Estimating Fresh Water Lens Aquifer Parameters Using Automated Parameter Estimation and Axisymmetric Flow and Transport Modeling

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ABSTRACT

In coastal aquifer settings, safe yield pumping rates for supply wells located within a fresh water lens must be set to rates that prevent salt water upconing and saline intrusion into the well field. Groundwater modeling to establish safe yield rates requires estimates of aquifer geometry and properties (e.g. horizontal and vertical hydraulic conductivity, porosity, dispersivity, and salt water transition zone depth and thickness), which in turn typically requires more computationally intensive modeling software (e.g. SEAWAT vs. MODFLOW). This computational burden, coupled with the inherent non-linearity of the problem may lead to challenges in parameter estimation.

In this study, a rapid parameter estimation approach was developed in which the inverse modeling code, PEST, was used with axisymmetric flow and transport modeling to automate the estimation of aquifer properties. A three-layer fresh water lens aquifer (the original model) was simulated to calculate data for use as "observations" in the parameter estimation process. Although the use of axisymmetric flow and transport modeling required simplification of the modeling domain, model-run-time efficiency was improved by approximately three orders of magnitude.

Axisymmetric flow and transport modeling should be applied only when the conceptual model will allow the model domain to be simplified into two-dimensional cylindrical coordinates. This cannot always be done due to aquifer heterogeneity that may not be adequately described in a two-dimensional axisymmetric model. Furthermore, in an axisymmetric model domain, the extraction / injection well must be placed in the center of the cylinder, with no additional extraction wells defined elsewhere in the model.

Results demonstrate the potential for coupling of axisymmetric flow and transport modeling with automated parameter estimation to provide an efficient tool for estimating aquifer parameters which could then be used to estimate sustainable pumping rates in fresh water lens aquifers. Although demonstrated for a fresh water lens aquifer, this flow and transport method can likely be applied to any well pumping above a saline zone.

INTRODUCTION

Communities for which groundwater is a major source of water supply must carefully manage the resource by striking a balance between meeting community water demands while avoiding deleterious hydrologic and environmental impacts. In certain coastal aquifers, water supply wells are located in proximity to a zone of laterally encroaching salt water, or are screened a short distance above a fresh water / salt water interface. A determination of safe yield must account for the potential for groundwater withdrawals to introduce saline water into the well field, resulting in unacceptable water quality and fouling the aquifer in the vicinity of the well field.

In many coastal environments, only a thin fresh water lens is available for water supply purposes. These lenses of fresh groundwater buoyantly "float" over saline water. The lenses form as fresh water recharges the aquifer via precipitation and infiltration into the saline environment. The formation of a fresh water lens aquifer is illustrated here using a hypothetical ocean island with saline groundwater (Figure 1). The island groundwater is then recharged with fresh water via precipitation and infiltration over a long period of time resulting in a fresh water lens aquifer (Figure 2). The interface between the lens of fresh groundwater and saline groundwater is a transition zone that may be thin or many feet thick.

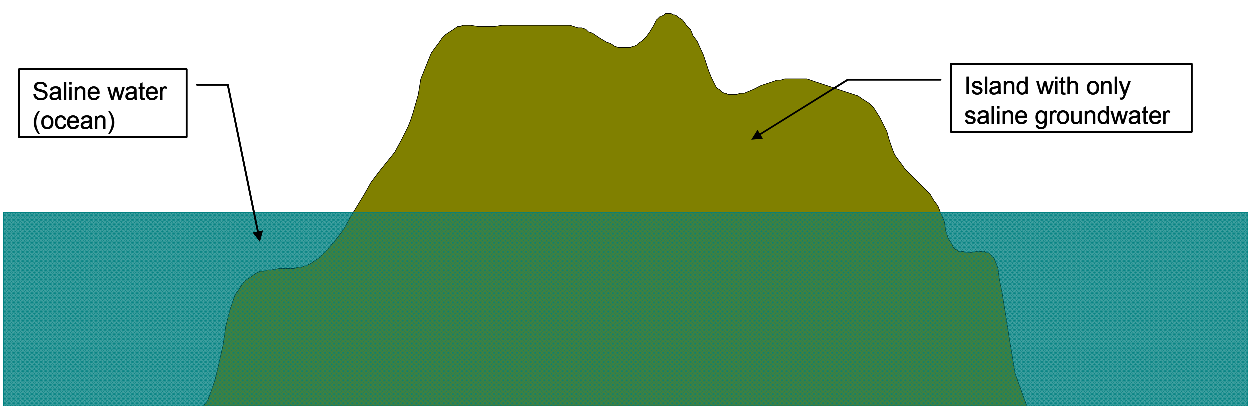

Figure 1 Cross section of a hypothetical ocean island with saline groundwater

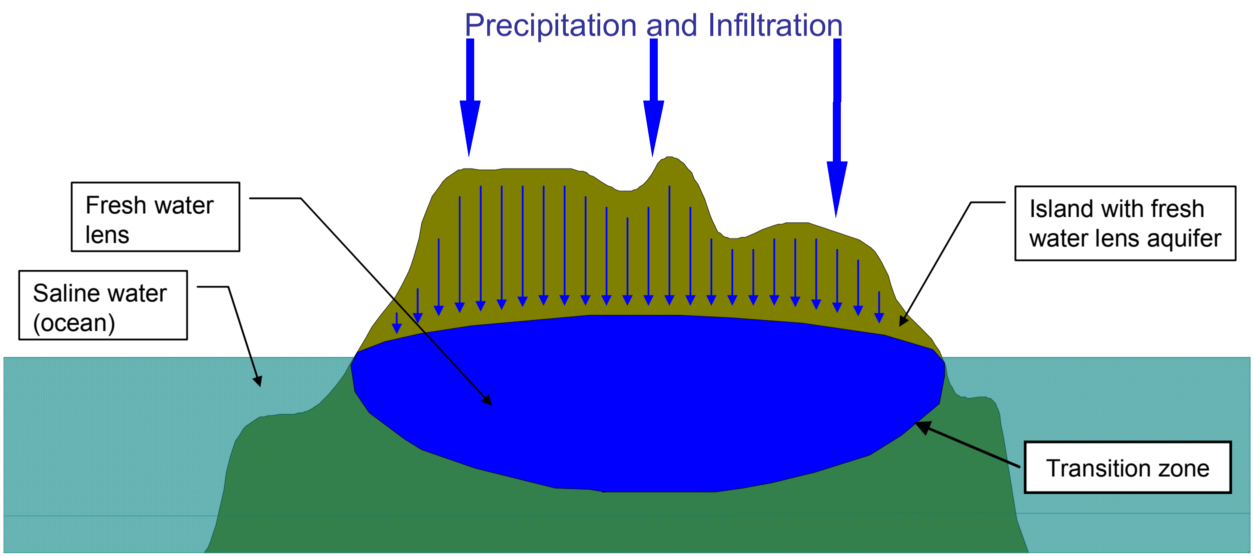

Figure 2 Cross section of a hypothetical ocean island with a fresh water lens

When groundwater is pumped from a fresh water lens at a greater rate than recharge can replenish it, two important conditions occur in the vicinity of the well. First, beneath the well screen, the transition zone between the fresh groundwater and the saline groundwater migrates upward. The upward migration of the transition zone due to pumping of the fresh water lens is called salt water upconing. Second, with prolonged pumping the lens becomes thinner. Both of these effects are depicted in Figure 3. If these conditions persist, upconing of saline groundwater can occur at the well, thereby fouling it.

