XVIII International Conference on Water Resources
CMWR 2010
J. Carrera (Ed)

CHARACTERIZATION OF THE BOUNDARY CONDITIONS IN AN AQUIFER MODEL: A BOUNDARY DATA COMPLETION METHOD

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Key words: inverse problem, advanced numerical methods, hydrogeologic resources, model predictions

Summary. This contribution concerns the identification of the boundary condition data on an unaccessible part of a domain boundary, by using overspecified data on another part this boundary which can be easily obtained. This problem happens in groundwater flows with any types of porous media and even in saturated and homogeneous porous medium. The associated forward problem is governed by Darcy equations. Sensitivity of the recovered boundary data against physical and numerical parameters will be discused.

1 INTRODUCTION

Since last decades, numerical simulations in hydrogeology have developed rapidly and filled a substantial gap in the prediction of groundwater flows. But those simulations may remain inaccurate due to the lack of knowledge of hydrogeologic parameters in the medium or flow variables information like hydraulic head or discharge on the boundaries. Inverse problem methods have been extensively used as an appropriate tool for the prediction of hydrogeologic parameters like hydraulic conductivity or porosity in complement to in-field measurements. Extended reviews of inverse methods for hydrogeologic parameters may be found in Carrera[6], De Marsily[7], McLaughlin[11], Yeh[14]

Still, estimation of hydraulic head and discharge at boundaries using inverse problems is more unusual, but may worth some consideration as complement of in-field measurement campaign which may be expensive or even impracticable.

Inverse problems for the recovery of data and its derivatives on boundaries have been successfully applied to a wide range of physical and engineering subjets: electrostatic tomography for crack detection (Santosa[12]), displacement and stress analysis in linear elasticity (Baranger[3], Andrieux[1] and Bonnet[5]), flux characterisation in heat transfer (Andrieux[2], Kozlov[10]) and leaks identification in fluid mechanics problems (Escriva[8], Belhachmi[4]). Standard illposed inverse problems on boundaries are formulated with overspecified data on one boundary's part and missing data on its complementary part, they are called Cauchy problem or data completion problem. Among the different methods, one consists in reformulating the illposed problem as two wellposed ones, as detailled in Andrieux[2]. Then the solution is the one which minimize an error gap functional between the two wellposed solutions. The inherent variational formulation of this method makes it appropriate for finite element methods and efficient optimisation technics like trust-region Newton method.

We apply this methodology to a hydrogeologic configuration inspired from work by Konikow[9] who predicted long term polluants dispersion in groundwater flow due to a leaky chemical pond under the Rocky Mountain arsenal in Colorado, US. Although being geometrically simplistic, our model keeps all the main hydrogeological caracteristics of the real case flow as simulated by Konikow[9], like boundary conditions and sources and sinks.

In the next section, the physical and mathematical layout of the forward simulated flow will be presented with emphasis on an appropriate equation scaling. Cauchy problem or data completion method is described in section three. Some results concerning the hydrogeologic application are detailled in section four, and conclusions and perspectives are sumed up in section five.

2 PHYSICAL AND MATHEMATICAL LAYOUT

2.1 Forward problem formulation

As mentioned before, the physical setup is derived from a hydrological model of a confined saturated alluvial aquifer flow in two dimension. The model setup is directly inspired from a test case in SUTRA code developped by Voss[13], itself derived from early work of Konikow[9]. The porous media is supposed undeformable with isotropic homogenous properties (hydraulic conductivity tensor $\mathbf{K} = K_0\mathbf{Id}$ and porosity ε_0). The flow is driven by the mass conservation equation and momentum conservation equation of motion which reduces to Darcy's equation. The geometry, with boundary condition data, is sketched on figure 1. The governing equations under the former assumptions may be written as follows:

$$\varepsilon_0 \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{\mathbf{q}}) = \mathcal{Q} \tag{1}$$

$$\vec{\mathbf{q}} = -\mathbf{K}\vec{\nabla} h = -K_0 \vec{\nabla} h \tag{2}$$

with ρ the density field, $\vec{\mathbf{q}}$ the specific vector flux or specific discharge, h the hydraulic head and $\mathcal{Q}$ a given distribution of sources and sinks. Under consideration of horizontal, steady and incompressible flow ($\rho = \rho_0$), the equations 1 and 2 reduce to a unique Poisson-like equation on the hydraulic head, which may be written as follows:

