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The differential system method for parameter identification; unconfined aquifer case

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We present the applicability of differential system (DS) method for identification of hydraulic conductivity and effective porosity in a phreatic aquifer. In the original setting, the first step of the DS system is to solve an overdetermined algebraic system in the least squares sense. A natural extension of the method is to pose a least squares problem in an appropriate functional space. We show an improvement of the identification by considering the least square problem in the space of square integrable functions in the time variable for a finite interval.

Keywords: inverse problem, phreatic aquifer, hydraulic conductivity, effective porosity, numerical modelling

1. Introduction

We consider an isotropic phreatic aquifer that satisfies Dupuit assumption and for which Darcy's law and the two-dimensional approximation hold. Thus the flow is modelled by the Boussinesq equation [1]:

$$\frac{\partial}{\partial x}\left(K(h-\eta)\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K(h-\eta)\frac{\partial h}{\partial y}\right)=n_{\mathrm{e}}\frac{\partial h}{\partial t}-f, \tag{1}$$

where $h(x, y, t)$ is the elevation of the aquifer free surface (piezometric head, or hydraulic potential), $\eta(x, y)$ is the elevation of the bottom of the aquifer, $f(x, y, t)$ is the source term, representing a vertical flux, positive if downward. The model parameters are hydraulic conductivity $K(x, y)$, and effective porosity $n_{\mathrm{e}}(x, y)$.

Given $K(x, y)$ and $n_{\mathrm{e}}(x, y)$, the direct problem consists of solving the partial differential equation (1) for h, subject to appropriate initial and boundary conditions. Here we are concerned with the following *inverse problem*: given p flow conditions for times t_i, $i = 1, 2, \ldots, p$, determine the model parameters $K(x, y)$ and $n_{\mathrm{e}}(x, y)$. For a

fixed t, a flow condition is a set of data $h(x_m, y_n, t)$, and $f(x_m, y_n, t)$, $m = 1, 2, , \ldots, M$, $n = 1, 2, \ldots, N$.

A method to deal with this sort of inverse problem is for instance the output least squares method; see [2,9]. This method requires a subroutine to solve the direct problem. Since hundreds of direct problems may have to be solved during the optimization of the model parameters, the output least squares method has a tendency to become computationally expensive.

For the confined aquifer case, Parravicini et al. [6] and Giudici et al. [5] proposed a direct method based on the solution of a Cauchy problem that allows for the determination of both transmissivity T and storativity S, when the potentials and source terms are given for three different flow conditions, at least one of them transient. Vázquez et al. [8] developing further the method show the advantages of using more than three flow conditions. The method essentially consists of writing the differential equation for each one of the flow conditions. Forming the set of equations as a first order partial differential system in the unknown T and an algebraic system in the unknown S. Therefore the name DS method (for Differential System method).

In this work we develop the DS method for the identification of hydraulic conductivity, $K(x, y)$, and effective porosity $n_e(x, y)$ for phreatic aquifers. We will show that the main features of the method are preserved, in particular, for the inversion no a priori knowledge of effective porosity is needed and, moreover, the identification of hydraulic conductivity does not depend upon it.

Direct methods involving Cauchy problems for parameter identification in diffusion equations are not new. Consider for instance a confined aquifer in the stationary case, namely,

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right) = -f. \tag{2}$$

To identify transmissitivity me may follow the approach in [3,7] and consider (2) as a first order PDE on the unknown T. The equation is solved by the method of characteristics, in this case, they are the flow lines of h and the solution is obtained by integrating along each flow line. The solution is unique if T is known along a curve Γ transversal to all flow lines. The method, although mathematically viable, is not practical since values of T along such a curve Γ are seldom known. Moreover, computing characteristics may not be very efficient. In contrast, the Cauchy problem to solve in the DS method requires only the value of transmissitivity (or conductivity) at a single location in the aquifer. Also, we shall see that the method is path independent.

The outline of our work is as follows.

In section 2 the inverse problem of interest is formulated and its solution by the DS method is developed. This section describes the main theoretical aspects of the method.

In order to verify the applicability of the DS method, a synthetic but realistic aquifer is presented in section 3. The data necessary for inversion is generated by solving a direct problem. The method of discretization is a balance cell model and finite differences.

In section 4 we deal with the numerical implementation of the DS method. In the first step of the method we require to solve linear systems in the unknowns $\partial K/\partial x$, $\partial K/\partial y$, n_e when the points (x_m, y_m) are fixed. The systems are overdetermined and ill-conditioned. The solution is found in the least squares sense using the *QR* factorization with Householder transformations. Next we integrate the resulting Cauchy problem along optimal paths to minimize error propagation.

It will become apparent that it is natural to consider the least squares problems that arise in the first step of the DS method in more general Hilbertian norms. This extension is presented in section 5, as well as the numerical implementation.

We conclude our exposition with a section entitled Comments and conclusions. Here we review the features of the DS method and discuss some problems for future work.

2. The continuous inverse problem

In order to show how the DS method applies to a phreatic aquifer; let us describe the method with explicit reference to an isotropic phreatic aquifer described by equation (1). For simplicity assume that the aquifer bottom coincide with the datum ($\eta(x, y) = 0$) then:

$$\frac{\partial}{\partial x}\left(Kh\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(Kh\frac{\partial h}{\partial y}\right) = n_e\frac{\partial h}{\partial t} - f. \tag{3}$$

Consider equation (3) and suppose that the source term $f(x, y, t_i)$, the potential $h(x, y, t_i)$ and its time derivative $\partial h(x, y, t_i)/\partial t$ are known as a function of space, at p different times t_i, $i = 1, 2, \ldots, p$. A set of data is given by these functions, so p sets of data are assumed to be known.

