Calibration of a Density-Dependent Groundwater Flow Model of the Lower West Coast Floridan Aquifer System

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ABSTRACT
A three dimensional density dependent groundwater model was developed as a predictive and interpretive tool for the Lower West Coast Floridan aquifer system using a modified version of SEAWAT-2000 (Langevin et al. 2003). This paper describes an automated calibration procedure for this model, the Lower West Coast Floridan Aquifer System Model (LWCFAS), using pilot points, regularization and the prior information option from PEST (Doherty 2004). A stepwise approach, starting with the least known parameter, was used to optimize three decision variables: vertical hydraulic conductivity of the confining units, storage and horizontal hydraulic conductivity of the aquifers. This approach allows for manageable computer run times while allowing the decision variables to improve in each step. A finer resolution model that meets calibration targets is achieved after calibrating a coarser model with PEST.

INTRODUCTION
The ever-increasing population of south Florida has put a strain on water supplies, which are mostly taken from the surficial and intermediate aquifer systems. Alternative water sources are being sought to curb the pressures exerted on present water supplies and to guarantee the long term survival of the Everglades. The South Florida Water Management District (SFWMD) initiated the development of the Lower West Coast Floridan Aquifer System (LWCFAS) Model in cooperation with Florida Atlantic University to investigate possible alternative water sources. The active zone is defined, when possible, as larger than the Lower West Coast (LWC) Planning Area, such that a buffer zone is created around the study area. Vertically, the model includes the three major aquifer systems that underlie southern Florida: the surficial aquifer system (SAS), the intermediate aquifer system (IAS), and the Floridan aquifer system (FAS); however, the model focuses on the IAS and FAS. The hydrostratigraphy follows that laid out by Reese and Richardson (2004). The only hydrologic stress is groundwater extraction and/orinjection.

This paper describes an automated calibration procedure that uses a series of steps, resulting in three versions of the LWCSFAS Model. The quasi-steady-state model was initiated to generate initial conditions and boundary conditions for the transient models. Two transient models were developed; the first model was created for semi-automatic calibration with a coarser resolution, and the second model was created with a finer resolution for predictions. These models are herein referred to as: Q3K-CP, T12K-UNCP and T3K-UNCP and correspond to a quasi-steady-state coupled model with a 3,000 ft by 3,000 ft resolution, a transient uncoupled model with a 12,000 ft by 12,000 ft resolution and a transient uncoupled model with a 3,000 ft by 3,000 ft resolution. The T3K-UNCP Model is the final product of the calibration approach.

MODEL DESIGN
A modified version of SEAWAT-2000 was selected for the LWCFAS Model. This version includes the UGEN (Restrepo et al., 2001) and HBXY (Restrepo et al., 2006) packages to handle data efficiently and interpolate boundary conditions. A combination of no-flow, constant head and general-head boundaries were used in this particular model. The western boundary coincides with the Gulf of Mexico. In the top and bottom model layers, constant head boundaries are

specified for all cells. In Layers 2 through 11, constant head boundaries are specified for the southern-most and western-most active cells in coastal regions along the Gulf and Florida Bay. The eastern (following a groundwater divide) and northern model boundaries contain general head boundaries for Layers 2 and 3 and no-flow boundaries for Layers 4 to 11.

CALIBRATION METHOD

PEST, a nonlinear, least-square, inverse modeling program developed by Doherty (2004) was used to auto-calibrate the LWCFAS Model, along with some manual calibration. This approach uses pilot points (PPs) and regularization parameterization scheme with SVD-Assist.

Q3K-CP Version of Model

The purpose of the Q3K-CP Model was to generate initial conditions and refine boundary conditions for the transient models. When the coupled model was initially executed, unreasonable values of concentration and hydraulic conductivities were needed to maintain the head in the model domain and keep the model stable. The Gulf boundary was refined during several manual, trial-and-error calibration runs until the surface around the boundary was smooth (e.g., avoiding significant gradients). The depiction of the Gulf boundary is hypothetical due to the unknown nature of the western boundary conditions; however, the Gulf boundary is located 60,000 feet off-shore, away from the main study area.

Predetermined ranges for initial input values were set by a combination of site-specific data or literature-cited values (Freeze and Cherry 1979). For this modeling effort, transient potentiometric heads were selected as calibration targets. Targets included daily and random samples from monitoring wells with time series consisting of frequent observations (i.e., 14,788 total weekly observations in 65 wells from Layers 2 through 10) over a maximum of five years.

T12K-UNCP Version of Model

For the LWCFAS Model transient calibration, in order to have reasonable running times, the original quasi-steady-state 3,000 feet by 3,000 feet model was aggregated into a coarser model with a resolution of 12,000 feet by 12,000 feet; this model was run uncoupled and has 12 layers, 72 rows, 37 columns and 260 weekly stress periods. In the decision process for the calibration, computer time for a simulation was also taken into consideration.

For the transient, uncoupled calibration, a stepwise calibration approach was used. The first step estimated the decision variables at PPs at a coarser resolution. The algorithm based upon sequential optimization steps increased the number of PPs to produce spatial disaggregation of the domain. This procedure was followed since a large model is being calibrated and PEST is a very calculation intensive program. In this approach, the same type of objective function was used. Transient calibration was undertaken to determine sequentially: vertical hydraulic conductivity in the confining layers (K_z), then the specific storage (S_s) of aquifer systems, and finally the horizontal hydraulic conductivity (K_x).

