OPTIMAL ESTIMATION OF HYDRAULIC CONDUCTIVITY AND BOUNDARY CONDITION UNDER STEADY-STATE SIMULATION

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Summary. The first step of aquifer parameter and dependent variable estimation based on hydraulic modeling is generally to choose the best steady-state condition for the set time period. This situation will occur when the hydraulic head variation for observed wells is at minimum. The aim of this study was to use and develop a finite-difference groundwater model, MODFLOW 2000, to define the best parameter estimation when all residual errors are at minimum for different cases considering accurate confidence intervals and sensitivity analysis. Ten different steady-state conditions were obtained during the given time period with no recharge. All these steady-state conditions were simulated and analyzed using the groundwater model for the study area. Based on the resulting confidence intervals it appears that results are statistically robust and optimal estimated parameters were selected based on minimum groundwater level change ($dh$) for successive months.

INTRODUCTION

A way to recover scarce water resources in arid and semiarid areas is to use artificial recharge of groundwater. Due to very small fresh water resources in the Gareh-Bygone Plain (GBP) in hyper-arid southern Iran, a floodwater spreading system was established between 1983 and 1987. However, after 25 years from its operation there has still not been any quantitative evaluation for the performance of the recharge system. As for most groundwater systems, hydraulic conductivity, recharge, and other aquifer variables cannot be measured directly in an accurate way. In general, the first step in estimation of aquifer parameters and dependent variables by groundwater models is to choose the best steady-state condition during a given time period. Also, calibration periods should be carried out for several different years to better estimate the hydraulic conductivity and boundary conditions for steady-state.

One way to simplify the model calibration is to choose steady-state time intervals when aquifer parameters such as storativity and storage coefficient can be ignored. The estimated parameters can then be transferred to transient or unsteady models. In steady-state intervals the heads in observation wells and the flow rates are almost constant over time. However, in reality this situation is not common. Thus, as an approximate method, steady-state condition in the groundwater system could be assumed during time intervals when there is a minimum hydraulic head variation for the observation wells. Due to uncertainties in data, the estimated parameters obtained from groundwater model calibration are generally uncertain. Therefore, the estimated parameters must be presented with certain confidence intervals.

The general objective of the present work is to apply and evaluate the above general methodology for the GBP groundwater system with limited field observations. Consequently, partial objectives are to find the best steady-state condition to estimate the aquifer parameters such as hydraulic conductivity by using the defined boundary conditions in order to analyze the model precision and model sensitivity.
DESCRIPTION OF STUDY AREA AND OBSERVATIONS
The Unconfined Gareh-Bygone Aquifer

The study area is located 200 km southeast of Shiraz city, in southern Iran (28°34´ and 28°41´N, 53°52´ and 54°00´E at an altitude of 1140 m above mean sea level; Fig. 1). According to the FAO climate classification, this region is extremely dry with a mean annual precipitation of 243 mm and the Class A Pan evaporation about of 3200 mm per year. The GBP is a 6000 ha expanse with colluvial soils and old debris cones of low slope covered with aeolian sand. The thickness of the aquifer ranges from practically zero at the foothills to about 43 m at the center of the GBP. The upper 12 m alluvium contains fine sand and gravel. The deeper layers consist of medium and coarse sand, gravel, and stones of different size, up to 0.4 m in diameter.

Figure 1 Location of study area in southern Iran.

A floodwater spreading system (FSS) to artificially recharge of groundwater was established in this area between 1983 and 1987 on about 2000 ha. This system diverts surface runoff from ephemeral rivers to the plain which then infiltrates and recharges groundwater and improves the vegetation cover. Despite the artificial recharge by the FSS, over-exploitation of groundwater has lead to a water table drop of about 8 m during the last 10 years in the study area (Fig. 2b).

Observations

In the GBP, hydraulic head has been recorded monthly since 1993 by the Fasa District Water Organization. Observations from four wells located within the GBP during 14 years between 1993 and 2007 were used in this study. Two ephemeral rivers, Bisheh-Zard and Tchah-Qootch, are the main sources of surface water for the GBP in the case of flood that come from the upper catchments named Bisheh-Zard and Tchah-Qootch sub basins, to the GBP. These were completely dry during the simulation period.

