Joint inversion of steady-state hydrologic and self-potential data for 3D hydraulic conductivity distribution at the Boise Hydrogeophysical Research Site

Salvatore Straface a,b,⇑, Francesco Chidichimo a, Enzo Rizzo b, Monica Riva c, Warren Barrash d, André Revil e,f, Michael Cardiff g,1, Alberto Guadagnini c

a Dipartimento Difesa del Suolo, Università della Calabria, Rende (CS), Italy
b Hydrogeosite Laboratory, CNR-IMAA, Tito - Marsico Nuovo (PZ), Italy
c Dipartimento di Ingegneria Idraulica, Ambientale, Infrastrutture Viarie, Rilevamento, Politecnico di Milano, Milano, Italy
d Center for Geophysical Investigation of the Shallow Subsurface, Boise State University, Boise, ID, USA
e Department of Geophysics, Colorado School of Mines, Golden, CO, USA
f ISTerre, CNRS, UMR 5559, Université de Savoie, Equipe Volcan, Le Bourget du Lac, France
g Department of Civil and Environmental Engineering, Stanford University, Stanford, CA, USA

ARTICLE INFO

Article history:
Received 7 June 2010
Received in revised form 3 June 2011
Accepted 13 July 2011
Available online 23 July 2011
This manuscript was handled by P. Baveye, Editor-in-Chief

Keywords:
Inverse problem
Multiple Indicator Kriging
Self potential

SUMMARY

We combine sedimentological, hydraulic and geophysical information to characterize the 3D distribution of transport properties of an heterogeneous aquifer. We focus on the joint inversion of hydraulic head and self-potential measurements collected during an extensive experimental campaign performed at the Boise Hydrogeophysical Research Site (BHRS), Boise, Idaho, and involving a series of dipole tests. While hydraulic head data obtained from piezometric readings in open wells represent a depth-averaged value, self-potential signals provide an estimate of the water table location. The aquifer is conceptualized as a multiple-continuum, where the volumetric fraction of a geo-material within a cell of the numerical flow model is calculated by Multiple Indicator Kriging. The latter is implemented on the basis of available sedimentological information. The functional format of the indicator variograms and associated parameters are estimated on the basis of formal model identification criteria. Self-potential and hydraulic head data have been embedded jointly within a three-dimensional inverse model of groundwater flow at the site. Each identified geo-material (category) is assumed to be characterized by a constant hydraulic conductivity. The latter constitute the set of model parameters. The hydraulic conductivity associated with a numerical block is then calculated as a weighted average of the conductivities of the geo-materials which are collocated in the block by means of Multiple Indicator Kriging. Model parameters are estimated by a Maximum Likelihood fit between measured and modeled state variables, resulting in a spatially heterogeneous distribution of hydraulic conductivity. The latter is effectively constrained on the sedimentological data and conditioned on both self-potential and borehole hydraulic head readings. Minimization of the Maximum Likelihood objective function allows estimating the relative weight of measurement errors associated with self-potential and borehole-based head data. The procedure adopted allowed a reconstruction of the heterogeneity of the site with a level of details, which was not obtained in previous studies and with relatively modest computational efforts. Further validation against dipole tests which were not used in the inversion procedure supports the robustness of the results.

1. Introduction

A key-problem in aquifers characterization is the requirement of a large number of direct and high resolution measurements of system parameters and state variables. Measurements of state variables typically include the drawdown induced in observation boreholes by pumping tests. This method is intrusive and consequently the hydrological system is perturbed by drillings. Geophysical approaches instead aim at using non-intrusive techniques to obtain a large amount of information on subsurface and with moderate costs. In the last few decades hydrologists have increasingly resorted to hydrogeophysical information to estimate groundwater flow parameters (Purvance and Andricevic, 2000; Slater and Lesmes, 2002; Binley et al., 2005; Yeh et al., 2008; Hördt et al., 2009; Koestel et al., 2009).
A key innovation in this field is based on the passive measurements of the self-potential generated by (1) ground water flow through a so-called electrokinetic coupling (Fournier, 1989; Birch, 1993; Birch, 1998; Aubert and Atangana, 1996; Jardani and Revil, 2009) and (2) electro-chemical processes associated with gradients of the chemical potentials of charge carriers (ionic species and electrons) in the pore water (e.g., Naudet et al., 2004; Revil et al., 2005). A general theory of all these effects has been developed by Revil and Linde (2006), and Revil et al. (2009, 2010). In the self-potential approach, the measured response is a function of unknown source of electrical currents and resistivity structure. Therefore, there is an inherent ambiguity when interpreting the self-potential data when the earth resistivity is unknown. This difficulty can be solved upon merging different kinds of measurements obtained from other non-intrusive techniques, Direct Current (DC) and Electromagnetic (EM)-based electrical resistivity tomography, seismic method and geothermal measurements (Jardani and Revil, 2009) or borehole data (Straface et al., 2010).

