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The benefit of using data on canal seepage and tracer concentration in aquifer parameter estimation

E. ZECHNER, D. GENEREUX & J. SAIERS

Geology Department, Florida International University, Miami, Florida 33199, USA
e-mail: eric.zechner@unibas.ch

Abstract We evaluate the benefit of using field data on groundwater fluxes to canals and pore-water solute concentrations, in addition to data on hydraulic head, to estimate model parameters for groundwater flow. The field site was a 100 km^2 area of the Biscayne Aquifer in southeast Florida. A total of seven models were calibrated to different combinations of 196 observations of groundwater head, 56 measurements of seepage between the aquifer and canals, and 196 measurements of pore-water chloride concentration. Each of the calibrated models was evaluated by testing its ability to predict the spatial and temporal variability in groundwater head and canal discharge during a 10 day canal drawdown experiment. The results of the simulations demonstrate that: (a) the models calibrated solely on hydraulic head measurements predict data on hydraulic heads and water fluxes poorly; (b) the models calibrated solely on seepage fluxes predict accurately, only if the number of parameters estimated in the calibration is restricted; and (c) the models calibrated on at least two types of data (e.g. hydraulic head and seepage fluxes) exhibit good predictive capability, regardless of the number of parameters estimated.

INTRODUCTION

Numerical models are used widely to study problems related to groundwater flow. Within the last decade, the use of automated inverse techniques to estimate model parameters that govern groundwater flow and solute transport have become more common. Inversion techniques usually involve adjusting values of aquifer parameters so that solutions to the groundwater flow equation match field data on hydraulic head. This procedure often results in solution non-uniqueness and instability, high correlation between optimal parameters, and large standard errors in the parameter estimates. One way to better constrain flow and transport models is to include field observations, in addition to hydraulic head, to calibrate the model. Results of published studies suggest that data on fluxes at head-dependent boundaries (Poeter & Hill, 1997; Hill *et al.*, 1998) and pore-water solute concentrations (e.g. Wagner & Gorelick, 1987; Keidser & Rosbjerg, 1991; Anderman *et al.*, 1996) can be used in conjunction with inverse techniques to more accurately specify values of aquifer parameters. Most of this work has been performed on synthetic aquifers. We assume inverse techniques that take advantage of data on water fluxes and solute concentrations have not been applied extensively to real aquifer systems because of the lack of reliable measurements on exchange between groundwater and surface water, together with the lack of data sets on the spatiotemporal distribution of solute concentrations in aquifers.

Our study area is located in southeast Florida along the eastern border of Everglades National Park. At this site, we have collected time series data on hydraulic head, water fluxes at canal boundaries, and chloride concentrations in groundwater and in canal water. We use these data in different combinations to calibrate numerical models of coupled groundwater flow and solute transport. Because the "true" parameter values are unknown in a natural aquifer, we evaluate the parameter sets determined from the different calibrations by predicting the results of a 10 day canal drawdown experiment (Genereux & Guardiario, 1998). The work presented here is the first study incorporating field observations of hydraulic heads, boundary fluxes, and pore-water tracer concentrations in a fully coupled, three-dimensional, groundwater-flow and solute-transport inversion.

HYDROGEOLOGICAL SETTING

The Biscayne Aquifer is the sole-source aquifer for more than four million people in southeast Florida and is considered one of the most permeable and productive aquifers of North America. Our study site is located approximately 50 km southwest of Miami in the C-111 basin of the Florida Everglades (Fig. 1). In this area, the unconfined aquifer reaches a thickness of nearly 15 m; the mean hydraulic conductivities exceed 0.1 m s^{-1} due to strongly developed secondary porosity. The highly permeable formations making up the Biscayne Aquifer, the Miami Limestone and the underlying Fort Thompson Formation, are separated with a 0.3 m thick micritic layer of very low permeability. Groundwater flow in the Biscayne Aquifer is strongly linked to canal water levels, which are controlled to meet flood control, water supply, and environmental objectives.