MODEL DESIGN

A conceptual groundwater model represents the groundwater system in a simplified way. Unrealistic results are often due to over-simplification and/or lack of detailed observations. Hence, in groundwater modeling it is important that the conceptual model is well represented by a valid hydrogeologic system and well defined boundary conditions for the study area. A widely used commercial groundwater flow model MODFLOW-2000 within the GMS software was selected to simulate and define the parameter estimation and boundary conditions. The GBP with 6000 ha was discretized into uniform square grids with side length 250 m into a finite-difference three-dimensional model. Geological investigation prepared from well logs showed that the GBP could be represented by
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only one layer with a red clay bedrock boundary at the bottom. Four observation wells were used to build the conceptual model for a fourteen-year period. Due to the limited number of observation wells and homogeneity of the geologic formation in the GBP, the Thiessen method was used to define the representative zones around each observation well (Z1, Z2, Z3, and Z4). The model was calibrated with observed hydraulic head at the observation wells in each zone.

**Steady-state groundwater conditions**

Todd and Mays\(^9\) stated that steady flow implies that no change occurs with time. This situation will occur when the hydraulic head variation for observed wells is at minimum. The partial-differential equation for groundwater flow used in MODFLOW is\(^8\):

\[
\frac{\partial}{\partial x} \left[ K_{xx} \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial y} \left[ K_{yy} \frac{\partial h}{\partial y} \right] + \frac{\partial}{\partial z} \left[ K_{zz} \frac{\partial h}{\partial z} \right] + W = S_s \frac{\partial h}{\partial t} 
\]  

where \(K_{xx}, K_{yy}, \) and \(K_{zz}\) are hydraulic conductivity along the \(x, y,\) and \(z\) coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity (\(L/T\)); \(h\) is the potentiometric head (\(L\)); \(W\) is a volumetric flux per unit volume representing sources and/or sinks of water, with \(W<0.0\) for flow out of the groundwater system, and \(W>0.0\) for flow in (\(T^{-1}\)); \(S_s\) is the specific storage of the porous material (\(L^{-1}\)); and \(t\) is time (\(T\)). Equation (1) is solved using the finite-difference method in which the groundwater flow system is divided into a grid of cells. The finite-difference equation for a cell is\(^8\):

\[
CR_{i,j,k} \left( h_{i,j,k-1}^m - h_{i,j,k}^m \right) + CR_{i,j,k} \left( h_{i,j,k+1}^m - h_{i,j,k}^m \right) + CC_{i,j,k} \left( h_{i-1,j,k}^m - h_{i,j,k}^m \right) + CC_{i,j,k} \left( h_{i+1,j,k}^m - h_{i,j,k}^m \right) + CV_{i,j,k} \left( h_{i,j,k-1}^m - h_{i,j,k}^m \right) + CV_{i,j,k} \left( h_{i,j,k+1}^m - h_{i,j,k}^m \right) + P_{i,j,k} h_{i,j,k}^m + Q_{i,j,k} = SS_{i,j,k} \left( DELR_j \times DELC_i \times THICK_{i,j,k} \right) \left( h_{i,j,k}^m - h_{i,j,k-1}^{m-1} \right)
\]  

where \(h_{i,j,k}^m\) is head at cell \(i,j,k\) at the time step \(m\) (\(L\)); \(CV, CR,\) and \(CC\) are hydraulic conductance, or branch conductance, between node \(i,j,k\) and a neighboring node (\(L^2/T\)); \(P_{i,j,k}\) is the sum of coefficients of head from source and sink terms (\(L^2/T\)); \(Q_{i,j,k}\) is the sum of constants from source and sink terms, with \(Q_{i,j,k}<0.0\) for flow out of the groundwater system, and \(Q_{i,j,k}>0.0\) for flow in (\(L^3/T\)); \(SS_{i,j,k}\) is the specific storage (\(L^2\)); \(DELR\) is the cell width of column \(j\) in all rows (\(L\)); \(DELC\) is the cell width of row \(i\) in all columns (\(L\)); \(THICK_{i,j,k}\) is the vertical thickness of cell \(i,j,k\) (\(L\)); and \(r^m\) is the time at the time step \(m\) (\(T\)). To designate hydraulic conductance between nodes, as opposed to hydraulic conductance within a cell, the subscript notation ‘\(1/2\)’ is used.

