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Key Points:

- We estimate drawdowns caused by hydraulic testing to characterize a complex aquifer system
- We employ a numerical groundwater model to calculate natural heads to de-trend head measurements
- We introduce a corrective factor to remove errors that arise in the modeling and measuring process

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Automatic Calibration of Groundwater Models With Bias Correction and Data Filtering: Working With Drawdown Data

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Abstract The drawdown response to a hydraulic stress contains crucial information to characterize an aquifer. Modeling drawdowns is far easier than modeling heads because they are subject to homogeneous (zero) internal sink/sources, and boundary and initial conditions. The problem lies on the fact that drawdowns are not measured directly but derived from measurements of head fluctuations. Resulting drawdowns may suffer persistent inaccuracies in complex systems with uncertain long-acting external stresses, so that they are affected not only by errors in head measurements, but also in estimates of the natural head evolution. This hinders the use of drawdowns in groundwater models, and forces modelers to employ absolute heads and soft information. In this context, we present a method to filter systematic errors in drawdown data during the calibration of a groundwater model. To do this, we introduce a bias correction term in a composite inverse problem that combines a natural head model with a drawdown model. Since these two models share the same parameters, a two-stage iterative optimization algorithm is developed to jointly estimate the bias, natural trends, and parameters. The method is illustrated by a synthetic example in a heterogeneous aquifer. The example shows that the method converges to the best conditional estimate even when absolute head data is strongly biased. In the same example, we demonstrate that the use of biased absolute head data in the traditional inverse problem can also provide good fittings but, in this case, the bias leads to an incorrect estimation of the transmissivity field.

1. Introduction

Hydraulic tests are typically used to characterize aquifers by analyzing the aquifer response to a known imposed stress. The term test is used here in a broad sense, including any perturbation to the normal functioning of the aquifer, such as pumping tests, stream-stage tests, or in general known water production periods. In any of these cases, the aquifer response to pumping or other hydraulic perturbations contains valuable information about the conceptual model and hydraulic properties (e.g., Domenico et al., 1997; Freeze & Cherry, 1979; Gringarten et al., 2008; Renard, 2006; Trabucchi et al., 2018). The response must be not only properly measured but also processed and interpreted to extract such information. The procedure usually involves fitting water level changes or drawdown to a mathematical model.

The definition of drawdown is well-known, simple and intuitive, but we want to briefly recall it to argue why modeling drawdowns, rather than heads, in the context of transient model calibration may be the best choice for aquifer test interpretation. Drawdown is defined as the difference between two heads: $s = h_n - h$, where h is the actually observed head resulting from the hydraulic test, and h_n is the natural head evolution (i.e., the head that would have been measured if the hydraulic test had not been performed). As a result, as we will show later, drawdown models enjoy homogeneous initial and boundary conditions (i.e., boundary and initial drawdowns are zero and boundary and internal sink/source terms are zero). This is advantageous because it avoids the problem of defining initial and boundary conditions during groundwater modeling (Renard, 2006). Only the stress that causes the drawdown, which should be well known, needs to be specified. At the same time, it allows one to avoid working with absolute heads, which are characterized by weak dependence on hydraulic properties and represent the solution to a differential equation with complex boundary and initial conditions (Renard, 2006). The downside of working with drawdowns lies on the fact that they do not inform directly about the functioning of the aquifer (i.e., where water comes from

or where does it flow to), but only about changes induced by their driving stress. These changes are most informative about transmissivity and storativity in the aquifer, whereas the overall aquifer functioning is controlled by recharge and boundary fluxes and heads, which control natural heads.

However, hydrogeologist often lack direct access to accurate drawdown data. Errors in head measurements and the inherent uncertainty associated with the natural head evolution of the system prevents an adequate estimation of drawdowns. Typical errors in head measurements (h) are those that propagate from inaccurate information on elevation data (datum), sampling procedure or measurement tools (Post & von Asmuth, 2013). These errors generally vary in space and can substantially affect the precision and interpretation of drawdown data and hydraulic gradients (Devlin & McElwee, 2007; Rau et al., 2019; Silliman & Mantz, 2000), increasing the uncertainty in hydraulic properties and the estimation of hydrogeological processes (Sweet et al., 1990). Since these errors are usually hard to recognize, making corrections is always a difficult task (Post & von Asmuth, 2013).

Actually, one of the reasons for working with drawdowns is that constant-in-time head errors are filtered away. The problem arises because error may also be transient. Transient errors may result from unknown external stresses, which typically affect natural heads (h_n), leading to hard-to-predict trends. Taking into account these external effects always deserves special attention during the analysis of hydraulic test data since the determination of the aquifer parameters should be based only on drawdown data derived from the hydraulic test. Actually, it is in this context of aquifer-test analysis that the concept of decomposing water levels into natural heads caused by external forces and drawdowns was initially developed. For short hydraulic tests and relatively large drawdowns, these transient external forces are usually negligible and h_n can be considered constant (typically equal to the initial head). But a de-trending time series analysis is usually required for long-term responses, or even for short term pumping tests when the magnitude of drawdown is comparable to natural head fluctuations (e.g., at distant observation wells; K. J. Halford, 2006; Maliva, 2016).