Let us introduce the notation:

$$\begin{aligned} f^i &\equiv f(x, y, t_i), \\ h^i &\equiv h(x, y, t_i), \\ \frac{\partial h^i}{\partial t} &\equiv \frac{h(x, y, t_i)}{\partial t}, \end{aligned}$$

then equation (3) gives:

$$\frac{\partial}{\partial x}\left(Kh^i\frac{\partial h^i}{\partial x}\right) + \frac{\partial}{\partial y}\left(Kh^i\frac{\partial h^i}{\partial y}\right) = n_e\frac{\partial h^i}{\partial t} - f^i.$$

Applying derivatives we obtain after some simplification

$$h^i\frac{\partial h^i}{\partial x}\frac{\partial K}{\partial x} + h^i\frac{\partial h^i}{\partial y}\frac{\partial K}{\partial y} - \frac{\partial h^i}{\partial t}n_e = -\overline{\Delta}h^i K - f^i,$$

where

$$\overline{\Delta}h^i = h^i \Delta h^i + \left(\frac{\partial h^i}{\partial x}\right)^2 + \left(\frac{\partial h^i}{\partial y}\right)^2.$$

Let us define

$$\mathbf{u} = (u_1, u_2, u_3) = \left(\frac{\partial K}{\partial x}, \frac{\partial K}{\partial y}, n_e\right). \tag{4}$$

And the vectors $\mathbf{z}$, $\mathbf{f}$ with components $\overline{\Delta}h^i$ and f^i, respectively.

Assuming that conductivity K is known, we have for a fixed point (x, y) the following linear system:

$$\mathbf{A}\mathbf{u} = -K\mathbf{z} + \mathbf{f}. \tag{5}$$

If $\text{Rank}(\mathbf{A}) = 3$, see remark below, then system (5) has a unique solution in the least squares sense given by

$$\mathbf{u} = -K\mathbf{a} + \mathbf{b}, \tag{6}$$

where the three component vector function $\mathbf{a}$ and $\mathbf{b}$ are the solution of the systems:

$$\begin{aligned} \mathbf{A}\mathbf{a} &= \mathbf{z}, \\ \mathbf{A}\mathbf{b} &= \mathbf{f}. \end{aligned} \tag{7}$$

Now, let us rewrite equation (6) recalling definition (4) and writing down the dependence upon x explicitly. We have the following system for the first two components of $\mathbf{u}$

$$\begin{aligned} u_1 &= \frac{\partial K}{\partial x} = -Ka_1 + b_1, \\ u_2 &= \frac{\partial K}{\partial y} = -Ka_2 + b_2. \end{aligned} \tag{8}$$

And the following equation for the third component of $\mathbf{u}$

$$u_3 = n_e = -Ka_3 + b_3. \tag{9}$$

The second step for identifying the parameters consists in considering the equations in (8) as a first order differential system for K.

To solve this differential system we need Cauchy data, that is, the assignment of conductivity at a point $\mathbf{x}^0 = (x_0, y_0)$ of the domain. The Cauchy problem to solve is the following:

$$\begin{aligned} u_1 &= \frac{\partial K}{\partial x} = -Ka_1 + b_1, \\ u_2 &= \frac{\partial K}{\partial y} = -Ka_2 + b_2, \\ K(x_0, y_0) &= K_0. \end{aligned} \tag{10}$$

The solution of system (10) under the appropriate regularity assumptions is unique, provided it exists. See the lemma in section 4 of [6].

The solution at a point $\mathbf{x} = (x, y)$ is found by choosing an appropriate path joining $\mathbf{x}$ with the initial point, and integrating (10) along it.

Indeed, let $\gamma(s)$, be a path joining $\mathbf{x}^0$ with $\mathbf{x}$

$$\gamma : [0, 1] \to \mathbb{R}^2, \qquad \gamma(0) = \mathbf{x}^0, \qquad \gamma(1) = \mathbf{x}.$$

Let $k(s) = K(\gamma(s))$, then

$$\frac{\mathrm{d}k}{\mathrm{d}s} = \nabla K\big(\gamma(s)\big)\frac{\mathrm{d}\gamma}{\mathrm{d}s} = \big(-K\big(\gamma(s)\big)a+b\big)\frac{\mathrm{d}\gamma}{\mathrm{d}s} = -a\frac{\mathrm{d}\gamma}{\mathrm{d}s}K\big(\gamma(s)\big) + b\frac{\mathrm{d}\gamma}{\mathrm{d}s}.$$

Here, $a \equiv \mathbf{a}(\gamma(s))$, and $b \equiv \mathbf{b}(\gamma(s))$. We are led to the initial value problem

$$\frac{\mathrm{d}k}{\mathrm{d}s} = -\left(a\frac{\mathrm{d}\gamma}{\mathrm{d}s}\right)k(s) + b\frac{\mathrm{d}\gamma}{\mathrm{d}s}, \qquad k(0) = K_0 \tag{11}$$

which is easily solved.

When conductivity has been evaluated, then equation (9) is used to obtain the effective porosity at every point of the domain.

Remark. Let us discuss the full rank condition of matrix A in (5). For confined aquifers in the stationary case, if two sets of data are given, say h^1 and h^2, the full rank condition means that the gradients ∇h^1, ∇h^2 of the potentials do not vanish and their equipotential lines do not overlap anywhere. This is fully discuss in [6]. Since linear independence of ∇h^1, ∇h^2 at a point (x, y) is equivalent to linear independence of $h^1\nabla h^1$, $h^2\nabla h^2$, the same physical condition implies the full rank condition for unconfined aquifers in the stationary case.

For aquifers in the transient case we need at least a transient flow condition. In this case a physical interpretation of the vectors

$$\left(\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}, -\frac{\partial h}{\partial t}\right)$$

for confined aquifers, or

$$\left(h\frac{\partial h}{\partial x}, h\frac{\partial h}{\partial y}, -\frac{\partial h}{\partial t}\right)$$

for unconfined aquifers, and its relation to the full rank condition is desirable.

In our case, we are content with the technical condition that the span of the row vectors

$$\left(h^i\frac{\partial h^i}{\partial x}, h^i\frac{\partial h^i}{\partial y}, -\frac{\partial h^i}{\partial t}\right), \quad i = 1, 2, \ldots, p,$$

is of dimension three.

3. A synthetic phreatic aquifer

The DS method, as described in the previous section, is applied to a synthetic but realistic example.

3.1. The numerical evaluation of the model parameters

Consider a regularly spaced lattice of nodes, each located at the center of a square cell, with sides parallel to the orthogonal Cartesian coordinate axes, and with spacing Δx along the x and y directions.

