Groundwater

Aquifer Characterization and Uncertainty in Multi-Frequency Oscillatory Flow Tests: Approach and Insights

by Jeremy R. Patterson[1] and Michael Cardiff[2]

Abstract

Characterizing aquifer properties and their associated uncertainty remains a fundamental challenge in hydrogeology. Recent studies demonstrate the use of oscillatory flow interference testing to characterize effective aquifer flow properties. These characterization efforts relate the relative amplitude and phase of an observation signal with a single frequency component to aquifer diffusivity and transmissivity. Here, we present a generalized workflow that relates extracted Fourier coefficients for observation signals with single and multiple frequency components to aquifer flow properties and their associated uncertainty. Through synthetic analytical modeling we show that multi-frequency oscillatory flow interference testing adds information that improves inversion performance and decreases parameter uncertainty. We show increased observation signal length, sampling frequency, and pressure sensor accuracy all produce decreased parameter uncertainty. This work represents the first attempt we are aware of to quantify effective aquifer parameters and their associated uncertainty using multi-frequency oscillatory flow interference testing.

Introduction

Characterizing the physical properties governing flow and transport, specifically transmissivity and storativity, in aquifers remains a fundamental challenge and active area of research in hydrogeology. This critical first step in all groundwater investigations has significant implications for groundwater resource management and contaminant remediation strategies. As such, there is a large body of literature exploring best practices for quantifying subsurface flow properties that can be largely grouped into four categories: (1) geophysical, (2) tracer, (3) core analysis, and (4) hydraulic. Cardiff et al. (2012) provide a thorough review of the various approaches within each category.

In this work, we focus on hydraulic characterization approaches, where aquifer flow properties are inferred by measuring pressure responses at discrete points throughout the aquifer in response to a natural or anthropogenic-induced pressure stimulus. The constant-rate pumping test and slug test, two common hydraulic characterization techniques, sample the aquifer at different scales, and thus estimate aquifer flow parameters which may differ by orders of magnitude depending on the level of heterogeneity present in the aquifer—the well-known "scale effect" (e.g., Bradbury and Muldoon 1990; Neuman 1990, 1994; Rayne 1994; Rovey and Cherkauer 1995; Sánchez-Vila et al. 1996; Schulze-Makuch et al. 1999). In this work, we discuss oscillatory flow interference testing, a hydraulic characterization approach capable of sampling an aquifer across a range of scales by changing the frequency of the introduced pressure perturbation (Cardiff et al. 2013).

The first attempt at leveraging oscillatory signals to characterize aquifer properties utilized diurnal river fluctuations to quantify the transmissivity of an alluvial aquifer (Ferris 1952). The first known use of non-natural periodic pressure signals proposed harmonic pulse testing to characterize petroleum reservoir permeability without interrupting production operations (Johnson et al. 1966), with the first field implementation occurring shortly thereafter (Kuo 1972). Following this, Black and Kipp (1981)

[1]Corresponding author: Department of Geoscience, University of Wisconsin-Madison, 1215 W. Dayton St., Madison, WI 53706; jpatterson7@wisc.edu

[2]Department of Geoscience, University of Wisconsin-Madison, 1215 W. Dayton St., Madison, WI 53706

Article Impact Statement: Multi-frequency analysis under oscillatory flow conditions improves effective parameter estimates and reduces parameter uncertainty.

Received May 2021, accepted August 2021.

doi: 10.1111/gwat.13134

developed the first analytical solutions to describe the expected steady-periodic response to oscillatory pressure stimulations from point and line sources in confined aquifer systems and investigated the distances across which measurable signals could be propagated. Building on this work, Rasmussen et al. (2003) developed analytical solutions for confined and leaky aquifer systems as well as aquifers with partially penetrating wells. This study presented formulas for separating hydraulic diffusivity into its component parts, transmissivity and storativity, by using oscillatory pressure data.

Oscillatory flow interference testing has many advantages over conventional hydraulic characterization techniques that are well documented in the literature (Fokker and Verga 2011; Cardiff et al. 2013; Bakhos et al. 2014; Guiltinan and Becker 2015; Rabinovich et al. 2015). For example, oscillatory flow interference testing samples an aquifer at multiple scales simply by varying the frequency of the pressure stimulation. Additionally, by alternating withdrawal and injection, oscillatory flow interference testing yields a net zero drawdown meaning that alterations to the flow field are negligible and follow-on testing can occur with minimal to no time waiting for aquifer recovery. While similar scaling could be achieved by changing the inter-well spacing or varying the time of a constant-rate pumping test, and thus the radius of influence, the aquifer must be allowed to recover to steady-state prior to follow-on testing, increasing the total time required for the characterization efforts.

In addition to the advantages presented above, oscillatory flow interference testing also benefits from the ability to extract the input signal from a noisy observation signal. In practice, data collected during aquifer characterization efforts can contain one or multiple sources of noise that obscure the signal such as: random instrument measurement error (i.e., white noise), linear trends associated with instrument drift, hydrologic noise such as periodic signals induced by earth tides or evapotranspiration, and discontinuities in the data (Bakhos et al. 2014). The interested reader is directed to Bakhos et al. (2014) for illustration of the various types of data noise. Using established signal processing techniques, attenuated and delayed stimulation signals recorded at an observation well are readily extracted from the noise and used to quantify aquifer flow parameters (Bakhos et al. 2014).

Despite the multiple advantages of oscillatory flow interference tests, their use in field settings remains limited. Field studies employing oscillatory flow interference testing described in the literature use multiple approaches to generate the pressure stimulation. One approach uses a pump in a water storage tank at the surface and another in the borehole to alternate pumping and injection flow rates in a periodic manner, creating a square signal centered around either a flow rate of zero or a constant background pumping rate (Rasmussen et al. 2003; Renner and Messar 2006; Salina Borello et al. 2019). Using this approach, the amplitude of the observation signal is controlled by the chosen pumping and injection flow rates. As an alternative to variable pumping rates, other studies have used oscillatory slug testing, where an electric motor raises and lowers a solid slug throughout the borehole to generate the periodic pressure stimulation, where the size of the solid slug moved through the water column controls the peak flow rates and resulting observation signal amplitudes (Becker and Guiltinan 2010; Guiltinan and Becker 2015). Similarly, Cardiff et al. (2020) used a surface motor connected to a down-hole piston to generate oscillatory flow in a screened interval between two packers. Last, Sayler et al. (2018) used a well-head pneumatic system to pressurize and depressurize the water column in a periodic manner. This approach produces the same effect of alternately injecting and pumping water from the aquifer without the need for additional pumps and water storage at the land surface, reducing water and equipment treatment requirements when testing contaminated aquifers.

The above-mentioned studies propose different approaches to quantify aquifer flow parameters using observation signals collected through oscillatory flow interference testing. Multiple studies used only borehole pressure measurements at stimulation and observation wells to estimate aquifer diffusivity by analyzing the amplitude ratio and phase ratio between the stimulation and observation wells (Black and Kipp 1981; Renner and Messar 2006; Becker and Guiltinan 2010; Sayler et al. 2018). Using this approach, the diffusivity cannot be separated into its component parts, transmissivity and storativity, due to the lack of flow-rate information from the pumping well, which provides the necessary additional constraint to quantify transmissivity (Black and Kipp 1981; Renner and Messar 2006). Leveraging flow rate and pressure data collected through oscillatory flow interference testing at the Savannah River Site, Rasmussen et al. (2003) developed approximate expressions relating relative amplitude ratio and phase delay to estimate aquifer diffusivity and transmissivity (Figure 1). Using the same approach, Guiltinan and Becker (2015) identified inter-well connectivity and quantified the flow properties of a fractured sedimentary bedrock aquifer. This inversion algorithm provides a straightforward approach to estimate aquifer flow parameters using oscillatory flow testing; however, in the event of phase wrapping when the phase offset between stimulation and observation signals exceeds 2π—this approach can return parameter estimates that are wrong by orders of magnitude (Cardiff and Sayler 2016).