Fluctuations affecting h_n can be classified as monotonic (e.g., long term trend), rhythmic (e.g., earth and sea tides), non-rhythmic (e.g., response to far away pumping), and singular (e.g., recharge event; K. J. Halford, 2006; Kruseman & de Ridder, 1991). Several filtering methods have been developed to remove rhythmic fluctuations from hydraulic head data (Calvache et al., 2016; Garcia et al., 2013; K. J. Halford, 2006; K. Halford et al., 2012; Zhang et al., 2014, among others). However, there are still not well-developed and consolidated methodologies to treat other fluctuations. In simple systems, h_n is typically estimated by fitting the head data measured prior to the hydraulic test to a linear or exponential function of time (Ferris et al., 1962; Maliva, 2016). Other methods estimate the temporal evolution of h_n by correlating h_n with the water level measured at a distant piezometer, by means of regression, provided that sufficient long pre- and post-test data is available (Kruseman & de Ridder, 1991), kriging (Alcolea et al., 2007; Gómez-Hernández et al., 1997) or neural networks (Coppola et al., 2005).

A more complete analysis can be carried out for de-trending purposes following K. Halford et al. (2012). In this case, the natural head solution is calculated as a linear combination of several time series (e.g., barometric pressure, tidal potential, recharge, external pumping), which are selected by a trial and error procedure aimed at minimizing the differences between h and h_n measured prior to the hydraulic test itself. Nevertheless, these de-trending approaches are quite laborious in complex systems and do not allow estimating natural heads for long time periods. In this case, one is usually forced to characterize the aquifer by developing a numerical groundwater model with head measurements h as observation data in the calibration procedure. This approach avoids most of the filtering problems but not those derived from systematic head measurement errors. Moreover, it requires to have an already good conceptual model of the system with detailed knowledge of the past aquifer stresses.

In this context, we propose a method for data filtering and aquifer characterization capable to: (i) filter the natural trend of hydraulic heads caused by external stresses that can otherwise mask the aquifer test response and complicate modeling efforts (estimate head changes or drawdown); (ii) correct errors derived from field measurements as well as model discrepancies or inadequacies; and (iii) automatically estimate hydraulic parameters through the solution of the inverse problem with drawdown response data. We apply these concept for transient model calibration. The article is organized as it follows. In Section 3, we present

the problem and the methodology. Then, we apply the method to a heterogeneous synthetic aquifer and analyze the results in Sections 4 and 5, where we also discuss some important aspects by comparing the method with traditional approaches. Finally, we highlight the most relevant conclusions in Section 6.

2. Background: Formal Definition of Drawdown

As mentioned in the introduction, we define drawdown as the difference between “natural heads,” h_n (i.e., those that would have occurred if no pumping test had been performed) and actual heads, h (i.e., those that have actually occurred in response to the pumping test and all other driving forces). Natural heads obey the flow equation,

$$S \frac{\partial h_n}{\partial t} = \nabla \cdot (\mathbf{T} \nabla h_n) + w, \quad \forall t > t_0 \quad \mathbf{x} \in \Omega, \quad (1)$$

subject to initial and boundary conditions

$$h_n = h_0, \quad t = t_0 \quad \forall \mathbf{x} \in \Omega, \quad (2)$$

$$\mathbf{T} \nabla h_n \cdot \mathbf{n} = \alpha (h_e - h_n) + q_e, \quad \forall t > t_0 \quad \mathbf{x} \in \Gamma, \quad (3)$$

where Ω is the flow domain and Γ its boundary, $\mathbf{n}$ is the unit normal vector, T is transmissivity, S is storage coefficient, w is the internal sink-source term (e.g., recharge), h_0 is the initial head, and h_e and q_e are the “external” heads and fluxes at the boundaries, respectively. The latter (h_e and q_e), as well as the sink/source term w can vary over time. α controls the type of boundary condition (α equals zero at prescribed flow portions of Γ , α equals ∞ at prescribed head portions, and, else, α is the leakage factor at mixed boundary condition portions of Γ).

Actual heads after pumping start, h , obey the same equation, except for the sink term due to pumping, that is

$$S \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{T} \nabla h) + w - \delta(\mathbf{x}_p) Q, \quad (4)$$

where Q is the pumping rate at $\mathbf{x}_p$ and δ is Dirac's delta. We assume that the test starts at t_i ($t_i > t_0$), so that Q is zero before t_i . This equation is subject to the same initial (Equation 2) and boundary (Equation 3) conditions as Equation 1.

We define drawdown as

$$s = h_n - h, \quad (5)$$

The equation governing s is obtained by simply subtracting Equation 4 from 1, which yields

$$S \frac{\partial s}{\partial t} = \nabla \cdot (\mathbf{T} \nabla s) + \delta(\mathbf{x}_p) Q, \quad (6)$$

The initial and boundary conditions are obtained as (Equation 2) and (Equation 3) minus their h counterparts, which we have not rewritten because they were identical. Therefore, the initial and boundary conditions of s are simply written as,

$$s = 0, \quad t = t_i, \quad (7)$$

$$\mathbf{T} \nabla s \cdot \mathbf{n} = -\alpha s. \quad (8)$$

Note that this definition requires the equation to be linear and time dependence of boundary conditions and internal sink-sources to be known. The advantage of defining drawdowns according to Equation 5 is that

Figure 1. Drawdown (s) is the difference between natural heads (h_n , black line, would have been observed without pumping) and the actual heads (h , red line). The evolution of natural heads may have to be modeled for proper calculation of drawdowns. Modeling may be hindered by bias (a) affecting measurements (h_m , circles).

all flow terms and external heads have vanished in Equations 6–8. That is, the drawdown model is identical to that of natural heads, but setting to zero all source terms, and boundary heads and fluxes. Only the type of boundary conditions, as specified by α , and the hydraulic test driving force (Q in 6) need to be kept. Note, also, that this definition allows one to relax the traditional requirements of pumping tests. That is, the aquifer does not need to be of infinite extent or be at steady-state conditions, etc. Obviously, the only problem is that this definition is based on an unobservable quantity, h_n . The problem is addressed in Section 3 below.