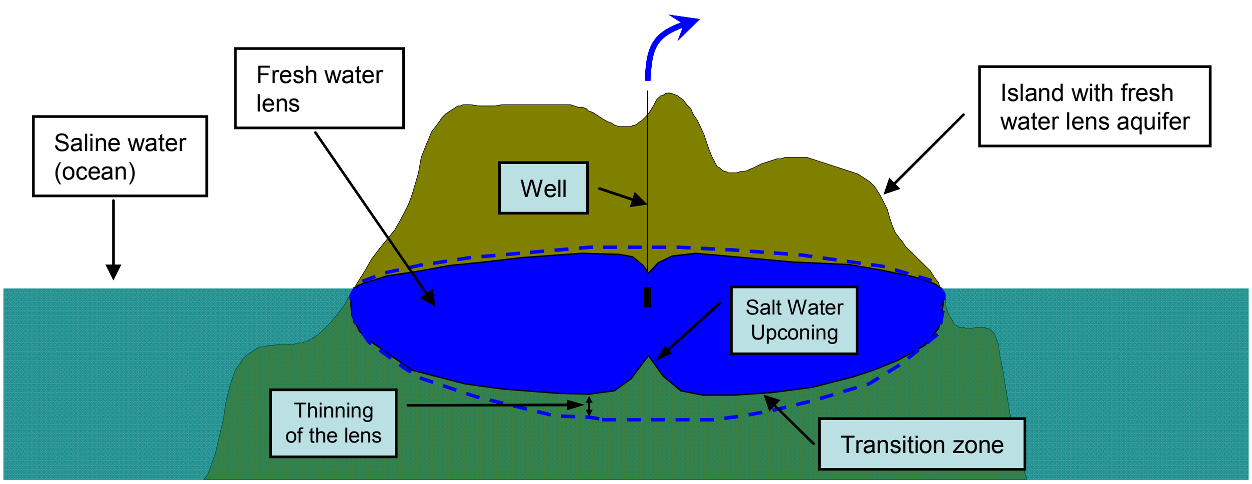

Figure 3 Cross section of a hypothetical ocean island with a pumping from a fresh water lens

Interaction among a number of parameters including the hydrologic properties of the aquifer and its extents, amount of recharge, and the transient nature of ocean boundaries (magnitudes of the tides, sea-level rise, etc.) determines the size of the fresh water lens and the thickness of the transition zone between the fresh and saline groundwater. The complexity of these interactions requires numerical modeling techniques to predict the influence of pumping on the transition zone and upconing in aquifers with thin lenses of fresh groundwater. These techniques can be used to predict the safe-yield pumping rates that minimize the amount of upconing, yet maximize the well yield. Accurate estimates of these parameters are important for the proper design of an extraction well and determining safe-yield pumping rates.

Cecan et al. (2008) suggest that the use of numerical flow and transport modeling to analyze pumping test data for a fresh water lens aquifer allows for more accurate estimates of aquifer parameters. This paper illustrates an automated method using PEST to estimate aquifer properties from pumping test data in an aquifer with a fresh water / salt water interface.

MODELING

Modeling a variable density flow environment, as in a fresh water lens aquifer setting, usually requires a more computationally intensive model that simulates density-dependent flow and transport. Three-dimensional variable density flow models such as SEAWAT (Langevin et al., 2008) or SUTRA (Voss 1984; Voss and Provost 2002) can be computationally demanding, resulting in long computation times. Inverse modeling requires numerous model simulations that increase computation times. Simplification of a model domain into two-dimensional axisymmetric space can reduce the computation time.

The term two-dimensional axisymmetric model space is used here to describe a vertical cross section of a cylinder. Therefore one lateral boundary of the model is the “center” of the island where the thickest fresh water lens formation occurs, and the other lateral boundary is the shore of the island. For figures in this paper, the center of the cylinder is to the left-hand side.

Langevin (2008) described a method of “tricking” SEAWAT into running an axisymmetric model. The scheme for using SEAWAT, MODFLOW, and / or MT3DMS in axisymmetric modeling is to modify several input parameters to account for the discrepancy between a rectangular geometry (upon which these programs are based) and a cylindrical geometry (Langevin, 2008). Essentially, this involves applying a factor of $r\theta$ to various model inputs, where r is the distance from the center of the cylindrical system to the center of the model cell where the property is being modified; and θ is the angle open to flow (usually 2π) (Langevin 2008). Properties or fluxes which generally need to be modified are (Langevin 2008):

- Horizontal hydraulic conductivity;
- Vertical hydraulic conductivity;
- Specific storage;
- Porosity
- Recharge; and
- Evapotranspiration.

Using this approach the fresh water lens aquifer system becomes much more computationally manageable. Furthermore, SEAWAT Version 4 (Langevin et al., 2008) allows the user to control whether the flow field after each iteration is recalculated based on a user specified tolerance for the maximum change in fluid density at any cell, the application of which could shorten model run times. Using SEAWAT Version 4 to solve an axisymmetric model of a fresh water lens yields run times that are more manageable from an inverse modeling perspective.

HYPOTHETICAL FRESHWATER LENS AQUIFER (THE ORIGINAL MODEL)

PEST was used to estimate the aquifer properties for a hypothetical fresh water lens aquifer simulated using a two-dimensional axisymmetric model in SEAWAT to examine the resulting computational savings. First, a hypothetical, axisymmetric model referred to herein as the "original model" was developed and included the creation of a fresh water lens. Then a pumping test was simulated to generate salt water concentrations in the transition zone and aquifer head data for later use as "observation data" in the PEST parameter estimation process.