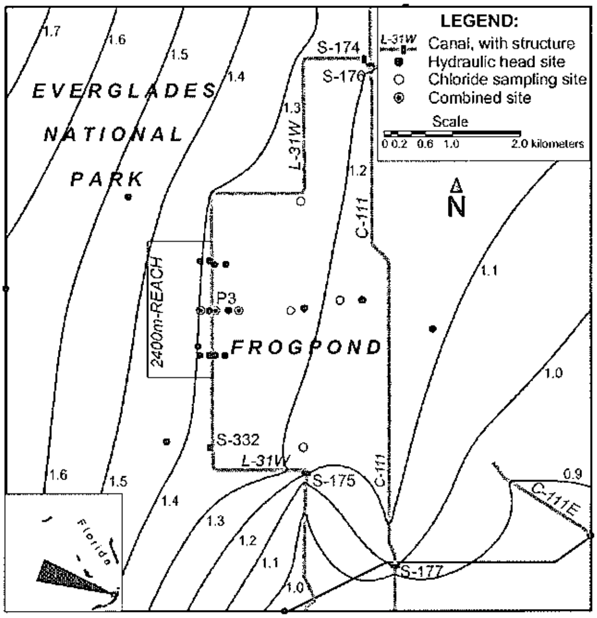

Fig. 1 Study site with canal boundaries and observation sites for hydraulic head, canal flow, and groundwater chloride concentration. The simulated piezometric surface corresponds to the end of June 1998.

DATA COLLECTION

Hydraulic head measurements were taken from 31 groundwater wells (Fig. 1). Fluxes between a defined canal reach and the aquifer were calculated from the difference of daily measured flows at upstream and downstream structures, or at nearby flow-calibrated, acoustic velocity meters. Water flux between canal and aquifer was calculated for the C-111 reach, between S-176 and S-177, and for the L-31W reach, between S-174 and S-175. (Fig. 1). Chloride concentrations were measured in water samples collected bimonthly from 14 wells in the Miami Limestone and the Fort Thompson Formations, and from water samples collected bimonthly from six locations within the C-111 and L-31W canals. Chloride concentrations in the groundwater west of L-31W canal remain relatively constant over the year at approximately 20 mg l^{-1}. Chloride concentrations in canal waters, however, show a higher variability. That is, the concentrations in both the L-31W and C-111 canals typically doubles from roughly 30 mg l^{-1} in February to approximately 60 mg l^{-1} in April. The response in the wells east of L-31W occurs with varying time delay and intensity, and depends on the distance from the canal and the location in either the upper or lower part of the aquifer. We used a transient chloride transport model in order to compare exactly the time-dependent simulated concentrations with the matching observations.

MODEL CALIBRATION

Automated model calibration was carried out with UCODE, a model-independent computer code developed by Poeter & Hill (1998). UCODE was combined with the application model codes MODFLOW (McDonald & Harbaugh, 1996) for groundwater flow, and MT3D (Zheng, 1990) for advective–dispersive solute transport in groundwater. The automated parameter estimation is posed as a nonlinear regression problem and is solved by minimizing a weighted least-squares objective function using a modified Gauss-Newton method (Hill, 1998). Groundwater flow and coupled chloride transport were simulated with a three-dimensional, two-layer finite difference model, discretized into a total of 21 836 cells, and covering a rectangular area of more than 100 km^2. Numerical solutions to both the flow and the transport equations were obtained for third-type conditions applied to all outer and inner boundaries of the rectangular problem domain. We found that numerical solutions to the flow and transport equations were the most sensitive to changes in the values of six parameters: the hydraulic conductivities of the Miami Limestone (K_{ML}) and the Fort Thompson Formation (K_{FT}), the specific yield of the Miami Limestone (S), the leakance between both layers (L), and the conductances per canal unit length of L-31W (C_{L31W}) and C-111 (C_{C111}). These parameters were adjusted in the inverse simulations, and we assumed that the values of these parameters did not vary spatially. The parameter with the lowest calculated sensitivity, C_{C111}, was kept constant in three out of our seven models (Table 1). We expected a possible improved model convergence with this reduction of estimated parameters.

The transient calibration model simulated a six month period from 18 February to 3 September, 1998. Initial values for three of the parameters were obtained from an analytical solution of a canal drawdown test (Genereux & Guardiario, 1998). These

Table 1 Flow and transport models identified on the basis of model number, calibration targets, and parameters estimated.

Model number	Calibration targets	Parameters estimated
1	Head (*H*)	K_{ML}, K_{FT}, S, L, C_{L31W}
2	Head	K_{ML}, K_{FT}, S, L, C_{L31W}, C_{C111}
3	Flux (*F*)	K_{ML}, K_{FT}, S, L, C_{L31W}
4	Flux	K_{ML}, K_{FT}, S, L, C_{L31W}, C_{C111}
5	Head, flux	K_{ML}, K_{FT}, S, L, C_{L31W}
6	Head, flux	K_{ML}, K_{FT}, S, L, C_{L31W}, C_{C111}
7	Head, flux, concentration (*C*)	K_{ML}, K_{FT}, S, L, C_{L31W}, C_{C111}

