Use of time series and harmonic constituents of tidal propagation to enhance estimation of coastal aquifer heterogeneity

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ABSTRACT

A synthetic two-dimensional model of a horizontally and vertically heterogeneous confined coastal aquifer system, based on the Upper Floridan aquifer in south Florida, USA, subjected to constant recharge and a complex tidal signal was used to generate 15-minute water-level data at select locations over a 7-day simulation period. “Observed” water-level data were generated by adding noise, representative of typical barometric pressure variations and measurement errors, to 15-minute data from the synthetic model.

Permeability was calibrated using a non-linear gradient-based parameter inversion approach with preferred-value Tikhonov regularization and 1) “observed” water-level data, 2) harmonic constituent data, or 3) a combination of “observed” water-level and harmonic constituent data. In all cases, high-frequency data used in the parameter inversion process were able to characterize broad-scale heterogeneities; the ability to discern fine-scale heterogeneity was greater when harmonic constituent data were used. These results suggest that the combined use of highly parameterized-inversion techniques and high frequency time and/or processed-harmonic constituent water-level data could be a useful approach to better characterize aquifer heterogeneities in coastal aquifers influenced by ocean tides.

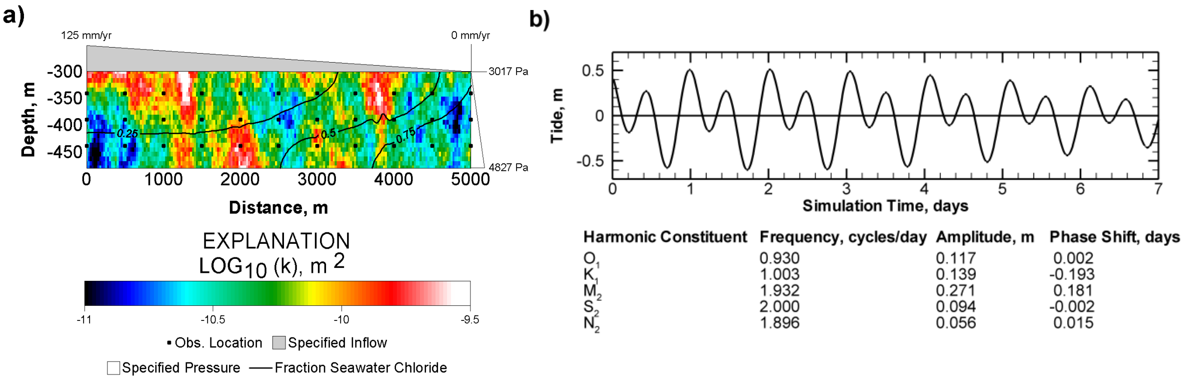
INTRODUCTION

Ocean tides are a combination of periodic constituents of different frequencies and amplitudes (Merritt, 2004), which cause a periodic fluctuation of an important boundary in coastal aquifers. In some settings, the tidal ranges can have magnitudes comparable to natural stresses, such as recharge events, and can be used to determine the hydraulic properties of coastal aquifers. The frequencies of tidal constituents are common to all ocean tides but the amplitudes and phase relations are characteristic of specific locations. The distance a tidal signal will propagate into a coastal aquifer is a function of hydraulic conductivity and the inverse of specific storage (hydraulic diffusivity). As a result, periodic head fluctuations in groundwater wells located close to the coast, resulting from tidal fluctuations, have been used extensively to estimate aquifer parameters (e.g., Ferris, 1951; Merritt, 2004).

Although tidal fluctuations have been used extensively to characterize aquifer properties, they have not been used with a highly parameterized numerical model to investigate heterogeneity in aquifer properties. The objectives of this study were to evaluate the use of “observation” data from a tidally-influenced synthetic coastal aquifer with a stochastically generated distribution of hydraulic conductivity to develop a calibrated model with highly-parameterized permeability and porosity fields. Because aquifer properties affect the amplitude and phase-shift of the tidal signal at specific locations in the aquifer (*e.g.*, observation wells), but not the frequency, harmonic constituent data are also used in the calibration process to improve the ability to resolve aquifer heterogeneities. The value of time-domain, harmonic constituent, and combined time-domain and harmonic constituent data is quantitatively evaluated to assess the relative value of these data.

