PARAMETER OPTIMIZATION AND UNCERTAINTY ANALYSIS OF AN INTEGRATED HYDROLOGIC MODEL

by

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Abstract. Automated calibration methods are increasingly more productive for refining groundwater models. Automated parameter calibration coupled with uncertainty analysis allows for quantitative skill assessment. The authors explore the use of a commercial package known as PEST in the groundwater pre-calibration of an integrated model of the Saddle Creek basin, an area characterized by extensive phosphate mining and rapid urbanization. PEST optimizes model calibration by minimizing the sum of squares difference between observed and modeled heads. Additionally, PEST calculates confidence limits for each optimized parameter. These confidence limits can be used to assess the relative uncertainty of individual parameters. This optimization process was used to simplify the hydraulic conductivity distribution of the Saddle Creek model from eight zones to one, and to suggest which of two conceptual models best represented the Floridan aquifer head distribution in the model.

Additional Key Words: model, calibration, optimization.

Introduction

Often, mining reclamation projects require the establishment of wetlands, the assessment of wet and dry season impacts, the improvement of hydrologic functioning, and the evaluation of design alternatives. Surface and groundwater models can be useful tools for addressing these requirements, and the usefulness of these models can be increased by improving the model calibration. This paper will describe the use of an automated calibration program for the pre-calibration of the groundwater component of an integrated surface water-groundwater model. Although only the groundwater component is addressed, these calibration programs are very general and may be applied to many different types of models.

Increasingly, groundwater modelers are taking advantage of programs that automate a portion of the calibration process. Programs such as PEST (Watermark Computing, 1999), UCODE (Poeter and Hill, 1999), and MODFLOWP (Hill, 1992) calculate the parameter values for a specified parameter distribution using a linear regression model that minimize an objective function, typically the sum-of-squares differences between observed and simulated heads. Along with the optimized parameter values, several sets of useful statistics are generated including parameter confidence limits, correlations, and sensitivities. With these statistics, calibration programs can be a valuable tool for evaluating the uncertainties associated with parameters that are used to model a real aquifer system.

Because parameter optimizing programs use linear regression and hence, assume that parameter variation is linear (at least in the vicinity of the optimized values), confidence limits can be calculated with a t- or F-test similar to an analysis of variance (Draper and Smith, 1981). The confidence interval, defined by an upper and lower 95 percent confidence limit, can suggest how well a particular parameter value is resolved. Spatial distribution of observation data, number of observations,

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Proceedings America Society of Mining and Reclamation, 2000 pp 694-699
DOI: 10.21000/JASMR00010694

https://doi.org/10.21000/JASMR00010694

contrast between parameters, and correlation with other parameters can affect the certainty of parameter resolution. Parameter values with wide confidence limits may be problematic. Wide confidence limits probably extend beyond the linearity assumption and, while the parameter value should remain suspect, the confidence interval is, most likely, exaggerated. Because the confidence limits are determined only by statistical procedures, the limits may exceed the possible values of some parameters.

Correlation between pairs of parameters can be a very useful indication of parameter reliability. Highly correlated parameters cannot be independently resolved without additional data. For example, recharge and leakance can be varied inversely to produce the same result. Without additional data, such as a flux measurement, only the ratio between recharge and leakance can be determined, not their absolute values.

This paper illustrates the use of one particular optimizing program, PEST, in evaluating surficial aquifer parameter distributions in the groundwater component of an integrated surface water-groundwater numerical model.

Conceptual Model

The area modeled is in Polk County of west-central Florida, which is located about 30 miles east of Tampa (Fig. 1). This area includes urban development, numerous lakes, agriculture, and extensive open-pit phosphate mining operations with active mines and closed mines in various states of reclamation. The surface water basins form the Saddle Creek watershed (SCW). Contained within the SCW is a reclaimed phosphate mine that is now a state recreation area, the Tenoroc Fish Management Area (Fig. 1). Tenoroc was used as an intensive data collection area for the modeling project.