Interpretation schemes that could model the self-potential field recorded during pumping tests have been developed (Revil et al., 2003; Rizzo et al., 2004; Titov et al., 2002; Titov et al., 2005; Jardani et al., 2009; Malama et al., 2009a,b). Data from several pumping tests can be combined and used in a tomographic fashion to characterize heterogeneity in the aquifer (for recent field examples see, Bohling et al., 2007; Li et al., 2007; Straface et al., 2007b; Cardiff et al., 2009). Recently, Straface et al. (2007a) used experimental hydraulic heads and self potential signals associated with a pumping test in an inverse model based on the Successive Linear Estimation (SLE) (Yeh et al., 1996), to estimate the transmissivity distribution of a small-scale aquifer. Bianchi Jannetti et al. (2010) extended the moment equations-based inverse method of Hernandez et al. (2003, 2006) to quasi-steady state flow conditions and presented its first application by using hydraulic heads and self potential signals collected during a pumping test at the Montalto Uffugo research site. In these cited works the authors used self-potential signals in a two-dimensional inverse modeling. Nevertheless, the self-potential method is able to locate the spatial distribution of electrical sources in the earth generated by the coupling electrokinetic mechanism. In other words, it provides a 3D estimate of the free surface location unlike borehole readings which provide a depth-averaged hydraulic head. In fact, even though a pumping test generates a velocity field in the aquifer, the pressure distribution within an observation well, located at some distance from a pumping well, is basically hydrostatic after pseudo-steady state conditions has been attained. Therefore, hydraulic head does not depend on the transducer vertical position, but attains a constant value representing, in that location, a depth-averaged quantity. On the other hand, the self-potential source inversion problem is highly non-unique. There are several possible distributions of sources that can fit the data equally. This dilemma is common to nearly all potential field inverse problems, and is exacerbated by the fact that measurement locations are often restricted to relatively few locations on the ground surface. Moreover, as with all geophysical techniques, data errors degrade our ability to interpret the measured signal. Common sources of self-potential measurement error can be associated with the degradation or drift of the measuring electrodes, poor contact between the electrode and soil, and cultural noise (Corwin, 1973; Perrier et al., 1997; Clerc et al., 1998; Petiau, 2000). As a consequence, joint inversion of self-potential and borehole based head data requires estimating the relative weight of the different data types adopted (Bianchi Jannetti et al., 2010).

In this context, a relevant question is how these two types of measurements can be combined within a three-dimensional inverse modeling approach. It is important to underline that many researchers are making a great effort to overcome the technological and interpretative limits to locate groundwater free surface via the self-potential method (Minsley et al., 2007). An alternative is represented by the approach proposed by Jardani and Revil (2009). In this work, the authors develop a joint inversion algorithm for Self Potential (SP) and temperature data in order to estimate hydraulic conductivity. They apply their methodology on a two-dimensional large scale real case, with 10 different zones (i.e., homogenous and anisotropic), conditioning the hydraulic conductivity on SP and Temperature. The application of their methodology to the Boise experiments should be possible but not straightforward. In fact, the difficulty is to apply this inversion algorithm to a 3D model, with the porous medium modeled as multiple continua (fully heterogeneous) and conditioning hydraulic conductivity only on SP (without any hydraulic head measurements) that is more highly unstable on this small scale. In this paper we adopt a joint inversion of hydraulic head and self potential measurements collected during an extensive experimental campaign performed at the Boise Hydrogeophysical Research Site (BHRS), Boise, Idaho, in June 2007. A previous study (Cardiff et al., 2009) estimated two-dimensional depth-averaged hydraulic conductivity variations at the BHRS using only the hydrologic data from the above-mentioned experimental field campaign. In this study, we estimate the three-dimensional distribution of the hydraulic conductivity \( k \) throughout the site by jointly inverting hydrologic and self-potential data while incorporating prior information from porosity and grain-size logs. We conceptualize the aquifer as a multiple-continuum, where the volumetric fraction of a geo-material within a cell of the numerical flow model is calculated by an application of Multiple Indicator Kriging (MIK). The latter is implemented on the basis of available stratigraphic information obtained from 18 wells and GPR reflection surveys at the site (Barrash and Reboulet, 2004). The functional form of the indicator variograms and associated parameters are estimated on the basis of formal model identification criteria (ICs). Each identified geo-material is assumed to be characterized by a constant hydraulic conductivity. The latter constitute the set of model parameters. The hydraulic conductivity associated with a numerical grid block is then calculated as a weighted average of the conductivities of the geo-materials which are found in the block according to the results of MIK. Model parameters are estimated by a Maximum Likelihood fit between measured and modeled state variables resulting in a spatially heterogeneous distribution of hydraulic conductivity, which is constrained on the sedimentological data and is conditioned on both self-potential and borehole hydraulic head readings.

2. The Boise Hydrogeophysical experiment

In June 2007, during the Summer field school on “Hydrogeophysics: Theory, Methods and Modeling”, a combined hydrogeophysical study including self-potential, electrical resistivity, and hydrologic data collection was performed at the Boise Hydrogeophysical Research Site. The primary aquifer stimulation during this study was a series of dipole pumping tests performed using the site’s fully penetrating wells. Detailed descriptions of the site, testing design, and field techniques can be found in Jardani et al. (2009), and Cardiff et al. (2009). Here, we briefly summarize the key elements which are directly relevant to our work.

The BHRS is located on a gravel bar adjacent to the Boise River, 15 km from downtown Boise, Idaho (Fig. 1). The aquifer at the BHRS consists of unconsolidated and unaltered Pleistocene to Holocene coarse fluvial deposits underlain by a red clay formation (Barrash and Reboulet, 2004). The thickness of the fluvial deposits is in the range of 18–20 m, and saturated thickness of the aquifer is generally about 16–17 m. The well field consists of 13 wells in the
central area (~20 m diameter) and five boundary wells about 10–35 m from the central area. The design and the method of well construction support a wide variety of single-well, cross-hole, and multiple-well hydrologic and geophysical tests for thorough three-dimensional characterization to determine the distributions of hydrodynamic and hydrodispersive properties of naturally heterogeneous aquifers. Further details about the geology of the site and available instrumentation are provided by Barrash and Clemo (2002).

The following paragraphs define some important details about the type of data available for site-characterization.

