laplace transformation provides the sought-after matrix flux potential Φ for the transient flow (Yuan and Lu, 2005):

$$\Phi(z,t) = \Phi_0(z) + 8D \exp\left[\frac{\alpha(L-z)}{2}\right]\sum_{n=1}^{\infty}\frac{(\lambda_n^2+\frac{\alpha^2}{4})sin(\lambda_n L)sin(\lambda_n z)}{2\alpha+\alpha^2 L+4L\lambda_n^2}G(t) \tag{6}$$

$$\Phi_0(z) = \frac{K_s\, exp\,[\alpha(\psi_b - z)]}{\alpha} + \frac{q_0}{\alpha}[\exp\,(-\alpha z) - 1] \tag{7}$$

$$G(t) = \int_0^t [q_0 - q_t(\tau)] \exp\left[-D\left(\lambda_n^2 + \frac{\alpha^2}{4}\right)(t-\tau)\right] d\tau \tag{8}$$

where $D = K_s/\{\alpha(\theta_s - \theta_r)\}$ is the diffusivity, λ_n is the nth positive root of the equation $\sin(\lambda L) + (2\lambda/\alpha)\cos(\lambda L) = 0$, $q_t(t)$ is the time dependent flux at the upper boundary and $\Phi_0(z)$ is the initial condition assumed to be the steady-state solution of the system. The actual flux can be approximated to any degree of accuracy by a suitable combination of functions (e.g. constant, linear, quadratic, exponential, sinusoidal) that make it possible to integrate Eq(8) in closed form.
After Φ has been evaluated, both pressure head and water content can be computed as $\psi = (1/\alpha)\, ln(\alpha\Phi/K_s)$ and $\theta = \theta_r + \alpha(\theta_s - \theta_r)\,\Phi/K_s$ respectively.

3. Algorithm for the boundary condition estimation

Rewriting Eq(7) as

$$\Phi_0(z)\xi(z) = C_1 + A_1(z) \tag{9}$$

makes it possible to express Eq(6) as

$$\Phi(z,t)\xi(z) = C_1 + A_1(z) + \xi(z)f(z,t) \tag{10}$$

where C_1 depends on $\psi|_{z=0}$ and $f(z,t)$ depends on the other parameters $q_t(t)$, α, D, L, but not on $\psi|_{z=0}$, that is:

$$\xi(z) = \frac{\alpha\, exp\,(\alpha z)}{K_s} \tag{11}$$

$$C_1 = \exp\,(\alpha\psi_b) \tag{12}$$

$$A_1(z) = \frac{q_0}{K_s}[1 - \exp\,(\alpha z)] \tag{13}$$

$$f(z,t) = 8D \exp\left[\frac{\alpha(L-z)}{2}\right]\sum_{n=1}^{\infty}\frac{(\lambda_n^2+\frac{\alpha^2}{4})sin(\lambda_n L)sin(\lambda_n z)}{2\alpha+\alpha^2 L+4L\lambda_n^2}G(t) \tag{14}$$

Since in inverse problems the lower boundary condition ψ_b is not known, it is convenient to approximate it using a simplified functional form dependent on a number of adjustable parameters, as already done in similar cases involving partial differential equations related to mass and heat conservation laws (Reverberi et al., 2013). Typically, the simpler the functional form, the higher the number of the parameters.
In this case a piecewise constant function of time is assumed for ψ_b, that is, the overall time range considered is divided into a number of time intervals in each of which ψ_b is constant. Obviously, any profile can be approximated to any desired degree of accuracy by increasing the number of intervals. The estimation problem consists in the identification of the constant values C_j in each time interval j.
Using a piecewise constant function implies the use of a first-type boundary condition in each interval. However, the estimation procedure would lead to equivalent results (within the limits of the approximations introduced) if different approximations are used (for instance, a piecewise constant value of the gradient). In this case, the availability of an analytic solution for the Dirichlet problem greatly simplifies the estimation task and is the main reason for using it.

At the end of the procedure showed in (Vocciante et al., 2015b) the general expression for the solution in the n-th interval $t_{n-1} \le t \le t_n$ is obtained.

$$\Gamma_n(z,t) = \Phi_n(z,t)\xi(z) = C_n + A_1(z) + \xi(z)\, g_{n-1}(z,t) + (C_1 - C_n)\xi(z)h_n(z) \tag{15}$$

$$h_n(z) = \frac{\left[\frac{A_1(z)}{\xi(z)} + g_{n-2}(z,t_{n-1})\right]\int_0^L \frac{1}{\xi(z)}\,dz}{\int_0^L \left[\frac{A_1(z)}{\xi(z)} + g_{n-2}(z,t_{n-1})\right]dz} \quad n \ge 2 \tag{16}$$

$$g_{n-1}(z,t) = \sum_{j=1}^{n-1} f\,(z, t_j - t_{j-1}) + f(z, t - t_{n-1}) \quad j \ge 1 \tag{17}$$

where $\xi(z) = \alpha/K_s\; exp\;(\alpha z)$, $C_n = exp\;(\alpha\psi_n)$ and $A_1 = q_0/K_s\,(1 - exp\;(\alpha z))$.