Normally, for a steady-state period, the storage term and therefore, the right hand side of Eqn. (1) and (2) is set to zero. Based on these equations and the difference in hydraulic head in a given zone for successive time intervals (\(dh>0\)) the system might be unsteady. Observed \(dh\) (hydraulic head change) during the simulation period was not absolutely zero but very small. Consequently, it was assumed that \(dh=0\) and this eliminates \(\partial h / \partial t\) from the equations. The assumption may result in a somewhat lower estimated conductance (\(C\)) or hydraulic conductivity (\(K\)) in the left hand side of the equations. Due to missing data for one of the observation well in some interval times, only ten different steady-state periods were selected during the total observation period when the absolute difference between heads for successive months was approximately close to zero (Fig. 2a).
Boundary conditions

Three different types of boundary conditions were defined for the study area 1) No-flow boundary was assigned to the northern part of the model area at the Gar Mountain range located in the northeastern part of GBP (Fig. 3). This mountain range is a part of upper catchment (Bisheh-Zard sub basin), which was created during the Mio-Pliocene time in the Agha Jari formation and floodwater comes from this catchment during flood periods to the GBP and spreads on the ground by the FSS. In addition, the area along Shur River of Jahrom, which is located at the western border of GBP, was defined as no-flow boundary. 2) Due to the observed hydraulic head close to the northern border of GBP (outside of model domain), this border was used as a general head boundary condition (Fig. 3). 3) According to the topography and bed rock map of GBP the general trend for groundwater flow is from northeast to southwest. Based on this, time-variant specified-head or changing-head boundary was defined along the south and southwest border of GBP (discharge area of groundwater; Fig. 3).

In addition, according to observed elevation head in pumping wells located in the southeast of GBP (adjacent aquifer), a changing-head boundary was assigned to this short border to recharge the GBP.

Due to the large hydraulic head at observation well number one (P1) as compared to the other observation wells it seems that, there is a direct connection between P1 and an external source. After analyzing satellite images and aerial photographs of the study area (Fig. 3), the existing geological map was modified with a fault affecting the hydraulic head at P1 (Fig. 3). In all cases, the results show that the fault is the main source of recharge to the GBP during steady-state conditions.

RESULTS AND DISCUSSION

To optimally estimate aquifer parameters and boundary conditions an objective function and confidence intervals were established. Hill and Tiedeman\textsuperscript{10} stated that parameters are estimated more precisely if the variance of objective function and confidence intervals is small. The calculation results show that the objective function is close to zero for all simulation periods (Table 1).
Figure 3 Satellite image of study area representing the upper catchment (Bisheh-Zard Sub Basin) of Gareh-Bygone Plain, floodwater spreading systems (FSS), observation wells (P1, P2, P3, and P4) and model domain.

Table 1 Comparison of the ten steady-state periods modeled with objective function, estimated horizontal hydraulic conductivities (K's) for each zone and average estimated horizontal hydraulic conductivity (Average K's) for entire area. The dh column represents the average differences of groundwater level changes for two successive months in all zones.