To aid in the establishment of boundary conditions and initial aquifer parameters, a regional model that incorporated the Saddle creek model domain was created. The regional model was based a model developed by the Southwest Florida Water Management District (SWFWMD). The SWFWMD model is a quasi-three dimensional MODFLOW model with four hydrostratigraphic units, all of which are fully or partially contained within the Saddle Creek watershed area. Figure 2 illustrates the sub-surface geology and the SWFWMD hydrostratigraphic units. The top unit, composed of sand, silty-sand and some clay, represents the surficial aquifer. The second unit contains a clayey confining bed which is missing or discontinuous in the north, including the Tenoroc and Saddle Creek area, but becomes continuous and thicker toward the south. As this unit thickens, an intermediate limestone aquifer develops. Below the second hydrostratigraphic unit is the top of the

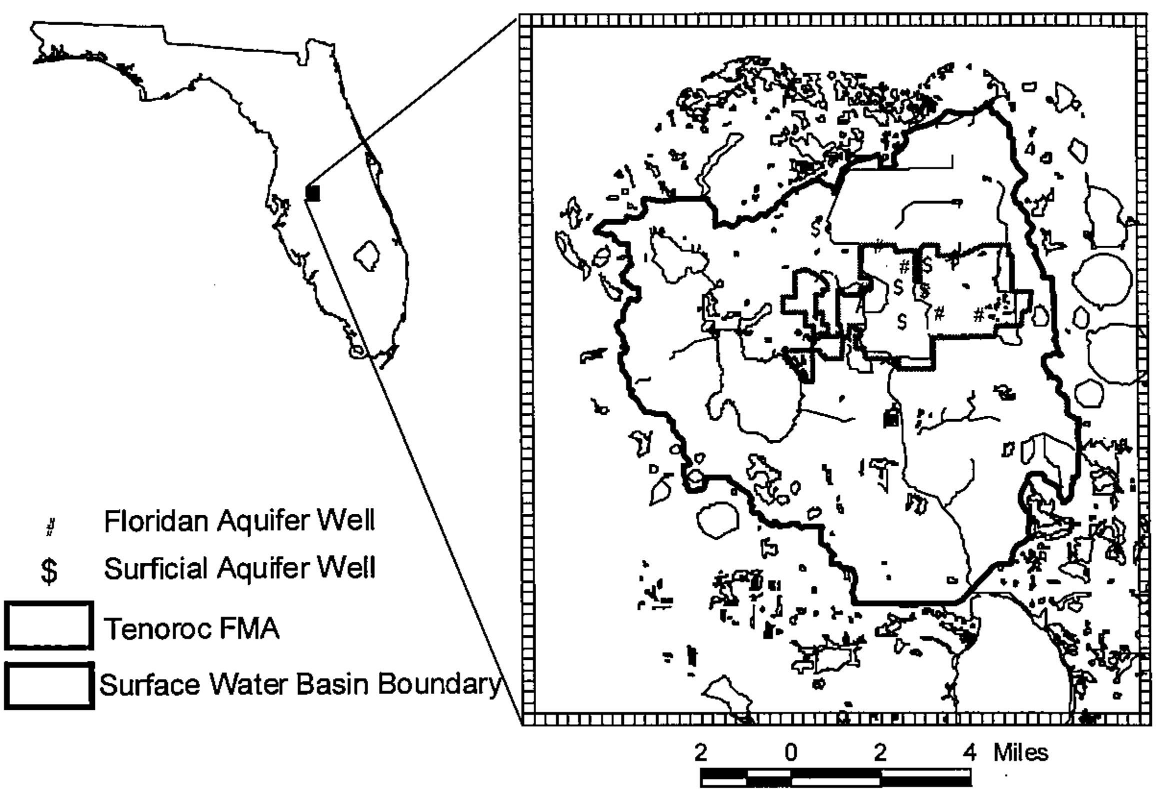

Figure 1. Site Location and Observation Wells

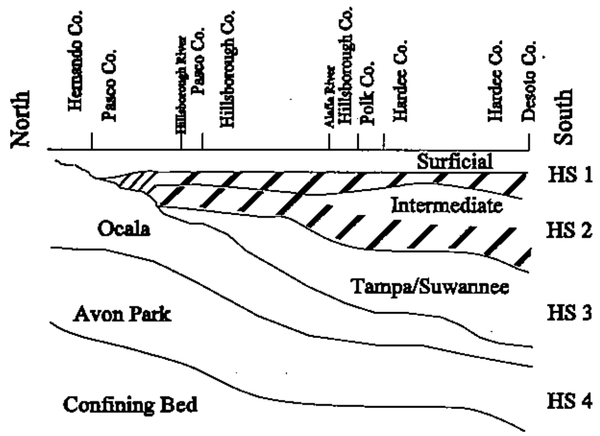

Figure 2. Subsurface geology and hydrostratigraphic units of the regional model.