Step 1. Initial conditions created by the Q3K-CP Model were used to start the transient calibration. PPs were located every 8 cells for a total of 27 per layer. The total number of PPs in a model simulation depends on the decision variables. The range of values for horizontal hydraulic conductivity was purposefully constrained, since it was the best available data. The optimal solution for the three decision variables was found using PEST. Several rounds of Step 1 were carried out until the solution did not change substantially and arrived to a minimum.

Step 2. The second step used the estimated parameters from Step 1 and increased the number of PPs to every 7 cells for a total of 36 per layer. The parameter space for K_x was kept very tight as described in Step 1. The optimal solution for the three decision variables was found again. One round of Step 2 was carried out. The objective function improved only for S_s and K_z.

Step 3. An additional round of runs was made to allow for refinement of the lower-layer parameters starting with the solution from Step 2. The PPs are located every 6 cells for a total of 49 PPs per layer. The objective function improved only for K_z.

In Layer 1, the original K_z was used with an upper limit defined as one order of magnitude of the starting value and three orders of magnitude for a lower limit. The limits for the other confining layers were set from 1.0E-9 to 2.E+1 and the initial values were based on the few published leakance values available. Values for S_s were derived from literature (Freeze and Cherry 1979) and ranged from 5.0E-06 feet-1 to 1.0E-4 feet-1. The upper and lower bounds of the horizontal conductivity were set to 35 percent above and below the initial data. The final results for K_x are relatively close to the field-measured data. In the current optimization procedure, two weights for the observations were used in all steps. For Layers 1 to 4, weights are equal to 1. For Layers 5 to 11, weights are equal to 8. These criteria put more weight to the focus area – Layers 5 to 12.

T3K-UNCP Version of Model

After the T12K-UNCP Model is calibrated through PEST, the T3K-CP Model was generated based on the estimated parameters from the T12K-UNCP Model. The purpose of the T3K-CP Model is to produce predictions using a finer grid resolution; this model did not undergo further calibration, but rather relies on the calibration from the coarser model.

CALIBRATION RESULTS

Calibration targets, for groups of observations per aquifer, within the model domain, are displayed in Figure 1 (for T12K-UNCP and T3K-UNCP Models).

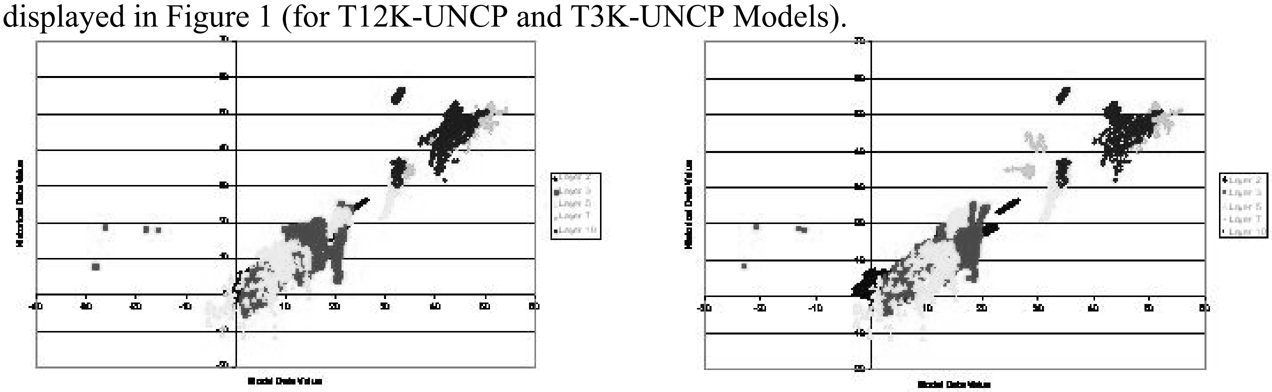

Figure 1.Calibration scatter plots for the T12K-UNCP and T3K-UNCP Models.

Table 1 provides the standard error and correlation coefficient (r-value) for each layer. The results indicate that there is a good linear relationship between the observed and simulated data for all layers for both models.

Table 1. Standard error and correlation coefficient for T12K-UNCP and T3K-UNCP Models.

Model Layer	Standard Error (ft)		Correlation Coefficient	
	T12K-UNCP	T3K-UNCP	T12K-UNCP	T3K-UNCP
3	4.12	3.99	0.75	0.76
5	3.50	4.97	0.95	0.91
7	1.68	5.34	0.97	0.91
10	6.99	7.40	0.40	0.32

CONCLUSIONS

This approach was applied to a regional model in a confined system. Model statistics indicate that the model does an acceptable job of matching the historical data. The combination of reasonable parameter distributions and a good fit between modeled values and field observations indicates that the model can be useful for evaluating regional groundwater issues where the concentration is not expected to change significantly over long periods of time. K_z is the most sensitive hydraulic parameter in the LWCFAS Model, followed by S_s and K_x. This is of utmost importance since the model has shown extensive spatial variability in the vertical conductance values. This approach allows for manageable computer run times while allowing the decision variables to improve in each step. A finer resolution model that meets calibration targets is achieved after calibrating a coarser model with PEST.

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