<table>
<thead>
<tr>
<th>Time period</th>
<th>Average dh (m)</th>
<th>Objective function</th>
<th>Z 1</th>
<th>Z 2</th>
<th>Z 3</th>
<th>Z 4</th>
<th>Average K's (m/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>St. state_1</td>
<td>-0.05</td>
<td>1.01×10^{-33}</td>
<td>0.063</td>
<td>0.117</td>
<td>0.052</td>
<td>0.159</td>
<td>0.097</td>
</tr>
<tr>
<td>St. state_2</td>
<td>+0.02</td>
<td>7.68×10^{-06}</td>
<td>0.017</td>
<td>0.230</td>
<td>0.013</td>
<td>0.070</td>
<td>0.082</td>
</tr>
<tr>
<td>St. state_3</td>
<td>-0.24</td>
<td>8.51×10^{-34}</td>
<td>0.052</td>
<td>0.153</td>
<td>0.054</td>
<td>0.111</td>
<td>0.092</td>
</tr>
<tr>
<td>St. state_4</td>
<td>+0.03</td>
<td>3.84×10^{-06}</td>
<td>0.082</td>
<td>0.108</td>
<td>0.099</td>
<td>0.107</td>
<td>0.099</td>
</tr>
<tr>
<td>St. state_5</td>
<td>-0.17</td>
<td>1.20×10^{-33}</td>
<td>0.056</td>
<td>0.177</td>
<td>0.084</td>
<td>0.044</td>
<td>0.090</td>
</tr>
<tr>
<td>St. state_6</td>
<td>-0.35</td>
<td>3.84×10^{-06}</td>
<td>0.088</td>
<td>0.028</td>
<td>0.276</td>
<td>0.012</td>
<td>0.101</td>
</tr>
<tr>
<td>St. state_7</td>
<td>-0.15</td>
<td>3.52×10^{-33}</td>
<td>0.048</td>
<td>0.012</td>
<td>0.230</td>
<td>0.002</td>
<td>0.073</td>
</tr>
<tr>
<td>St. state_8</td>
<td>-0.10</td>
<td>6.12×10^{-33}</td>
<td>0.060</td>
<td>0.018</td>
<td>0.302</td>
<td>0.002</td>
<td>0.095</td>
</tr>
<tr>
<td>St. state_9</td>
<td>-0.15</td>
<td>5.15×10^{-33}</td>
<td>0.053</td>
<td>0.017</td>
<td>0.278</td>
<td>0.002</td>
<td>0.087</td>
</tr>
<tr>
<td>St. state_10</td>
<td>-0.31</td>
<td>1.03×10^{-04}</td>
<td>0.033</td>
<td>0.015</td>
<td>0.234</td>
<td>0.0003</td>
<td>0.070</td>
</tr>
<tr>
<td>Total average</td>
<td>-0.14</td>
<td>1.18×10^{-05}</td>
<td>0.055</td>
<td>0.087</td>
<td>0.162</td>
<td>0.051</td>
<td>0.088</td>
</tr>
</tbody>
</table>

In addition, the estimated average hydraulic conductivities for all periods are similar. In the present study, the statistical distribution at the 95% confidence limits was used for the estimation of horizontal hydraulic conductivity within the four zones (Z1, Z2, Z3, and Z4). Figure 5c indicates that the confidence intervals for estimated hydraulic conductivities in all four zones and all steady-state periods are quite narrow and the estimated horizontal hydraulic conductivities in all periods and zones varied between 0.0003 and 0.3 m/day. Based on the resulting confidence intervals it appears that all estimated values are statistically robust. Due to similar estimated value and small value of objective function in
all model periods (Table 1), model verification was carried out for one more steady-state condition for the year 2008 with 2 more observation wells with more recent observations. In this case, two more steady-state simulations were carried out for the same time interval in which the model first, was calibrated only based on old observation wells and second, including old and new observation wells. According to the calibration and verification test, the model result shows that the $K$ value in both model runs are estimated close. Due to more observation wells in the model verification, the residual and objective functions are larger. On the other hand, the standard deviation in the case of verification is less. This is because of more input information to the model according to 6 observation wells. In addition, Model verification for 2008 gave a $K$ which is quite similar to the mean $K$ value resulting from the calibration.

The results of steady-state simulation show that the trend of groundwater flow in downstream area of the fault in GBP is generally from northeast to south/southwest. The steady-state groundwater flow is to a great extent influenced by water that comes from the upper catchment (Bisheh-Zard sub-basin) via the fault (Fig. 4). Nevertheless, the model results show that the hydraulic head at the fault is higher than the hydraulic head at both sides of the fault (north and south). Consequently, the fault influences and recharges both the north and the south part of GBP. The results show that there is no significant change in the groundwater level in zone 1 and zone 2 (area around P1 and P2) for all simulated years. This is because of the vicinity of these zones to the fault with direct recharge function. However, due to numerous pumping wells located in zone 3 and zone 4, the groundwater level has dropped significantly in these areas (Fig. 4).