Conceptual Model

The hypothetical or original model represents an approximately 517 foot thick aquifer with three hydrogeologic units (Figure 4). The model diameter is 14,000 feet, extending 7,000 feet in all directions from the pumping center. The uppermost hydrogeologic unit is approximately 75 feet thick and divided into 10 model layers of equal thickness. The value of hydraulic conductivity of the uppermost unit is 150 feet/day for both horizontal (K_h) and vertical (K_v) directions. The middle hydrogeologic unit is approximately 90 feet thick and is divided into 14 model layers of equal thickness. The value of K_h for the middle unit is 50 feet/day and K_v is 5 feet/day. The lower hydrogeologic unit is approximately 350 feet thick and is divided into 54 model layers of equal thickness. The value of K_h of the bottom unit is 25 feet/day and the value of K_v is 0.883 feet/day. The remaining input aquifer parameters are constant for all layers with specific storage (Ss) of 6.8×10^{-5} per foot, effective porosity of 0.25, specific yield (SY) of 0.25, longitudinal dispersivity (α_L) 3.0 transverse dispersivity (α_T) of 0.3, and vertical dispersivity (α_V) of 0.003.

The cylindrical island boundary conditions of the original model consisted of recharge (24 inches/year) applied to the uppermost layer and sea water salt concentration (35 g/L) and head (0.0 feet) applied at the shoreline (outer lateral boundary). The lower model boundary was considered no-flow (zero-flux). An initial head of 0.0 feet was applied to all model cells.

The original model simulated 200 years of recharge to produce a steady-state fresh water lens. At steady-state the fresh water lens thickness in the center of the island was approximately 200 feet thick, the fresh water / salt water transition zone was approximately 50 feet thick (Figure 5). Toward the outer lateral boundary, the fresh water lens and transition zone diminish to nearly 0 and approximately 10 feet, respectively.

For the purpose of determining the savings in run time between two-dimensional axisymmetric and three-dimensional rectangular model domains, a three–dimensional rectangular model of similar layering and with similar aquifer properties was constructed and used to simulate the formation of a fresh water lens. The three –dimensional rectangular model also contained 78 layers (like the axisymmetric model), but contained 103 rows and 103 columns resulting in 827,502 cells. The three-dimensional model was highly discretized to closely resemble the axisymmetric model and to accurately simulate the fresh water lens. A large amount of vertical discretization was needed to adequately simulate the 30- to 50-foot thick transition zone. Due to the large number of cells and transport properties selected, the computer run time of the three-dimensional model was about 45 days in a shared processor environment; whereas the run time of the axisymmetric model (which only had about 8,500 cells) was just under two hours in a non-shared processor environment. This difference in run times represents approximately three orders of magnitude. It is unlikely that meaningful parameter estimation analyses could have been performed with the full three-dimensional rectangular model. Thus, if a fresh water lens model can be simplified by converting it to a two-dimensional axisymmetric model, run times can be greatly reduced and parameter estimation becomes feasible.