Upper Floridan aquifer. The freshwater portion of the Floridan aquifer (the Upper Floridan) is separated into two hydrostratigraphic units, Model Layers Three and Four. Model Layer Three represents the Tampa/Suwannee Limestone and the Ocala Formation. The fourth hydrostratigraphic unit representing the lower portion of the Upper Floridan aquifer is comprised of the Avon Park Formation. For the regional and Saddle Creek models, the layer associated with the more productive Unit Four (Avon Park Formation) was assigned a transmissivity value of four times that of Unit Three. Fluxes into and out of hydrostratigraphic Unit Two, including the intermediate aquifer, were simulated by adjusting the leakance terms at the upper and lower boundaries. The intermediate aquifer does not exist (at least as a continuous unit) in the upper portion of the SCW and, therefore, the leakance and transmissivity values for Layer Two in that area reflect a confining unit only.

The regional model was calibrated to steady-state conditions using the average Floridan aquifer elevation from the 1989 U.S.G.S. potentiometric surfaces, the average of the monthly 1989 estimated groundwater withdrawals from SWFWMD, and a constant-head surficial aquifer estimated from surface water features.

The Saddle Creek model domain resides within the far-field model (Fig. 3) and initially used the same parameter distributions. The Saddle Creek study area is 14 by 16 miles. The model cell length was fixed at 1/4 mile, creating a 64x56 row by column grid with cell areas of 0.06 square mile each. The northern no-flow boundary coincides with that of the regional model; the other boundaries are head-dependant flux with conductances derived from the far-field model.

<u>Data Collection</u>

Data for the Saddle Creek model was collected over a 2 ½ year period beginning October 1996 thru March 1999. Data collected included precipitation from four rainfall stations and streamflow from U.S.G.S. gaging stations. SWFWMD provided lake stages, groundwater withdrawals, and Floridan aquifer elevation data from wells surrounding the model area. Extensive