3. Problem Statement and Methodology

3.1. Bias Correction

Let us consider the interpretation of a hydraulic test, the head response of which is affected by strong external effects that prevent a clear estimation of the change in hydraulic head produced only by the aquifer test. The aquifer test starts at time $t = t_i$. Hydraulic head evolution is recorded at several observation points before and during the test. We wish to filter head data to obtain drawdowns, that is, the aquifer response to the aquifer test at the observation points, and use the resulting filtered data to calibrate a groundwater model. In the following, we will show that these two processes (filtering and calibration) are not independent from one another and should therefore be treated jointly.

Let us start by defining the time series of drawdown data from Equation 5 as the change in groundwater head with respect to natural head conditions determined by the head solution resulting from all system stresses taking place in the aquifer rather than the hydraulic test itself,

$$\mathbf{s} = \mathbf{h}_n - \mathbf{h}_m, \quad (9)$$

where $\mathbf{h}_m$ is the time series of head measurements at observation points, and $\mathbf{h}_n$ is the time series of natural head solutions at observation points.

The proposed method is based on assuming that the best approach for estimating $\mathbf{h}_n$ is a groundwater model itself, since it incorporates the underlying physics in the problem. However, this poses important challenges since both $\mathbf{s}$ and $\mathbf{h}_n$ depend on the unknown model, which is not exempt from uncertainties. As a result, flow models often exhibit systematic errors in the temporal evolution of heads simulated at specific points. These systematic discrepancies can be mainly attributed to two sources of errors: model bias and errors in field measurements. Model bias at observation points stems from structural and parametric uncertainties. That is, uncertainties associated with the underlying physics of the problem, which are not properly represented in the conceptual model (e.g., unknown recent past stresses, initial and boundary conditions and so on), and uncertainties associated with the spatial distribution of aquifer parameters such as the transmissivity, which is known to vary orders of magnitude even in moderately homogeneous systems. At the same time, errors in head measurements (e.g., elevation data) can also generate systematic discrepancies between flow models and observations. The accuracy of the spatial position information can emphasize these errors, from which we could obtain, for example, wrong flow directions (or gradient), possibly inconsistent with the boundary conditions set in the model.

To overcome these difficulties, we propose to estimate drawdowns using a bias correction term (Figure 1) defined by an unknown vector $\mathbf{a}$ of biases at every observation point,

$$\mathbf{s}_e = \mathbf{h}_n - \mathbf{h}_m + \mathbf{a}, \quad (10)$$

The inverse problem is then posed as an optimization procedure aimed at finding not only the parameters, but also the correction terms that provide a good model fit. Carrera and Neuman (1986) and Hill (1992) already recognized the need of minimizing the biases between observed and simulated time series. Still, automatic calibration procedures nowadays consider parameter calibration only, without the incorporation/quantification of bias correction.

3.2. Calibration

In this section, we formalize the inclusion of the bias correction term in the automatic calibration process. Calibration of groundwater models through optimization methods typically minimize an objective function that contains a formal goodness of fit criterion, often the weighted sum of square head errors, and a regularization term that accounts for prior parameter information (e.g., Carrera & Neuman, 1986). In this case, considering that drawdown is estimated by Equation 10, the model with bias correction is $\mathbf{h}(\mathbf{p}) + \mathbf{a}$ and the objective function can be written as,

$$F(\mathbf{p}, \mathbf{a}) = F_h(\mathbf{p}, \mathbf{a}) + \lambda F_p(\mathbf{p}), \quad (11)$$

where

$$F_h(\mathbf{p}, \mathbf{a}) = (\mathbf{h}(\mathbf{p}) - \mathbf{h}_m + \mathbf{a})^t \mathbf{V}_h^{-1} (\mathbf{h}(\mathbf{p}) - \mathbf{h}_m + \mathbf{a}), \quad (12)$$

$$F_p(\mathbf{p}) = (\mathbf{p} - \mathbf{p}_m)^t \mathbf{V}_p^{-1} (\mathbf{p} - \mathbf{p}_m). \quad (13)$$

Here, $\mathbf{p}$ is the vector of model parameters, λ is the plausibility factor, $\mathbf{h}(\mathbf{p})$ is the groundwater model solution evaluated at the observation points at multiple observation times, $\mathbf{p}_m$ is the vector of prior information about the parameters, and $\mathbf{V}_h$ and $\mathbf{V}_p$ the corresponding covariance functions of errors in heads and parameters, respectively. From this, the calibration-optimization procedure can be formulated as a minimization problem, i.e., finding the set of parameters and bias correction terms that minimize the objective function,

$$(\hat{\mathbf{p}}, \hat{\mathbf{a}}) = \arg \min_{(\mathbf{p}, \mathbf{a})} F(\mathbf{p}, \mathbf{a}). \quad (14)$$

We note that the bias correction prevents systematic errors to control the objective function, which may preclude a good estimation of parameters and/or a good model fit.