Nodes are labelled with the ordered pair of integer numbers (m, n), $m = 1, 2, \ldots, M$, $n = 1, 2, \ldots, N$, so that the pair (m, n) represents the node $x(m, n) = m\Delta x\mathbf{i} + n\Delta x\mathbf{j}$, where the vectors $\mathbf{i}$ and $\mathbf{j}$ are the unit vectors.

Recalling the discrete conservative scheme with finite differences for the unconfined aquifer [1] then the model parameters that need to be identified are easily pointed out.

Consider an interior cell $B(m, n)$ of the discrete domain of the aquifer. The integral balance equation for $B(m, n)$ is the following:

$$\begin{aligned} &n_e(m,n)\big(h^i(m,n) - h^{i-1}(m,n)\big)\frac{(\Delta x)^2}{\Delta t_i} \\ &\quad = -F^i(m,n) + (KD^*)\big((m,n),(m+1,n)\big)\big(h^i(m+1,n) - h^i(m,n)\big) \\ &\qquad + (KD^*)\big((m,n),(m-1,n)\big)\big(h^i(m-1,n) - h^i(m,n)\big) \\ &\qquad + (KD^*)\big((m,n),(m,n+1)\big)\big(h^i(m,n+1) - h^i(m,n)\big) \\ &\qquad + (KD^*)\big((m,n),(m,n-1)\big)\big(h^i(m,n) - h^i(m,n-1)\big), \end{aligned} \tag{12}$$

where $F^i(m, n)$ is the integrated source term over $B(m, n)$, and

$$(KD^*)\big((m,n),(m+1,n)\big) = \frac{2K(m,n)K(m+1,n)}{K(m,n)+K(m+1,n)}\frac{(h^{i-1}(m+1,n)+h^{i-1}(m,n))}{2},$$

$$(KD^*)\big((m,n),(m-1,n)\big) = \frac{2K(m,n)K(m-1,n)}{K(m,n)+K(m-1,n)}\frac{(h^{i-1}(m-1,n)+h^{i-1}(m,n))}{2},$$

$$(KD^*)\big((m,n),(m,n+1)\big) = \frac{2K(m,n)K(m,n+1)}{K(m,n)+K(m,n+1)}\frac{(h^{i-1}(m,n+1)+h^{i-1}(m,n))}{2},$$

$$(KD^*)\big((m,n),(m,n-1)\big) = \frac{2K(m,n)K(m,n-1)}{K(m,n)+K(m,n-1)}\frac{(h^{i-1}(m,n-1)+h^{i-1}(m,n))}{2}$$

which is a formulation of the multiple cells models [1].

The choice of space and time intervals Δx and Δt_i is based on geometrical factors and frequency of measurements, which depend upon the goals of the forecasting model.

The discrete parameters that appear in equation (12) are the internode conductivity $K((m, n), (m', n'))$ and the cell effective porosity $n_e(m, n)$. These are the discrete model

parameters relevant for the description of groundwater flow at the given, fixed, space and time scales.

Therefore, the goal of the discrete inverse problem for the case of unconfined aquifers is the determination of the internode conductivity and the effective porosity of the cell.

3.2. Generation of synthetic data

The synthetic phreatic aquifer that we consider is divided into a square regular lattice of cells, with $M = N = 9$, $\Delta x = 25$ m. Conductivity is constant on each cell and is given by

$$K(m,n) = \big((18 - 3n) + 10m\big) \cdot 0.000005 \text{ m}^2/\text{s}.$$

Since the domain is divided into zones of constant conductivity and the regular spacing of the cells, the internode conductivities, denoted with $K((m,n),(m\prime,n\prime))$, are the harmonic mean of the cell values.

Effective porosity is constant on each cell as well and is given by

$$\eta_e(m,n) = \frac{2(10-m)n/((10-m)+n)}{30.0}.$$

Dirichlet boundary conditions for the piezometric head have been assigned at the border of the domain. They do no vary with time. The values, in meters, are shown in table 1.

The initial conditions for the piezometric head are given by the solution of a steady-state forward problem corresponding to the source term given by

$$F(m,n) = -\big((4.5-n)^2 + 2\big((10-m) - 5.5\big)^2\big) \cdot 0.0000001 \text{ (m}^3/\text{s)}$$

which represents leakage in the aquifer and is present in all the situations devised. For the synthetic aquifer the contour flows of the initial conditions for the piezometric head are shown in figure 1.

Table 1
Dirichlet boundary conditions for the piezometric heads (in meters).

m \ n	1	2	3	4	5	6	7	8	9
1	40.00	40.05	40.10	40.15	40.20	40.25	40.30	40.35	40.40
2	39.80	x	x	x	x	x	x	x	40.20
3	39.60	x	x	x	x	x	x	x	40.00
4	39.40	x	x	x	x	x	x	x	39.85
5	39.20	x	x	x	x	x	x	x	39.70
6	39.00	x	x	x	x	x	x	x	39.55
7	39.80	x	x	x	x	x	x	x	39.40
8	38.60	x	x	x	x	x	x	x	39.30
9	38.40	38.50	38.60	38.70	38.80	38.90	39.00	39.10	39.20

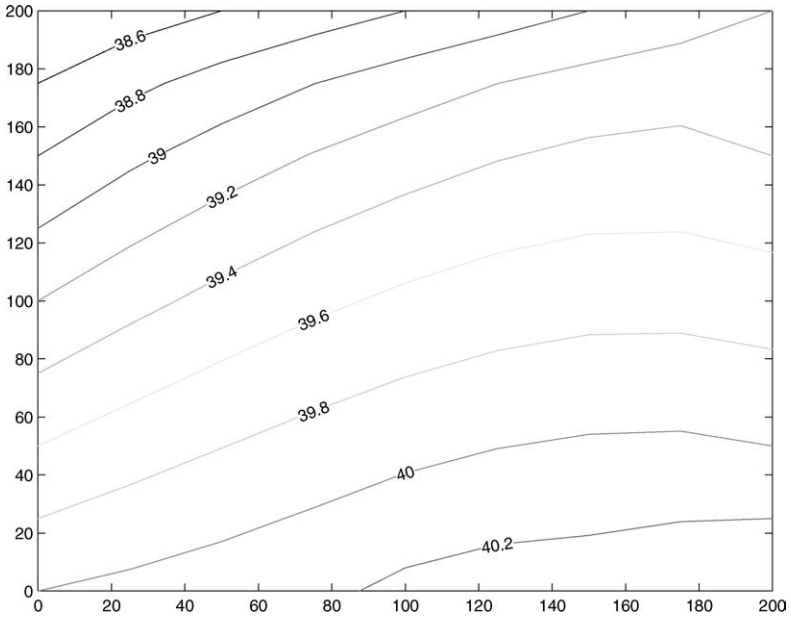

Figure 1. Contour maps of piezometric head, initial steady state ($t = 0$).