2.1. Hydraulic measurements

Ten dipole tests, in which water was pumped from one well and injected into another, and one traditional pumping test were performed. A high pumping rate of about 4 L/s was chosen for this highly conductive aquifer (an average hydraulic conductivity, $K_{ave} = 7.5 \times 10^{-4}$ m/s, has been estimated, see Fox, 2006 or Barrash et al., 2006) in order to produce head changes that were well discernible from instrument error. Preliminary modeling efforts suggested that a reasonable approximation to steady state would be reached after about 2–3 h of pumping, allowing a full set of drawdown and recovery data to be collected in a one-day for each test. The number and choice of specific well pairs for the dipole tests were determined using a time constraint of 10–12 days within which completion of the experimental campaign could be achieved and preliminary analytical modeling, on the basis of an homogeneous hydraulic conductivity, $K \approx 5 \times 10^{-4}$ m/s (Cardiff et al., 2009). Hydraulic data were collected throughout pumping and recovery phases using a combination of instruments. Fifteen vented pressure transducers were placed down-well to measure total head change for all wells, with the exception of X1, X3, and X5 (the wells located furthest from the central area (Fig. 1)). The responses of X1 and X5 were expected to be relatively slow to develop and were measured manually using electric tapes. Well X3 was outfitted with an in-well battery-powered logger for the duration of the experiment to allow continuous collection of both test-related water level changes (on weekdays) in addition to daily evapotranspiration (ET) signals (overnight and during the weekends). Additionally, well A1 was set up with a multilevel packer and port setup (absolute pressure sensor spacing 2 m) in order to collect some depth-dependent pressure change information, in pseudo-logarithmically spaced time increments. Boise River stage and river edge positions were measured manually to establish boundary condition control in conjunction with a pressure transducer placed in the river to monitor for possible stage changes during the testing period. The tests chosen included seven cross-site tests (B1–B4, B2–B5, B3–B6, C1–C4, C4–C1, C2–C5, and C3–C6) in addition to four other tests using non-opposite pairs of C wells. The pumping tests performed are summarized in Table 1. Overall, the majority of instruments worked as planned. As an example of the type of data collected, Fig. 2 reports histories of drawdown and raising of the water table during dipole test C5–C1.

2.2. Self-potential measurements

Self-potential signals were measured at the ground surface in the set of 89 electrodes depicted in Fig. 1 and in seven additional electrodes placed in boreholes. A reference electrode was placed 90 m from the region of investigation. Each in-ground nonpolarizing electrode was placed in boreholes. Each in-ground nonpolarizing electrode was placed inside a hole 10 cm deep and filled with a

Table 1

<table>
<thead>
<tr>
<th>Date</th>
<th>Test number</th>
<th>Extraction well</th>
<th>Injection well</th>
<th>Rate (L/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>June 18 2007</td>
<td>1</td>
<td>B6</td>
<td>B3</td>
<td>3.9</td>
</tr>
<tr>
<td>June 19 2007</td>
<td>2</td>
<td>B1</td>
<td>B4</td>
<td>4.2</td>
</tr>
<tr>
<td>June 20 2007</td>
<td>3</td>
<td>B5</td>
<td>B2</td>
<td>4.1</td>
</tr>
<tr>
<td>June 21 2007</td>
<td>4</td>
<td>C5</td>
<td>C2</td>
<td>4.1</td>
</tr>
<tr>
<td>June 22 2007</td>
<td>5</td>
<td>C6</td>
<td>C3</td>
<td>4.0</td>
</tr>
<tr>
<td>June 23 2007</td>
<td>6</td>
<td>C6</td>
<td>C5</td>
<td>1.7</td>
</tr>
<tr>
<td>June 24 2007</td>
<td>7</td>
<td>B6</td>
<td>Monopole</td>
<td>2.3</td>
</tr>
<tr>
<td>June 25 2007</td>
<td>8</td>
<td>C1</td>
<td>C4</td>
<td>4.2</td>
</tr>
<tr>
<td>June 26 2007</td>
<td>9</td>
<td>C4</td>
<td>C1</td>
<td>4.3</td>
</tr>
<tr>
<td>June 27 2007</td>
<td>10</td>
<td>C4</td>
<td>C3</td>
<td>4.3</td>
</tr>
<tr>
<td>June 28 2007</td>
<td>11</td>
<td>C5</td>
<td>C1</td>
<td>4.3</td>
</tr>
</tbody>
</table>
moistened bentonite and gypsum mixture to ensure good contact between the electrode and the ground, and stones were placed above the electrodes. Measurements of the self-potential signals were carried out with a Keithley 2701 multichannel voltmeter, and we used nonpolarizing Pb/PbCl₂ (Petiau) electrodes (Perrier et al., 1998). The voltmeter was connected to a laptop computer where the data were stored. All the electrodes were scanned during a period of 30 s. To account for drift effects associated with temperature changes, an additional reference electrode was located 50 m from the middle of the investigated region, and temperature of the packing medium around the reference electrode was measured periodically. According to SDEC (the company manufacturing the Petiau electrodes used in this study), the temperature dependence of these electrodes is 0.210 mV/°C. During the day, we measured variations of temperature ranging from a few degrees Celsius to 15 °C. A difference in temperature of 10 °C is responsible for a drift of the self-potential measurement of 2 mV, and therefore this effect cannot be neglected. Following Rizzo et al. (2004), a filtering operation has been used to improve the signal-to-noise ratio of these data and to correct the temperature drift.

2.3. Stratigraphic information

Stratigraphic information from wells drilling are included in a database containing location and local thickness of identified geo-materials within each column. Barrash and Clemo (2002) derived porosity values for each well by means of a neutron logs performed in each well at the BHRS at regular intervals (spacing 0.03 m) from the bottom of each well to the water table. The neutron-derived porosity logs at the BHRS indicate the occurrence of five hydrostratigraphic units across the central area of the well field. These subsurface units are also consistent with GPR reflection profiles (Peretti et al., 1999). Four of these units are cobble-dominated deposits and can be traced across the central portion of the site. The fifth unit is a channel sand that is continuous in the western part of the site and pinches out from the river to the central portion of the well field (Barrash and Clemo, 2002). Porosity from Units 1 and 3 have similar means, variances, and key vertical geostatistical descriptors and are considered to be similar (if not the same type of) hydrostratigraphic units based on the trends and statistics detected within porosity logs (Fig. 3). Units 2 and 4 also display similar porosity statistics and may be considered as similar hydrostratigraphic units, although they have dissimilar vertical geostatistical interpretations. Unit 5 is typically sand. Table 2 provides the elevations used as the basal contacts for each of the porosity units at the BHRS.