As the studies above illustrate, aquifer characterization using oscillatory flow interference testing leverages collected stimulation and observation signals with established analytical models to quantify effective aquifer flow parameters, often in a deterministic manner. While uncertainty quantification is well-established and frequently applied in the context of hydraulic and geophysical aquifer characterization (e.g., Linde et al. 2017), quantifying the uncertainty of estimated aquifer flow parameters under oscillatory flow conditions remains unexplored. Given that these flow properties provide inputs for predictive modeling simulations, understanding the uncertainty in these

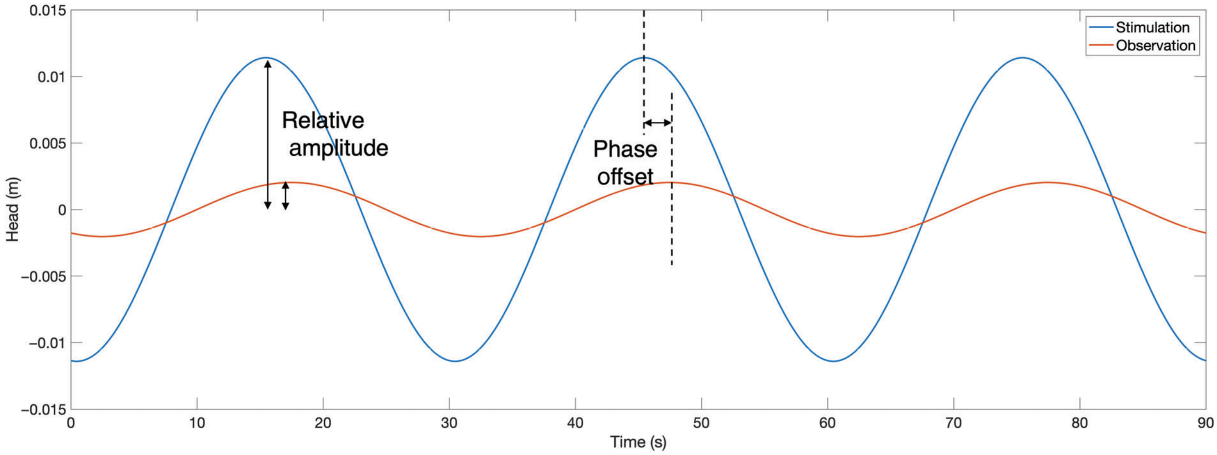

Figure 1. The stimulation signal (blue) represents the head measured at the stimulation well. The observation signal (orange), representing head measured at the observation well, is attenuated and offset relative to the stimulation signal. The relative amplitude and phase offset provide constraints to estimate aquifer diffusivity.

parameter estimates is critical for groundwater resource management and contaminant remediation strategies. Similarly, the effect of using multiple frequencies on reducing parameter uncertainty under oscillatory flow conditions remains an unexplored area in the literature. This points to a clear need for the development of a generalized inversion strategy that estimates aquifer flow parameters and quantifies the associated uncertainty using single and multiple frequency oscillatory flow interference testing.

In this work we build on established analytical solutions to develop a generalized gradient-based inversion workflow that improves on previous approaches in three ways. First, our approach provides an alternative analysis framework for oscillatory signals that simplifies data analysis and error propagation by working directly with extracted Fourier coefficients instead of the amplitude ratio and phase offset seen in previous works (Rasmussen et al. 2003; Renner and Messar 2006; Becker and Guiltinan 2010). Second, our approach allows for simultaneous inversion of multiple frequencies when quantifying effective flow properties. Last, the presented workflow directly relates data error to associated parameter uncertainty through linearized error propagation.

Mathematical Approach

In this section we present our mathematical approach through a workflow that estimates aquifer flow parameter estimates under uncertainty. For consistency and clarity, we employ the following terminology throughout the remainder of this manuscript. "Observation signal" refers to the timeseries of pressure measurements and associated noise collected at an observation well, "data" refers to the Fourier coefficients extracted through signal processing, "error" refers to the error associated with the extracted Fourier coefficient estimates resulting from observation signal noise, and "uncertainty" refers to the uncertainty in estimated aquifer flow parameters. The primary steps in our workflow are briefly described:

1. Signal processing: Using a least-squares approach, we directly relate the measured noisy observation signal to the extracted Fourier coefficients and the associated data error.
2. Optimization under uncertainty: Extracted Fourier coefficients are provided as data for a gradient-based Bayesian inversion providing optimal aquifer flow parameters as outputs.
3. Uncertainty quantification: Optimal aquifer flow parameters and data error are used to quantify parameter uncertainty through linearized error propagation—from observation signal noise, to data error, to aquifer parameter uncertainty.

Signal Processing

Here, we discuss our signal processing strategy to remove observation signal noise and extract the Fourier coefficients using an ordinary least squares approach as discussed by Bakhos et al. (2014). For the purposes of this analysis, we assume the signal has achieved a steady-periodic state. That is, the observation signal can be defined with a constant amplitude and phase and any initial transient effects associated with the onset of testing can be neglected. Further, we assume that the period of the stimulation signal is exactly known. If the stimulation period is not precisely known, application of a discrete Fourier transform to the observation signal can be used to extract the dominant period of the signal, allowing direct application of the following signal processing workflow (Bakhos et al. 2014).

As an illustrative example, consider a time series of head measurements at a specified distance (d) from the stimulation well, given by a linear combination of sinusoids and observational noise:

$$\boldsymbol{h}(d, \boldsymbol{t}) = \Phi_r \cos(\omega \boldsymbol{t}) - \Phi_i \sin(\omega \boldsymbol{t}) + \varepsilon(\boldsymbol{t}) \qquad (1)$$

where ω is the angular frequency in radians—which can be represented as $\omega = 2\pi/P$ where P is the stimulation period—Φ_r and Φ_i are the real and imaginary Fourier coefficients, respectively, and $\boldsymbol{\varepsilon}$ is the observation noise. Given this observation signal, we can write Equation (1) as a matrix system of equations where the Fourier coefficients are the only unknown (Equation 2).

$$h = X\boldsymbol{\Phi} + \epsilon, \quad X = \begin{bmatrix} \cos(\omega t_1) & \sin(\omega t_1) \\ \vdots & \vdots \\ \cos(\omega t_n) & \sin(\omega t_n) \end{bmatrix}, \quad \boldsymbol{\Phi} = \begin{bmatrix} \Phi_r \\ \Phi_i \end{bmatrix} \tag{2}$$

For the purposes of this example, we determine the Fourier coefficients for an observation signal with one frequency component; however, this analysis is easily extended to observation signals with multiple frequency components by expanding $\boldsymbol{X}$ and $\boldsymbol{\Phi}$ to include the additional sinusoidal terms and Fourier coefficients (Bakhos et al. 2014).

Taking a least-squares approach, the Fourier coefficients and their associated error are estimated as:

$$\widehat{\boldsymbol{\Phi}} = (X^T X)^{-1} X h \tag{3}$$

$$\boldsymbol{R} = \sigma^2 (X^T X)^{-1} \tag{4}$$

The misfit between the modeled signal using the optimal Fourier coefficients ($\boldsymbol{X}\widehat{\boldsymbol{\Phi}}$) and the observation signal ($\boldsymbol{h}$), provides an estimate of the variance (σ^2) of the observation signal noise ($\boldsymbol{\varepsilon}$). Last, we use linear theory to quantify the data error (i.e., covariance matrix [$\boldsymbol{R}$]) assuming $\varepsilon \sim \mathcal{N}(0, \sigma^2)$, following Bakhos et al. (2014).

Given a forward model that takes aquifer flow parameters as inputs and generates Fourier coefficients as outputs, we can create a gradient inversion algorithm that estimates the aquifer flow parameters that most closely match the data using the analysis approach described above. Further, using linearized error propagation we can quantify the uncertainty in these parameter estimates, and assess the quality of our linearization by contouring model misfits across a reasonably wide range of parameter values.

