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Seismic Waveform Tomography With Multicomponent Data at a Groundwater Contamination Site

by

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ABSTRACT

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This thesis develops an SH-wave version of frequency-domain, full waveform
tomography, and applies it, together with traditional acoustic waveform tomography, to a
multicomponent seismic data set acquired over a shallow contaminated aquifer at Hill Air
Force Base, Utah. The study combines the high resolution provided by waveform
tomography with inherent advantages of SH-wave imaging, such as reduced seismic
velocity and independence of pore fluid content. Presented are synthetic tests of the
method, its application to the field data, and interpretation of the resulting P- and S-wave
velocity models.

Synthetic tests reveal fundamental differences between acoustic and SH
waveform tomography, and demonstrate, together with the field data inversions,
 improved resolution for SH-wave imaging due to smaller velocities. High-resolution
velocity models from inversion of the field data are interpreted in terms of lithology and
water saturation, which are better constrained by the availability of both P- and S-wave
velocity.
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CHAPTER 1
INTRODUCTION

Fresh water shortages are likely to become a pressing issue as future population growth stresses current supplies (UN, 2006). Groundwater comprises the majority of available freshwater resources, and will be increasingly relied upon to meet growing demand in many regions (EPA, 2004; WBCSD, 2006). However, many vital groundwater aquifers are contaminated and require extensive remediation; the Environmental Protection Agency (EPA) has identified more than 1200 such sites in the United States (Moore et al., 1995). In many cases, knowledge of site-specific subsurface geology is essential for designing an efficient remediation program. Non-invasive geophysical imaging plays an important role in this regard, as it is often the most effective way to obtain spatially continuous interpretations of subsurface geologic properties.

Seismic techniques are gaining prominence for near-surface applications such as imaging of contaminated aquifers. Reflection seismic surveys are common for near-surface studies (e.g., Fradelizio et al., 2008; Francese et al., 2002). However, accurate velocity models are required for reflection processing, and they provide additional interpretative power of their own, therefore there is also a need for advanced inversion methods that directly estimate the subsurface seismic velocity field. Frequency-domain, full waveform tomography is a particularly effective inversion technique for obtaining high-resolution velocity models.
In 2005, Rice University acquired a 2D, nine-component (i.e., vertical, horizontal radial, and horizontal transverse components for each source and receiver) seismic survey at a shallow groundwater contamination site located at Hill Air Force Base (HAFB), Utah. Motivated by the resolving power of waveform tomography and expected advantages of SH-wave imaging, the objective of this study is to apply acoustic and SH-wave versions of waveform tomography to the vertical source-receiver and horizontal transverse source-receiver data components, respectively, and produce high-resolution maps of subsurface P- and S-wave velocity. It is believed that this is the first application of waveform tomography to an SH-wave field data set.

The aim of frequency-domain, full waveform tomography is to estimate a subsurface velocity model by inverting the amplitude and phase information in an observed frequency-domain waveform. These aspects of the data are more sensitive to scattering interactions with small-scale velocity perturbations than traveltime data, and therefore waveform tomography is able to provide significantly increased resolution beyond traveltime tomography techniques. However, waveform tomography is less robust and more computationally expensive than common traveltime methods. This study applies the frequency-domain full waveform tomography technique developed primarily by Gerhard Pratt (e.g., Pratt 1999). One of the first applications of the technique to real seismic data was from a physical-scale model with a crosswell-style acquisition geometry (Pratt, 1999). A companion paper (Pratt and Shipp, 1999) describes one of the first applications to field data, from a crosswell experiment in a layered sedimentary environment. Recently, waveform tomography has also been applied to surface seismic data sets in various environments; e.g., a realistic crustal-scale synthetic
model (Brenders and Pratt, 2007), a reflection/refraction survey of the shallow crust across the San Andreas Fault (Bleibinhaus et al., 2007), wide-aperture land data sets over thrust belts (Jaiswal et al., 2008; Ravaut et al., 2004), an ocean-bottom seismic data set at a subduction zone (Operto et al., 2006), a long-offset marine reflection/refraction data set for sub-basalt imaging (Chironi et al., 2006), and a marine reflection data set over a gas deposit (Hicks and Pratt, 2001). To the best of the author’s knowledge, the only previous applications to near-surface (i.e., upper 20 m of the subsurface) data used vertical seismic profile (VSP) and surface surveys at the current study site (Gao et al., 2006; Gao et al., 2007).