The transient regime is set up by a sudden start of some array of wells at $t = 0$. The array of wells are placed in the cells corresponding to the nodes: $(2, 2)$, $(3, 8)$, $(4, 8)$, $(6, 8)$, $(7, 8)$. At these nodes the source term during the transient regime is equal to $0.01\ \mathrm{m}^3/\mathrm{s}$.

Piezometric heads at different times are obtained by solving the forward problem with the reference parameters, the boundary and initial conditions, and the source term described above. The piezometric head is computed at the times in years

$$t_1 = 0.001, \quad t_2 = 0.0022, \quad t_3 = 0.0046, \quad t_4 = 0.0100.$$

The contour maps of the four transient flow situations are represented in figure 2.

4. Numerical implementation of the DS method

The sets of data used in the identification are given by $h(m, n, i)$, $(\partial h/\partial t)(m, n, i)$, $F(m, n, i)$, with $i = 0, 1, 2, 3, 4$. The time derivatives of the piezometric heads for the sets of data from 1 to 4 are evaluated with the backward differences.

There are two numerical problems to consider when implementing the DS method. First, the solution of the linear systems (7), and second, the integration of equation (11).

The systems (7) are overdetermined and ill-conditioned, the preferred algorithm is *QR* decomposition with Householder transformations.

To integrate equation (11) we use polygonal paths through the nodes of the lattice. Moreover, **a**, **b** are approximated by constants along internode segments and denoted

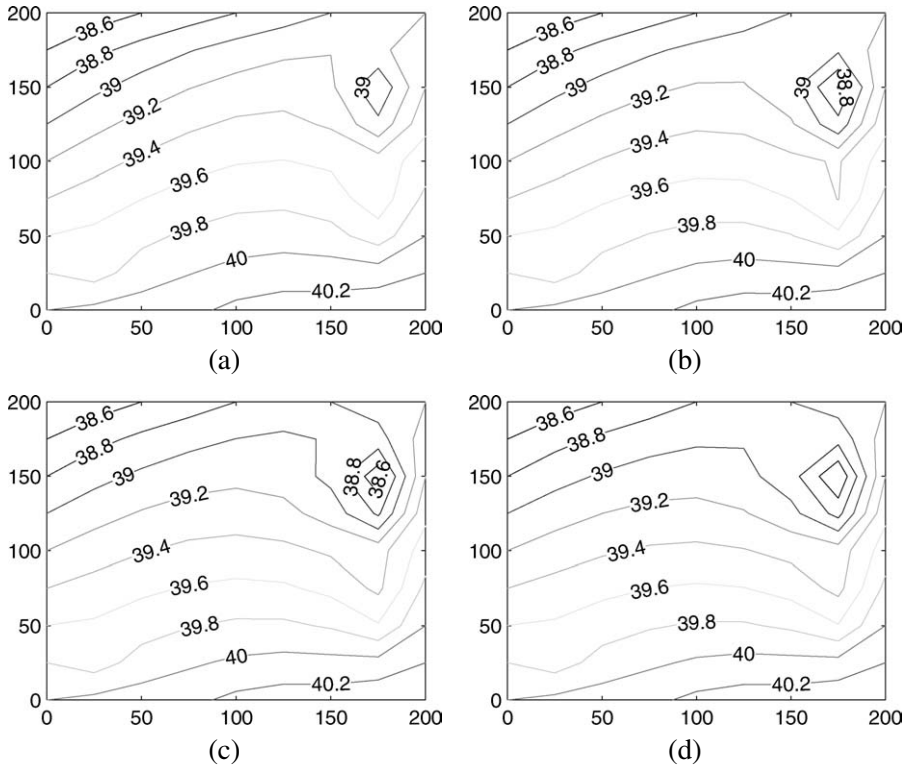

Figure 2. Contour maps of piezometric head at four flow situations: (a) situation 1, $t = 0.001$ year; (b) situation 2, $t = 0.0022$ year; (c) situation 3, $t = 0.0046$ year; (d) situation 4, $t = 0.0100$ year.

by a_A, b_A. In our case these are the averages of the corresponding **a**'s and **b**'s defining the segment. These quantities are scalars since between internode segments the path of integration is parallel to a coordinate axis.

It is possible to establish an a priori estimate for the difference between the true conductivity $k(s)$ and the identified conductivity $k_A(s)$.

In fact, following the proof of Gronwall's lemma we obtain

$$\begin{aligned}\left|k(s) - k_A(s)\right| \leqslant \exp\left(-\int_0^s a_A(r)\,\mathrm{d}r\right) \cdot \Bigg(&\left|k(0) - k_A(0)\right| \\ &+ \int_0^s \exp\left(\int_0^r a_A(p)\,\mathrm{d}p\right)\left|k(r)\right|\left|a(r) - a_A(r)\right| + \left|b(r) - b_A(r)\right|\mathrm{d}r\Bigg).\end{aligned}$$

This suggests that among the possible integration paths that join the node (m, n), where we want to compute conductivity, to the initial node (m_0, n_0) we should choose that one for which the sum $\sum_{(m_0,n_0)}^{(m,n)} |a_A|$, performed over all internode segments connecting the vertices of the path, is the smallest. The estimate above also suggests to select as initial node, the node with minimum norm of the first two components of **a**. In

Table 2
Identified conductivities $\times 10^{-4}$.