$$-\rho_0 K_0 \Delta h(x, y) = \mathcal{Q}(x, y) \tag{3}$$

An equivalent formulation is possible, averaging the tridimensional equation along the vertical and defining the transmissivity or hydraulic diffusivity as $T = bK_0$ (with b the aquifer thickness). The hydrogeological boundary conditions are the following (see figure 1): lateral frontiers (Γ_e and Γ_w) are assumed impervious ($\nabla h \cdot \vec{n} = 0$), constant hydraulic on the north side and a linear profil of hydraulic head, due to a river draining, on the south side. Two impervious rocky beds in the aquifer are introduced in the geometry. A leaky contaminant pond is included through a pointwise source of polluant and three sinks on a same row downstream reproduce a "draining wall". The sources and sinks are modelled as pointwise Dirac distributions of mass flow rate by volume unit $\mathcal{Q}_p^i$ with respectively positive and negative magnitude. The resulting forward or direct problem equations are:

$$-\rho_0 K_0 \Delta h(x, y) = \sum_{i=1}^{N_p} \mathcal{Q}_p^i \delta(x - x_i, y - y_i) \qquad \forall (x, y) \quad \text{in} \quad \Omega \tag{4}$$

$$\vec{\nabla} h(x, y) \cdot \vec{n} = 0 \qquad \forall (x, y) \quad \text{on} \quad \Gamma_w \cup \Gamma_e \tag{5}$$

$$h(x, y) = h_n \quad \forall (x, y) \quad \text{on} \quad \Gamma_n \tag{6}$$

$$h(x, y) = ax + b \quad \forall (x, y) \quad \text{on} \quad \Gamma_s \tag{7}$$

where Ω denotes the whole domain, $\partial\Omega = \Gamma = \Gamma_n \cup \Gamma_s \cup \Gamma_e \cup \Gamma_w$ its outer boundary, $\Gamma_N = \Gamma_e \cup \Gamma_w$ and $\Gamma_D = \Gamma_n \cup \Gamma_s$ are respectively Neumann and Dirichlet kind boundary conditions subsets.

2.2 Scaling of the forward problem equation

As the boundary data completion method is based on the measurement of an error functional, the method is sensitive to the range of variation of the forward problem solution and the conditionning of the laplacian operator in the Poisson equation. This has a direct impact on the convergency of the iterative minimisation algorithm of the error based functional. With an appropriate scaling of the equation, we expect a fair reduction of the iteration's count needed for minimisation. We'll show, through numerical experiments, that the equation scaling leads effectively to a drastically reduction of the needed iterations count for a given fixed tolerance.

The appropriate scaling relies on the definition of a reference values: L_{ref} a characteristic length in the horizontal plan and $\mathcal{Q}_{p_{ref}} = \rho_0 K_0 / L_{ref}$ a reference mass flow rate by volume unit:

$$\tilde{x} = \frac{x}{L_{ref}} \quad \tilde{y} = \frac{y}{L_{ref}} \quad \tilde{h} = \frac{h}{L_{ref}} \quad \tilde{\mathcal{Q}}_p = \frac{\mathcal{Q}_p}{\rho_0 K_0 / L_{ref}}$$

Then former equation (4) is then reduced to its dimensionless or scaled form:

$$-\tilde{\Delta}\tilde{h}(\tilde{x},\tilde{y}) = \sum_{i=1}^{N_p} \tilde{\mathcal{Q}}_p^i \delta(\tilde{x}-\tilde{x}_i, \tilde{y}-\tilde{y}_i) \tag{8}$$

This equation (without tilde notation) is used in the next section for the Cauchy problem or boundary data completion problem formulation.