The presented approach is equivalent to optimizing a given forward model to the amplitude and phase of a signal; however, optimizing the forward model to the extracted Fourier coefficients has multiple benefits. First, optimizing over the Fourier coefficients minimizes issues with phase nonuniqueness due to phase wrapping (Bakhos et al. 2014). Also, the forward and inverse relations between an observation signal and the extracted Fourier coefficients are linear in nature, allowing direct application of linear theory to reconstruct a noise-free signal, quantify data error, and quantify uncertainty in estimated flow parameters through linearized error propagation.

Optimization Under Uncertainty

As discussed above, Rasmussen et al. (2003) provide a set of approximate analytical solutions to estimate aquifer flow properties using the relative amplitude and phase offset of the observation signal with respect to the stimulation signal. Here, we present a gradient inversion under a Bayesian framework that relies on Fourier coefficients as forward model outputs to estimate the optimal aquifer flow properties.

To determine the optimal aquifer flow parameters, we minimize the following objective function, which is equivalent to maximizing the likelihood of aquifer flow parameters given the available data (Aster et al. 2018):

$$\min_{s} \frac{1}{2} \left(\boldsymbol{\Phi} - \boldsymbol{h}(\boldsymbol{s})\right)^{\mathrm{T}} \boldsymbol{R}^{-1} \left(\boldsymbol{\Phi} - \boldsymbol{h}(\boldsymbol{s})\right) \tag{5}$$

where $\boldsymbol{\Phi} = \begin{bmatrix} \Phi_r \\ \Phi_i \end{bmatrix}$ are the extracted Fourier coefficients, $\boldsymbol{h}(\boldsymbol{s})$ is the forward model that takes aquifer flow parameters ($\boldsymbol{s}$) as inputs and outputs Fourier coefficients, $\boldsymbol{R}$ is the $n \times n$ data error covariance matrix, and n is the number of data points (i.e., the number of extracted Fourier coefficients). For the case of multi-frequency inversion, $\boldsymbol{R}$ is a block-diagonal matrix where the diagonal is populated by the covariance matrix for each frequency component. To conduct this inversion, we apply the Levenberg–Marquardt algorithm, where we determine the gradient at each iteration by numerically approximating the Jacobian matrix with the updated parameters (Aster et al. 2018).

For the purposes of our analysis, we assume an uninformative prior during inversion, that is we assign equal probabilities to all possible parameter values. Our inversion returns the maximum of the posterior distribution, and because we assume the flow parameters are log-normally distributed, the maximum a posteriori probability is identical to the mean value of the posterior distribution (Aster et al. 2018). Also, we assume observation noise is unbiased with independent Gaussian errors. We impose a nonnegativity constraint on the estimated parameters by working with log-transformed parameters. We declare convergence when the relative change in objective function and relative change in parameter values between consecutive iterations is less than or equal to 1e-6.

Uncertainty Quantification

Finally, we discuss uncertainty quantification, the last step in our developed workflow. Following inversion, we use the determined optimal flow parameters as inputs to quantify parameter uncertainty through linearized error propagation. First, we numerically approximate the $m \times \cancel{m}$ n Jacobian matrix (i.e., parameter sensitivity matrix) by making small perturbations to the optimal parameters, where m is the number of optimal aquifer flow parameters quantified. Next, we use the Jacobian to calculate the parameter covariance matrix given by:

$$\mathrm{Cov}(\boldsymbol{s}^*) = \left(\boldsymbol{J}(\boldsymbol{s}^*)^{\mathrm{T}} \boldsymbol{R}^{-1} \boldsymbol{J}(\boldsymbol{s}^*)\right)^{-1} \tag{6}$$

where $\boldsymbol{J}$ is the Jacobian matrix at the optimal parameters, and $\boldsymbol{s}^*$ is the vector of optimal aquifer flow parameters (Aster et al. 2018). The diagonal elements of the parameter covariance matrix represent the posterior variance of the estimated aquifer flow parameters. Finally, we use the χ^2 distribution with m degrees of freedom to draw the bounds of the 95% confidence ellipse rotated and scaled by the eigenvalues and eigenvectors of the parameter covariance matrix, following Aster et al. (2018).

Synthetic Modeling Examples

Considering the practitioner with a finite amount of time to complete field experiments, here we present a practical synthetic application of the aquifer characterization workflow described above. In this work, we assume that each oscillatory flow interference test is conducted independently when signals of multiple frequencies are analyzed; therefore, the total test time is the sum of each individual test time. As an example, for the multi-frequency case with stimulation periods of 30 s, 90 s, and 180 s we consider oscillatory flow tests that run for a total of 12 periods, yielding a 6-min test at 30 s period, 18-min test at 90 s period, and 36-min test at 180 s period for total testing time of 60 min. Using this approach, we investigate a range of total test times to understand how the number of full periods (i.e., signal length) in the observation signal used during analysis affects aquifer flow parameter uncertainty.

We start with a base case scenario using input parameters representative of a field-scale characterization effort in a confined—and possibly leaky—sedimentary bedrock aquifer (Table 1). We selected instrument error and sampling frequency to be consistent with the capabilities of equipment commonly employed in industrial and academic settings. Next, we conduct a brief sensitivity analysis to understand how improvement in observation signal recording and choices made during experimental design affects parameter uncertainty. Specifically, we explore how changes in inter-well spacing, sampling frequency, observation signal noise, and total test time impact the uncertainty of the estimated aquifer flow parameters. This analysis improves the current understanding of oscillatory flow interference testing and supports decision-making during field experiment planning so that aquifer characterization efforts can be pursued in the most cost-effective and time-efficient manner while minimizing parameter uncertainty.

Synthetic Data

To more closely match field conditions, we generate noisy synthetic data in a series of three steps. First, we generate the noise-free signal (Equation 1) using the Fourier coefficients determined by applying the base case input parameters (Table 1) to the appropriate forward model. Next, we add random noise to the true signal, assuming independent and identically distributed Gaussian noise with zero mean and 0.01 m standard deviation (σ). This signal represents the raw time series that would be collected at surrounding observation wells during oscillatory flow interference testing. Finally, we employ the least-squares approach described in the signal processing workflow to extract the Fourier coefficients from the observation signal and compute the associated data error covariance matrix.

Table 1

Base Case Modeling Input Parameters for the Fully Confined and Leaky Confined Aquifer Conceptual Models

Parameter	Value	Units
Radial distance (r)	10	m
Diffusivity (log): $\ln(D)$	2	$\ln(m^2/s)$
Transmissivity (log): $\ln(T)$	−8	$\ln(m^2/s)$
Leakance (log): $\ln(L)$ (Leaky case only)	−21	$\ln(s^{-1})$
Assumed observation signal noise (σ)	0.01	m
Sampling frequency	8	Hz

Note: The base case scenario includes three single frequency and three multi-frequency stimulation signals.

Confined Aquifer System

First, we apply our workflow to a fully confined synthetic aquifer system using the analytical model described given by equation 6 in Rasmussen et al. (2003), which outputs Fourier coefficients for a given set of aquifer flow parameters. The assumptions of the analytical model are identical to those of the Theis solution, with the constant pumping rate being modified to a sinusoidal pumping rate. Specifically, we assume the aquifer is fully confined with a constant saturated thickness across an infinite areal extent. Further, we assume that the aquifer is at steady-state prior to testing with no head change at infinite distance, and the well is fully penetrating creating purely radial flow. Finally, we assume the aquifer flow properties are homogeneous and isotropic (Theis 1935). Under this conceptual model, we use the generated synthetic data to invert for transmissivity (T) and storativity (S), which then allows diffusivity to be determined. Recognizing that practitioners have finite time to available for testing, we employ stimulation periods of 30 s, 90 s, and 180 s. This represents the shortest practical stimulation periods that generate measurable signals at observation wells while testing the aquifer at multiple scales.