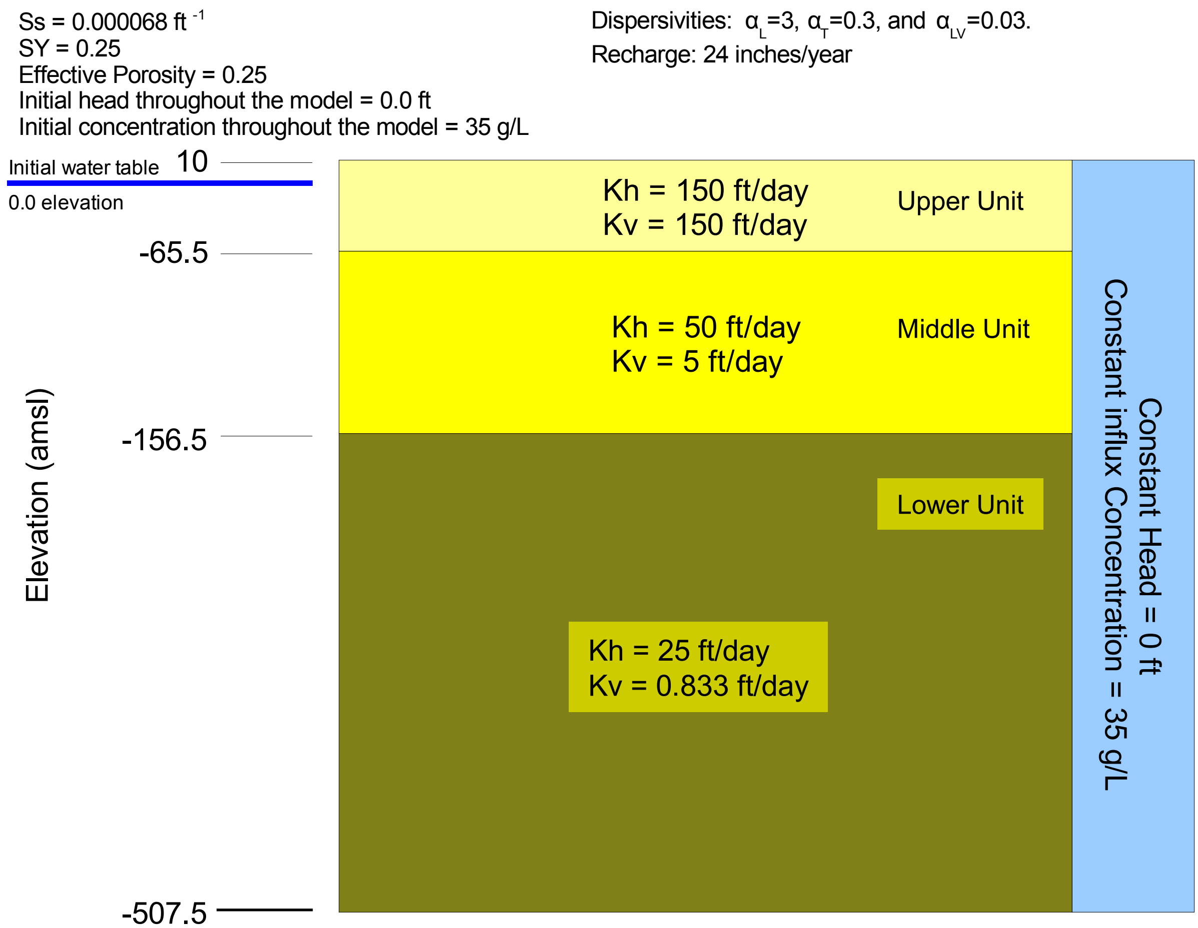

Figure 4 Cross section of the original model listing the aquifer properties

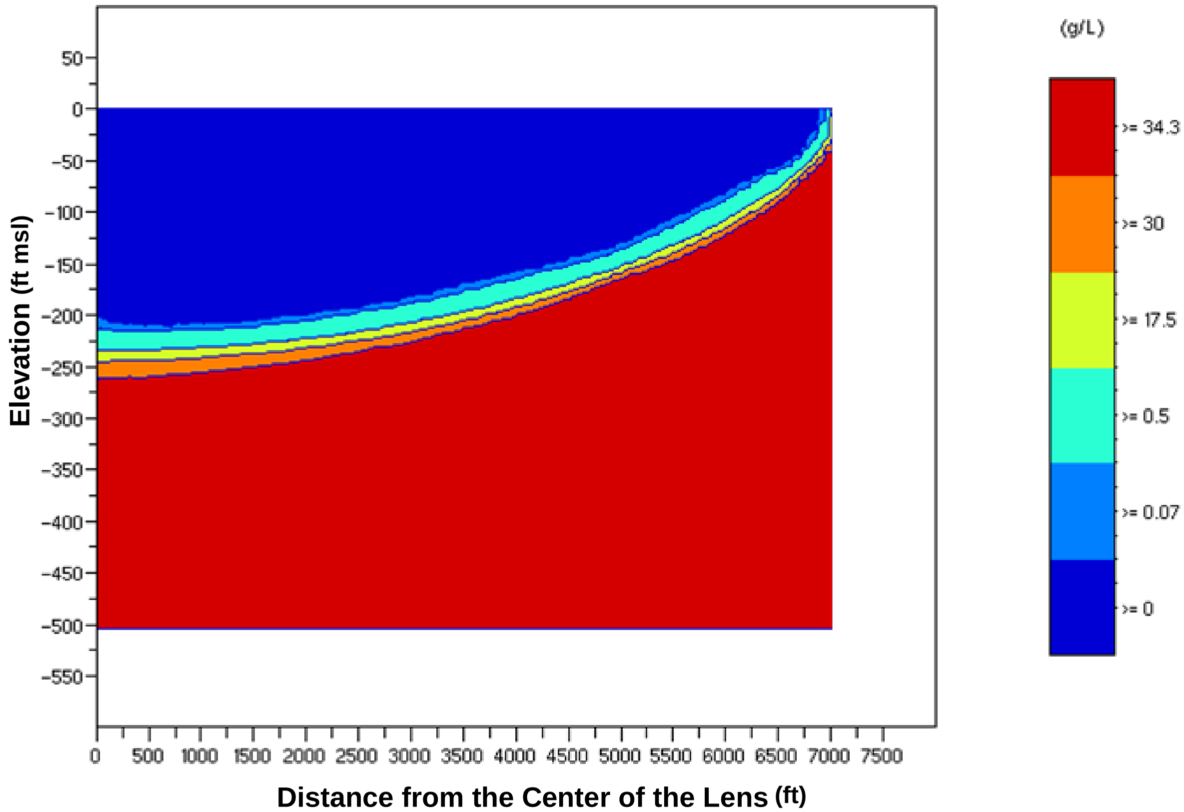

Figure 5 Cross section of the simulated fresh water lens from the original model after 200 years of simulation

Simulated 10-Day Pumping Test

After creation of the fresh water lens, a 10-day pumping test was simulated using the original model. The pumping well was placed at the center of the model by necessity of the axisymmetric conditions. The pumping well screen is partially penetrating and was placed in the upper hydrogeologic unit at a depth between 30 and 60 feet. There were 26 partially penetrating observation well screens located within all three hydrogeologic units with depths ranging between 0 and 300 feet as shown in Figure 6. The nearest observation well screen was located at a radial distance of 8 feet from the pumping well and the farthest was 4,125 feet from the pumping well. The approximate top of the fresh water / salt water transition zone is shown on Figure 6. Note that the deepest wells are screened within the transition zone.

Figure 7 shows the log-log plot of drawdown vs. time from each observation well over the 10-day period. These values of drawdown were used as “observation data” in the subsequent PEST simulations. Figure 8 shows the salt concentration over time for each observation well.

The deepest observation wells within the transition zone contain the highest salt concentrations of approximately 35 g/L. The observation wells screened at the top of the transition zone have salt concentrations of approximately 5 g/L. The observations wells within the middle and upper hydrogeologic units have salt concentrations of 0 g/L. The calculated drawdown and concentration data generated from this the 10-day pumping test were used as the "observed" data in the PEST optimization run described below.

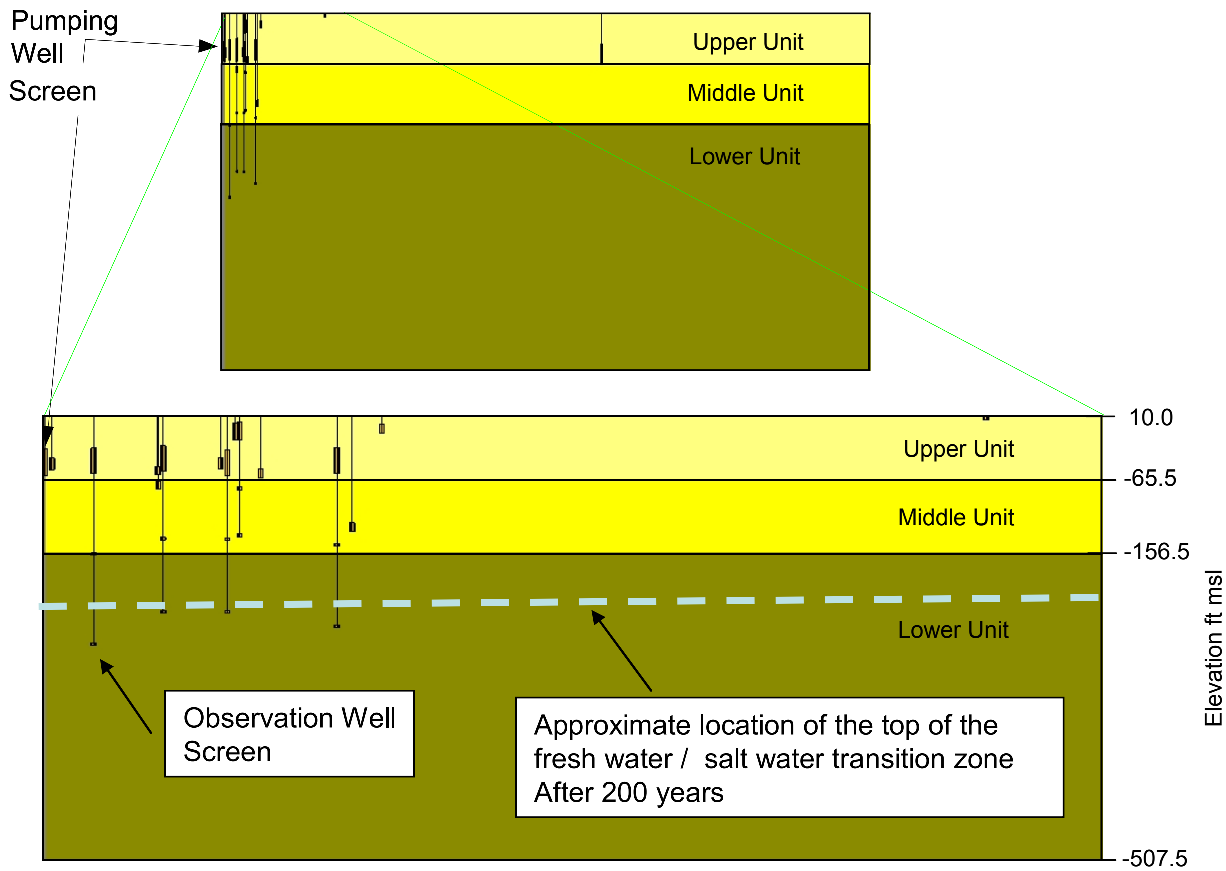

Figure 6 Pumping and monitoring well locations within the original axisymmetric model