METHODS

SUTRA-MS (Hughes and Sanford, 2004) was used to develop a model of a synthetic confined coastal aquifer (fig. 1a). The model was composed of 4,623 nodes and 4,400 equal-sized quadrilateral elements. The horizontal permeability (k_h) distribution of the aquifer was stochastically generated using a spherical variogram model with a mean k_h of 2.62×10^{-11} m^2 and a range of 5,000 m (fig. 1a). A horizontal to vertical permeability ratio (k_h / k_v) of 10 was used. Porosity (ε) in the original model was related to k_h using the Kozeny-Carman equation (Bear, 1978) and a length scale characteristic of permeable carbonate aquifers (0.01 m). A constant fluid and matrix compressibility of 4.47×10^{-10} and 1×10^{-8} $[kg/(m^2 \cdot s)]^{-1}$, respectively, were used. Hydraulic diffusivity ranged from 0.5 to 86 m^2/s with a mean value of 8.1 m^2/s. A linear recharge rate, ranging from 125 to 0 mm/yr, was applied to the top edge of the model (fig. 1a). A specified pressure boundary representing a hydrostatic, coastal boundary was applied to the right edge of the model (fig. 1a). No flow boundaries were assigned to the left and bottom edges of the model.



Harmonic Constituent	Frequency, cycles/day	Amplitude, m	Phase Shift, days
O_1	0.930	0.117	0.002
K_1	1.003	0.139	-0.193
M_2	1.932	0.271	0.181
S_2	2.000	0.094	-0.002
N_2	1.896	0.056	0.015

Figure 1. a) Model domain, boundary conditions, synthetic horizontal permeability, steady-condition factional seawater concentrations, and observation locations used. b) Harmonic constituents and resulting tidal fluctuations applied to the specified pressure boundary on the right edge of the model.

Initial pressure and fractional chloride concentrations for the synthetic model were generated using specified pressure nodes based on a sea-level elevation of 0.0 m and specified recharge rates (fig. 1a). A complex tidal signal, composed of the 5 most significant diurnal (O_1 and K_1) and semi-diurnal (M_2, S_2, and N_2) harmonic constituents, was applied to the synthetic model at specified pressure boundaries (fig. 1b). The synthetic model was then run for a 7-day period using a 15-minute timestep length. Water-level data were extracted from the synthetic model at 33 regularly spaced locations in the model domain (fig. 1a). Measurement "noise" was added to the water levels extracted from the synthetic model to represent realistic field conditions and calculated as the sum of Gaussian measurement error (±0.005334 m) and observed atmospheric pressure changes (±0.001 m) for a 7-day period beginning on July 1, 2009 at Virginia Key, Florida, USA. Fractional chloride concentration and fluid density data were not evaluated because of the short 7-day simulation period.

The automated, non-linear gradient-based parameter inversion code PEST was used to calibrate k_h in the models (Doherty, 2010). A k_h / k_v of 10 and the same Kozeny-Carman relation used to relate k_h and ε in the synthetic model was applied during model calibration. The models were parameterized using a pilot point in every model element and soft-knowledge using preferred-value Tikhonov regularization was used to make the inverse problem tractable. A total of 673 time-domain "observations" were used at each of the 33 observation locations. Harmonic constituent data at the 33 observation locations included amplitude data for each harmonic constituent calculated using a least-squares approach (Merritt, 2004). The tradeoff between adherence to the Tikhonov condition and the model fit to "observed" data was set at 0.40 m^2, which is equal to the sum of squares error (SSE) of the measurement error.

RESULTS AND DISCUSSION

The calibrated k_h fields for models calculated using a time-domain and/or harmonic constituent data are shown in figure 2. In all cases, the calibrated k_h field resulted in a calculated SSE error less than 0.5 m^2 for the time-domain "observations". Differences between the synthetic and calibrated k_h values are generally within ±1/3 an order of magnitude of the synthetic k_h (table 1) even though the strength of the tidal signal is reduced by more than 90% over most of the model domain. The discrepancy between the synthetic and calibrated k_h increased slightly between a distance of 0 and 1,000 m where attenuation of the tidal signal is greatest (generally less than 2% of the tidal signal).