Following the idea that drawdown response contains information about parameters within the aquifer that is more valuable and with less measurement errors than absolute heads, we propose a new objective function with two terms. The contribution associated with the discrepancy between simulated and observed natural heads before the start of the hydraulic test F_{h_n} , and the contribution of drawdown errors during the hydraulic test itself F_s (including the recovery stage).

$$F(\mathbf{p}, \mathbf{a}) = F_{h_n}(\mathbf{p}, \mathbf{a}) + F_s(\mathbf{p}, \mathbf{a}) + \lambda F_p(\mathbf{p}), \quad (15)$$

where

$$F_{h_n}(\mathbf{p}, \mathbf{a}) = (\mathbf{h}_n(\mathbf{p}) - \mathbf{h}_m + \mathbf{a})^t \mathbf{V}_h^{-1} (\mathbf{h}_n(\mathbf{p}) - \mathbf{h}_m + \mathbf{a}), \quad t < t_i, \quad (16)$$

$$F_s(\mathbf{p}, \mathbf{a}) = (\mathbf{s}(\mathbf{p}) - \mathbf{s}_e)^t \mathbf{V}_s^{-1} (\mathbf{s}(\mathbf{p}) - \mathbf{s}_e), \quad t \geq t_i, \quad (17)$$

Introducing (Equation 10) into (Equation 17) we have

$$F_s(\mathbf{p}, \mathbf{a}) = (\mathbf{s}(\mathbf{p}) - \mathbf{h}_n(\mathbf{p}) + \mathbf{h}_m - \mathbf{a})^t \mathbf{V}_s^{-1} (\mathbf{s}(\mathbf{p}) - \mathbf{h}_n(\mathbf{p}) + \mathbf{h}_m - \mathbf{a}), \quad t \geq t_i, \quad (18)$$

This formulation deserves several considerations. First, the evaluation of the objective function $F(\mathbf{p}, \mathbf{a})$ requires two different flow models. One standard model to simulate the natural evolution of the system $\mathbf{h}_n(\mathbf{p})$ (without the hydraulic test), and another to simulate the drawdown response $\mathbf{s}(\mathbf{p})$ to the hydraulic test. These two models share the same parameters and therefore the problem cannot be in general decomposed into two separate entities, which is the normal practice nowadays. Second, written this way, the covariance matrix of drawdown errors can express that drawdown data or changes in heads can be measured more

accurately than absolute heads, if necessary. Third, the method is only applicable to linear problems. One option for non-linear problems (e.g., if T is a function of h) is to linearize the equation by treating the properties as time dependent (e.g., substituting $T(h)$ by $T(h^{k-1})$, where h^{k-1} is the head in the previous inversion iteration, which requires storing all heads from the previous iteration).

3.3. Algorithm

The strategy used to solve the optimization problem given by 14 is that of an iterative two-stage optimization process. It consists in taking the system to a first mid-step position during which the bias correction is determined by assuming that the parameters are known. Then, we use the estimated bias correction to take the system to its final stage by minimizing drawdown errors through parameters estimation. These two stages are repeated until convergence. Formally, the procedure can be written as

$$\mathbf{a}^{k+1/2} = \arg \min_{(\mathbf{a})} F_{h_n}(\mathbf{p}^k, \mathbf{a}^k) \quad t < t_i, \quad (19)$$

$$\mathbf{p}^{k+1} = \arg \min_{(\mathbf{p})} F_s(\mathbf{p}^k, \mathbf{a}^{k+1/2}) + \lambda F_p(\mathbf{p}^k) \quad t > t_i, \quad (20)$$

where k denotes the iteration index.

Before initializing the process, we assume that we have collected all available information to develop an initial conceptual model of the system. We assume as well that we have performed a hydraulic test and collected field data before and during the test (e.g., head measurements and stresses data, such as pumping rates or weather data). With these assumptions, the algorithm consists in the following steps, also illustrated in Figures 2 and 3:

1. Initialize the process at $k = 0$, defining $\mathbf{p}^0$.
2. Solve the natural head model to get $\mathbf{h}_n^k = \mathbf{h}_n(\mathbf{p}^k)$.
3. Estimate the bias corrective factor $\mathbf{a}^{k+1/2}$ minimizing $F_{h_n}(\mathbf{p}^k, \mathbf{a}^k)$ at each observation point and for $t < t_i$.
4. Compute drawdowns as $\mathbf{s}_e^k = \mathbf{h}_n^k - \mathbf{h}_m + \mathbf{a}^{k+1/2}$.
5. Develop the drawdown model and calibrate $\mathbf{p}^{k+1}$ with computed drawdowns $\mathbf{s}_e^k$, by minimizing $F_s(\mathbf{p}^k, \mathbf{a}^{k+1/2}) + \lambda F_p(\mathbf{p}^k)$ at each observation point and for $t > t_i$.
6. Convergence check: if $\|\mathbf{p}^{k+1} - \mathbf{p}^k\| < \epsilon_p$ and $\|\mathbf{s}^{k+1} - \mathbf{s}^k\| < \epsilon_s$, where ϵ_p and ϵ_s are the convergence tolerances of parameters and drawdowns respectively, the iterative process end; else go to step 2.