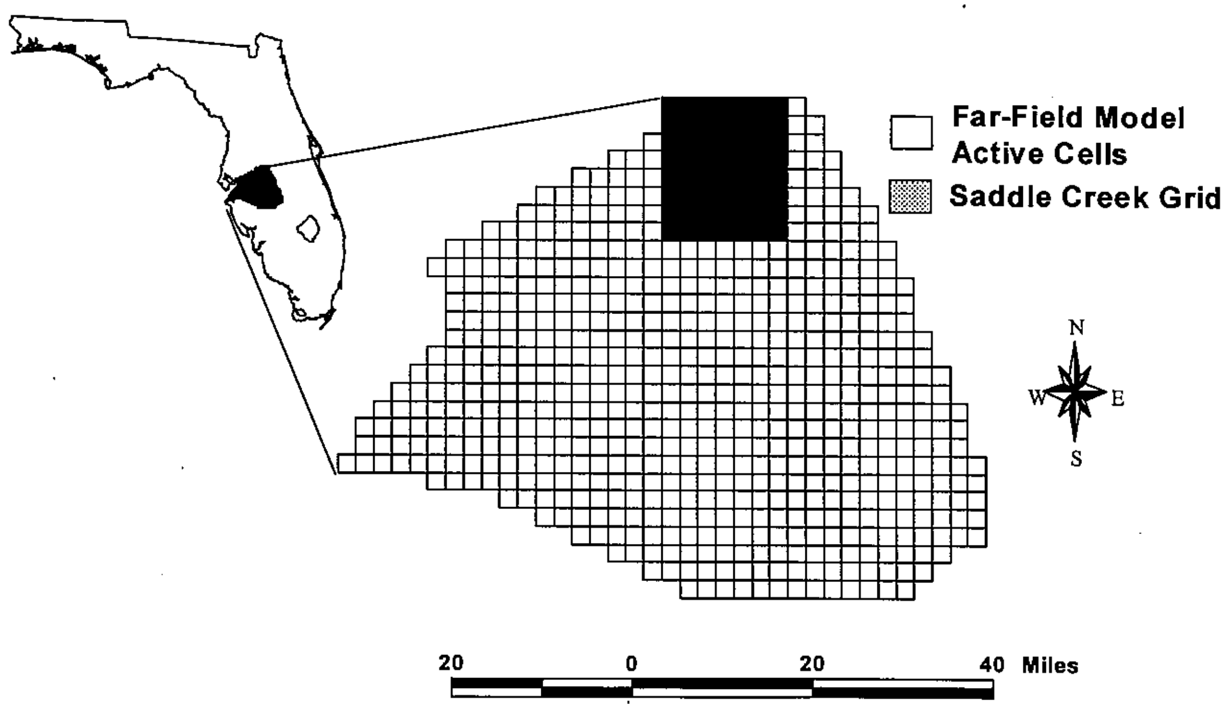

Figure 3. Far-Field Model and Saddle Creek Model

additional data were collected within the Tenoroc Fish Management Area (FMA). To monitor groundwater elevations, a network of wells was used, consisting of four surficial wells installed for this project and one U.S.G.S. surficial well, and five existing Floridan wells remaining from the mining operation and one U.S.G.S Floridan well (Fig. 1). To monitor surface water conditions, seven streamflow stations and five lake staff gages were installed.

Calibration programs require a data set with which to compare simulation results, in this case water level elevations in each aquifer were used. A monthly time series was developed for each of the twelve wells (six surficial and six Floridan) that were measured during the two and a half year data collection period. Because the wells were clustered together, a second set of aquifer elevations was created. From the monthly SWFWMD Floridan well survey, a Floridan aquifer surface was created by interpolating existing water level data using the Arc/Info TIN function. From the TIN, Floridan elevations at 20 points scattered throughout the model domain were interpolated for each monthly time step. Because the Floridan aquifer is highly transmissive, the interpolated heads should provide a reasonable approximation of the Floridan surface. To adjust for the difference in reliability between the measured and interpolated heads, measured heads were given a weight three times greater than interpolated heads. The total number of observations over the 30 month simulation period was 919 of which 319 were actual water level observations.

Recharge estimates for the groundwater model were derived from the surface water model; therefore, the recharge distribution was not an optimized parameter. This flux estimate provided an additional constraint on the groundwater model.

Optimization Results

To explore how PEST (or other calibration programs) can be used to evaluate alternative conceptual models, two of the questions that arose during the calibration process will be addressed: 1) Can a physically-based parameter distribution such as county soil maps or mining landforms be used to represent the surficial aquifer? 2) If a distribution of large head residuals can be improved by adjusting more than one parameter, which parameter is the best choice?

Physically-based Parameter Distribution

Models seem to provide better predictive results when a minimum number of different distributions of parameters are employed (Freyberg, 1988). Models may reproduce observations closely with a complex network of odd-shaped parameter zones clustered around wells. However, when new observations or different stresses, such as increased groundwater withdrawals, are added, the model reliability decreases – often substantially. One of the benefits of optimization programs is that a model containing many zones of a parameter can be simplified by combining zones with similar optimized values and sensitivities producing a more generalized solution.

The regional model used a hydraulic conductivity value of 10 ft/day for all of layer one. With the finer resolution of the Saddle Creek model, it was proposed that a generalized discretization based on a physical property may provide a more accurate model. Soil types and (or) mined landforms seemed to be a reasonable possibility. The Bureau of Mining and Reclamation of the Florida Department of Environmental Protection maintains a database of mined landforms. These primary landforms are coded as clay settling areas, sand tailings areas, mined-out areas, hydraulically-mined areas and other. These basic landforms, however, do not have consistent effects on the groundwater flow system. Clay settling areas may be constructed on unmined land where they do not affect the flow of groundwater but do limit infiltration, or they may be filled into a mine pit where they act as barriers to groundwater flow. Similarly, sand tailings may be on mined, unmined, or clay settling areas, each with a different, or possibly no effect, on the groundwater flow system. For this reason, only mined-out areas, which incorporate mined land and associated mine pits, were used with the soil types. Mined out areas were assigned to soil type code 150. Figure 4 illustrates the distribution of soils identified in