**Figure 4** Simulated head (m) and groundwater flow direction for the experimental area during the year 1996.04.15

**Sensitivity analysis**

According to Fig. 5, the sensitivities display a generally increasing trend with time that may be due to increase in pumping from groundwater during recent years. The latest four time periods, have high sensitivities for observations but moderate parameter sensitivities. In time periods 7 to 10 there is larger variation in observation and parameter sensitivities and $K$ values. In these periods the zones with lowest observation sensitivities have high parameter sensitivities and least $K$ values and there is a weak balance between the parameter and observation sensitivities in the different zones. In addition, there is a big difference between the $K$ values in various zones and the highest absolute average $dh$ values (Table 1). Therefore, the $K$ values in these periods cannot be reliable. On the other hand, when there is a balance between observation and parameter sensitivity in each zone or less difference between these in the given zone, better $K$ values can be derived. For example, in time periods 7 to 10 there is large difference between the parameter and observation sensitivity in zones 3 and 4, $K$ values are either very high or near zero. But for these periods and zone 2, lower differences between the observation and parameter sensitivity means a more logical $K$ value. By accepting that time periods 1 to 6 are better estimated with less differences between zone fluctuations in sensitivities, it can be derived that:

For $K1$ the best periods are 5 and 6 and between them period 5 is better for its lower average $dh$ value (Table 1). For $K2$ the best time period between 1 to 6 is time period 6 with less difference
between the sensitivities for zone 2. For $K3$ the time period 2 is the best which has the highest sensitivities and lowest differences. For $K4$ the second time period is the best with lowest sensitivity difference and the highest sensitivities.

Figure 5  Groundwater model simulations in ten different steady-state conditions. (a) model sensitivity to the observations, $P1$ to $P4$, (each time period contains four observation wells); (b) model sensitivity to the parameters, $K1$ to $K4$, (each time period contains four different zones to estimate hydraulic conductivity); (c) estimated value and its confidence interval for four zones in each steady-state condition.

Also it is argued that for the case that there is a considerable difference between the observation and parameter sensitivities the $K$ values are proportional to the observation sensitivity minus parameter sensitivity for a given zone. When the observation sensitivity is less than the parameter sensitivity, the $K$ values tend to be small and close to zero. And for the case that the observation sensitivity is considerably larger than the parameter sensitivity, the $K$ values are large and larger than the $K$ for other zones.

CONCLUSIONS

The present study has shown that optimal parameter estimation and boundary condition can be defined by a steady-state groundwater model for unconfined aquifer with high precision and reliability. This approach makes a fast simulation and determined aquifer parameters appear reliable. One of the disadvantages of steady-state modeling is its limitation in estimation of aquifer parameters such as specific yield, recharge rate, etc. In this study data from four observation wells were used to simulate the 6000 ha unconfined aquifer based on precision and reliability of estimation. The estimated values were optimized according to the model sensitivity to observations and parameters. The result shows that in case of minimum difference between observation and parameter sensitivities and minimum groundwater level changes during successive intervals, $dh=0$, optimal steady-state parameter estimation
and boundary condition can be defined. For all simulations periods, the confidence intervals were at minimum and the model could estimate the parameters based on observation data. Therefore, based on these results, limited number of observations may still provide relevant information for robust parameter estimation. During steady-state groundwater flow with no recharge from surface water, the system is mainly recharged by the fault crosses the northern part the aquifer and groundwater flow direction is from northeast to south and southwest. The range of hydraulic conductivities for alluvial fans may vary from 0.001 to 1 m/day\(^{11}\). The average estimated hydraulic conductivity resulting from modeling the observations was about 0.1 m/day. The parameter estimation method and suggested boundary condition could be applied for the Gareh-Bygone Aquifer to understand the groundwater flow system better. These parameters can hopefully be transferred to a transient model to estimate other aquifer parameters and groundwater behavior in a similar area. In addition, the approach appears promising and could be applied to other aquifer and groundwater systems to define the best steady-state conditions and optimal parameter estimation.

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