3 CAUCHY PROBLEM LAYOUT

Let consider the following adimensioned Cauchy problem. Hereafter, we denote by: Γ_m ($=\Gamma_n$) the boundary where the overspecified data are known or measured, Γ_u ($=\Gamma_s$) the boundary where the data have to be identified, Γ_b ($=\Gamma_e \cup \Gamma_w$) the boundary where natural boundary condition is specified.

$$\begin{cases} -\Delta h = \mathcal{Q} & \text{in} \quad \Omega \\ \vec{\nabla} h \cdot \vec{n} = 0 & \text{on} \quad \Gamma_b \\ h = F_m & \text{on} \quad \Gamma_m \\ h = H_m & \text{on} \quad \Gamma_m \end{cases} \tag{9}$$

The method developped by Andrieux[1,2] and Baranger[3] is based on a simple idea which consist in splitting the Cauchy problem into two wellposed ones. The first problem takes into account the known Dirichlet data and the unknown Neumann one, the second problem takes into account the known Neumann data and the unknown Dirichlet one, such that:

$$\mathcal{P}_1 = \begin{cases} -\Delta h_1 = \mathcal{Q} & \text{in} \quad \Omega \\ \vec{\nabla} h_1 \cdot \vec{n} = 0 & \text{on} \quad \Gamma_b \\ h_1 = H_m & \text{on} \quad \Gamma_m \\ \vec{\nabla} h_1 \cdot \vec{n} = \eta & \text{on} \quad \Gamma_u \end{cases} \quad and \quad \mathcal{P}_2 = \begin{cases} -\Delta h_2 = \mathcal{Q} & \text{in} \quad \Omega \\ \vec{\nabla} h_2 \cdot \vec{n} = 0 & \text{on} \quad \Gamma_b \\ \vec{\nabla} h_2 \cdot \vec{n} = F_m & \text{on} \quad \Gamma_m \\ h_2 = \tau & \text{on} \quad \Gamma_u \end{cases} \tag{10}$$

The following step of this method is to build an error functional on the pair (η, τ) using a seminorm E. Indeed, h_1 and h_2 are obviously equal only when the pair (η, τ) meets the real data (F_u, H_u) on the boundary Γ_u. We propose then to solve the data completion problem via the following minimization:

$$\begin{cases} (F_u, H_u) = arg\min_{\eta,\tau} E(\eta,\tau) \\ with \ (h_1, h_2) \ solution \ of \ (\mathcal{P}_1, \mathcal{P}_2) \end{cases} \quad \text{with} \quad E(\eta,\tau) = \frac{1}{2}\int_\Omega (\nabla h_1 - \nabla h_2)^2 \tag{11}$$

Using the properties of the h_1 and h_2, it is straightforward to derive an alternative expression of the E functional:

$$E(\eta,\tau) = \frac{1}{2}\int_{\Gamma_u} (\eta - \vec{\nabla} h_2.\vec{n})(h_1 - \tau) + \frac{1}{2}\int_{\Gamma_m} (\vec{\nabla} h_1.\vec{n} - F_m)(H_m - h_2) \tag{12}$$

This expression shows that the error between the two fields h_1 and h_2 can be expressed equivalently by an integral involving only the boundary of the domain Ω. Let's remark the following properties: $E(\eta,\tau)$ reaches its minimum for $h_1 = h_2 + Cte = h$, where h is the unique solution to our data recovering problem, $E(\eta,\tau)$ is convex, quadratic and positive with a minimum equal to zero. We can also observe that $E(\eta,\tau)$ involves integrals on the whole boundary of the domain. Furthermore, the two fields h_1 and h_2 solutions of (10) are truly coupled via the error energy-like functional. Furthermore, the alternative form (12) of the error functional, makes possible the comparison of the proposed approach with more classical least square error methods : Here both Neumann and Dirichlet errors are naturally mixed and no dimensional factor is needed for that purpose. The Dirichlet error is weighted by the Neumann one. In this approach the Neumann and Dirichlet missing data are treated simultaneously, whereas other approaches require the evaluation of $\nabla h.n$ from h by numerical differentiation.
The minimization problem introduced needs the evaluation of the gradient of E. The components of this gradient can be computed in an efficient way by using the adjoint state method, for more details see Andrieux[1,2] and Baranger[3]. This method makes possible to evaluate the gradient in any direction using only the determination of two adjoint fields v_1 and v_2.