There is a sizeable body of work demonstrating the efficacy of waveform tomography for various field data applications, however very little of it concerns near-surface surveys. Furthermore, it is believed that all previous field data applications inverted single-component data based on a visco-acoustic wave equation. Extending the method to SH-wave data sets provides information on a second elastic parameter in the earth, the rigidity, which may enhance interpretation of subsurface lithology and pore fluid saturation. In addition, there are several inherent advantages of SH-waves over P-waves for near-surface imaging (e.g., Goforth and Hayward, 1992; Young and Hoyos, 2001; Jarvis and Knight, 2002; Rabbel et al., 2004). P-wavefields contain strong water table reflections, which can interfere with reflections from geologic interfaces. Furthermore, the P-wavelength increases significantly below the water table, degrading resolution, because the bulk compressibility of unconsolidated sediment is highly dependent on pore fluid content. In contrast, SH-waves are almost unaffected by pore fluid, eliminating these problems inherent to P-waves. Finally, the acoustic wave
equation is unable to predict certain aspects of a real vertical-component data set, such as Rayleigh waves and P-SV converted waves, which restricts the useable portion of the observed wavefield. The SH-wave equation, on the other hand, predicts all aspects of a pure SH-wavefield, which may allow for inversion of a longer seismic coda.

The next section is a brief overview of the waveform tomography method, with emphasis on the salient points regarding extension of the method to SH-waves and practical inversion strategy. This is followed by background information on the HAFB field site, including relevant near-surface geology and previous geophysical surveys. Results of traveltime tomography using the field data are then described. Synthetic waveform tomography tests comparing the acoustic and SH-wave methods are covered next. The synthetic tests demonstrate a small difference in depth sensitivity due to fundamental differences in the interaction of acoustic and SH-waves with subsurface velocity perturbations. However, a much more prominent effect is the improvement in resolution obtained by using SH-waves with their lower velocities. The application of waveform tomography to the field data is then described, and the resulting high-resolution models are interpreted for lithologic and water-saturation features in the contaminated aquifer. The availability of both P- and S-wave velocity models significantly improves interpretative capability. The thesis closes with a discussion on the strengths and limitations of the waveform tomography models, with some proposed actions that could be taken in the future to improve the SH-wave method introduced here.
CHAPTER 2

METHODOLOGY

The theoretical background of frequency-domain, full waveform tomography forward modeling and inversion is developed extensively in Stekl and Pratt (1998) and Pratt et al. (1998). The following is a brief overview of this background, emphasizing extension of the method to the SH wave equation. The reader is referred to the above literature for a rigorous development of the method, and Appendix 1 for a derivation of the full details of the SH-wave forward modeling and inversion relations, equations 2 and 5.

The acoustic and SH wave equations are given in the time domain by equations 1a and 1b respectively, for a source signature $f(x,t)$ (Marfurt, 1984):

\[
\nabla \cdot \left( \frac{1}{\rho} \nabla u \right) - \frac{\partial}{\partial t} \left( \frac{1}{\lambda} \frac{\partial u}{\partial t} \right) = f(x,t), \tag{1a}
\]

\[
\nabla \cdot (\mu \nabla u) - \frac{\partial}{\partial t} \left( \rho \frac{\partial u}{\partial t} \right) = f(x,t), \tag{1b}
\]

where the wavefield variable $u(x,t)$ is pressure and transverse displacement in the acoustic and SH-wave cases respectively, $\rho$ is density, and $\lambda$ and $\mu$ are Lame's parameters, which are calculated from specified density and seismic velocity models. To simplify the problem, density is often assumed to be proportional to the fourth root of velocity (Gardner et al., 1974). The similarity of the two wave equations motivates the extension of the acoustic waveform tomography algorithm to SH-waves. By taking a Fourier transform and a spatial finite-difference approximation, the wave equations,
equations 1a and 1b, can be written in a general matrix form for a given angular frequency $\omega$:

$$\mathbf{Su}(\omega) = \mathbf{f}(\omega),$$  \hspace{1cm} (2)

where $\mathbf{u}$ and $\mathbf{f}$ are complex-valued vectors representing the frequency-domain wavefield and source signature at a set of subsurface nodes, and $\mathbf{S}$ is a complex-valued impedance matrix that depends on frequency and subsurface elastic parameters (Lame parameters and density). For a given frequency and subsurface velocity model, once the impedance matrix is calculated and inverted (typically with an LU decomposition), the wavefield at every node can be readily calculated for multiple source terms. This is a significant computational advantage of frequency-domain modeling over time-domain methods. The form of the impedance matrix is slightly different depending on whether acoustic or SH-waves are modeled, but the process is the same.