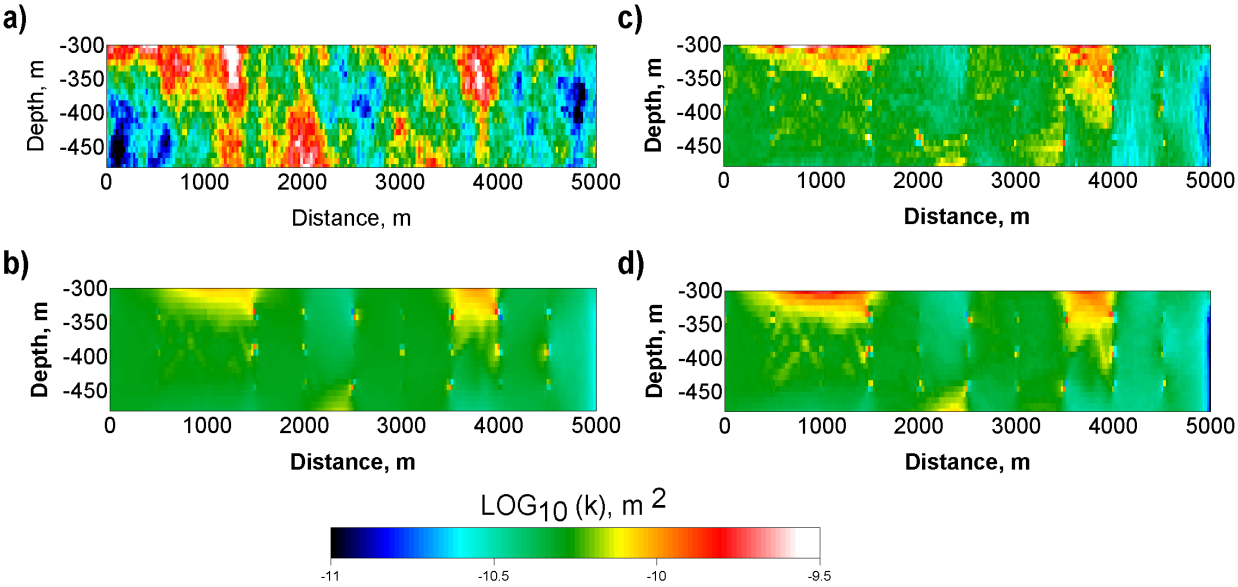


Figure 2. a) Synthetic and calibrated horizontal permeability for models calibrated using b) time-, c) frequency-, and d) combined time-domain and harmonic constituent data.

Large-scale heterogeneity is resolved when the model is calibrated with the time-domain data and the combined time-domain and harmonic constituent data. Small-scale heterogeneity is resolved when the model is calibrated with the harmonic constituent data. The variability of the k_h field is closest to the synthetic k_h field when harmonic constituent data are used to calibrate the model (table 1).

CONCLUSIONS

For the simulations evaluated, the approach was able to resolve aquifer heterogeneity throughout the domain even though the tidal signal strength is reduced by more than 90% over most of the model domain. In general, it appears the information contained in the harmonic constituent data was sufficient to enhance calibration of the model to a similar level of precision as the time-domain data and resolve more of the variability present in the synthetic permeability field. The use of time-domain and harmonic constituent data in the calibration process improved the ability to resolve the permeability field over the model calibrated using only the time-domain data, but did not capture the variability of the model calibrated just with the harmonic constituent data.

Because handling large numbers of parameters and observations is memory intensive, another advantage of using harmonic constituent data is that it reduces the number of observations used to calculate the SSE evaluated as part of the objective function minimization process used by the parameter inversion process. In this case, it reduced the number of observations from 22,209 to 165 without reducing the ability to calibrate the model.

The results of this numerical evaluation suggests that high-frequency water-level data, processed harmonic constituent data, and regularized inversion techniques can be used to calibrate highly-parameterized permeability fields for coastal aquifers with observable tidal fluctuations. Using this strategy with saltwater intrusion models shows promise for improving the reliability of predictions, which are often highly dependent on aquifer heterogeneity.

Table 1. Statistical measures of model errors and calibrated horizontal permeability fields

Simulation	**Sum of Square Errors, m^2**	**$\log_{10}(k_h)$ error Standard Deviation, m^2**	**$\log_{10}(k_h)$ Mean, m^2**	**$\log_{10}(k_h)$ Standard Deviation, m^2**
Synthetic	0.40	0.00	-10.3	0.296
Time-domain	0.39	0.29	-10.3	0.086
Harmonic constituent	0.47	0.26	-10.3	0.15
Time-domain and Harmonic	0.44	0.26	-10.3	0.13

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