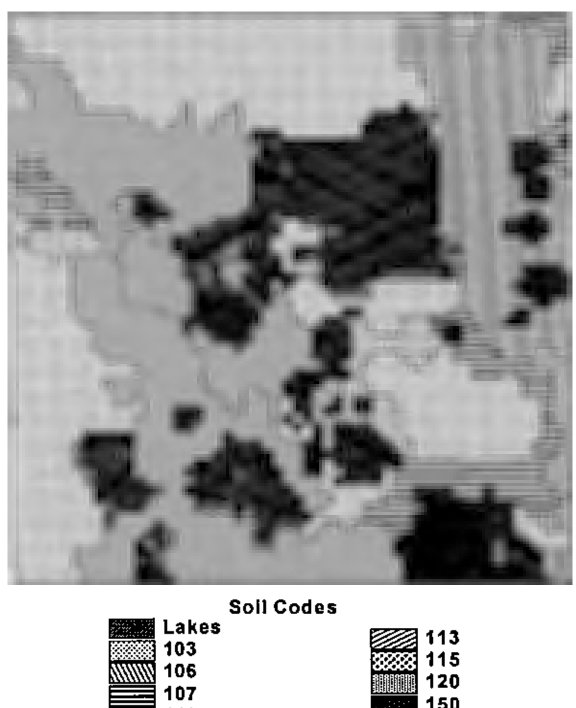

Figure 4. Soil-Type Distribution

the model area. Each of the eight different soil types was assigned a leakance, hydraulic conductivity, and specific yield parameter. PEST was used to optimize these parameter values.

The optimization results are summarized in Table 1. Parameters were named by soil code preceded by 'h' for hydraulic conductivity, 'l' for leakance, and 's' for specific yield. Parameter correlations were low, which is necessary to fix reasonable confidence limits on estimated values. The parameters with highest correlation coefficients were h107 and l107 at 0.67 and s106 and s113 at 0.61. However, there were few parameter values which differed enough from the others to justify a separate distribution. All of the hydraulic conductivity values were within the most restrictive confidence interval, as were all of the leakance values, and all but one of the specific yield values. Also, many of the confidence intervals, especially the hydraulic conductivity and specific yield, were quite broad. Thus, the soil classification distribution was not employed.

Table 1. Soil-type Optimization (feet and day units)

Param	Est. Value	95% Confidence		Sens
		Lower	Upper	
h103	14	-58	85	0.08
h106	8	-665	681	0.04
h107	4	-1012	1020	0.02
h110	11	-12	34	0.62
h113	17	-565	599	0.02
h115	9	-1287	1305	0.01
h120	1	-503	505	0.64
h150	13	-14	40	0.46
l103	1.4e-04	6.0e-05	3.5e-04	94
l106	1.5e-04	2.0e-05	9.7e-04	58
l107	1.1e-04	0	1.4e-02	6
l110	1.6e-04	1.0e-04	2.3e-04	77
l113	1.5e-04	8.0e-05	3.0e-04	114
l115	1.6e-04	0	4.7e-01	8
l120	1.8e-04	5.0e-05	6.3e-04	62
l150	1.4e-04	1.0e-04	2.0e-04	66
s103	0.09	-0.12	0.30	72
s106	0.09	-0.69	0.87	32
s107	0.02	-2.63	2.67	4
s110	0.10	0.04	0.16	136
s113	0.10	-0.08	0.29	199
s115	0.41	-1.85	2.68	2
s120	0.11	-0.36	0.58	51
s150	0.10	0.05	0.15	153