The first optimization can be seen as curve-fitting the head data $\mathbf{h}_m$ observed at a given point prior to the hydraulic test with a known natural head solution $\mathbf{h}_n$ by minimizing the vertical displacement between $\mathbf{h}_m$ and $\mathbf{h}_n$ (the bias correction, considered as a constant over time). Estimating the bias as constant, we are assuming that the trend (but not necessary the absolute value) of head measurements and that of calculated natural heads is correct. We are neglecting errors due to possible head measurement drifts and those derived from not knowing some natural head drift. The resulting bias correction factor $\mathbf{a}$ is then used, jointly with the natural head solution and head measurements, to estimate the drawdown $\mathbf{s}_e$ during the hydraulic test period. The second optimization is the solution of the inverse problem written in terms of drawdowns (just calculated). Estimated parameters $\mathbf{p}$ are then employed to update the natural head model. At first glance, the procedure for estimating $\mathbf{a}$ seems similar to those in which time series are explicitly adjusted to remove the bias. But differences arise as $\mathbf{a}$ is estimated using calculated $\mathbf{h}_n$ which depends on hydraulic parameter estimates. As parameter estimates improve throughout the iterations, $\mathbf{h}_n$ improves and the bias changes, leading to improved drawdown estimates. The iterative process will stop when no more relevant changes are seen in drawdown calculation. In the following, we show that this iterative procedure converges to the true solution while removing model bias and measurement errors.

Figure 2. Schematic description of the proposed method. The final outputs from the iterative process are highlighted in dark red: de-trended and corrected drawdown s_e and aquifer parameters p .

4. Application

We investigate the capabilities of the proposed method and some of its most important aspects. For this purpose, we build a synthetic heterogeneous aquifer characterized by long-acting multiple stresses and we simulate a hydraulic test (4.1). We then use the simulated head values obtained at few points to test the proposed method. Systematic errors were added to the simulated head values to bias the head measurements (4.2). We finally compare these results with those obtained from the use of absolute head data in the traditional inverse modeling approach. In this case, biased and non-biased absolute head data are used (4.3). The latter provides an ideal parameter estimation solution, as we consider that errors in head measurements are zero.

4.1. Synthetic Scenario

We consider a rectangular synthetic aquifer with dimensions of $30 \times 30 \text{ km}^2$ (Figure 4). The flow model is implemented in TRANSIN, a free finite element code developed by Medina & Carrera (2005). The domain is discretized in 8,032 triangular elements. The size of the elements is 0.25 km in the hydraulic test area and gradually increases toward the domain boundaries. The model simulates the fluctuation history of

Figure 3. Drawdown estimation. On the left, biased heads measured in the field (red dots) and simulated natural head h_n calculated by means of a flow model (black dash line). On the right, bias correction a is added and the drawdown s_e during hydraulic test ($t \geq t_i$) is underlined (green arrow).

hydraulic heads over a period of 1,740 days, discretized in 787 time-steps. A variable time-step increment adjusted to stress conditions is used to properly simulate rapid head changes.

The decimal log of transmissivity is considered to vary in space following a multi-Gaussian random space function model characterized by an isotropic spherical covariance function with zero mean and a variance of one. The integral scale is 4 km. One realization of a sequential Gaussian simulation generated with SGEMS (Remy et al., 2009) was chosen to represent the transmissivity field (Figure 4). The storage coefficient is assumed constant in the whole domain, i.e., $S = 0.0001$. The East and West boundaries are impermeable. The North and South boundaries are characterized by prescribed hydraulic heads. Boundary heads increase monotonically (but not linearly) from 35 to 35.5 m during the simulation in the North boundary (presented in Figure 5), whereas head is constant ($h = 30$ m) at the South. Head fluctuations during the simulation are caused by three important rainfall events and five production wells operating in the area with variable flow rates. The location of these wells is shown in Figure 4.

A network of 16 monitoring piezometers are installed in the area and start recording water levels at time $t_m = 540$ days with a constant sampling period of 10 days. For each piezometer, water level measurements are biased by adding a uniform random noise $[-0.2, 0.2]$ and an arbitrary positive systematic error $B(\mathbf{x})$ to the simulated heads. The imposed systematic errors $B(\mathbf{x})$ are given in Figure 4. The operation of all production wells after a time $t_i = 790$ days generates an important stress to the aquifer under monitoring conditions

Figure 4. Aquifer system domain. Left, transmissivity field, location of pumping wells (white stars), point measurements of transmissivity (white circles). Right, location of pilot points (black dots) and observation points (red circles with a diameter proportional to the bias of head measurements).

Figure 5. Anthropogenic and natural factors that cause head changes in the aquifer. Above, the pumping rate time series of the five wells installed in the area. Below, the time series representing the rainfall events (left axis) and the North boundary head evolution (right axis).

(see Figure 5). Consequently, the period (t_i, t_f) is considered to act as a hydraulic test from which one wishes to characterize the aquifer.