Table 2

<table>
<thead>
<tr>
<th>Well</th>
<th>Aquifer bottom elevation (m)</th>
<th>Unit1 top elevation (m)</th>
<th>Unit2 top elevation (m)</th>
<th>Unit3 top elevation (m)</th>
<th>Unit4 top elevation (m)</th>
<th>Unit5 top elevation (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>832.1</td>
<td>834.0</td>
<td>840.1</td>
<td>843.0</td>
<td>847.2</td>
<td>847.6</td>
</tr>
<tr>
<td>B1</td>
<td>832.4</td>
<td>834.5</td>
<td>841.2</td>
<td>843.8</td>
<td>847.9</td>
<td>–</td>
</tr>
<tr>
<td>B2</td>
<td>830.8</td>
<td>833.4</td>
<td>839.0</td>
<td>841.5</td>
<td>847.4</td>
<td>–</td>
</tr>
<tr>
<td>B3</td>
<td>831.7</td>
<td>834.6</td>
<td>838.6</td>
<td>841.5</td>
<td>847.5</td>
<td>–</td>
</tr>
<tr>
<td>B4</td>
<td>832.4</td>
<td>835.0</td>
<td>838.4</td>
<td>841.9</td>
<td>846.7</td>
<td>847.6</td>
</tr>
<tr>
<td>B5</td>
<td>830.8</td>
<td>834.0</td>
<td>838.8</td>
<td>843.7</td>
<td>846.2</td>
<td>847.4</td>
</tr>
<tr>
<td>B6</td>
<td>831.2</td>
<td>833.9</td>
<td>840.0</td>
<td>842.0</td>
<td>846.6</td>
<td>847.6</td>
</tr>
<tr>
<td>C1</td>
<td>831.4</td>
<td>833.8</td>
<td>838.0</td>
<td>842.7</td>
<td>847.6</td>
<td>–</td>
</tr>
<tr>
<td>C2</td>
<td>831.0</td>
<td>834.0</td>
<td>838.4</td>
<td>842.6</td>
<td>847.6</td>
<td>–</td>
</tr>
<tr>
<td>C3</td>
<td>831.0</td>
<td>834.3</td>
<td>840.3</td>
<td>843.7</td>
<td>847.1</td>
<td>847.3</td>
</tr>
<tr>
<td>C4</td>
<td>830.9</td>
<td>834.4</td>
<td>840.9</td>
<td>844.0</td>
<td>845.8</td>
<td>847.6</td>
</tr>
<tr>
<td>C5</td>
<td>831.6</td>
<td>832.7</td>
<td>840.6</td>
<td>842.9</td>
<td>845.7</td>
<td>847.4</td>
</tr>
<tr>
<td>C6</td>
<td>831.3</td>
<td>834.2</td>
<td>839.4</td>
<td>842.1</td>
<td>846.7</td>
<td>847.3</td>
</tr>
</tbody>
</table>

* Unit 5 top is limited by position of water table for porosity log measurements.

Table 3

Lithological categories classified in BHRS (Barrash and Reboulet, 2004).

<table>
<thead>
<tr>
<th>Lithological categories</th>
<th>Average porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 Sand</td>
<td>0.429</td>
</tr>
<tr>
<td>4 Pebble- and cobble dominated units</td>
<td>0.232</td>
</tr>
<tr>
<td>3</td>
<td>0.172</td>
</tr>
<tr>
<td>2</td>
<td>0.241</td>
</tr>
<tr>
<td>1 Basalt</td>
<td>0.182</td>
</tr>
</tbody>
</table>

Six different lithological categories, derived from core samples collected during wells drilling, have been finally classified in the BHRS (Barrash and Clemo, 2002; Barrash and Reboulet, 2004) and are reported in Table 3. These data constitute our base of reference for the reconstruction of the internal architecture of the system on the basis of a multiple continua approach.
3. Theoretical background

3.1. Aquifer characterization as an overlapping continuum

A variety of studies suggest the importance of honoring geological features and information in hydrogeologic modeling (e.g., Webb, 1995; Scheibe and Freyberg, 1995; Webb and Anderson, 1996; Ritzi et al., 1994, 1995, 1996; Boggs and Adams, 1992; Boggs et al., 1992; Rehfeldt et al., 1992; Lee et al., 2007 and references therein). Increasingly powerful aquifer characterization techniques are available at various stages of development (Jardani and Revil, 2009), so that the approximate boundaries between regions where different geo-materials occur can sometimes be reliably characterized by geophysical surveying techniques. Errors associated with boundary locations can be derived (in principle) through geostatistics. Techniques which are available to describe the spatial variability of the properties and attributes of the host porous matrix from geologic observations and local measurements include continuous geostatistical models, discontinuous facies models (e.g., Indicator or Gaussian-Threshold models, Markov chain model), or genetic models. De Marsily et al. (2005) offer an insightful review focusing on (stochastic) composite models to characterize heterogeneous porous media in terms of disjoint units (or litho-facies) within which hydraulic attributes (typically porosity and hydraulic conductivity) can be spatially variable is presented by Winter et al. (2003).

Sometimes block geometries cannot be characterized because adequate hydrogeological and geophysical data are not available or because there is not sufficient resolution to determine boundaries. In this case, models that can be adopted to reflect the composite nature of the system include multiple-continua approaches. These models have typically been used to quantify the exchange of mass and momentum between fractured and matrix phases in fractured media. The idea is conceptually similar to that imbued in stationary models with multi-modal distributions. It relies on the adoption of a random indicator function, \( I(x) \), to designate the membership of a point \( x \) in material \( M_i \). Materials (continua) \( M_i \) are allowed to overlap in multiple-continua models. The possibility of such a co-existence of various materials at the same point \( x \) relies on the idea that a point in the continuum description of porous media represents a volume that can be comprised of several materials \( M_i \).

Here, we characterize the distribution of materials at the site in the spirit of multiple-(overlapping) continua concepts. We use the stratigraphic information presented in Section 2.3 and adopt successive applications of Indicator Kriging to provide an estimate of the probability of occurrence of each geo-material within the blocks of the numerical grid adopted to solve the groundwater flow problem. The procedure we adopt is detailed in the following.