values were 1.7×10^{-1}, 4.7×10^{-2}, and 8.3×10^{-3} m s^{-1} for K_{ML}, K_{FT}, and C_{L31W}, respectively. The starting value for C_{C111} was set to 1.2×10^{-2} m s^{-1} due to the 50% wider canal profile compared to L-31W. Starting estimates for S and L were 0.15 and 3.0×10^{-2} s^{-1}, respectively. The total number of observations used for the model calibrations were: (a) 196 hydraulic heads of the upper Miami Limestone, (b) 56 seepages of the canals L-31W and C-111, and (c) 196 chloride concentrations in both formations of the Biscayne Aquifer. Measurements of hydraulic heads (*H*), seepage fluxes (*F*), and pore-water chloride concentrations (*C*) were used to estimate the parameters of seven different models (Table 1).

CALIBRATION RESULTS

The optimal parameter values differ significantly depending on the types of data used in the calibration (Fig. 2). For example, the range in best-fit values of L is greater than eight orders of magnitude. Only optimal values of K_{ML} and C_{L31W} differ between calibrated models by less than an order of magnitude. The 95% parameter confidence intervals are generally smaller for models with larger numbers of adjustable parameters (Fig. 2). Compared to parameter confidence limits calculated for the inverse simulations

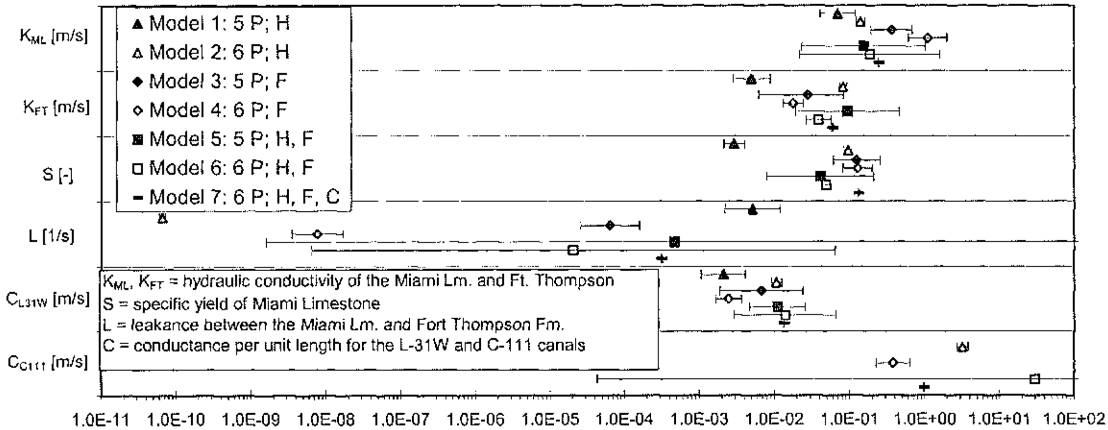

Fig. 2 Calibrated final parameter values and 95% confidence intervals. Models 1–7 differ in the number of estimated parameters (*P*), and measurement types used for the calibration (*H*: hydraulic head, *F*: seepage flux, and *C*: chloride concentration).

with one and two calibration targets (i.e. Models 1–6), the confidence limits calculated for the inverse simulation with three calibration targets (i.e. Model 7) are considerably smaller and suggest a higher likely accuracy of the estimates (Hill, 1998).

MODEL EVALUATION

Each of the seven models was evaluated by comparing predicted and measured values of hydraulic head and canal seepage taken during a canal drawdown test on L-31W. The accuracy of the prediction is quantified by comparing the sum of weighted-squared residuals for each measurement type, and the sum of the weighted-squared residuals for all measurement types. The drawdown test in canal L-31W was performed over 10 days in January 1996 between the structures S-174 and S-175 (Genereux & Guardiario, 1998). The hydraulic head response to the 0.4 m drop in canal stage was measured in 27 wells. Observations of groundwater seepage into canals were obtained by measuring canal flows (a) with Doppler acoustic velocity meters on both ends of a 2400 m reach on L-31W (see Fig. 1), (b) between gates S-174 and S-175 on L-31W, and (c) between gates S-176 and S-177 on C-111. A total of 511 hydraulic head and 67 flux measurements were collected.