Figure 2 shows parameter uncertainty results across a range of scenarios. Through linearized error propagation, we find that uncertainty in estimated transmissivity is consistently greater than storativity, with the exception of the shortest stimulation period under single frequency inversion (Figure 2). Further, our results indicate that uncertainty in estimated storativity remains approximately equal at all but the shortest stimulation period for a given total test time, including multi-frequency inversion (Figure 2). In contrast, our analysis shows that uncertainty in estimated transmissivity decreases with increasing stimulation period when conducting single frequency inversions, while the uncertainty associated with multi-frequency inversions are approximately equivalent for a given signal length (Figure 2).

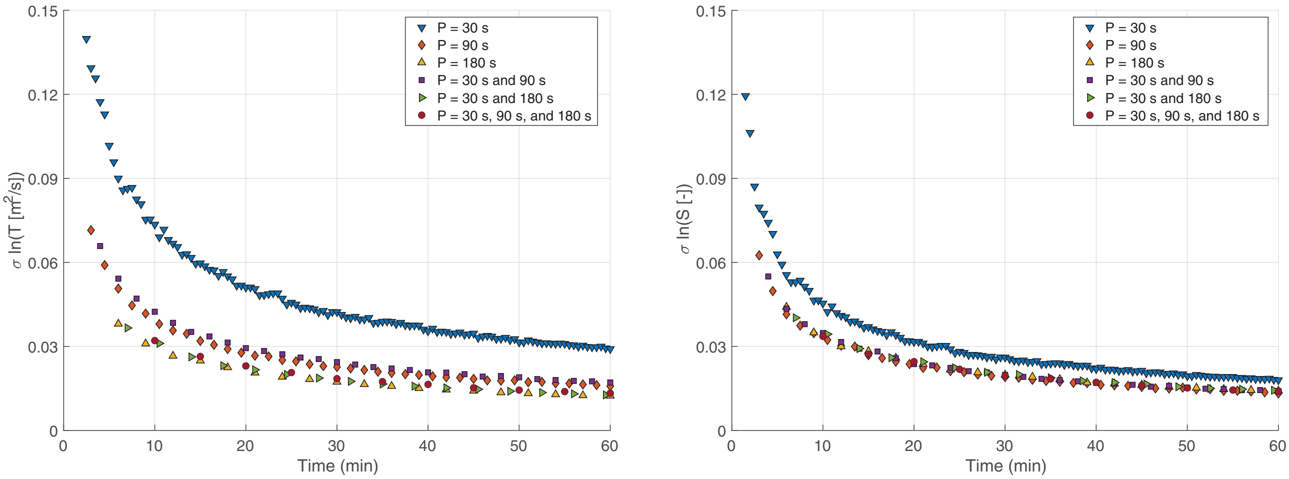

Figure 2. Transmissivity (left) and storativity (right) uncertainty—the square root of the diagonal elements of the parameter covariance matrix (Equation 6)—as a function of signal length across all single frequency and multi-frequency inversions analyses.

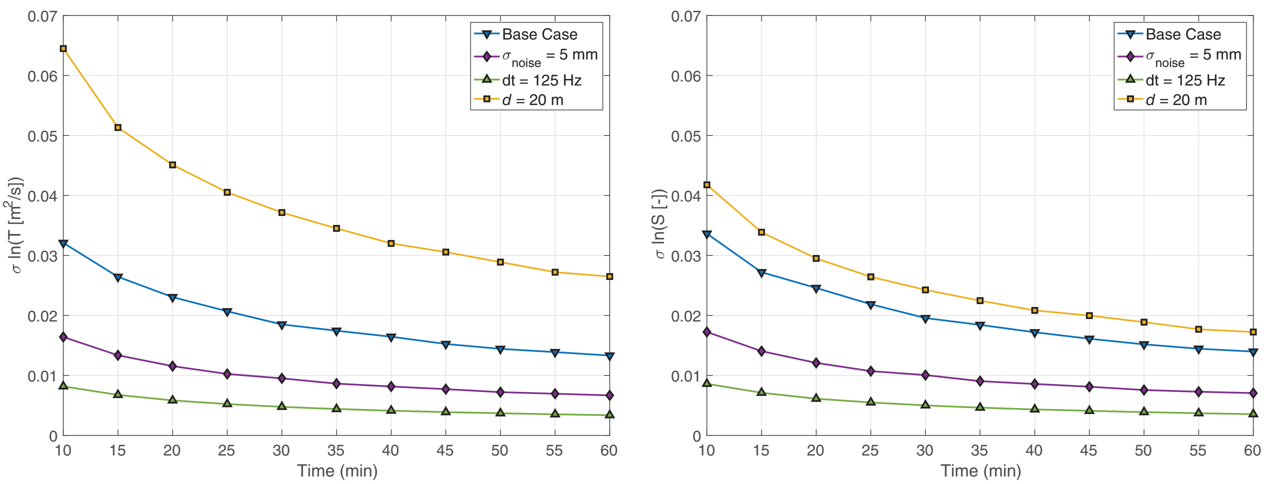

Figure 3. Transmissivity (left) and storativity (right) uncertainty sensitivity analysis with stimulation periods of 30 s, 90 s, and 180 s. Yellow squares represent increased inter-well spacing, green triangles represent increased sampling frequency, and purple diamonds represent decreased observation signal noise. Increasing distance increases uncertainty while increased sampling frequency has the largest impact on uncertainty reduction.

To understand the impact of experimental design and equipment capabilities on the uncertainty of estimated aquifer flow parameters, we explore how observation signal length (i.e., total test time), inter-well spacing, observation signal sampling frequency, and observation signal noise changes parameter uncertainty compared to the multi-frequency baseline scenario with 30 s, 90 s, and 180 s stimulation periods. Analogous to results presented by Bakhos et al. (2014), we find that uncertainty in estimated transmissivity and storativity decrease approximately exponentially with increased signal length (Figure 2). Further, our sensitivity analysis indicates that increasing the sampling frequency produces the largest decrease in parameter uncertainty under oscillatory flow conditions (Figure 3). In contrast, we observe an increase in parameter uncertainty at inter-well spacing (Figure 3), a trend that holds across all explored stimulation periods (Figure S1). Specifically, we note a one order of magnitude increase in parameter uncertainty with a 20-m inter-well spacing and 30-s stimulation period (Figure S1)—this scenario represents the case where the inter-well spacing exceeds the maximum propagation distance for signals of this frequency. However, complementing the 30-s stimulation period with an intermediate or long stimulation period signal in a multi-frequency inversion produces lower parameter uncertainty than any of the single frequency inversions with increased inter-well spacing at a 30-s stimulation period (Figure S1).

Further exploring the advantages of multi-frequency inversion during aquifer characterization, we contour the log-transformed model misfit relative to the base case true model, across a wide range of reasonable parameter values. Single frequency analysis shows a well-defined global minimum associated with the true parameters that elongates along the storativity axis and contracts along the transmissivity axis with increasing stimulation period