$$\frac{\partial E(\eta,\tau)}{\partial \eta}.\delta\eta = -\int_{\Gamma_u} v_1 \delta\eta \quad and \quad \frac{\partial E(\eta,\tau)}{\partial \tau}.\delta\tau = -\int_{\Gamma_u} (\eta - \nabla h_2.n - \nabla v_2.n)\delta\tau \tag{13}$$

where the associated adjoint problems are:

$$\left\{\begin{array}{lll} \triangle v_1 = 0 & \text{in} & \Omega \\ v_1 = 0 & \text{on} & \Gamma_m \\ \vec{\nabla} v_1.\vec{n} = \vec{\nabla} h_2.\vec{n} - \eta & \text{on} & \Gamma_u \end{array}\right. \quad and \quad \left\{\begin{array}{lll} \triangle v_2 = 0 & \text{in} & \Omega \\ v_2 = 0 & \text{on} & \Gamma_u \\ \vec{\nabla} v_2.\vec{n} = \vec{\nabla} h_1.\vec{n} - F_m & \text{on} & \Gamma_m \end{array}\right. \tag{14}$$

4 APPLICATION AND RESULTS

4.1 Aquifer flow analysis: forward and inverse problem

First, we present a general overview of the simulated forward aquifer flow problem on figure 3(a). The unscaled physical parameters for the reference case are the following: $K_0 = 2.5\ 10^{-4} m/s$, $\rho_0 = 998 kg/m^3$, $h_n = 250m$, $a = 2.5\ 10^{-3}$, $b = 17.5m$, $\mathcal{Q}_p^1 = 28.2 kg/(m^3 s)$, $\mathcal{Q}_p^{2,3,4} = -5.65 kg/(m^3 s)$ and $L_{ref} = 2\ 10^4 m$. The flow streams from the north face to the south side, mainly parallel to the impervious lateral sides and locally deflected by the rocky beds and crosswise hydraulic gradient due to a river stream. A separated flow is observed in the near region of the source, modelling the leaky contaminant pond. After postprocessing through the integration of a passive scalar convection-diffusion equation with constant injection concentration source ($C = 1000$) at the leaky source, we represent the isoconcentration field, the separated zone is clearly shown by the plume of the contaminant, delimited by isocontour $C = 240$ (see figure 3(b)).

The data completion inverse problem results are reported on figures 4(a) and 4(b): hydraulic head and discharge profil (normal derivative) on the south side of the domain are compared to the forward reference problem in both cases: scaled and unscaled equation. Good agreement is obtained with the reference solution corresponding to the linear hydraulic head profil specified in eq. 7. and except from corner effets near $x = 0$ and $x = 0.8$ no major difference exists between the two scaled and unscaled data completion problem. Those errors are difficult to avoid in data completion problems, as corners are mesh resolution dependant and illposedness prevent from good mesh convergency.

4.2 Numerical sensivity of the method

Besides of the general flow features, we carried out a numerical sensivity analysis of the inverse data completion problem, in particular minimisation algorithm cost, comparing scaled (eq. 4) and unscaled (eq. 8) equation. As shown on figure 2, the scaling improves greatly the iterations count needed for the minimisation algorithm, i.e. trusted-region Newton method. For a fixed tolerance criterion ($tol_{func} = 10^{-12}$), in the scaled case, the criterion is satisfied with very few iterations (up to 5) and steep slope convergency. Besides additional computations with $K_0 = 100K_0$ and finer mesh ($h = h/5$) show almost independancy of the iterations count against those parameters. Whereas for the unscaled equation, global number of iteration is more than one fold for the reference scaled case (up to 68) and strongly dependant of physical parameter K and mesh size (up to 180). Other results not reported here, with finer meshes and other values of hydraulic conductivity, show the similar trends.

5 CONCLUSION

In this contribution, we present a method for inverse problems on boundaries, called data completion or Cauchy problem, with application in hydrogeology problems. The methodology is applied on a fully satured confined aquifer flow governed by Darcy law. We focus on the effect of an appropriate scaling of the governing equation: numerical results show a strong influence of the scaling on the minimisation of error gap functional in the reformulated Cauchy problem: Mesh size and hydraulic conductivity dependency is almost removed with proper scaling. Inverse problem, which are usually very sensitive to numerical and physical parameters should be reformulated with scaled equations before solving.