The goal of waveform tomography is to find the optimal model parameter vector $\mathbf{p}$ (typically representing seismic velocity at some subset of nodes in the subsurface), which minimizes the scalar objective function, or data misfit:

$$E(\mathbf{p}) = \frac{1}{2} \delta \mathbf{d}' \delta \mathbf{d}^*, \hspace{1cm} (3)$$

where $\delta \mathbf{d}$ is a vector of the frequency-domain residual between the observed data and predicted wavefield at each receiver for a given frequency, and superscripts $t$ and $*$ represent the vector transpose and complex conjugate respectively. In this work, a local descent gradient inversion method is used to iteratively update the model parameters:

$$\mathbf{p}^{(k+1)} = \mathbf{p}^{(k)} - \alpha^{(k)} \nabla_\mathbf{p} E^{(k)}, \hspace{1cm} (4)$$

where $k$ is the iteration number, $\nabla_\mathbf{p}$ is the gradient operator with respect to the model parameter vector, $\mathbf{p}$, and $\alpha$ is an estimated step length, see Pratt et al. (1998) for details.
The gradient is computed with an efficient back-propagation technique developed initially by Tarantola (1984):

\[
(\nabla_i E)_i = \text{Re} \left\{ u' \left[ \frac{\partial S'}{\partial \phi} \right] (S^{-1})' \delta d' \right\}.
\] (5)

The gradient for the \( i \)th model parameter (i.e., the velocity update at a specific node) is calculated in several steps. First, the inverse impedance matrix is used to forward model the wavefield in the current velocity model. The resulting data residual vector is treated as a source and multiplied by the inverse impedance matrix to produce a back-propagated wavefield (i.e., the last two factors in the gradient calculation, equation 5). The back-propagated wavefield is correlated (i.e., multiplied in the frequency domain) with a virtual source described as the interaction of the incident modeled wavefield \( u \) with a hypothetical velocity perturbation (i.e., the derivative of the impedance matrix).

Differences between the acoustic and SH-wave methods are almost entirely contained in the entries of the impedance matrix, \( S \), and the derivative matrix in the gradient calculation, equation 5. Other differences between the techniques, such as treatment of free surface reflections and anelastic attenuation, are special cases not considered in this study. The reader is referred to Appendix 1 for a full derivation of the entries in the impedance and derivative matrices for both the acoustic and SH-wave cases.

Waveform tomography is a nonlinear iterative process, and therefore accurate convergence requires a reasonably accurate initial estimate of the true subsurface velocity field. More precisely, the initial model must predict arrival times within a half-cycle of the seismic waveform. The initial model is typically obtained from traveltime tomography, which provides a robust and accurate low-wavenumber velocity model. The above iterative inversion is then performed for a single frequency (or group of nearby
frequencies), producing an updated velocity model. The process is repeated sequentially for increasing frequency groups, gradually updating the model with finer features as the frequency under consideration increases. Between each frequency group inversion, the best-fit source signature is calculated for the most recent velocity model (e.g., Pratt, 1999). Unlike many traveltime tomographic methods that converge to the simplest model satisfying observed data within a specified error bound, the stopping criteria for waveform tomography are more qualitative. As frequency increases so does nonlinearity of the inversion, and thus model updates for higher frequency components may be more unstable and error-prone. The exact stopping point is judged qualitatively, and is typically based on when further model updates lack consistency with existing features in the model, or when further inversion does not continue to reduce the objective function.
3.1. Background

The field site, Operable Unit 2 (OU-2), is located at Hill Air Force Base (HAFB), in northern Utah (Figure 3.1). Near the northeast edge of the base, OU-2 occupies a fluvial terrace roughly 90 m above the Weber River Valley, a rural area dependent on groundwater for its fresh water supply (Dana, 2004).