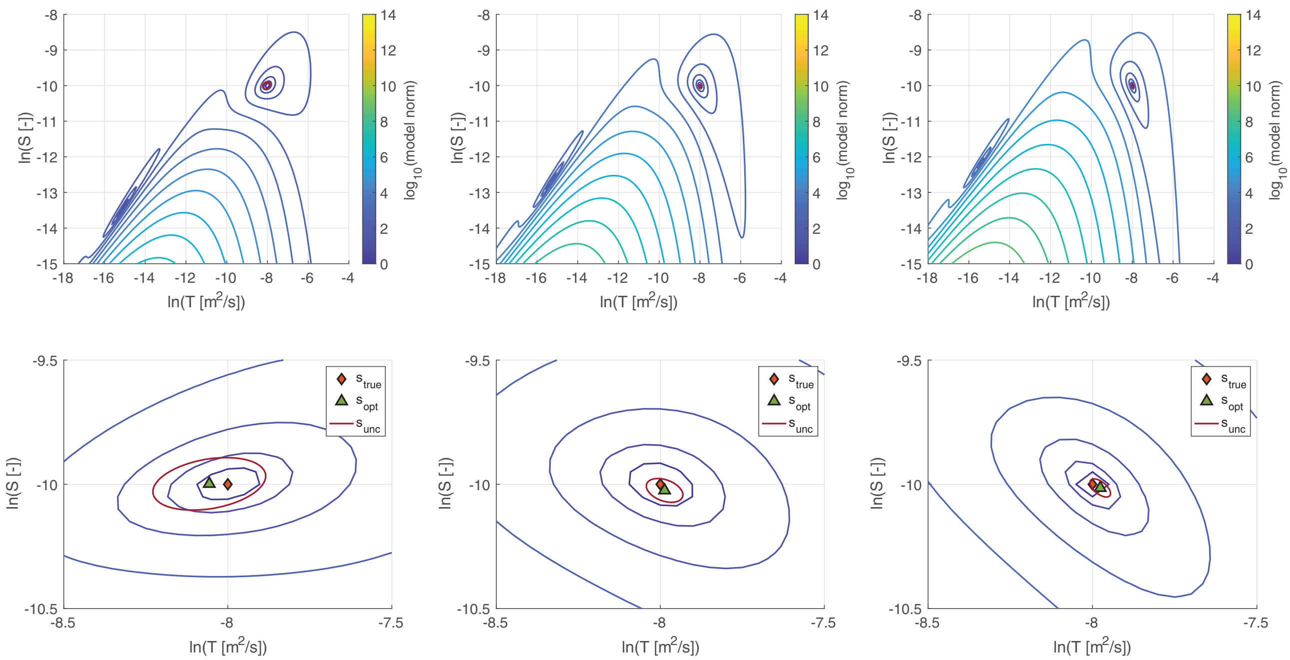

Figure 4. Model misfit contours (top row) with zoomed in view at global optimum (bottom row) showing optimal and true parameters within 95% confidence ellipse for single frequency inversions at stimulation periods of 30 s (left), 90 s (center), and 180 s (right). Parameter uncertainty decreases with increasing stimulation period using single frequency inversion.

Table 2
Optimal Parameters and Objective Function Values (Equation 5) for All Stimulation Periods at the Global and Local Minima

Period (s)	$\ln(T_{opt})$	$\ln(S_{opt})$	Global minimum $\log_{10}$ (misfit)	$\ln(T_{opt})$	$\ln(S_{opt})$	Local minimum $\log_{10}$ (misfit)
30	−8.0	−9.9	−0.42	−15.1	−13.5	−0.42
90	−7.9	−10.0	−0.06	−15.3	−12.7	−0.06
180	−7.9	−10.0	0.28	−15.4	−12.1	0.28
30 and 90	−8.0	−9.9	−0.82	−15.3	−12.7	2.44
30 and 180	−7.9	−10.0	−0.32	−15.4	−12.1	2.40
30, 90, and 180	−8.0	−9.9	−0.49	−15.4	−12.1	3.62

(Figure 4). We see that our inversion converges at the global minimum with the true model parameters lying inside the 95% confidence ellipse (Figure 4). Further, our single frequency analysis reveals a well-defined local minimum at decreased transmissivity and storativity values associated with the first phase wrap (Figure 4). We note that the local minimum decreases in size along the transmissivity axis and shifts to higher storativity values with increasing stimulation period (Figure 4). Under single frequency analysis, model misfits at the local minimum are equivalent to misfits at the global minimum (Table 2), motivating the use of multiple frequencies during analysis.

Similar to the single frequency analysis, our multi-frequency analysis again shows a well-defined global optimum centered at the true aquifer parameters that elongates along the storativity axis relative to the lowest frequency component used during inversion (Figure 5). Utilizing a multi-frequency observation signal, we note that the inversion converges to more accurate optimal parameters and a 95% confidence ellipse that is reduced in size relative to the single frequency inversions (Figure 5). The local minimum seen in the single frequency analysis persists under multi-frequency analysis with notable differences. First, the location of the local minimum does not shift throughout the parameter space with different permutations of frequency components (Figure 5). Next, we note a significant decrease in the size of the local minimum compared with the single frequency analysis (Figure 5). Last, there are fewer misfit contours defining the local minimum and the misfit value of the contours are larger compared to our single frequency analysis (Figure 5). To illustrate this point, we strategically change the initial parameters for inversion, which directs convergence to the local minimum, and we evaluate the objective function at these optimal parameters. This analysis shows greater than two orders of magnitude difference in misfit using multi-frequency analysis compared to the single frequency analysis (Table 2).

Leaky Aquifer System

We now apply our workflow to a synthetic leaky confined aquifer system using the analytical model described given by equation 14 in Rasmussen et al. (2003), which outputs Fourier coefficients for a given set of aquifer flow parameters. Under this conceptual framework, we invoke the same assumptions used for the fully confined conceptual model. Further, we assume the aquifer is bounded by an aquitard on both sides with a source of water on the opposite side of one aquitard. The leaky aquitard is

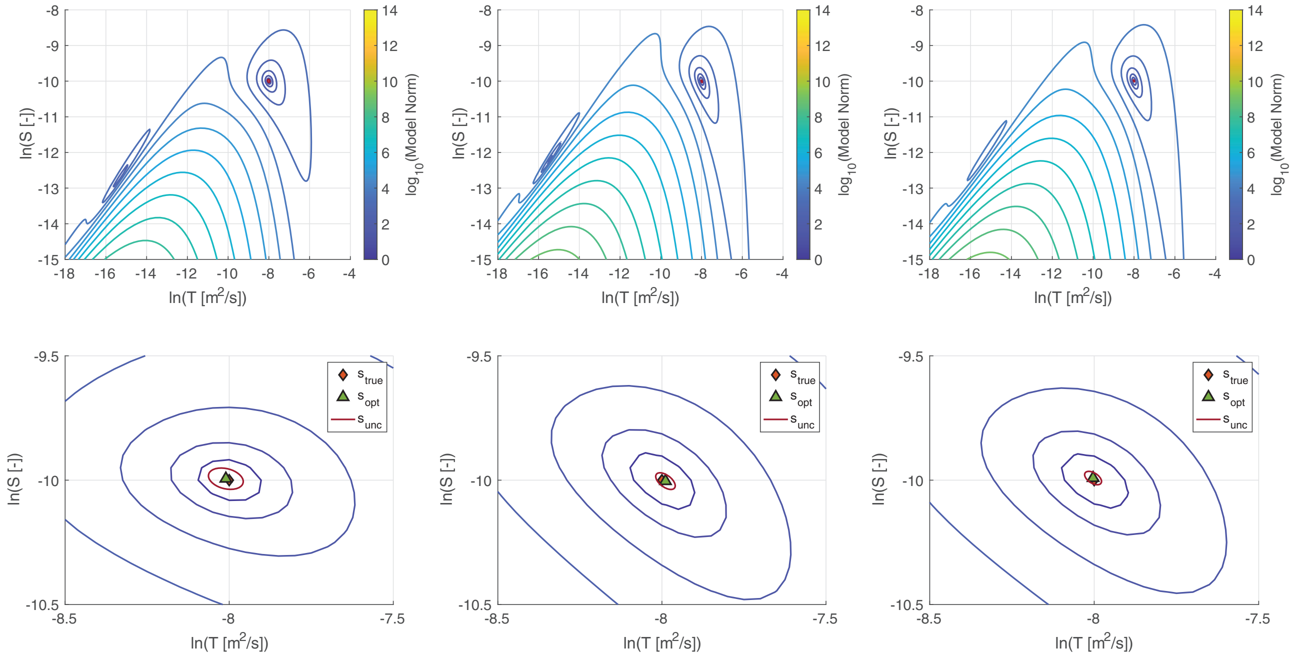

Figure 5. Model misfit contours (top row) with zoomed in view at global optimum (bottom row) showing optimal and true parameters within 95% confidence ellipse for multi-frequency inversion analyses at stimulation periods of 30 s and 90 s (left), 30 s and 180 s (center), and 30 s, 90 s, and 180 s (right). The 95% confidence ellipse is smaller for all multi-frequency analyses as compared to their respective single frequency results.

assumed to be incompressible with no horizontal flow component (Hantush and Jacob 1955). Under this conceptual model, we estimate transmissivity, storativity, and aquitard leakance (L). Due to the large contrast in aquifer transmissivity and aquitard leakance, longer stimulation periods are required to generate the vertical gradients necessary to induce vertical flow through the confining unit; therefore, we increased the stimulation periods to 3600 s, 5400 s, and 7200 s under this conceptual model.