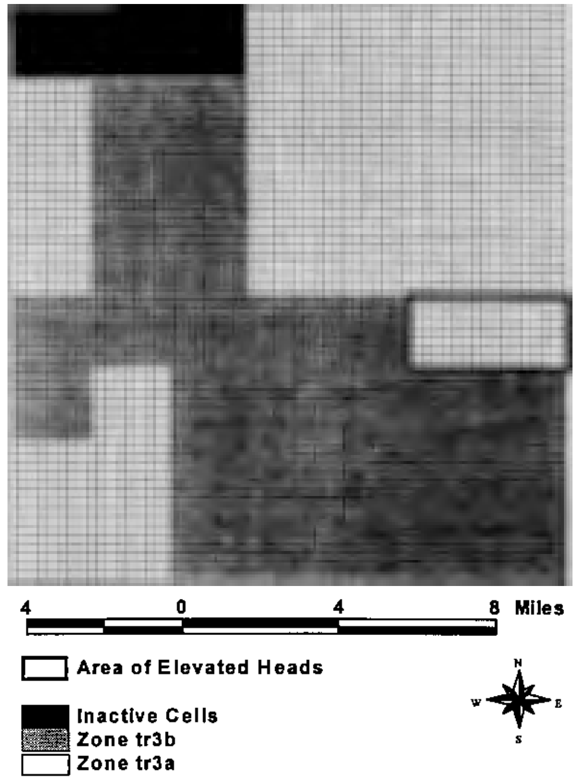

Figure 5. Initial Floridan Transmissivity Parameter Zonation from the Regional Model

Parameter Selection

Frequently during calibration, a pattern of head residuals can be improved by altering the distribution of one or more parameters. With an optimizing program, different parameter distributions can be easily compared. During calibration, it was noticed that one area of the model-calculated heads exceeded observed heads in the Floridan aquifer layers by almost six feet (Fig 5). To correct this problem, two obvious choices were available: create a new zone of lower leakance over the area or alter the transmissivity of the Floridan layers.

Table 2 contains the optimization results before the two alternative options were tested. The total sum-of-squares residual was 24655. For the first option, a low leakance zone was added above the elevated head area (l214) and a new optimization was run. The problem heads were reduced by approximately two feet. Table 3 contains the optimization results. The total sum-of-squares residual has been reduced to 24027, but the optimized leakance value for parameter l214 is very low and the confidence interval spans 126 orders of magnitude. Also, the sensitivity for this parameter is very low compared to the other parameters, indicating that the model is very insensitive to this parameter at this value.

To effect option two, the Floridan transmissivity in the boxed area of Figure 5 (where the heads were elevated) was changed from the higher transmissivity parameter tr3a to the lower transmissivity parameter tr3b. Table 4 shows the results of this modification. The optimized values are realistic, the sum-of-squares error is 24070, the same as the above option but the confidence intervals are all relatively narrow and the sensitivities are similar. Of the two options, this appears to be more reasonable.

Table 2. Initial Transmissivity and Leakance Optimization (feet and day units)

Param	Est. Value	95% Confidence		Sens
		Lower	Upper	
l201	1.6e-04	1.3e-04	1.9e-04	199
l212	1.0e-03	8.4e-04	1.2e-03	112
l213	5.0e-05	2.0e-05	1.5e-04	183
tr3a	21656	16831	27865	131
tr3b	6205	5309	7252	399

Table 3. Additional Low Leakance Zone Optimization (feet and day units)

Param	Est. Value	95% Confidence		Sens
		Lower	Upper	
l201	1.6e-04	1.3e-04	2.0e-04	185
l212	1.0e-03	7.6e-04	1.3e-03	112
l213	5.2e-05	3.3e-05	8.1e-05	179
l214	4.2e-07	1.8e-70	9.8e+56	0.20
tr3a	27954	22462	34790	132
tr3b	6460	5473	7624	430

Table 4. Final Transmissivity and Leakance Optimization (feet and day units)

Param	Est. Value	95% Confidence		Sens
		Lower	Upper	
l201	1.6e-04	1.3e-04	1.9e-04	186
l212	1.0e-03	8.4e-04	1.2e-03	112
l213	5.2e-05	2.0e-05	1.4e-04	176
tr3a	26834	20582	34985	132
tr3b	6460	5541	7532	430

Conclusion

Automated calibration, or more appropriately parameter optimization, programs can be a useful tool to more efficiently and reliably calibrate groundwater models. Also, and perhaps more importantly, these programs can provide a means to objectively evaluate different conceptual models. As modeling becomes more important in the resource allocation and environmental assessment decision-making process, modelers should not only present well-calibrated models, they should also provide some indication of the level of confidence or predictive ability which may be expected of their models. These tools can be an aid in achieving that goal.

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