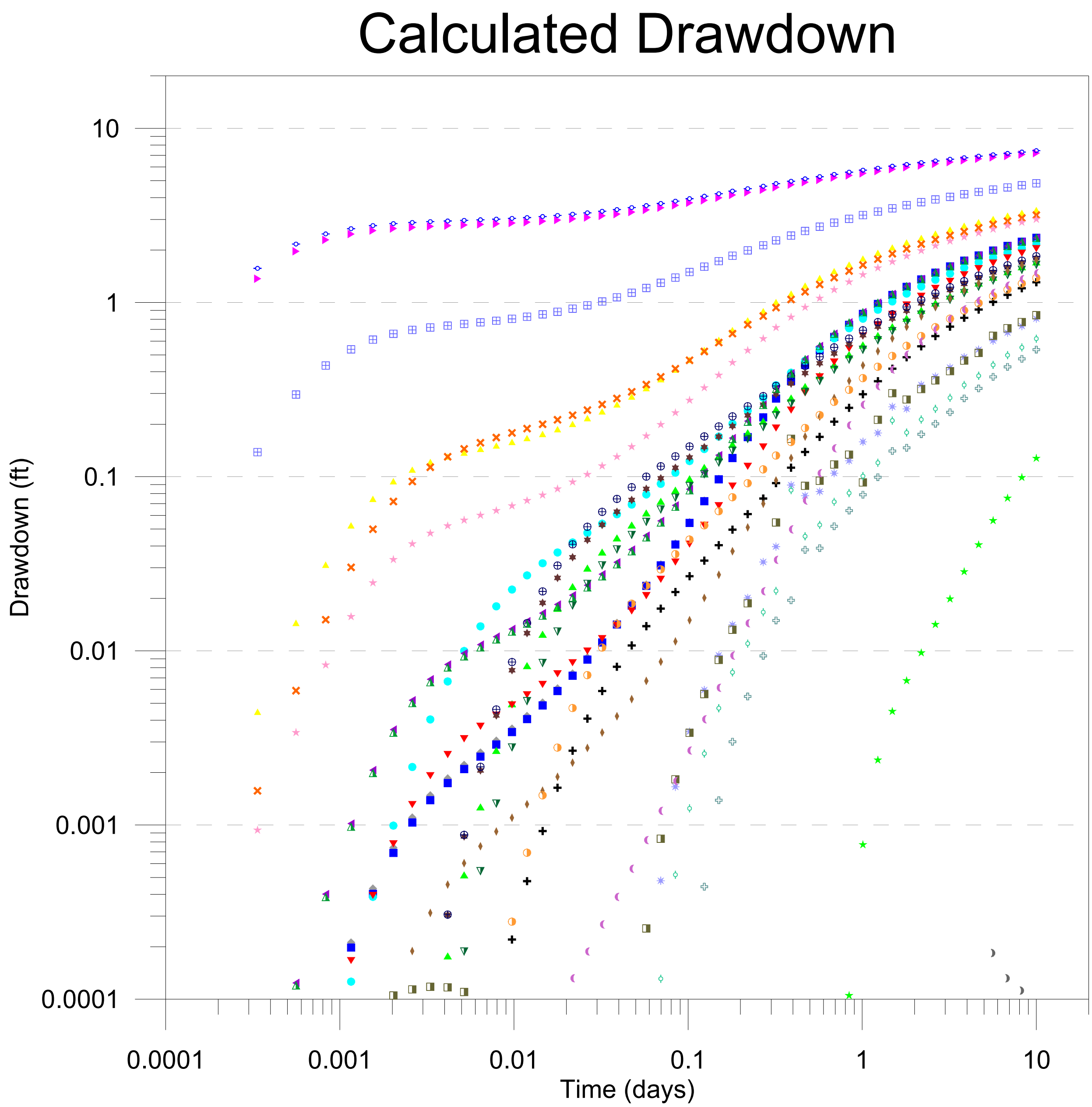

Figure 7 Simulated drawdown of a 10-day pumping test from the original axisymmetric model