1. Stratigraphic and sedimentological information are analyzed and grouped into \( n \) main classes. Each one of these identifies a material type. Here, we adopt the data and results of Barrash and Clemo (2002) and Barrash and Reboulet (2004) and rely on the identification of \( n = 6 \) categories, i.e., 6 geo-materials, identified as \( M_i \) (\( i = 1, 2, \ldots, 6 \)).

2. We start upon assigning a value of the indicator, \( I = 1 \), to samples where material \( M_i \) is observed, while assigning \( I = 0 \) to locations where other samples are available.

3. Three-dimensional indicator variography is then performed. Resulting sample variograms are interpreted and modeled by different theoretical variograms and key geostatistical parameters (sill, range, nugget, anisotropy pattern) are identified for each class.

4. Indicator Kriging is performed. Kriged values of the indicator coincide with the estimated probability of finding \( M_i \) within each block.

5. The procedure is repeated upon assigning a value of the indicator, \( I = 1 \), to samples associated with material \( M_i \), while setting \( I = 0 \) to locations where other samples are available. Kriged values of the indicator coincide with the estimated probability of occurrence of \( M_i \) within each block.

6. This is repeated in sequence to identify block-volumetric fractions of \((n - 1)\) materials. The volumetric fraction of material \( n \) is finally calculated as the complement to unity for each grid block.

The hydraulic conductivity value of a grid block \( K_j \) is then calculated as a weighted average of the conductivities of materials occurring in the block \( k_j \) according to the following expression:

\[
K_j = \sum_{i=1}^{n} \frac{I_{ik_j} \cdot k_i}{j = 1, \ldots, N_j}
\] (1)

where \( l \) is the estimated percentage of the materials in a block, \( j \) indicates the position of a specific grid block and \( N_j \) is the number of grid blocks. For simplicity, we assume that each material is associated with a uniform hydraulic conductivity. In our application, these result in six hydraulic conductivity values which are calibrated in the inverse modeling procedure presented in Section 3.2.2.

3.2. Inverse modeling with multiple data sources

We consider steady-state groundwater flow in a randomly heterogeneous domain. The flux vector \( q(x) \) and the hydraulic head \( h(x) \) obey the continuity equation and Darcy’s Law subject to given forcing terms (sources and boundary conditions) where \( x \) is a vector of spatial coordinates. We write:

\[
h_{j} = h_{j0} + \varepsilon_{j} \quad j = 1, \ldots, N_{p}
\] (2)

\[
h_{i} = h_{i0} + \varepsilon_{i} \quad i = 1, \ldots, N_{b}
\] (3)

where, \( h_{j0} \) is the unknown true value of the vertically average hydraulic head, \( h_{j0} \), at measurement point \( x_{j} \); \( \varepsilon_{j} \), its measurement value obtained by borehole reading, \( \varepsilon_{j} \), the corresponding zero-mean measurement error; \( h_{i0} \) is the unknown true value of the location of the water table, \( h_{i0} \), at measurement point \( x_{i} \); \( \varepsilon_{i} \), its measurement value, as obtained by self-potential interpretations, \( \varepsilon_{i} \), the corresponding zero-mean measurement error; \( N_{p} \) and \( N_{b} \) are the number of available measurements of head and self-potential, respectively.

Following the work of Carrera and Neuman (1986) we assume (a) lack of space correlation between measurement errors of \( h_{i} \) and \( h_{c} \); (b) \( \varepsilon_{j} \) and \( \varepsilon_{i} \) being multivariate Gaussian; (c) the covariance matrix of measurements errors, \( C_{hp} \) and \( C_{hc} \):

\[
C_{hp} = \sigma_{hp}^{2} \sigma_{hp} \quad C_{hc} = \sigma_{hc}^{2} \sigma_{hc}
\] (4)

to be known up to the positive statistical parameters \( \sigma_{hp}^{2} \) and \( \sigma_{hc}^{2} \), which are typically unknown and need to be estimated during inversion; and (d) lack of spatial cross-correlation between measurement errors of \( h_{p} \) and \( h_{c} \). The latter assumption renders the known symmetric positive-definite matrices \( \sigma_{hp} = \sigma_{hp} \) and \( I \) (Identity matrix).

In the absence of direct measurements of hydraulic conductivity at the scale of interest, the Maximum Likelihood estimate of the values of hydraulic conductivity associated with each material are obtained by minimizing the negative log likelihood criterion (Carrera and Neuman, 1986; Medina and Carrera, 2003)
$\text{NLL} = \frac{R_{hP}}{\sigma_{hP}^2} + \frac{R_{hE}}{\sigma_{hE}^2} \ln |V_{hP}| + \ln |V_{hE}| + N_{hP} \ln \sigma_{hP}^2 + N_{hE} \ln \sigma_{hE}^2$

$+ (N_{hP} + N_{hE}) \ln 2\pi$ (5)

Here, $N_{hP}$ and $N_{hE}$ are defined as:

$R_{hk} = (h_{hk}^m - h_{hk}^p) / \sqrt{V_{hk}^p |V_{hk}^m|}$ \quad $k = P, E$ (6)

$h_{hk}^m$ is the vector of measurements of type $k$, $h_{hk}^p$ is a vector of modeled state variables of type $k$. If the statistical parameters $\sigma_{hP}^2$ and $\sigma_{hE}^2$ are known, minimizing Eq. (5) is equivalent to minimizing the following general least squares criterion:

$R = R_{hP} + \mu R_{hP}$ (7)

where $\mu$ is the relative weight between measurement errors

$\mu = \frac{\sigma_{hE}^2}{\sigma_{hP}^2}$ (8)

In the common case where these statistical parameters are unknown, they could in principle be estimated jointly with the estimates of materials' conductivities by minimizing Eq. (5). However, such estimation is likely to be unstable (Carrera and Neuman, 1986). We therefore follow recent works of Hernandez et al. (2006) and Bianchi Jannetti et al. (2010) by minimizing Eq. (7) with respect to the vector of hydraulic parameters for selected values of $\sigma_{hP}^2$ and $\sigma_{hE}^2$. We then improve upon these values as described below and repeat the process iteratively until all parameters converge to within predetermined tolerance levels.