m \ n	2	3	4	5	6	7	8
2	4.728	3.964	4.300	3.692	3.552	3.410	3.315
3	3.703	3.503	3.377	3.242	3.103	2.968	2.839
4	3.191	3.041	2.921	2.788	2.653	2.519	2.204
5	2.736	2.584	2.461	2.330	2.198	2.065	1.591
6	2.281	2.126	1.998	1.867	1.739	1.609	1.074
7	1.826	1.663	1.529	1.399	1.276	1.151	0.080
8	1.366	1.194	1.049	0.916	0.788	−0.587	−0.483

Table 3
Relative errors for identified conductivity.

m \ n	2	3	4	5	6	7	8
2	0.0278	0.1091	0	0.1103	0.1120	0.1142	0.1041
3	0.0968	0.1132	0.1114	0.1119	0.1133	0.1142	0.1128
4	0.1136	0.1186	0.1148	0.1150	0.1157	0.1161	0.1839
5	0.1176	0.1239	0.1209	0.1209	0.1210	0.1212	0.2766
6	0.1226	0.1324	0.1315	0.1317	0.1306	0.1301	0.3684
7	0.1307	0.1470	0.1506	0.1520	0.1494	0.1473	0.9333
8	0.1460	0.1768	0.1932	0.2032	0.2118	1.6911	1.6893

practice, if one has K given at more than one point, then among these points one should choose the one with minimal norm of the first two components of **a** as initial point.

We are led in the language of combinatorial optimization to a shortest path problem. The problem is to connect the initial node (m_0, n_0) with all nodes in the lattice at minimum cost. Here the cost between consecutive nodes is the corresponding $|a_A|$. The optimal paths are computed by means of the classical Dijkstra's algorithm.

With the criterion above, we choose $(2, 4)$ as the initial node. In table 2 we show the identified conductivities.

At first sight the prediction is close to the true values except at the nodes $(8, 7)$ and $(8, 8)$ where we have meaningless predictions. Table 3 presents relative errors, which shows that the errors away from these nodes are acceptable.

We now present the corresponding tables for the effective porosity. The predictions are given in tables 4 and 5.

As expected there are meaningless predictions at the nodes $(8, 7)$ and $(8, 8)$. The relative errors are in table 5.

We have presented a numerical comparison of the predicted parameters, conductivity and porosity. More important for the management of the aquifer, is to verify that with the predicted parameters it is possible to recover the evolution of the aquifer. This evolution is better understood graphically, we plot the contour lines of the different flow situations (solid line) for the piezometric head, and the contour lines using the identified parameters of the corresponding piezometric head (dashed line). See the initial condition in figure 3.

Table 4
Identified porosity in inner nodes.

m \ n	2	3	4	5	6	7	8
2	0.0494	0.0716	0.0867	0.0830	0.0873	0.0910	0.0978
3	0.0793	0.0918	0.0999	0.1082	0.1160	0.1231	0.1909
4	0.0805	0.1001	0.1145	0.1266	0.1379	0.1483	0.2580
5	0.0829	0.1057	0.1238	0.1395	0.1542	0.1667	0.1520
6	0.0831	0.1083	0.1290	0.1474	0.1656	0.1833	0.3278
7	0.0829	0.1090	0.1308	0.1508	0.1722	0.1949	0.5521
8	0.0827	0.1083	0.1288	0.1479	0.1684	−0.1641	−0.2139

Table 5
Relative errors for identified porosity.

m \ n	2	3	4	5	6	7	8
2	0.2590	0.1052	0.0250	0.1282	0.1268	0.1224	0.0831
3	0.0082	0.0819	0.1261	0.1344	0.1300	0.1206	0.3122
4	0.0939	0.1239	0.1415	0.1457	0.1383	0.1261	0.4510
5	0.1291	0.1545	0.1641	0.1630	0.1519	0.1425	0.2592
6	0.1685	0.1881	0.1935	0.1891	0.1718	0.1488	0.4341
7	0.2011	0.2217	0.2293	0.2246	0.2007	0.1649	1.2183
8	0.2244	0.2556	0.2754	0.2791	0.2633	1.6595	1.8021

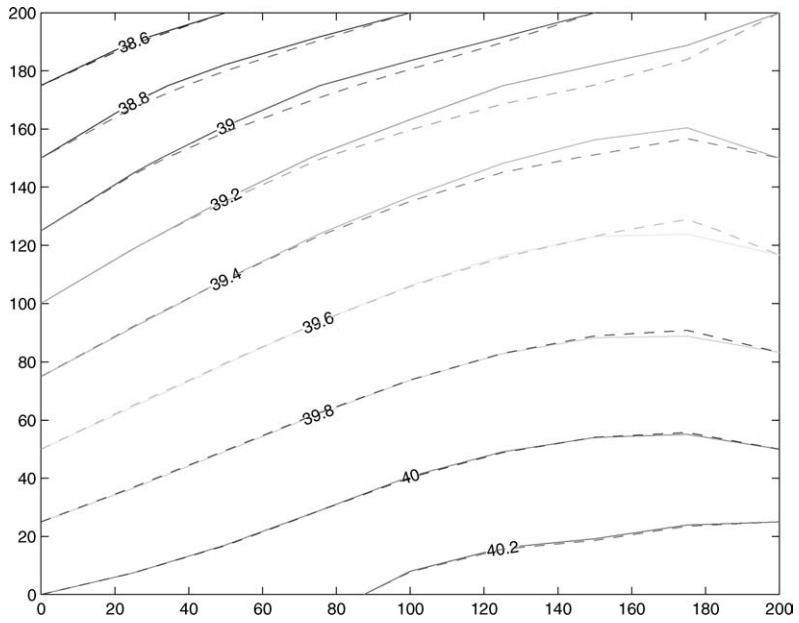

Figure 3. Contour maps of piezometric head initial steady state. Solid lines – synthetic, dashed lines – predicted.