We assume to know 2 point measurements of transmissivity (shown in Figure 4), a rough estimation of the storage coefficient ($S = 0.01$), the true head values of the southern boundary ($h = 30$ m), and two head measurements taken at different times in the northern boundary ($h(t_m) = 35$ m and $h(t_f) = 35.5$ m).

4.2. The Filtering-Corrective Method

Our method requires two groundwater models, the natural head model that represents the natural trend of heads and the drawdown model. The specific features of these models for the application of the filtering-corrective method proposed are described below:

Naturalheadmodel. The initial transmissivity field $T^{k=0}(\mathbf{x})$ is estimated by ordinary kriging using the two available measurements (T_1 and T_2). For this, we assumed that the geostatistical model is perfectly known. The initial storage coefficient is set to $S^{k=0} = 0.01$ (Figure 6). Boundary conditions are identical to those of the true model, except that northern head is assumed to increase linearly over time, from $h(t_0) = 35$ m to $h(t_f) = 35.5$ m. In order to represent a typical scenario, we consider that the initial condition of the model is unknown (Gupta et al., 2012; Seck et al., 2015). To handle this, following the normal practice, we go back in the past with the model for a time period prior to the calibration period to attenuate the spurious transient response given by possibly wrong initial conditions. Thus, the model simulates the fluctuation history of natural heads h_n from $t_0 = 240$ to $t_f = 1,740$ over a period of 1,500 days. The pumping history at time $t < t_0$ is unknown and consequently initial heads at $t = t_0$ are determined by a blind steady-state solution (without considering extractions or recharge stresses). The time and spatial discretization coincide with those of the synthetic scenario. Rainfall events and pumping well extractions control the transient natural head

evolution. We consider the two recharge events and pumping rates up to $t = t_i$ shown in Figure 5, which are identical to those of the synthetic scenario. In the optimization process, we consider h_n and h_m data from t_m to t_i . We build the diagonal matrix $\mathbf{V}_h$ assigning a unit weight to all available observations, except for the last two measures closest to time t_i , to which a weight of 10 is assigned. In this way we want to ensure drawdowns to be almost zero at the beginning of the hydraulic test.

Drawdown model. The model simulates the fluctuation history of drawdown over a period of 950 days (from $t_i = 790$ to $t_f = 1,740$), discretized in 186 time-steps. Time and spatial discretization coincide with those of the synthetic scenario. Boundary and initial conditions are easily set as discussed in Section 2: no flow boundaries (*East* and *West*) do not change, prescribed head boundaries (*South* and *Northern*) are prescribed zero head boundaries, and the initial drawdown is zero everywhere. Only pumping rates during hydraulic test period (from t_i to t_f) are considered. They are simulated prescribing the flow rate with time according to Figure 5. The optimization process is carried out applying both the classical inverse problem (zonal parametrization) and the regularized pilot points method (Alcolea et al., 2006), with 225 pilot points uniformly distributed throughout the model area (shown in Figure 4). The former is used for storage coefficient estimation, as the parameter is spatially homogeneous, while the latter is used to estimate the transmissivity field through conditional estimation. We employ the same geostatistical model as before. The covariance function $\mathbf{V}_s$ is constructed by assigning a unit weight to all observations while the plausibility term is $\lambda = 1$.

It could be rightfully argued that structural model errors in this synthetic example are modest. They are restricted to the neglecting of small scale variability, the erroneous initial condition and the time variability of the North boundary heads. These types of uncertainties are frequent. But other sources of model error may also affect real models: flow dimension (the Dupuit approximation may not be valid), model extent (location of boundaries often uncertain), etc. We have opted for relatively simple errors so as to facilitate the discussion and because model errors are usually reduced during the modeling process, which would be hard to reproduce in a synthetic example.

4.3. Traditional Calibration with Head Data

We use absolute biased head measurements h_m in the traditional inverse modeling approach for estimating hydraulic parameters and compare the results with the ones obtained from the application of the proposed method. The model simulates the fluctuation history of hydraulic heads over a period of 1,500 days, from t_0 to t_f . Time and spatial discretization coincide with those of the synthetic aquifer. Initial and boundary conditions as well as the initial hydraulic parameters are the same as those used for the natural head model. Since we simulate the overall behavior of the system, we consider all the stresses that affect the aquifer: recharge events and production wells, including the hydraulic test pumping rates (Figure 5). We calibrate the model employing two different sets of head observations: the biased head measurements used in the natural head model, and the exact head measurements obtained directly from the true aquifer simulation. In both cases, the model is calibrated in the time period between t_m and t_f .

5. Results and Discussion

5.1. Overall Performance

We start by analyzing the overall performance of the proposed method. Figure 6 displays the transmissivity field and drawdown estimates obtained at three iterations (0, 1, and 7) of the two-stage optimization method. The figure also compares these results with the true solution. We first note that the process converges in just seven iterations. The most important change in the parameter estimates (including drawdown) occurs in the first iteration. The storage coefficient decreases two orders of magnitude approaching the real value, and the transmissivity field considerably changes in terms of both spatial patterns and absolute values toward the true solution. In subsequent iterations, S and $T(\mathbf{x})$ improve but field patterns are maintained. Comparison with the true solution points out that the method can identify the overall trends of transmissivity variation. The final drawdown estimates obtained after seven iterations resemble the true solution, except in the central eastern area of the domain.