We solve the three-dimensional flow problem with the widely used and thoroughly tested finite difference MODFLOW software (Hill et al., 2000). Model details are provided in Section 6. For given $\sigma_{hP}^2$ and $\sigma_{hE}^2$, we minimize Eq. (7) using the iterative Levenberg–Marquardt algorithm PEST implemented in the public domain (Doherty, 2002).

The minimization algorithm computes an updated parameter estimate $K_i$ of the (unknown) true vector of hydraulic conductivities, $K$, and a Cramer–Rao lower bound approximation for the covariance matrix, $Q$, of the corresponding estimation errors (Carrera and Neuman, 1986); the latter is evaluated according to:

$Q = \sigma_{hP}^2 |V_{hP}^m J_{hP}| + \mu \sigma_{hE}^2 |V_{hE}^m J_{hE}|^{-1}$ (9)

where $J_{hk}$ ($k = E, P$) is a Jacobian matrix of derivatives of the state variable (water level or vertically integrated heads) with respect to $K$, evaluated at $K_{hr}$ (see also Medina and Carrera, 2003). Next, $K_{hr}$ is projected onto the finite difference grid of MODFLOW via the algorithm presented in Section 3.1. The iterative process continues until $R$ in Eq. (7) stabilizes to within a desired tolerance.

In essence, our inverse process iterates between the estimation of hydraulic and statistical parameters. Each iteration starts by adopting the most recent estimates of the statistical parameters, $\sigma_{hP}^2$ and $\sigma_{hE}^2$. It then proceeds by estimating hydraulic parameters through the minimization of (7) and adopting the Cramer-Rao lower bound as an estimate of its covariance matrix $Q$. Next, we obtain an estimate of the weight $\mu$ by minimizing (with respect to $\mu$) that between the following functions which defines it most sharply:

1. NLL in (5)
2. The Kashyap (1982) Bayesian model selection criterion

$\text{KIC} = \text{NLL} + N_{hP} \ln \left( \frac{N_{hP} + N_{hE}}{2\pi} \right) - \ln |Q|$. (10)

We follow this by ML estimation of $\sigma_{hP}^2$ according to

$\sigma_{hP}^2 = \frac{R_{hP}}{N_{hP} + N_{hE}}$ (11)

and of $\sigma_{hE}^2$ based on the definition of $\mu$.

### 4. Geostatistical analysis of lithostratigraphic information

Spatial variability of the material types was analyzed by three-dimensional indicator variography, along the lines of Section 3.1. Sample directional three-dimensional variograms of the indicators have been reconstructed. The results are summarized in Table 4. The analysis of the data allowed interpreting a spatial variability pattern associated with sample horizontal variograms exhibiting no clear evidence of directional anisotropy while the vertical range resulted significantly smaller than its horizontal counterpart. Table 4 also indicates that there is a directional dependence of the variograms sill. This might be associated with (a) occurrence of a zonal anisotropy in the system (Isaaks and Srivastava, 1989) and (b) direction undersampling of the complete range of variability. Selection of the variogram models was performed as follows: (1) key parameters associated with a given variogram model were calibrated on the basis of a maximum likelihood fit between sample and model variograms; (2) the Kashyap’s selection criterion, $\text{KIC}$, was then adopted for model selection. Figs. 4–8 illustrate our results by depicting the calculated experimental variograms and the adopted interpretative models. The Kriging algorithm is implemented by means of the widely used suite GSLIB (Deutsch and Journel, 1998), upon considering the occurrence of the detected zonal anisotropy. Kriged values are associated with the center of elements of the computational grid described in Section 6.

### 5. Reconstruction of water table by means of self-potential measurements

Under steady-state conditions, Jardani et al. (2009) demonstrated, inverting the Poisson equation in a probabilistic (Bayesian) framework and using also the available potentiometric data in the inverse problem, that self potential signals exhibit a linear relationship with the saturated thickness of the aquifer, according to

$\phi(r) \approx \phi_0 - C(e - h(r)) = C(h(r) - h_0)$ (13)

Here, $C$ is the electrokinetic conversion coefficient ($\text{V/m}$) associated with hydraulic head variations, $\phi_0$ is the electrical potential ($\text{V}$) at vector location $r$, and $h_0$ ($\text{m}$) is the hydraulic head where the reference electrode is placed. The assumption of a linear relationship between the saturated thickness of the aquifer and the measured self potential signals allows performing an estimation of the water table depth by means of an application of Kriging with external drift (Delhomme, 1979; Galli and Meunier, 1987; Ahmed and de Marsily, 1987; Troisi et al., 2000). In this sense, the Kriging with external drift may be considered as an extension of Kriging with a trend model in which self-potential variable is assumed to reflect the spatial trends of the hydraulic head variability up to a linear rescal-
ing of units, or in a way more general Kriging with external drift can be considered a special case of the Bayesian interpolation without constraints (Linde et al., 2007). As pointed out by Straface et al. (2010), in the Kriging with external drift method secondary variable (self-potential) is assumed to reflect the spatial trends of the hydraulic head (primary variable) distribution up to a linear rescaling of units within small search neighborhoods. In this sense the value of coupling coefficient may be considered locally constant within the search neighborhoods. In order to implement Kriging with external drift on \( h(x) \), values of \( \phi(x) \) should be available at

![Fig. 4. Category 1 – (a) vertical and (b) horizontal variogram (m²) vs. lag distance (m).](image1)

![Fig. 5. Category 2 – (a) vertical and (b) horizontal variogram (m²) vs. lag distance (m).](image2)

![Fig. 6. Category 3 – (a) vertical and (b) horizontal variogram (m²) vs. lag distance (m).](image3)
each point where $h(x)$ should be estimated together with values of $\varphi$ at all points where $h$ data are available. If these values of $\varphi(x)$ are not directly available at all required locations, they may be determined in advance by an ordinary Kriging implementation. A variogram model for $\varphi(x)$ is inferred from the available data and cross-validated according to a standard-check procedure (Isaaks and Srivastava, 1989; Deutsch and Journel, 1998). It is important to underline that, while previous methods proposed like the semiempirical, the tomographic and the simplex algorithms (Revil et al., 2003; Rizzo et al., 2004), need to estimate, by means of laboratory tests, the value of the electrokinetic coupling coefficient $C$, application of Kriging with external drift does not require prior knowledge of this term because it is estimated directly by means of Kriging system equations (Straface et al., 2010).