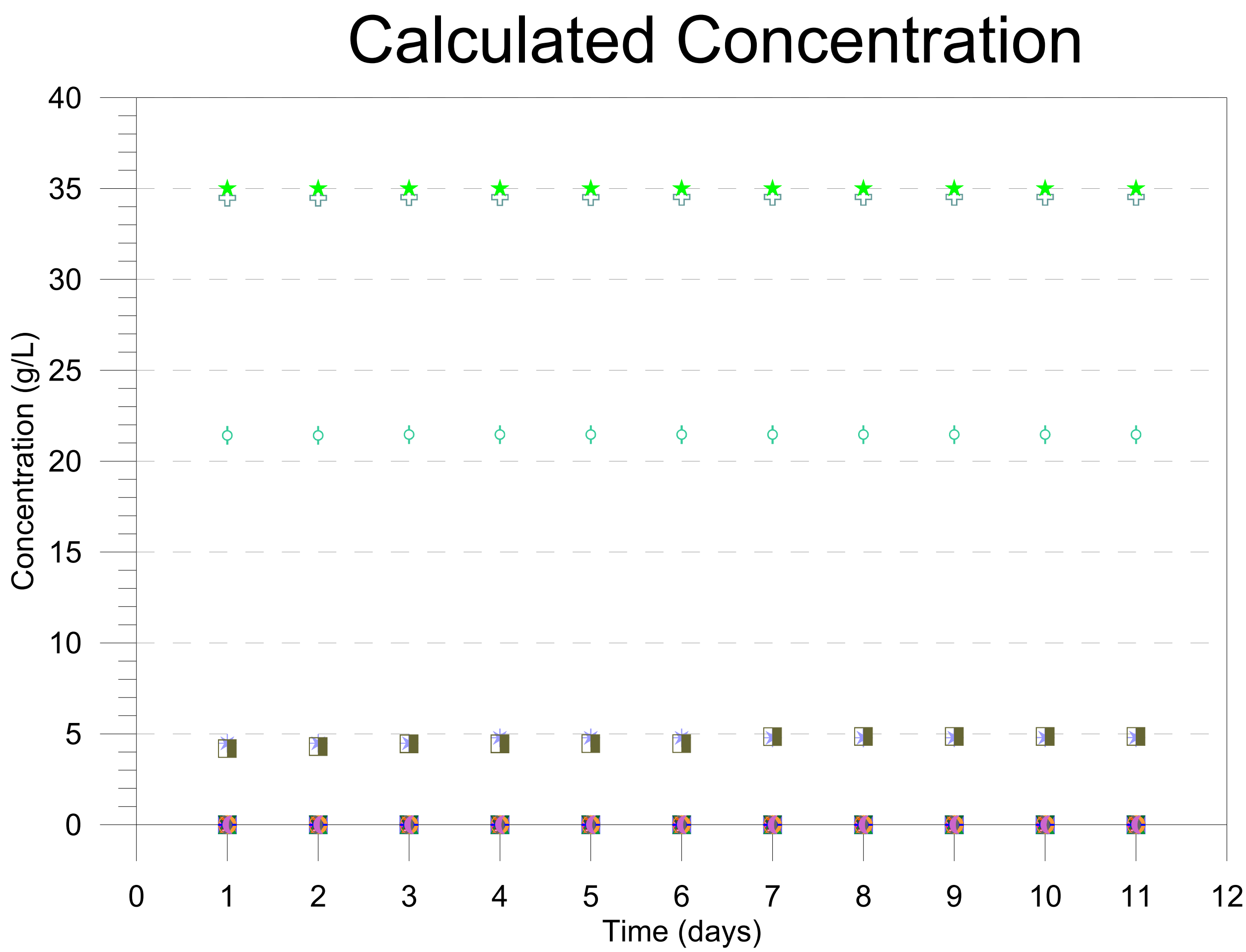

Figure 8 Simulated concentration of a 10-day pumping test from the original axisymmetric model

PARAMETER ESTIMATION USING AN AXISYMMETRIC MODEL

The PEST parameter optimization modeling process was applied to the vertical anisotropy (K_h/K_v) of the axisymmetric model by using the 10-day pumping test "observation data" as optimization targets. The vertical anisotropy is described by two parameters, K_h and K_v. Because the upper hydrogeologic unit is isotropic with respect to hydraulic conductivity (K_h/K_v=1), five aquifer parameters were optimized. The values of K_h and corresponding values of K_h/K_v are listed on Table 1 and include the original model parameters, the initial PEST aquifer parameter values, and the final, optimized aquifer parameter values.

The PEST optimization completed 28 iterations and, for this relatively simple model, resulted in estimating parameter values that matched the original model values well (Table 1). It appears that the largest difference between the original and optimized values occurred for the lower hydrogeologic unit. This is likely due to the fact there are far fewer observation wells screened in this unit and that head values in the lower hydrogeologic unit changed by the smallest amount during the 10-day test thereby making the value of hydraulic conductivity in the lower unit less sensitive to parameter changes. Figure 9 is a plot of the heads and salt concentrations of the original model vs. the heads and concentrations of the final PEST optimized model. There is excellent agreement between the two as seen by the data falling along the 1:1 line.

Table 1 Table of the original parameter values, initial parameter values used in the PEST run, and the optimized parameter values from the PEST run

Parameters	Original Model	Initial PEST Values	Final PEST Optimized Values
Horizontal hydraulic conductivity (K_h) of upper unit (ft/day)	150	100	149.5
Horizontal hydraulic conductivity (K_h) of middle unit (ft/day)	50	100	47.6
Horizontal hydraulic conductivity (K_h) of lower unit (ft/day)	25	100	38.0
Vertical hydraulic conductivity anisotropy of upper unit (K_h / K_v)	1	1	1.1
Vertical hydraulic conductivity anisotropy of middle unit (K_h / K_v)	10	10	17.1
Vertical hydraulic conductivity anisotropy of lower unit (K_h / K_v)	30	30	26.4

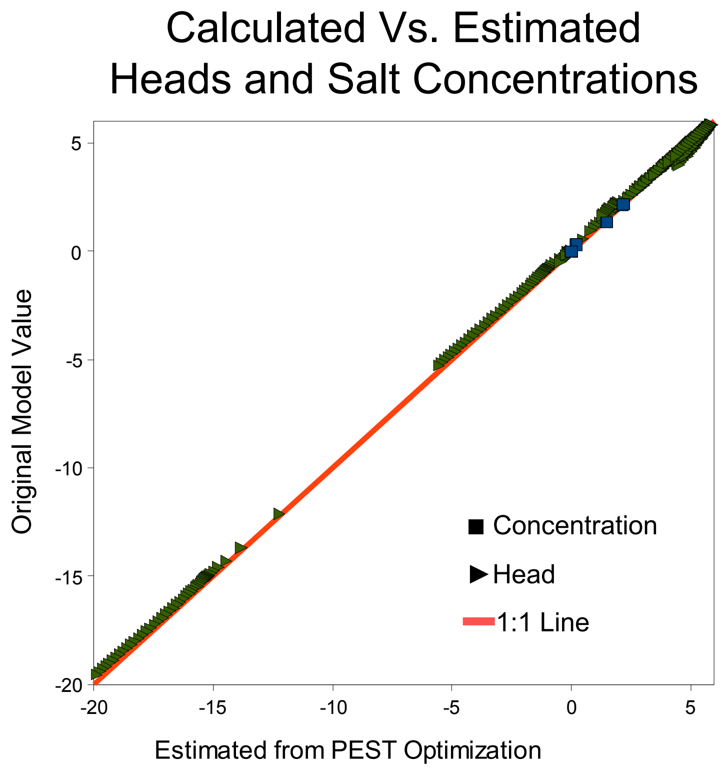

Figure 9 Calculated vs. estimated heads and salt concentrations

The parameter values varied throughout the 28 iterations as PEST optimized the parameters. The PEST optimizations were performed on weekends and nights using between 3 to 10 workstations (depending on availability) over the course of about three weeks. The total calculation time required to complete the parameter estimation was approximately 10 days for the axisymmetric model. It would not have been possible to perform a similar parameter estimation exercise for the three-dimensional rectangular model of this fresh water lens aquifer because of the length of the simulation times discussed previously.

Figure 10 is a graph showing the variation of K_h for all 28 iterations. The values of K_h show very little variations after 15 iterations. Figure 11 is a graph showing K_h/K_v which also shows very little variation in the upper and middle hydrogeologic units after 15 iterations. Anisotropy in the lower hydrogeologic unit does not vary much through the process, likely due to the limited number of observation wells and the small variations in head and salt concentration over the 10-day pumping test.