The estimated transmissivity map is smooth because the pilot point method is coupled with conditional estimation. Small-scale variations cannot be properly represented by the conditional estimation pilot point

Figure 6. Sequence of estimated hydraulic parameters (T and S) and drawdown fields along the iterative process. The top row contains the initial data ($k = 0$, i.e., the hydraulic parameters used at the beginning of the modeling phase for the natural head model). The next two rows contain the results of the first ($k = 1$) and last ($k = 7$) iterations, respectively. The “real” aquifer data are plotted in the bottom row for comparison purposes. The estimated aquifer behavior (drawdown) resemble the real one. At the same time, the zones of high and low permeability are well captured, even if conditional estimation is not capable of reproducing small scale variability.

method. Still variability patterns are well captured in the central portion and become more blurred toward the boundaries for several reasons. First, no observation points are available, so that there is a strip of domain that remains “unforked” (i.e., without observations on both sides) near the boundaries. Second, even if observations had been available at the boundary, transmissivity estimates would have remained uncertain because drawdowns are less informative about transmissivity. Near no flow boundaries, the normal

Figure 7. Comparison of the three calibrations (A, top row, traditional inversion with noisy and biased measurements; B, middle row, same with exact measurements; and, C, proposed method). The comparison is made in terms of estimated transmissivity (decimal logarithm) $\log_{10} T$ error histograms (left column), transmissivity fields (middle column) and measured (dots) and computed (red line) hydrographs at one observation point (right column). The hydrograph fits are analogous, but error histograms for the “ideal” (exact head data) top row and the proposed method are smaller than with traditional inversion.

component of the gradient is zero regardless of the transmissivity value. Near zero drawdown boundaries, drawdown will be small regardless of the transmissivity value. Observations near the boundary can be relevant to understand the type of boundary condition and to understand natural heads, but they are not very informative about transmissivity. Comparing the estimated S and $T(\mathbf{x})$ with estimates obtained using directly head data may be more appropriate than comparing them with true values.

Figure 7 displays the estimated transmissivity fields and histograms of errors obtained by the use of head data in the traditional inverse modeling approach. The traditional approach with exact (non-biased and error free) head measurements provides the “best” estimate of the transmissivity field conditioned to head data and transmissivity values because in this case head errors were neglected. Therefore, we could qualitatively state that the estimated field recovers all the information contained in the data. The filtering-corrective method yields results that are similar to this best solution, which allows us to conclude that the method is capable of properly filtering systematic errors in head data without sacrificing fitting accuracy. On the contrary, the traditional approach with biased head measurements converges to an incorrect solution of the transmissivity field with an important overestimation of transmissivity in extensive areas of the domain. Note though that the goodness-of-fit is still similar. These results are supported by quantitative measures given by the histograms of the transmissivity error, which is defined by $\epsilon(\mathbf{x}) = \ln T^{\text{true}}(\mathbf{x}) - \ln T^{(7)}(\mathbf{x})$.

Figure 8. Drawdowns (above) and natural heads (below) calculated along the iterative process in observation well OW12 are presented. Real solutions (red dots) are also plotted for comparison purposes.

The filtering-corrective method and the traditional approach with exact measurements follow a normal distribution centered close to zero with a standard deviation of about $\sigma \approx 0.9$. Instead, the traditional approach with biased measures exhibit an asymmetric distribution centered at $\mu = -0.23$ with $\sigma = 1.1$.

In sum, results demonstrate that the filtering-corrective method should be the choice for groundwater modeling calibration when head measures are systematically biased. In this case, the method is capable to automatically de-trend natural heads and estimate drawdown data for accurate aquifer characterization. Otherwise, caution should be taken when dealing with systematic head errors in groundwater models since these errors can lead to a poor estimation of transmissivity even when a good fit is obtained. Results also show further evidence of what is already known, namely that a model cannot be trusted just for having a good fit.

5.2. Natural Heads, Drawdowns, and Bias Correction

We analyze the evolution of the estimated natural head, drawdown, and bias correction obtained by the filtering-corrective method to get further insight. Figure 8 displays the natural heads and drawdown hydrographs at one observation well for several iterations. Consistently with previous results, the first iterations ($k = 0, 1, 2$) exhibit a great improvement. The estimated natural head approach the real solution, never reaching it because of systematic errors, but reproducing well the relative head variations in the system.

This is actually a very nice feature of the method proposed, i.e., we can remove the bias and calibrate the model only through relative heads. In general, small discrepancies can be observed at early times (up to time t_m) due to a poor representation of the initial condition in the natural head model but an almost constant error is displayed for longer times $t > t_m$ (Figure 8). These model errors partially reflect that head observations are systematically biased. Most importantly, the estimated drawdown data converge satisfactorily to the real solution (Figure 8), meaning that both modeling and measurement errors have been corrected. It is important to underline that in general, the broader and more correct the knowledge of stresses (in particular those that generate long transient responses), the better the estimate of natural heads. A poor definition of the stresses could rebound on hydraulic parameter estimates, without affecting the quality of the calibration (Figure 7). An additional note of caution is required regarding the impact of high frequency head fluctuations on long-term large scale models as the one discussed here. Typically, they are driven by fluctuating stresses (Earth or sea tides, daily fluctuations in pumping, barometric pressure, etc.) that are rarely included in models because they are hard to model, because their impact is relatively small, because they dissipate quickly, because they reflect local parameters that may not be relevant for large scale models, and because they are filtered away when averaging dense time series data. Still, they may be relevant in numerous occasions: when drawdowns are small (low Q/T ratio or distant piezometers), specially for short term, or when measurements are scattered, so that averaging them is not possible. A number of methods are available in such cases (Del Val, 2020; Garcia et al., 2013; K. Halford et al., 2012).