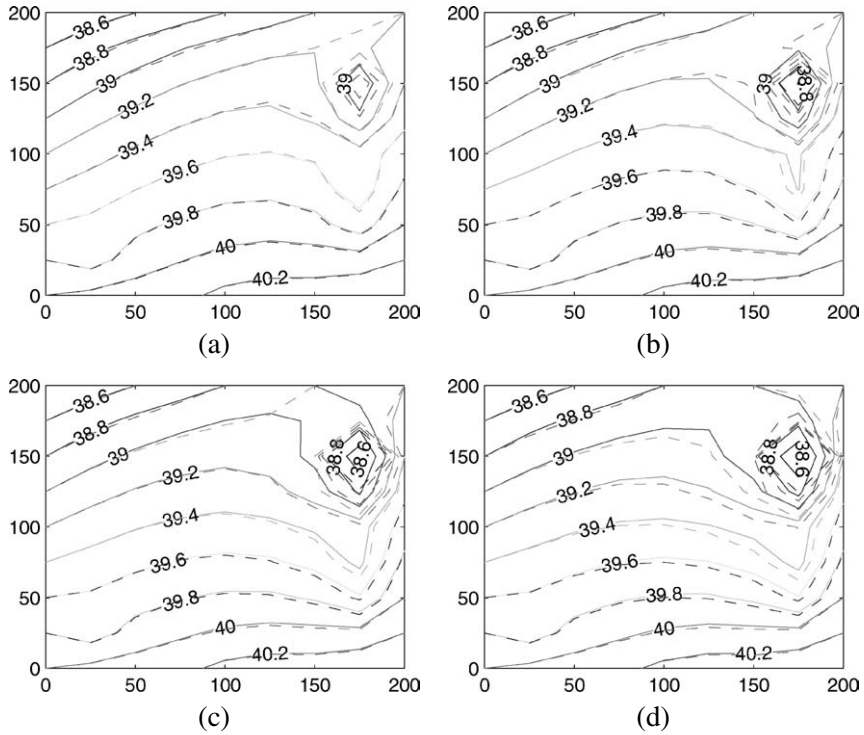

Figure 4. Contour maps of piezometric head at four flow situations: (a) situation 1, $t = 0.001$ year; (b) situation 2, $t = 0.0022$ year; (c) situation 3, $t = 0.0046$ year; (d) situation 4, $t = 0.0100$ year. Solid lines – synthetic, dashed lines – predicted.

The predictions for the transient flow situations are in figure 4. We observe that the prediction of aquifer evolution is satisfactory. This in spite of the poor identification of parameters near the nodes (8, 7) and (8, 8). We remark that in the nodes (8, 7) and (8, 8) where we have meaningless predictions we have interpolated by the values of the parameters in the nodes (8, 6) and (7, 8), respectively.

4.1. Some numerical aspects of the DS method

The reader may agree that the ideas that support the DS method are simple. However, its numerical implementation is a delicate matter.

In forming the linear systems (7) it is necessary to approximate the gradients and laplacian of the piezometric head, as well as time derivatives. The choice of space and time intervals, Δx and Δt_i, is based on the geometry and dimension of the aquifer, on the location and areal density of the piezometers, and on the frequency of measurements. Hence, the principles of numerical differentiation by finite differences may not be valid. This, together with the small variations of the potential in aquifer flow, make the numerical approximation of derivatives highly sensitive.

The other numerical problem of interest is the integration of the Cauchy problem (10). A naive, yet natural approach, is to start with an arbitrary initial node, and

to compute conductivity in a given node, integrate along the shortest polygonal path. It can be verified that the conductivity values are far from correct. We have carried out the same experiment for confined aquifers with similar results. We conclude that the choice of the path of integration by the optimal criterion stated above is a must. The error propagation is significant.

In our particular example, the integration paths to compute conductivity at the nodes (8, 7) and (8, 8), are the longest. This explains in part, the meaningless predictions at these nodes, and the poor predictions in some of their neighbors.

4.2. On inverse crimes

Let us quote Colton and Kress [4] on *inverse crimes*. In order to avoid trivial inversion of finite-dimensional problems, for reliably testing the performance of an approximation method for the inverse problem it is crucial that the synthetic data be obtained by a forward solver which has no connection to the inverse solver under consideration. It is apparent that with our direct solver and the DS method, this criterion is satisfactorily met. We have borrowed this methodology from previous works on confined aquifers, e.g., [8].

5. An alternative approach to the DS method

5.1. The continuous problem

Let us proceed as in section 2 and consider equation (3) in the form

$$h\frac{\partial h}{\partial x}\frac{\partial K}{\partial x} + h\frac{\partial h}{\partial y}\frac{\partial K}{\partial y} - \frac{\partial h}{\partial t}n_{\mathrm{e}} = -\overline{\Delta}hK - f,$$

where

$$\overline{\Delta}h = h\Delta h + \left(\frac{\partial h}{\partial x}\right)^2 + \left(\frac{\partial h}{\partial y}\right)^2.$$

As before define

$$\mathbf{u} = (u_1, u_2, u_3) = \left(\frac{\partial K}{\partial x}, \frac{\partial K}{\partial y}, n_{\mathrm{e}}\right).$$

Let us fix (x, y) again. In this case we assume that h, ∇h, $\overline{\Delta}h$ and f are known in (x, y, t) for $t \in I = [0, T]$, and belong to $L^2(0, T)$.

Recall that

$$L^2(0, T) = \left\{\varphi\colon \int_0^T \left|\varphi(t)\right|^2 \mathrm{d}t < +\infty\right\}$$

with inner product

$$\langle \varphi, \psi \rangle = \int_0^T \varphi(t)\psi(t)\,\mathrm{d}t$$

and induced norm

$$\|\varphi\|^2 = \langle \varphi, \varphi \rangle = \int_0^T \left|\varphi(t)\right|^2 \mathrm{d}t.$$

Consider the map

$$\mathcal{L} : \mathbb{R}^3 \to L^2(0, T)$$

given by

$$\mathcal{L}(u_1, u_2, u_3) = h\frac{\partial h}{\partial x}u_1 + h\frac{\partial h}{\partial y}u_2 - \frac{\partial h}{\partial t}u_3 + \overline{\Delta}hK + f.$$

We seek to minimize

$$\mathcal{R}(u_1, u_2, u_3) = \frac{1}{2}\left\|\mathcal{L}(u_1, u_2, u_3)\right\|^2.$$

Assuming that K is known, the minimum satisfies $\nabla\mathcal{R}(u_1, u_2, u_3) = 0$, which leads us to a system

$$\mathbf{Au} = -K\mathbf{z} + \mathbf{f}. \tag{13}$$

If $\mathrm{Rank}(\mathbf{A}) = 3$ this system has a unique solution given by

$$\mathbf{u} = -K\mathbf{a} + \mathbf{b},$$

where the three component vector function $\mathbf{a}$ and $\mathbf{b}$ are the solutions of the systems

$$\mathbf{Aa} = \mathbf{z}, \qquad \mathbf{Ab} = \mathbf{f}. \tag{14}$$

Once we solve these algebraic systems, we mimic the second step in the DS method as in section 2.