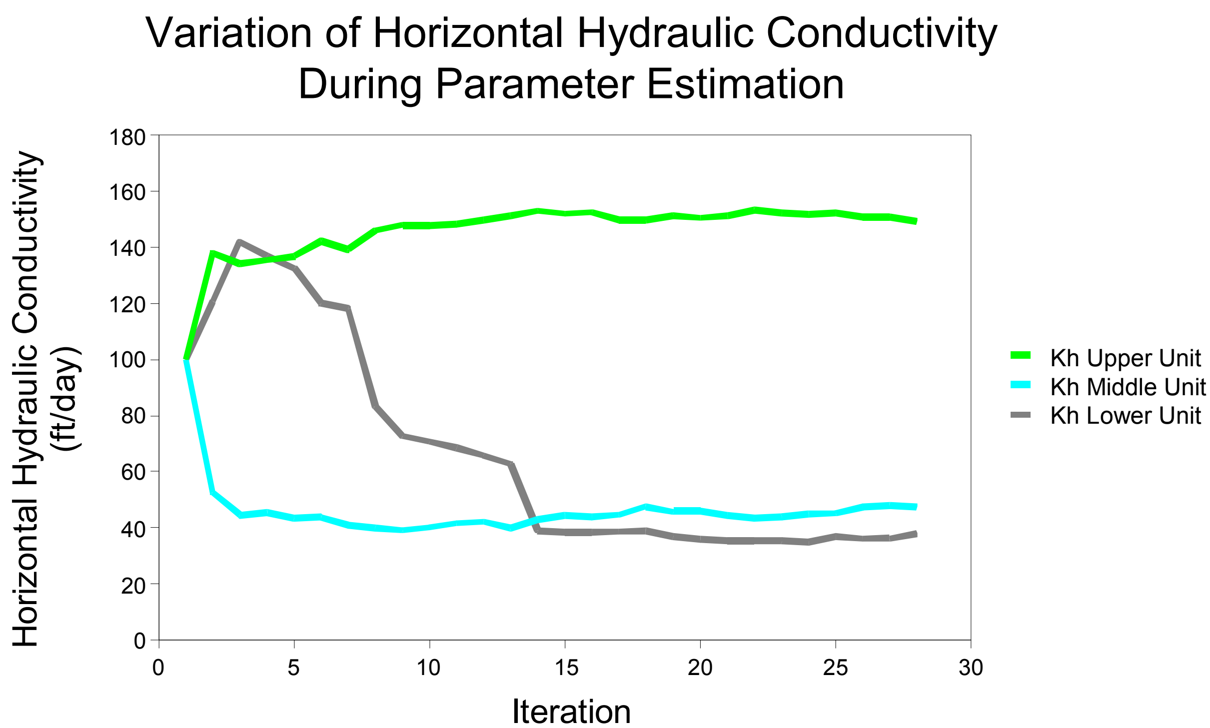

Figure 10 Variation in horizontal hydraulic conductivity for each PEST iteration

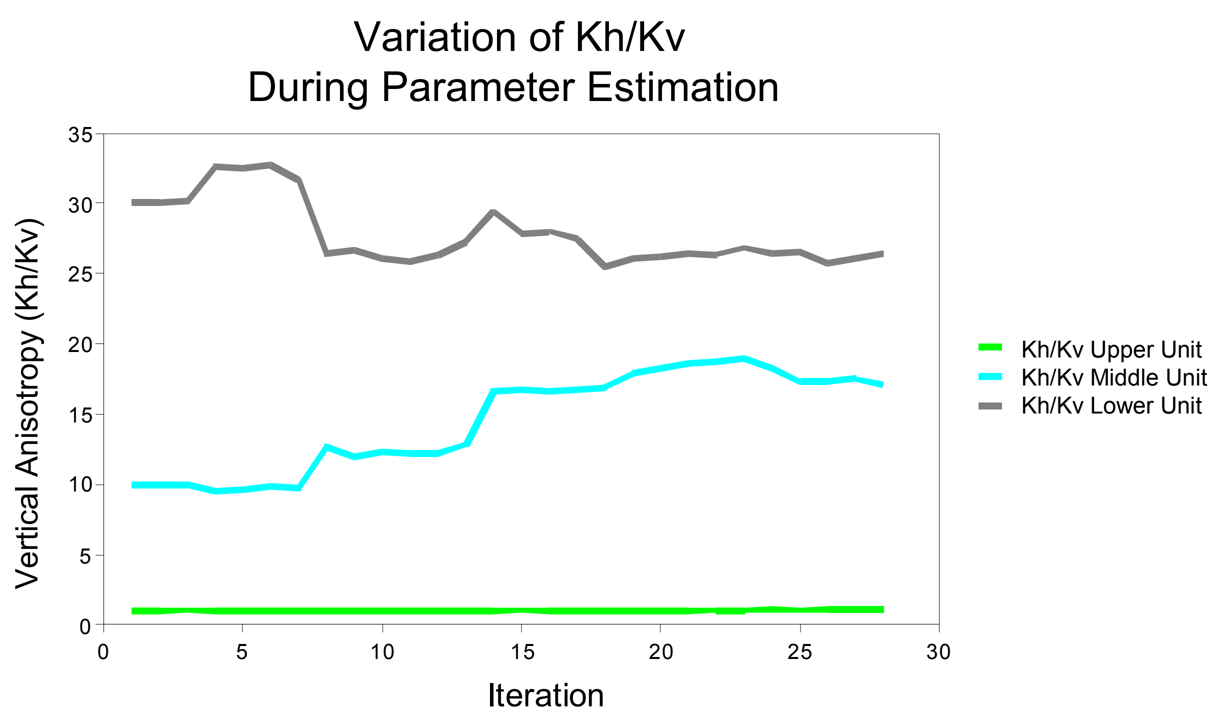

Figure 11 Variation of K_h/K_v for each PEST iteration

Discussion

There were two observation groups contributing to the objective function for the PEST run:

1. Concentration; and
2. Head.

The PEST optimization effectively lowered the objective function from 6,060 to 110 in the 28 iterations (Figure 12). As depicted in Figure 12 the concentration contribution to the objective function is rather small, whereas the head contribution to the objective function predominates.

The parameter sensitivities for each iteration are plotted in Figure 13. Figure 13 shows that the PEST inversion is most sensitive to the values of K_h of the three layers and that the most sensitive parameter is K_h of the upper unit where most of the observations are located. However, the inversion is somewhat sensitive to K_h/K_v of the lower unit, comparable to the sensitivities of K_h within the upper and middle units in the later optimization iterations. The inversion is weakly sensitive to the K_h/K_v of the upper and middle units. The larger differences between the original and optimized values shown in Table 1 correspond to the variables with smaller sensitivities (i.e. the parameters with smaller sensitivities did not match as well as those with a higher sensitivity).