The reconstruction of the water table was performed using the GSLIB library (Deutsch and Journel, 1998). An isotropic exponential variogram model with a sill equal to 1.6 mV$^2$ and a range value of 9.0 m was inferred for measured self-potential signals in the horizontal plane. Fig. 9 shows the experimental and modeled variogram inferred for $\varphi$. Ordinary Kriging was then performed for self-potential over a regular two-dimensional grid, with a size of 0.5 m, covering the site. At this point, the self-potential variogram model was cross-validated by implementing the ordinary Kriging to re-estimate self-potential values at points where experimental values of $\varphi$ were available and so calculating the estimation error. The residual variogram, $\gamma_k(h)$, was then inferred from pairs of $h$-values that are unaffected (or only slightly affected) by the trend, i.e., from data pairs such that $\varphi(x) = \varphi(x + h)$, and kriging with external drift was run for $h$ over the same 2D grid. Fig. 10 depicts...
the distribution of the location of the water table obtained with the described procedure.

6. Inverse flow model at Boise Hydrogeophysical Research Site

6.1. Description of the numerical model

Three-dimensional modeling of the BHRS has been performed under steady state flow conditions. The horizontal dimensions of the heterogeneous model domain are 60 m \( \times \) 60 m while the associated depth is 21 m. The model is vertically discretized by means of 60 layers with uniform thickness of 0.35 m. Each layer is discretized by a regular grid of 14,400 square cells having a side of 0.5 m. Simulations have been performed by imposing a mixed boundary condition along the boundary of the 60 m \( \times \) 60 m computational domain. The mixed boundary condition has been obtained by extending the size of the simulation region from 60 m up to 500 m from the well-field center (at this distance it had been verified experimentally that head changes were negligible) and is of the form:

\[
K \nabla h = N_0 + C(h_b - h)
\]

where the flux \( N_0 \) is equal to zero, \( C \) is the average conductance of the region comprised between the 60 m \( \times \) 60 m domain and the extended one (Fig. 1), \( h_b \) is the constant hydraulic head value imposed on the boundary of the enlarged domain and \( h \) is the hydraulic head value on the 60 m \( \times \) 60 m numerical model domain. The head distribution within the enlarged domain has been estimated by projecting a planar trend surface obtained from water levels measured during the two weeks before the dipole tests and has been adopted to estimate the values of \( h_b \) in the mixed boundary condition. The conductance value \( C \) has been calculated by assuming the aquifer comprised within the two domains (Fig. 1) to be homogeneous with an average hydraulic conductivity corresponding to that reported by Fox (2006) and Barrash et al. (2006).

SP signals acquired during our dipole test, provide information on the late-time part of the experiment, when pseudo-steady state regime is reached. It is well known that, during this regime, hydraulic heads are subjected to space–time variations while head gradients are time independent. This implies that one can represent drawdown increments (i.e., \( \Delta h(x, x_0) = h(x_0) - h(x) \)) by means of a steady state flow equation. In our case, we compute drawdown increments, \( \Delta h(x, x_0) \), relative to that recorded at an observation electrode positioned at location \( x_0 \), which is farthest from the pumping and injection wells outside of the investigated area. These quantities constitute our state variable measurements in (6).

6.2. Results of the Inversion

Here, we present the results of the inversion of the test termed C5(Extraction)/C1(Injection) in Table 1. Data collected during the dipole tests are obtained in two different ways: direct sampling within observation wells, and derived measures from self potential acquisition. With reference to self-potential measures, since the linear relationship between electrical and hydraulic information is effective under the hypothesis of small water table variations (Straface et al., 2010), estimates of water table are affected by a generally unquantifiable error in the proximity of the pumping and injection wells. For all these reasons, the strength of measurement errors is estimated according to the procedure explained in Section 3.2. From an operational standpoint, we select five values of \( \mu \) \( (\mu = 0.1, 1, 3, 5, 10) \) for our inversion. These represent a wide range...
of variability of the relative importance of the measurement errors associated with the two types of data available. For each value of \( l \) the steady state flow inversion is performed and the optimum value of \( l \) is identified by applying the methodology described in Section 3.2. Fig. 11 depicts the values of \( KIC \) and \( NLL \) associated with the selected values of \( l \). The observed ability of \( KIC \) to identify the statistical parameters included in (4) is consistent with previous observations of Hernandez et al. (2006), Riva et al. (2009), and Bianchi Jannetti et al. (2010), in the context of the inversion of mean groundwater flow equations. The optimization process returns a standard deviation of ±4.6 cm for the electrodes and ±2.7 cm for piezometric readings at wells, which are consistent, given the three-dimensional model configuration, the available lithological information and the degree error associated to water table elaboration (Section 5).

The optimum set of hydraulic parameters estimated at the value of \( l \) associated with the minimum value of \( KIC \) is reported in Table 5. A qualitative analysis of the consistency of inversion results against previously published geological observations can then be performed. Two vertical transects crossing the wells C5–A1–C2 and B1–A1–A4 have been carried out in which hydraulic conductivity value of a model grid block has been calculated as a weighted average of the estimated hydraulic conductivity values of Table 5. Fig. 12 shows the estimated vertical distribution of heterogeneity at BHRS after the calibration of data from Dipole Test C5–C1. Because of the linear combination of the estimated hydraulic conductivities, the resulting maps present a different permeability range with respect to the one obtained in Table 5. In the transect C5–A1–C2, the boundaries between the five stratigraphic units derived from porosity logs and obtained on the basis of Table 2 are available up to a depth of about 15 m, the juxtaposition to the reconstructed conductivity field, indicates a good agreement between the two types of reconstructions (Fig. 12).