5.2. *Numerical implementation*

Throughout the development of the DS method with L^2-norm, we assumed that the functions involved were known for all times. In practice this is not the case, instead we have observations for a finite number of time situations, that is, we know, $h(m, n, i)$, $(\partial h/\partial t)(m, n, i)$, $F(m, n, i)$, with $i = 0, 1, \ldots, p$. The time derivatives of the piezometric heads for the sets of data from 1 to p are evaluated with the backward differences.

First, we have to solve the linear system (13). When using the L^2-norm, the system reads

$$\begin{bmatrix} \langle hh_x, hh_x\rangle & \langle hh_x, hh_y\rangle & \langle hh_x, -h_t\rangle \\ \langle hh_x, hh_y\rangle & \langle hh_y, hh_y\rangle & \langle hh_y, -h_t\rangle \\ \langle hh_x, -h_t\rangle & \langle hh_y, -h_t\rangle & \langle h_t, h_t\rangle \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = -K \begin{bmatrix} \langle hh_x, \overline{\Delta}h\rangle \\ \langle hh_y, \overline{\Delta}h\rangle \\ \langle -h_t, \overline{\Delta}h\rangle \end{bmatrix} + \begin{bmatrix} \langle hh_x, f\rangle \\ \langle hh_y, f\rangle \\ \langle -h_t, f\rangle \end{bmatrix}. \tag{15}$$

The components of the system (15) are integrals in t, these are approximated numerically by interpolating with linear functions at time t_1, t_2, t_3 and t_4. The system is again ill-conditioned and solved with the QR decomposition as before.

There is no change when integrating the corresponding Cauchy problem.

5.3. Parameter identification

Next we present the tables of the identified parameters, as well as the tables of errors. First, in table 6 we show conductivity.

Observe that in contrast with the previous identification, we have at the nodes (8, 7) and (8, 8) realistic predictions.

Let us look at table 7 for the corresponding porosity values.

Observe that in the location of a well, node (4, 8), we have an unrealistic prediction. Better conclusions can be drawn by looking at the tables of relative errors (tables 8 and 9).

By inspection, we conclude that identification of conductivity with the L^2-norm is better than before. Observe that we have a different initial node.

Predictions for porosity are not as satisfactory, see table 9.

Finally, figures 5 and 6 show that the aquifer evolution is predicted correctly in spite of the poor prediction of porosity in some nodes. Here is only necessary to replace the value of the parameters in the node (4, 8). We selected the node (4, 7).

Table 6
Identified conductivities with L^2-norm ($\times 10^{-4}$).

m n	2	3	4	5	6	7	8
2	4.4862	3.9205	3.7462	4.1500	3.8883	3.9260	3.8837
3	3.3731	3.2169	3.3963	3.3391	3.4282	3.4562	3.9994
4	2.9931	2.9692	3.0534	3.1052	3.1719	3.2235	1.8989
5	2.6070	2.5867	2.6039	2.5786	2.6065	2.7521	2.9904
6	2.2083	2.1595	2.1299	2.0631	2.0395	2.0921	2.8693
7	1.7829	1.7124	1.6448	1.5453	1.4644	1.3907	1.1815
8	1.3479	1.2543	1.1516	1.0156	0.86843	0.56974	0.51823

Table 7
Identified porosities with L^2-norm.

m n	2	3	4	5	6	7	8
2	0.0650	0.0716	0.0841	0.0492	0.0875	0.1066	0.1137
3	0.0668	0.0858	0.0022	0.0892	0.1239	0.1479	0.1679
4	0.0786	0.0437	0.0815	0.1193	0.1586	0.1980	3463.0
5	0.0229	0.0677	0.1028	0.1320	0.1705	0.2335	0.3026
6	0.0557	0.0838	0.1120	0.1394	0.1784	0.2470	0.3109
7	0.0626	0.0896	0.1161	0.1411	0.1738	0.2235	0.2510
8	0.0655	0.0927	0.1178	0.1383	0.1562	0.1214	0.2378

Table 8
Relative errors for conductivities with L^2-norm.

m n	2	3	4	5	6	7	8
2	0.0247	0.1190	0.1288	0	0.0279	0.0197	0.0497
3	0.1773	0.1856	0.1062	0.0852	0.0205	0.0317	0.2498
4	0.1686	0.1394	0.0747	0.0142	0.0573	0.1310	0.70321
5	0.1590	0.1231	0.0700	0.0269	0.0426	0.1711	0.3593
6	0.1506	0.1186	0.0740	0.0404	0.0198	0.1309	0.6879
7	0.1510	0.1218	0.0862	0.0635	0.0238	0.0302	0.0155
8	0.1575	0.1350	0.1141	0.1169	0.1316	0.3297	0.2597

Table 9
Relative errors for porosities with L^2-norm.

m n	2	3	4	5	6	7	8
2	0.0253	0.1051	0.0534	0.4831	0.1253	0.0283	0.0661
3	0.1651	0.1425	0.9807	0.2862	0.0709	0.0568	0.1541
4	0.1160	0.6177	0.3886	0.1947	0.0089	0.1667	0.19478
5	0.7600	0.4580	0.3060	0.2078	0.0622	0.2009	0.4750
6	0.4432	0.3718	0.3003	0.2334	0.1082	0.1467	0.3602
7	0.3963	0.3599	0.3160	0.2743	0.1930	0.0422	0.0084
8	0.3857	0.3628	0.3374	0.3259	0.3167	0.5122	0.1081