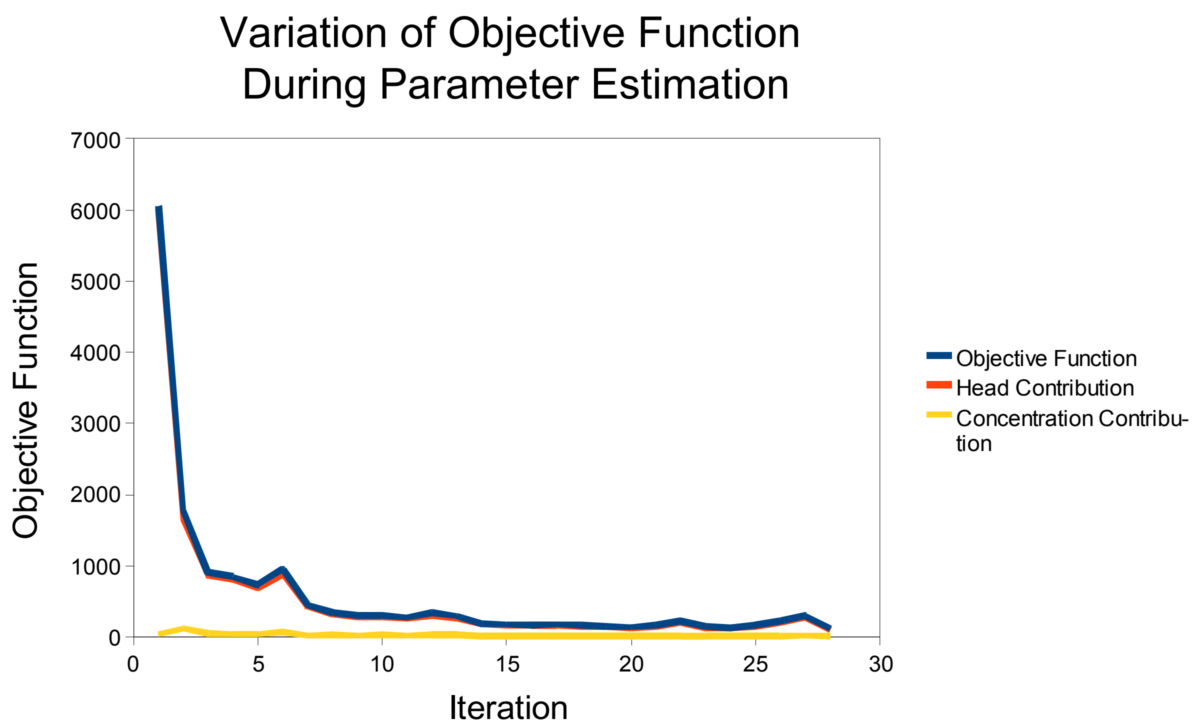

Figure 12 Variation of objective function for each PEST iteration

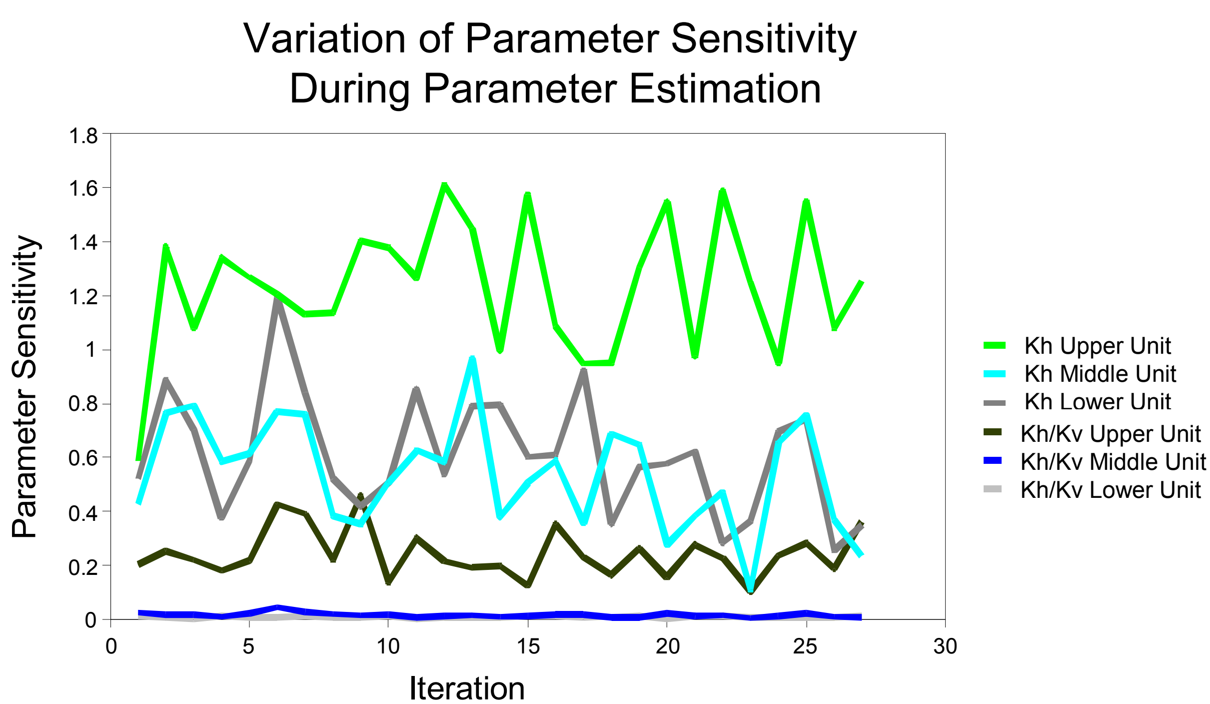

Figure 13 Variation of parameter sensitivity for each PEST iteration

CONCLUSIONS

Results demonstrate the potential for coupling of axisymmetric flow and transport modeling with automated parameter estimation to provide an efficient tool for estimating aquifer parameters which could then used to estimate safe yield pumping rates in fresh water lens aquifers. Although demonstrated for a fresh water lens aquifer, this method can likely be applied to any well pumping above a saline zone.

This approach presents an automated way to use PEST for optimization of aquifer parameters in a relatively short period of time, provided that the problem can be simplified for axisymmetric flow and transport simulation. By using axisymmetric flow and transport modeling in SEAWAT Version 4, model run times can be reduced such that parameter estimation becomes more manageable.

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