We then compare the spatial distribution of depth-average conductivities against that obtained by Cardiff et al. (2009) by means of a two-dimensional inversion on the basis of hydraulic tomography data. Fig. 13 shows that the depth averaged log-conductivity distribution obtained in our work displays some key features which are consistent with the results obtained by Cardiff et al. (2009). In both cases, the aquifer is characterized by lower permeability areas on the Western region of the field (left side of Fig. 13a and b). The system then tend to display a sequence of more permeable geomaterials moving towards the Eastern side. It is interesting to note that the distribution of depth-averaged conductivities obtained on the basis of a three-dimensional flow model is associated with less pronounced horizontal variations than those resulting from the inversion of a two-dimensional flow model. A relatively large conductivity variability is instead observable along vertical slices (Fig. 12), consistently with pronounced stratification observed at the site.

Table 5

<table>
<thead>
<tr>
<th>Lithological categories</th>
<th>Hydraulic conductivities</th>
<th>Uncertainties</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1.33 \times 10^{-5} m/s</td>
<td>\pm 2.52 \times 10^{-5} m/s</td>
</tr>
<tr>
<td>4</td>
<td>2.42 \times 10^{-4} m/s</td>
<td>\pm 1.67 \times 10^{-4} m/s</td>
</tr>
<tr>
<td>3</td>
<td>1.94 \times 10^{-4} m/s</td>
<td>\pm 1.27 \times 10^{-4} m/s</td>
</tr>
<tr>
<td>2</td>
<td>2.18 \times 10^{-4} m/s</td>
<td>\pm 2.16 \times 10^{-4} m/s</td>
</tr>
<tr>
<td>1</td>
<td>5.59 \times 10^{-5} m/s</td>
<td>\pm 2.08 \times 10^{-5} m/s</td>
</tr>
<tr>
<td>0</td>
<td>4.00 \times 10^{-12} m/s</td>
<td>\pm 8.97 \times 10^{-12} m/s</td>
</tr>
</tbody>
</table>

Fig. 12. Two vertical transects crossing the wells B1–A1–A4 and C5–A1–C2 showing the estimated vertical distribution of hydraulic conductivity (m/s) at BHRS. In the second transect, is showed a stratigraphical comparison between the inverse modeling result and the one derived from the neutron porosity logs at the BHRS.
Finally, we validate our inverse modeling results upon simulating all the remaining dipole tests on the calibrated three-dimensional conductivity field. As an example of the quality of the results obtained, Fig. 14 depicts the observed and modeled depth averaged head values obtained at steady-state for dipole tests C4(Extraction)/C3(Injection) and C1(Extraction)/C4(Injection), which represent the best and worst validation results, respectively. As a complement to these results, Fig. 14 shows also a scatterplot of the observed and modeled (steady-state) drawdown for the complete set of dipole tests. The simulation of the experimental tests not included in the inversion procedure, returned hydraulic head values close to the observed one (the correlation coefficient with the unitary slope factor line is about 0.97).

7. Conclusions

We combined the use of sedimentological, hydraulic and hydrogeophysical information to characterize a three-dimensional heterogeneous aquifer. We focused on the joint inversion of

---

*Fig. 13. Estimate of depth averaged log-conductivity field from (a) 3D inverse modeling of BHRS field using hydraulic and geophysical data, and (b) 2D inverse modeling of BHRS field using hydraulic data (Cardiff et al., 2009).*
sedimentological (porosity), hydraulic head and self-potential observations collected at the Boise Hydrogeophysical Research Site (BHRS), Boise, Idaho, during an extensive series of tests. The aquifer was conceptualized as a multiple-continuum, where the volumetric fraction of a geo-material within a cell of the numerical flow model has been calculated by Multiple Indicator Kriging (MIK). The latter was implemented on the basis of available sedimentological information obtained from porosity measurements performed by means of neutron probe acquisition. Self potential and hydraulic head data have been embedded jointly within a three-dimensional (pseudo-steady state) inverse model of groundwater flow at the site. Each identified geo-material was assumed to be characterized by a constant hydraulic conductivity. The hydraulic conductivity associated with a numerical block was then calculated as a weighted average of the conductivities of the geo-materials which were found in the block according to the results of MIK. Model parameters were estimated by a Maximum Likelihood fit between measured and modeled state variables resulting in a spatially heterogeneous distribution of hydraulic conductivity, which was constrained on the sedimentological data and conditioned on both free surface location derived from self-potential signals and depth-averaged hydraulic head obtained from borehole readings. Minimization of the ML objective function allowed estimating the relative weight of errors associated with self-potential and borehole-based data.

The procedure adopted allowed a three-dimensional reconstruction of the heterogeneity of the site with a level of detail which was not obtained in previous studies and relatively modest computational efforts. Further validation against dipole tests which were not used in the inversion procedure supports the robustness of the results.

It is important to underline that the technological and interpretative limits associated with the identification of the subsurface lithology by means of neutron probe acquisition and location of the free surface via self-potential are surmountable, e.g., by jointly using resistivity information as described by Jardani and Revil (2009). Consequently, in spite of these limitations, the procedure adopted in this paper, can represent a useful instrument for real heterogeneous aquifers characterization and for predictive analysis of their behavior.

Acknowledgements

The field experiment was supported by PRIN2006 – Project “Statistical estimation of heterogeneity in complex randomly heterogeneous geologic media”, EPA grants X-96004601-0 and X-96004601-1 and by NSF grant DMS-0934680. M. Cardiff was also supported during his PhD program at Stanford by an NSF Graduate Research Fellowship. Significant help during the field experiments was provided by participants in the Boise State and Calabria Universities “Hydrogeophysics: Theory, Methods, and Modeling” summer program: Steve Berg, Francesco Chidichimo, Agnès Crespy, Carlyle Miller, Harry Liu, Timothy Johnson, Domenico Sorbo, Leah Steinbrunn, and Jianwei Xiang. We thank Frédéric Perrier for the use of his non-polarizing electrodes.

References