Using single frequency oscillatory flow interference testing to characterize the flow properties of the leaky aquifer system creates an ill-posed parameter estimation problem with more unknown parameters than data. Linear inverse theory suggests that our inversion will be nonunique with multiple sets of parameters fitting the data equally well, and using an uninformed prior we have no extra information to help constrain (i.e., regularize) the inversion within an expected range of parameter values (Aster et al. 2018). Using a grid search across a reasonably wide parameter space, we identify the range of parameters that yield a data misfit $\leq$5e-4 (Figure 6). Using the type-curve analysis presented in Rasmussen et al. (2003) as a framework, we see that if we know or make a reasonable guess at the aquitard leakance, we can identify the aquifer flow parameters with a nonlinear trade-off between transmissivity and storativity (Figure 6). Further, we observe multiple levels of parameter nonuniqueness with nonlinear relationships between transmissivity and leakance as well as storativity and leakance (Figure 6). These results motivate the use of multiple frequency components as additional constraints during inversion under the leaky conceptual model.

The single frequency analysis discussed above indicates that multi-frequency inversion is necessary to accurately and uniquely identify aquifer flow parameters of a leaky confined aquifer. Using multiple frequency components, our inversion converges to optimal aquifer flow parameters with a 95% confidence ellipsoid that encompasses the true model parameters (Figure 7). Consistent with the confined analysis, we note the size of the 95% confidence ellipsoid decreases with increasing stimulation period in the multi-frequency analysis (Figure 7). Compared to our uncertainty analysis using a fully confined conceptual model (Figure 2), we observe that uncertainty in diffusivity and transmissivity increases under the leaky conceptual model (Figure 8).

Similar to the fully confined modeling discussed above, we conduct sensitivity analysis to explore the effect of observation signal length, inter-well spacing, sampling frequency, and observation signal noise on parameter uncertainty under a leaky conceptual model. Using an observation signal with stimulation periods of 3600 s, 5400 s, and 7200 s for the sensitivity analysis, we find that increased sampling frequency produces the greatest decrease in parameter uncertainty, while increased inter-well spacing leads to an increase in parameter uncertainty (Figure 9), consistent with our fully confined analysis (Figure 3). Consistent with our confined analysis and Bakhos et al. (2014), our results show decreasing uncertainty with increasing signal length (Figure 9).

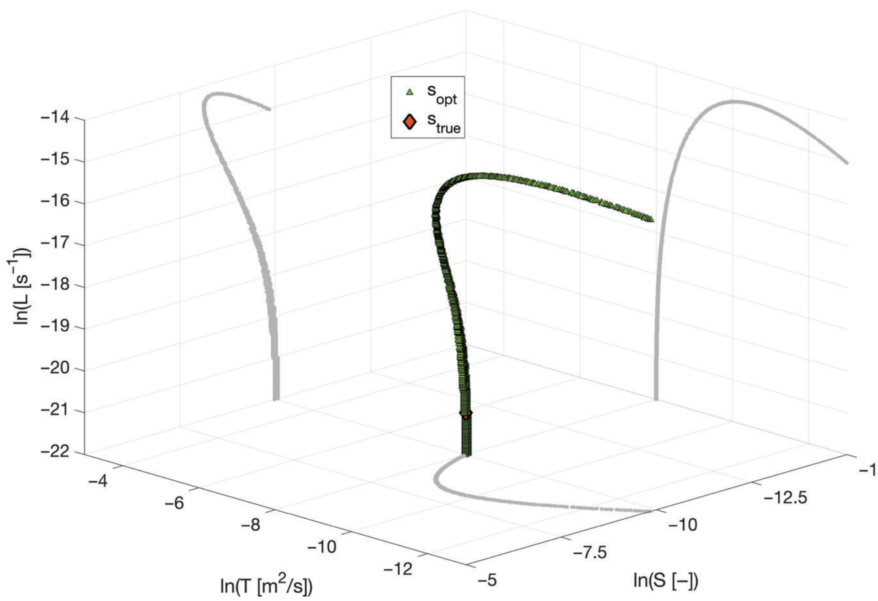

Figure 6. The range of parameters that fit the extracted Fourier coefficients equally well for an observation signal with one frequency component. Gray circles represent two-dimensional projections onto the respective plane and green diamonds represent the three-dimensional parameter vectors.

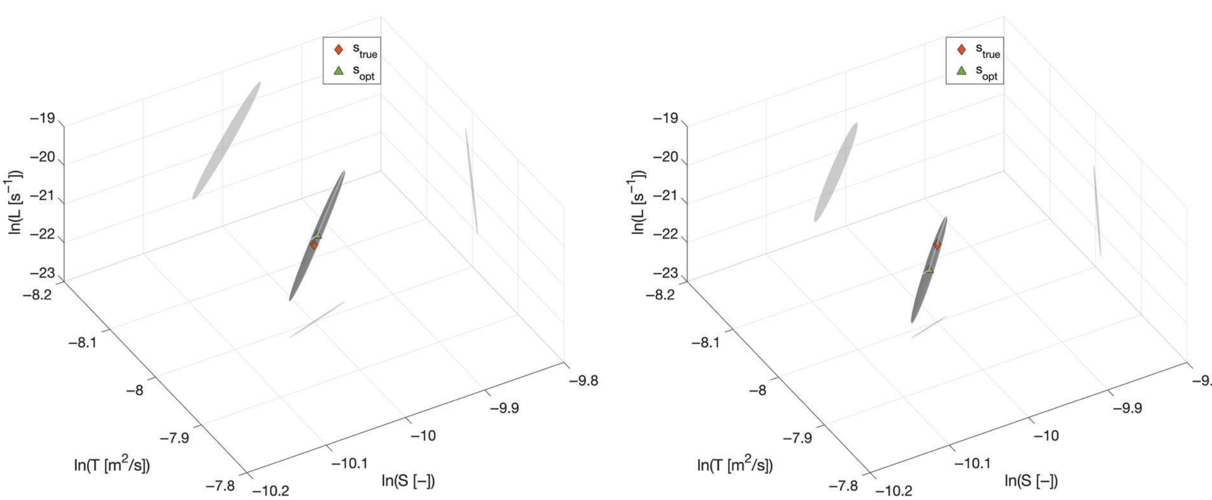

Figure 7. Parameter 95% confidence ellipsoid from multi-frequency inversion with 3600 s and 5400 s stimulation periods (left) and 3600 s and 7200 s stimulation periods (right). Reduced ellipsoid size illustrates the effect of low-frequency components on uncertainty reduction.

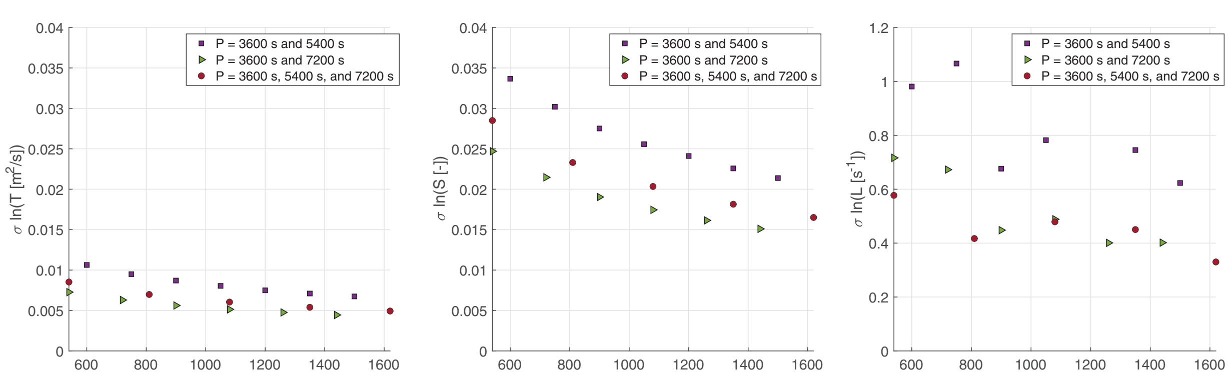

Figure 8. Transmissivity (left), storativity (center), and leakance (right) uncertainty using multi-frequency inversion, showing significant improvement relative to single frequency analysis. Note the change in vertical scale with leakance uncertainty (right).