Extension of this method to more complex geometries and full tridimensional domains is considered: for this goal, lowering iteration's count in minimisation algorithms is decisive, as finer meshes are needed for full geometric complexity. Application of data completion to mixed formulation of Stokes equation or Darcy law with heteoregeneous and anisotropic hydraulic conductivity field is also considered.

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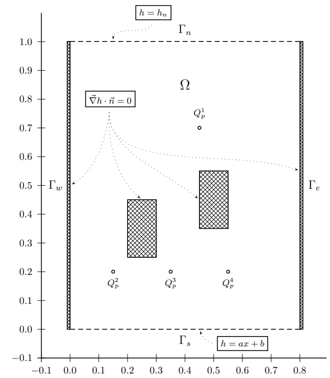


Figure 1: Geometry setup with scaled variables

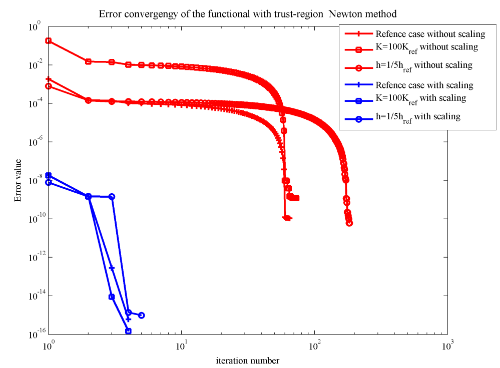
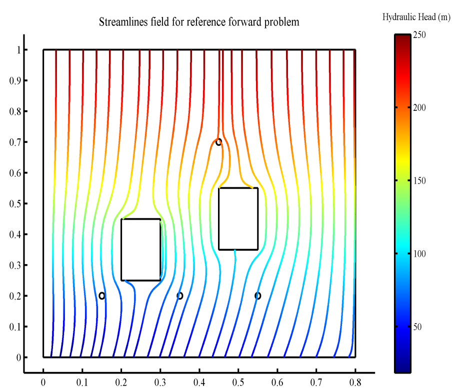
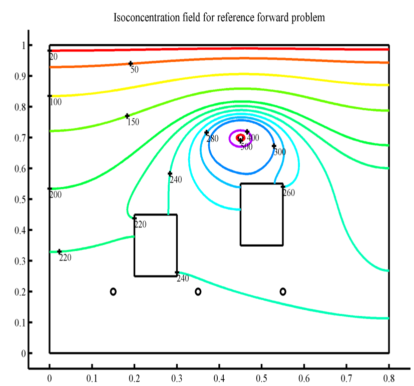


Figure 2: Convergency of trusted-region Newton method with and without equation scaling

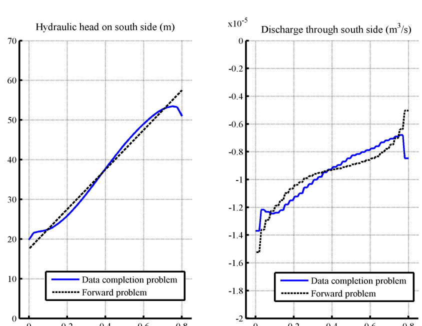


(a) Streamlines field

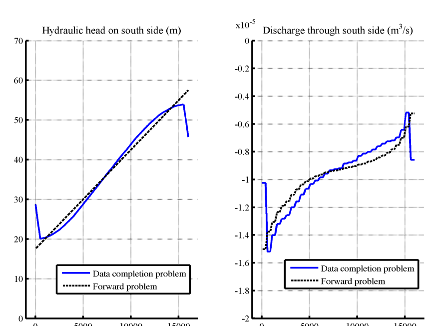


(b) Isoconcentration field

Figure 3: Forward reference solution



(a) Scaled reference solution



(b) Unscaled reference solution

Figure 4: Hydraulic head and discharge on south side