We find that the predictive capability of the model is a strong function of the types of data used in the calibration (Fig. 3). The residual sum of squares is greatest for Models 1 and 2 indicating that parameters derived from calibrations based solely on head measurements cannot be used to predict groundwater flow in the canal drawdown experiment. The predictive capabilities of the models calibrated solely on flux (i.e. Models 3 and 4) depend on the number of parameters estimated in the calibration; in the six-parameter calibration, the match between observations and predictions is poor, but in the five-parameter calibration, model-data agreement is excellent. Models calibrated on both measurements of hydraulic head and fluxes (i.e. Models 5 and 6), closely predict the results of the drawdown test, and are outperformed only by Model 7,

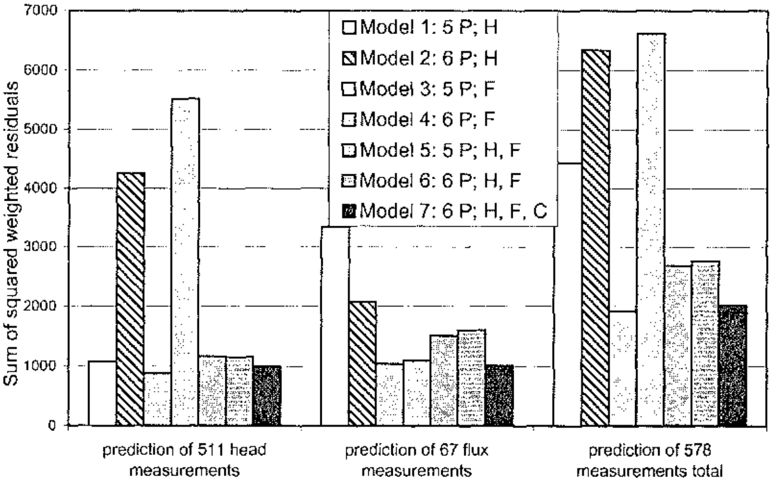

Fig. 3 Sum of weighted squared residuals for the drawdown test prediction of 511 hydraulic head and 67 canal seepage flux measurements.

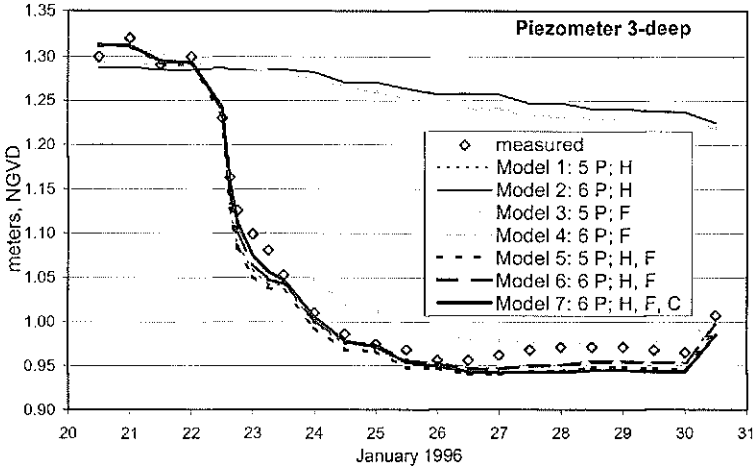

Fig. 4 Comparison of observed and model-calculated hydraulic heads. Piezometer 3-deep bottoms in the Fort Thompson Formation.

which was calibrated on all three types of observation—hydraulic head, fluxes, and pore-water chloride concentrations. The predictive capabilities of each model, as quantified by the residual calculations, are mirrored in the predictions of the individual well hydrograph that was measured during the drawdown experiment (Fig. 4). The piezometer 3-deep is screened in the lower layer of the Biscayne Aquifer. Models 2 and 4 are not able to reproduce the well response to the drop in stage in the canal cutting solely through the upper layer. This is due to the fact that these two models estimated a leakance between layers, which is several magnitudes lower than in the other calibrated models (see Fig. 2).

SUMMARY AND CONCLUSIONS

We compared seven groundwater models calibrated against different combinations of hydraulic head, canal seepage fluxes, and pore-water chloride concentrations. Automated inverse techniques were used for the groundwater flow and coupled solute transport model calibrations. Each of the seven models was evaluated by comparing predicted and measured values of hydraulic head and canal seepage taken during a 10 day canal drawdown test of L-31W. We find that predictions of groundwater flow are in serious error if they are based on parameters obtained from models calibrated solely on hydraulic heads. Parameters could be estimated more accurately and the uncertainty in the fitted parameters could be reduced by using data on groundwater fluxes to canals, and pore-water chloride concentration in the calibration process. Although our results were derived for a permeable limestone aquifer, we believe that the techniques tested in this work will be applicable for estimating aquifer parameters in a wide variety of hydrogeological settings. Our results also demonstrate that a fairly simple model of a complex hydrogeological environment can perform accurately if the appropriate calibration data are chosen.

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