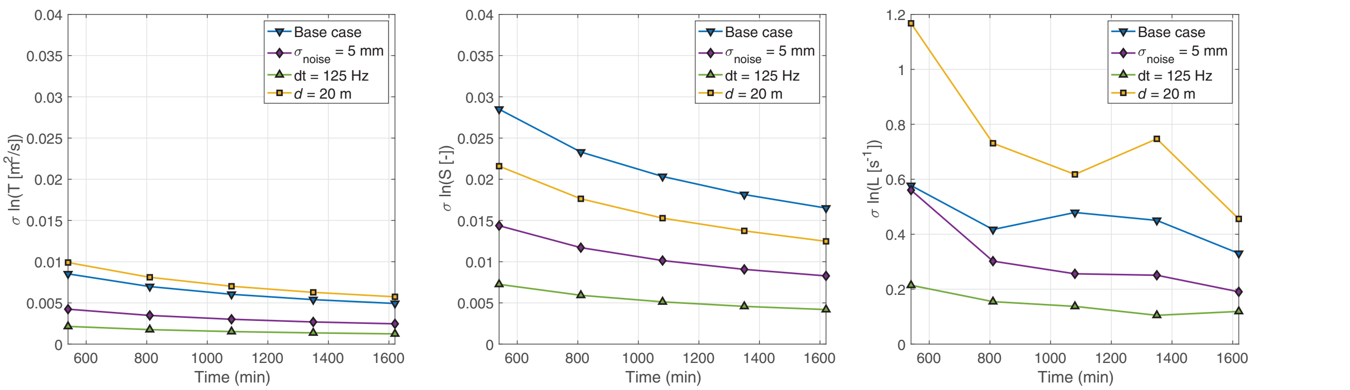

Figure 9. Transmissivity (left), storativity (center), and leakance (right) uncertainty sensitivity analysis with stimulation periods of 3600 s, 5400 s, and 7200 s. Yellow squares represent increased inter-well spacing, green triangles represent increased sampling frequency, and purple diamonds represent decreased observation signal noise. Increasing distance increases uncertainty while increased sampling frequency has the greatest impact on uncertainty reduction. Note the change in vertical scale with leakance uncertainty.

Discussion and Conclusions

This work presents a generalized aquifer characterization workflow that uses oscillatory flow interference testing to estimate aquifer flow properties and their associated uncertainties. The presented analytical modeling studies are designed to represent an average aquifer characterization effort at the field scale with aquifer parameters that are characteristic of confined sedimentary bedrock aquifers. The presented workflow is easily adaptable to numerical and field aquifer characterization studies across a range of scales and lithologies.

This work demonstrates the first effort to estimate aquifer flow parameters in a leaky aquifer system using single- and multi-frequency oscillatory flow interference testing. Previous efforts utilized type-curve analysis to determine if measured pressure responses were consistent with the predicted pressure response of a leaky aquifer at a given leakance value (Rasmussen et al. 2003). Our analysis shows that while a single-frequency oscillatory flow interference test is not able to uniquely identify all parameters, multi-frequency oscillatory flow interference testing provides additional information that allows estimation of aquifer flow parameters and aquitard leakance. This finding further supports the assertion that employing multiple frequencies during oscillatory flow testing provides additional information about aquifer flow parameters (Cardiff et al. 2013). Adapting our workflow to a leaky confined model is beneficial not only to aquifers assumed to have leaky confining layers, but also fractured bedrock aquifers where the surrounding porous media has sufficient primary porosity and hydraulic conductivity to promote fluid exchange along pressure gradients between the fracture and porous media.

Aquifer characterization through oscillatory flow interference testing does present new issues that should be considered during inversion. First, the large area of parameter space with no observable gradient represents the range of parameters where the observation signal is indistinguishable from observation noise due to attenuation (Figures 4 and 5). Inversion iterations or initial parameter guesses located in this region of the parameter space make no progress and ultimately converge to inaccurate optimal parameters with unreasonably large uncertainties, due to the lack of gradient. Further, phase wrapping is a concern during oscillatory flow testing analysis that can lead to inaccurate parameter estimates (Cardiff and Sayler 2016), which manifests as a local minimum in the parameter space (Figures 4 and 5). Our findings show that the use of multi-frequency flow testing reduces the size of this local minimum and produces significantly greater data misfit (Table 2), further demonstrating the additional information provided when multiple testing frequencies are employed. Additionally, based on our visualizations of the parameter misfit space we employ a simple strategy of providing initial parameter guesses of higher than expected transmissivity and lower than expected storativity to improve inversion performance. Employing these approaches, we consistently achieve optimal parameter estimates within uncertainty bounds of the true aquifer parameters (Figures 4 and 5).

The characteristic length, or penetration depth (d_p) under oscillatory flow conditions, of diffusion processes scales according to $d_p \propto \sqrt{DP}$ (Turcotte and Schubert 2002; Renner and Messar 2006; Becker and Guiltinan 2010). The significant increase in parameter uncertainty seen in our confined sensitivity analysis at a stimulation period of 30 s, illustrates the effect of inter-well spacings that exceed the penetration depth of an oscillatory flow test (Figure S1). Though a small pressure signal propagates beyond the penetration depth, instrument capabilities dictate the identifiability of the signal within the noise (Renner and Messar 2006). These results highlight the care needed during the planning stages of aquifer characterization efforts to ensure readily identifiable signals are measurable at observation wells. In light of this, we advocate the use of simple initial modeling tools (e.g., Cardiff and Barrash 2015) during test design to ensure the selection of proper stimulation periods and pumping magnitudes.

Modeling simulations that output prediction uncertainty are critically important for decision-making related to groundwater resource management and contaminant remediation strategies (Linde et al. 2017). These predictive modeling simulations rely on uncertainty in parameter inputs, providing the motivation to conduct aquifer characterization studies that yield parameter estimates with the smallest possible uncertainty. Our sensitivity analysis shows that, under oscillatory flow testing conditions, increasing the sampling frequency yields the largest decrease in parameter uncertainty. The increased sampling frequency allows us to more accurately determine when the peak of a specific wave passes the observation well, thereby decreasing data uncertainty and thus parameter uncertainty. Although decreasing the variance of the observation signal noise decreases parameter uncertainty, sensors capable of high-resolution pressure measurements (e.g., fiber-optic pressure sensors with millimeter scale measurement error) are not widespread and remain expensive.

The presented multi-frequency analysis represents an area of promising future research, motivating the development of multi-frequency oscillatory flow interference testing with stacked stimulation periods. In our work, we assume that each frequency represents an individual oscillatory flow test; however, theoretically it would be possible to use multiple stimulation signals, each at different frequencies, to generate a single observation signal at surrounding wells to estimate aquifer flow properties and quantify their uncertainty. Under specified time constraints, this would allow longer signals to be collected thereby further reducing parameter uncertainty as seen through previous studies and this work (Bakhos et al. 2014). That said, stacking of multi-frequency signals is likely to increase the error associated with the Fourier coefficients for each individual frequency component. To date, the use of stacked stimulation periods for oscillatory flow testing has not been explored in numerical or field studies and remains a promising direction for building on this work. Modern pressure stimulation techniques, such as computer-controlled air pressure valves, may make signal stacking more accessible than prior stimulation approaches, making this a promising area of future research.