Figure 9. For each observation well, the evolution of the absolute difference between imposed error $B(x)$ and estimated bias correction $a(x)$ is presented. Throughout the iterations, in some wells the corrective factor get closer and finally approaches $B(x)$. Others present an estimated bias that initially tends to $B(x)$ but finally converges to another value (e.g., OW8 and OW12). The difference that remains probably acts as correction for errors not related to $B(x)$, as, for example, modeling errors.

Due to its importance in the overall process and its dual role in dealing with measurements and model errors, we analyze the evolution of the correction term $a(x)$ during the iterative process. For this purpose, we show in Figure 9 the evolution of $\Delta = |B(x) - a(x)|$ with the number of iterations at each observation well. Results show an important decrease of Δ in the first iterations during which model parameters are being actively adjusted based on relative heads. After a few iterations, the parameters reach a final solution and Δ seems to stabilize to a constant value. In

some cases, for example, in observation wells OW1, OW5, and OW6, the correction term $a(\mathbf{x})$ approaches to $B(\mathbf{x})$, meaning that model errors no longer affect the estimated natural head in these zones. However, an appreciable difference remains in other observation wells. Most of them are located in the north-eastern part of the domain where boundary conditions control the outcome of the model. Here, the correction term $a(\mathbf{x})$ accounts also for structural model errors (neglecting small scale variability, errors in initial conditions and time dependence of North boundary head) that cannot be resolved.

5.3. Discussion

The proposed method can be viewed as splitting the complex modeling problem (model construction and parameter estimation) into two simpler problems: the natural heads model, which is sensitive to boundary and initial conditions, and the drawdowns model, which is sensitive to aquifer parameters within the model domain. While drawdowns have been widely used in groundwater hydrology, primarily for pumping test interpretation, the proposed method allows generalizing the problem to large scale regional models. In this context, the method is similar to what K. J. Halford and Jackson (2020) term “stress-response models,” which isolate the response of portions of the model to known stresses, thus facilitating model construction. The question may be raised as to when is this splitting favorable and whether solving the full problem might be better. We do not have a straight answer to this, but we feel that two criteria should be followed: knowledge and sensitivity. First, stresses should be well known for the drawdown (stress-response) model to be reliable. Second, sensitivities should be quite well separated for the problem to converge. The natural heads model is primarily sensitive to boundary and initial conditions. The drawdowns model is basically sensitive to hydraulic parameters within the model domain and, possibly, the type of boundary condition, but not the actual value of boundary heads and fluxes.

6. Conclusions

Systematic errors in drawdown data driven by uncertain past stresses and errors in head measurements typically hinder the use of drawdown data in complex aquifer systems. We have presented a filtering-corrective method for automatic calibration of groundwater models that is capable of detrending natural heads and correcting head measurements with a bias correction term. This procedure is shown to improve drawdown estimates and, consequently, the estimated properties of the aquifer. The method combines a natural head model with a drawdown model in the same inverse problem. Since these two models depend on the same parameters, a two-stage iterative optimization algorithm has been developed to jointly estimate the bias and the parameters.

Among the features of the proposed method we highlight the following findings:

- First, the use of a groundwater natural head model for h_n estimation. Instead of using statistical methods or data from distant wells, we have chosen to calculate h_n , necessary to de-trend head measurements, through a numerical flow model. Applying the proposed method is thus possible to take into consideration aquifer heterogeneity and the different influence that stresses have on observation points, given the spatial variability of the hydraulic parameters.
- The correction term $a(x)$ is crucial for a good estimation of drawdowns. Basically, we trust the relative variations of both calculated natural heads and head measurements, but not their absolute values that are therefore corrected applying the bias correction.
- Dividing the process into two groundwater models made it possible to attenuate the effect of uncertainties associated with the definition of boundary and initial conditions in the natural head model.
- At the same time, no uncertainties characterize boundary and initial conditions in the drawdown model, where hydraulic properties have to be estimated. Thus, the optimization process is not directly affected by these uncertainties.

The comparison with traditional approach also highlighted some interesting and other well-known aspects of inversion.

- Applying the proposed method has allowed us to reach the same quality of results that could be obtained if we had used exact (not-biased) field measurements, which is practically impossible.
- Trying to calibrate a flow model with wrong (biased) observation data could lead to very good fits, with parameters that are far from the true ones.
- The inverse problem is a very powerful tool for aquifer characterization, but results may be affected by errors in observation data and conceptual model. Therefore, results consistency should be always checked with independent information.

The fact that the corrective term is properly estimated improves the quality of both natural head measurements and models. This is important because drawdowns are relevant for estimating hydraulic parameters (T and S), but by themselves contain no information of where and how much groundwater flows from/to, which is the ultimate goal of modeling.

Data Availability Statement

All data used was synthetically generated. The paper provides all the information needed to replicate them. If the reader has any data-related inquiries, please contact the corresponding author.

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