At this point, given the vector of experimental data Φ' measured at the surface, the vector c of the boundary conditions C_n could be estimated using the usual least squares method, which in our case provides the minimisation problem $\|Ac - b\|^2 = min$ where $b = \Phi' - (\frac{A1(L)}{\xi(L)} + g)$ and A is a sparse matrix of dimension $[n \times k]$, with n the number of intervals and k the total number of measurement. As showed in (Vocciante et al., 2015b), in this case no regularization techniques are needed in the reconstruction procedure, since the approximations introduced have also regularized the solution: the particular structure of the matrix A, which is such that the data in the j-th time interval affect only the values of C_1 and C_j, determines the well-posed nature of the reconstruction observed.

4. Estimation in case of unknown parameters

In case one or more non-linear unknown parameters are contained in the mathematical model of the phenomenon, it is still possible to use the approach shown above. The parameter estimation procedure can in fact be modified to accommodate the estimate of these additional parameters. In this case, the least squares method provides the following minimization problem for the estimation of the parameters $\{H|c\}$

$$\|\Phi' - \Omega(H) - A(H)c\|^2 = min \tag{18}$$

A general optimisation algorithm with respect to the set $\{H|c\}$ would considerably reduce the efficiency of the regression algorithm, due to the difficulty of determining suitable starting values and to the possibility of multiple local minima.
However, these difficulties can be overcome if the principle of relative optimality is applied, which in our case provides optimal values of the vector c for every value of the non-linear parameter H

$$c = \left(A^T(H)A(H)\right)^{-1} A^T(H)[\Phi' - \Omega(H)] \tag{19}$$

or $c = A^+(H)[\Phi' - \Omega(H)]$ (where $A^+(H)$ is the pseudoinverse of A) if the matrix $A(H)$ is not full rank. Thus, the computation of the non-linear parameter can be carried out by minimising the objective function

$$\|\{\Phi' - \Omega(H)\} - A(H)A^+(H)\{\Phi' - \Omega(H)\}\|^2 =$$

$$\left\|P_A^\perp\{\Phi' - \Omega(H)\}\right\|^2 = \left\|P_A^\perp(H)\delta(H)\right\|^2 = min \tag{20}$$

where $P_A^\perp = \{\Phi' - \Omega(H)\} - A(H)A^+(H)$ is the projector on the orthogonal complement of the column space of $A(H)$ with respect to one parameter only.
The typical Gauss-Newton step in the iterative procedure for the estimation of the non-linear parameter is given by (Golub and Pereyra, 1973)

$$H_{n+1} = H_n - \tau_n \left[D\left(P_A^\perp(H_n)\delta(H_n)\right)\right]^+ P_A^\perp(H_n)\delta(H_n) \tag{21}$$

where the operator D is the Fréchet derivative of matrices and τ_n is an interpolation-extrapolation factor used to locate the minimum of the objective function in the direction $\left[D\left(P_A^\perp(H_n)\delta(H_n)\right)\right]^+ P_A^\perp(H_n)\delta(H_n)$.

Furthermore, indicating the variance of the data with σ^2, $\sigma^2\left[D\left(P_A^\perp(H_n)\delta(H_n)\right)\right]^+$ provides an estimate of the variance of the parameter H, once convergence at H^* has been attained.

For the regression procedure to be completely described, even if this is not the case due to the well-posed nature of the reconstruction achieved through the above-explained procedure, a further aspect should be taken into account.

Whenever the matrix $A(H)$ is rank deficient, which is generally the case due to the ill-posed nature of inversion problems like (15)-(17), the evaluation of the pseudoinverse matrix $A^{+}(H)$, generally tackled using the approach suggested by Tikhonov and Arsenine (1976), can lead to unsatisfactory results when a non-linear parameter is considered in the estimation procedure. This can be true even if the Morozov's discrepancy principle (Morozov, 1984) is used to determine the Tikhonov parameter ω in the identification of a suitable regularization matrix Ψ.

Indeed, an unsuitable value of ω could be compensated by a biased estimate of the non-linear parameter H since there might be a large number of combinations of $\{\omega|H\}$ that predict the same statistical properties of the data. Rather, additional constraints dependent on the particular conditions of the experimentation should be added to the optimisation problem, like the use of a combination of tridiagonal and pentadiagonal matrix for Ψ according to the strategy originally recommended by Twomey, (1963).

5. Conclusions

The temporal profiles of pressure and water content at a certain depth can be determined using measurements made at the surface provided an inverse solution of Richards' equation is employed.

We have shown how to obtain a suitable approximation of such solutions, based on the assumption of piecewise constant profiles. The performances of the resulting algorithm have been shown in (Vocciante et al., 2015b). Here we have shown a generalization of this approach, which allows accommodating of unknown non-linear parameters in the estimation procedure making use of the method of separation of variables due to Golub and Pereyra (1973). Finally, we highlighted the further complications that normally result from this kind of extension, since the presence of a biased estimate of the non-linear parameter can considerably complicate the eventual regularization process.

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