Acknowledgments

This work was supported by funding through NSF-EAR 1654649 “CAREER: Understanding Transport Processes in Fractured Sedimentary Rock Through Multi-Frequency and Multi-Method Investigations”, and through the Wisconsin Department of Natural Resources Contract “Oscillatory Testing and Interpretation at Three Sites in Waushara County.” The authors wish to thank three anonymous reviewers, Dr Leonard Konikow and Dr Charles Andrews, for their comments and feedback which greatly improved the quality of this work. The code used to generate this analysis is available for download at https://zenodo.org/record/5165335#.YQx67y2caCM.

Authors' Note

The authors do not have any conflicts of interest or financial disclosures to report.

Supporting Information

Additional supporting information may be found online in the Supporting Information section at the end of the article. Supporting Information is generally *not* peer reviewed.

Figure S1. Sensitivity analysis uncertainty results under a fully confined conceptual model for all single frequency and multi-frequency analyses.
Figure S2. Sensitivity analysis uncertainty results under a leaky confined conceptual model for all multi-frequency analyses.

References

Aster, R.C., B. Borchers, and C.H. Thurber. 2018. *Parameter Estimation and Inverse Problems.* Boston, MA: Elsevier.

Bakhos, T., M. Cardiff, W. Barrash, and P.K. Kitanidis. 2014. Data processing for oscillatory pumping tests. *Journal of Hydrology* 511: 310–319. https://doi.org/10.1016/j.jhydrol.2014.01.007

Becker, M., and E. Guiltinan. 2010. Cross-hole periodic hydraulic testing of inter-well connectivity. In *Thirty-Fifth Workshop on Geothermal Reservoir Engineering.* Stanford, CA: Stanford University.

Black, J.H., and K.L. Kipp. 1981. Determination of hydrogeological parameters using sinusoidal pressure tests: A theoretical appraisal. *Water Resources Research* 17, no. 3: 686–692. https://doi.org/10.1029/WR017i003p00686

Bradbury, K.R., and M.A. Muldoon. 1990. Hydraulic conductivity determinations in unlithified glacial and fluvial materials. In *Ground Water and Vadose Zone Monitoring*, ed. D. Nielsen, and A. Johnson, West Conshohocken, PA: ASTM International. https://doi.org/10.1520/STP23404S

Cardiff, M., and C. Sayler. 2016. Strategies for avoiding errors and ambiguities in the analysis of oscillatory pumping tests. *Journal of Hydrology* 540: 1016–1021. https://doi.org/10.1016/j.jhydrol.2016.06.045

Cardiff, M., and W. Barrash. 2015. Analytical and semi-analytical tools for the design of oscillatory pumping tests. *Groundwater* 53, no. 6: 896–907. https://doi.org/10.1111/gwat.12308

Cardiff, M., Y. Zhou, W. Barrash, and P. K. Kitanidis. 2020. Aquifer imaging with oscillatory hydraulic tomography: Application at the field scale. *Groundwater* 58, no. 5: 710–722. https://doi.org/10.1111/gwat.12960.

Cardiff, M., T. Bakhos, P.K. Kitanidis, and W. Barrash. 2013. Aquifer heterogeneity characterization with oscillatory pumping: Sensitivity analysis and imaging potential. *Water Resources Research* 49, no. 9: 5395–5410. https://doi.org/10.1002/wrcr.20356

Cardiff, M., W. Barrash, and P.K. Kitanidis. 2012. A field proof-of-concept of aquifer imaging using 3-D transient hydraulic tomography with modular, temporarily-emplaced equipment. *Water Resources Research* 48, no. W05531. 1–18. https://doi.org/10.1029/2011WR011704

Ferris, J.G. 1952. *Cyclic Fluctuations of Water Level as a Basis for Determining Aquifer Transmissibility.* U.S. Geological Survey Ground Water Note 1. Washington, DC: U.S. Geological Survey. https://doi.org/10.3133/70133368

Fokker, P.A., and F. Verga. 2011. Application of harmonic pulse testing to water–oil displacement. *Journal of Petroleum*

Science and Engineering 79, no. 3–4: 125–134. https://doi.org/10.1016/j.petrol.2011.09.004

Guiltinan, E., and M.W. Becker. 2015. Measuring well hydraulic connectivity in fractured bedrock using periodic slug tests. *Journal of Hydrology* 521: 100–107. https://doi.org/10.1016/j.jhydrol.2014.11.066

Hantush, M.S., and C.E. Jacob. 1955. Non-steady radial flow in an infinite leaky aquifer. *Eos, Transactions American Geophysical Union* 36, no. 1: 95–100.

Johnson, C.R., R.A. Greenkorn, and E.G. Woods. 1966. Pulse-testing: A new method for describing reservoir flow properties between wells. *Journal of Petroleum Technology* 18, no. 12: 1599–1604. https://doi.org/10.2118/1517-PA

Kuo, C.H. 1972. Determination of reservoir properties from sinusoidal and multirate flow tests in one or more wells. *Society of Petroleum Engineers Journal* 12, no. 06: 499–507. https://doi.org/10.2118/3632-PA

Linde, N., D. Ginsbourger, J. Irving, F. Nobile, and A. Doucet. 2017. On uncertainty quantification in hydrogeology and hydrogeophysics. *Advances in Water Resources* 110, December: 166–181. https://doi.org/10.1016/j.advwatres.2017.10.014

Neuman, S.P. 1994. Generalized scaling of permeabilities: Validation and effect of support scale. *Geophysical Research Letters* 21, no. 5: 349–352.

Neuman, S.P. 1990. Universal scaling of hydraulic conductivities and dispersivities in geologic media. *Water Resources Research* 26, no. 8: 1749–1758.

Rabinovich, A., W. Barrash, M. Cardiff, D.L. Hochstetler, T. Bakhos, G. Dagan, and P.K. Kitanidis. 2015. Frequency dependent hydraulic properties estimated from oscillatory pumping tests in an unconfined aquifer. *Journal of Hydrology* 531: 2–16. https://doi.org/10.1016/j.jhydrol.2015.08.021

Rasmussen, T.C., K.G. Haborak, and M.H. Young. 2003. Estimating aquifer hydraulic properties using sinusoidal pumping at the Savannah River site, South Carolina, USA. *Hydrogeology Journal* 11, no. 4: 466–482. https://doi.org/10.1007/s10040-003-0255-7

Rayne, T.W. 1994. Variability of Hydraulic Conductivity in Sandy Till: The Effects of Scale and Method. Ph.D. thesis, University of Wisconsin-Madison.

Renner, J., and M. Messar. 2006. Periodic pumping tests. *Geophysical Journal International* 167, no. 1: 479–493. https://doi.org/10.1111/j.1365-246X.2006.02984.x

Rovey, C.W., and D.S. Cherkauer. 1995. Scale dependency of hydraulic conductivity measurements. *Groundwater* 33, no. 5: 769–780.

Salina Borello, E., P.A. Fokker, D. Viberti, F. Verga, H. Hofmann, P. Meier, K.-B. Min, K. Yoon, and G. Zimmermann. 2019. Harmonic pulse testing for well monitoring: Application to a fractured geothermal reservoir. *Water Resources Research* 55, no. 6: 4727–4744. https://doi.org/10.1029/2018WR024029

Sánchez-Vila, X., J. Carrera, and J.P. Girardi. 1996. Scale effects in transmissivity. *Journal of Hydrology* 183, no. 1–2: 1–22.

Sayler, C., M. Cardiff, and M.D. Fort. 2018. Understanding the geometry of connected fracture flow with multiperiod oscillatory hydraulic tests. *Groundwater* 56, no. 2: 276–287.

Schulze-Makuch, D., D.A. Carlson, D.S. Cherkauer, and P. Malik. 1999. Scale dependency of hydraulic conductivity in heterogeneous media. *Groundwater* 37, no. 6: 904–919. https://doi.org/10.1111/j.1745-6584.1999.tb01190.x

Theis, C.V. 1935. The relation between the lowering of the piezometric surface and the rate and duration of discharge of a well using ground-water storage. *Eos, Transactions American Geophysical Union* 16, no. 2: 519–524.

Turcotte, D.L., and G. Schubert. 2002. *Geodynamics.* New York, NY: Cambridge University Press.