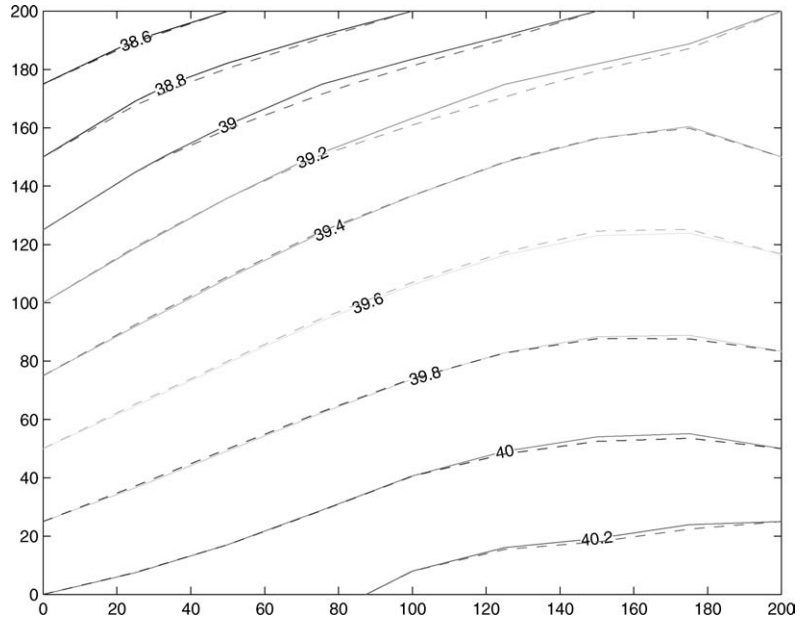

Figure 5. Contour maps of piezometric head initial steady state. Solid lines – synthetic, dashed lines – predicted.

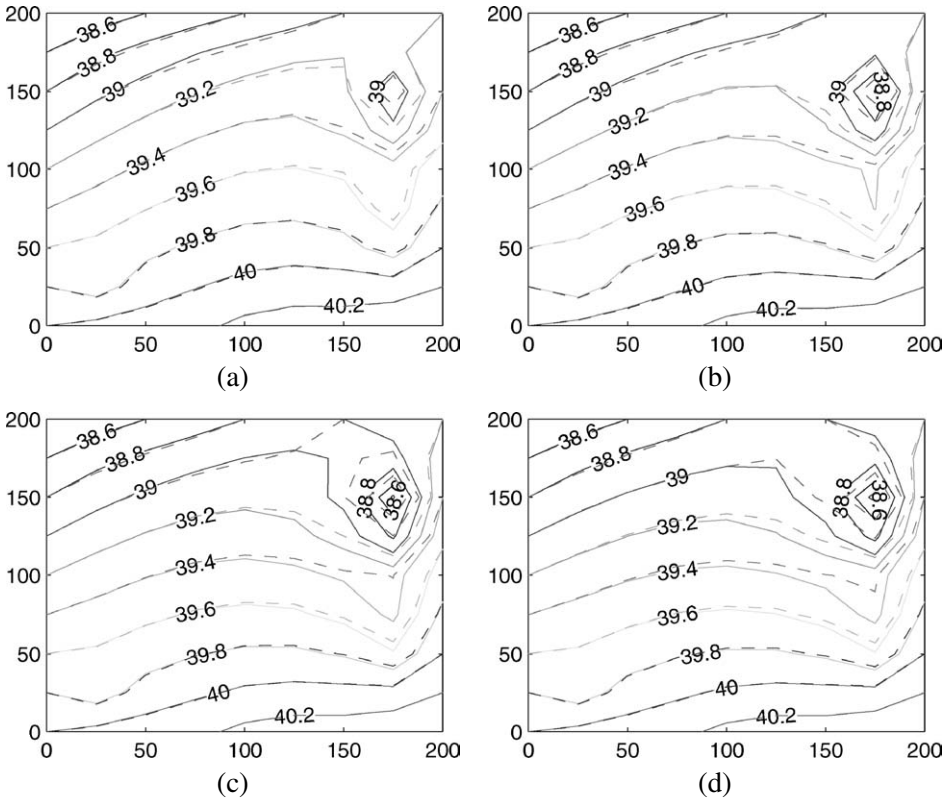

Figure 6. Contour maps of piezometric head at four flow situations: (a) situation 1, $t = 0.001$ year; (b) situation 2, $t = 0.0022$ year; (c) situation 3, $t = 0.0046$ year; (d) situation 4, $t = 0.0100$ year. Solid lines – synthetic, dashed lines – predicted.

We remark that the solution of the direct problem was also carried out without modifying the identified parameters, that is, without disregarding the meaningless predictions. The results are similar. To simulate a physically correct model, it is necessary to replace those incorrect values using some technique of interpolation. We have chosen the simplest one.

6. Comments and conclusions

The DS method, like any other inverse method in geophysics, needs high quality data. Thanks to recent improvements in instrumentation, it is nowadays possible. However, data have to be carefully analyzed before its use for inverse methods. Also, it is fundamental to collect independent sets of data.

The DS method can be applied to small subregions of an aquifer and identifies the parameters directly at the scale determined by the spacing of the observation points where data are collected.

Some other features of the method are:

(i) it uses those measurable quantities that are usually collected in aquifers under control or that can be interpolated from these,

(ii) no prior information on effective porosity is required,

(iii) no initial guess of the unknown parameters is required,

(iv) no forward problem solutions are needed,

(v) the identification of hydraulic conductivity does not depend upon effective porosity, even when only transient data are used,

(vi) the internode hydraulic conductivity and cell effective porosity are ready-to-use parameters for the numerical implementation of the forward problem with conservative schemes,

(vii) takes into account several flows with different directions, all over the aquifer, using data on the whole flow field.

It can be seen that the solutions of the systems (7) and (14) are almost identical in a significant number of nodes. This suggests that there is a unique Cauchy problem associated with the DS method. Consequently, it appears that the main problem in the method, is the approximation of the functions **a** and **b** in the systems (7) and (14). It is our intention to supply the theory supporting this approximation as well as an error analysis of the method. Also of interest is to correct the solution of both, inverse and forward problems, in the neighborhood of wells.

In real problems there is some noise added to the data. In [8] it is shown that the DS method provides good answers, even when noise is involved, in the case of confined aquifers. An extension to unconfined aquifers is required. Our preliminary results are promising.

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