In the past, OU-2 was used as a disposal site for chlorinated organic solvents, which subsequently seeped down into a shallow aquifer (USAF, 1998). These toxic solvents are classified as dense nonaqueous phase liquids (DNAPLs) based on their behavior in the subsurface, which is illustrated schematically in Figure 3.2. DNAPL is denser than groundwater and relatively insoluble, thus it tends to sink down through the aquifer and pool as a free liquid phase above low-permeability features, either at topographic lows at the aquifer base or heterogeneity within the aquifer itself. There, the contaminant slowly dissolves, producing a long-lived toxic plume that can degrade regional groundwater quality. It is important to understand the topography of the aquifer base and identify low-permeability features within the aquifer so that in situ remediation can be targeted at potential DNAPL traps (Intera, 1997).
Figure 3.1:
Aerial view of the field site, Operable Unit 2 (OU-2), located near the northeast edge of Hill Air Force Base (HAFB). Contamination from OU-2 affects the nearby Weber River Valley, a rural area dependent on groundwater. The base is located in northern Utah (inset) west of the Wasatch Range and east of Great Salt Lake.
3.2. Geology

HAFB is located in the eastern Lake Bonneville basin, west of the Wasatch Range and east of Great Salt Lake. Lake Bonneville was the larger pre-cursor to the modern Great Salt Lake prior to the late Pleistocene, when the lake shrank rapidly due to increasing aridity and other factors (Currey, 1980). Deposition of near-surface sediment at HAFB occurred during this regression, in a lacustrine deltaic environment where the Weber River flowed into Lake Bonneville. The relatively high-energy Weber River carried fairly coarse-grained sediment as it flowed out of the nearby Wasatch Range.
There are two formations of interest to the groundwater problem at HAFB: the Provo Formation at the surface and the underlying Alpine Formation. The Alpine Formation is a thick silty clay deposited in relatively deep water during the Bonneville highstand prior to about 14,000 years ago, when the Lake Bonneville shoreline was at the base of the Wasatch Mountains to the east of HAFB (Figure 3.3). The Provo Formation was deposited in shallower water during the Provo stand (roughly 14,000 to 12,500 years ago); the high-energy environment resulted in deposition of a heterogeneous mixture of interbedded sands and gravels with some silts and clays (Currey, 1980). Small-scale slumping features add to the complexity of the Provo Formation (Dana, 2004). The high level of Provo heterogeneity, demonstrated by rapid lithologic variation over short distances (Figure 3.4), greatly increases the difficulty of both seismic imaging and groundwater remediation within the Provo Formation.

From a hydrogeologic standpoint, the Provo Formation comprises an unconfined aquifer, sealed below by the Alpine clay aquiclude. Pump tests at OU-2 estimate an average porosity of 27% and hydraulic conductivity ranging from 13.0 to 35.4 m/day for the Provo aquifer, while the measured hydraulic conductivity of $9 \times 10^{-6}$ m/day for the Alpine Formation effectively prevents groundwater flow (Dana, 2004; Intera, 1997). In 2005, borehole measurements at OU-2 estimated the average water table at roughly 10 m depth; however, the water table is variable depending on precipitation and remediation activity, and subsurface water saturation is characterized by a smoothly increasing profile rather than a sharp boundary (Fradelizio, 2007). Provo Formation thickness at OU-2 ranges from 2-15 m, and exhibits a north trending paleochannel feature incised in the Alpine clay surface (Figure 3.5). The DNAPL contaminant is expected to collect at low-
permeability heterogeneities within the Provo aquifer or at low points in the base of the paleochannel. Therefore, the objective of an ongoing seismic imaging program at OU-2 has been to aid remediation activities by mapping the topography of the paleochannel base and identifying lithologic variations in the Provo Formation.

Figure 3.3: Aerial photograph showing local geomorphology at HAFB, including ancient Lake Bonneville shorelines. The modern Great Salt Lake shoreline is out of the image to the west. Late Pleistocene deposition at OU-2 (site marked by the yellow star) occurred during the Bonneville (prior to 14,000 years ago) and Provo (14,000 – 12,500 years ago) stands. The Weber River was the dominant source of depositional material carried out of the Wasatch Range. Image resolution is 32 m (modified from USGS, 1997).
Figure 3.4:
Lithology logs from the northern part of OU-2 (see Figure 3.5) illustrate heterogeneity in the Provo Formation paleochannel (modified from USAF, 1998).
Figure 3.5:
Contour map of the depth to Alpine clay estimated by kriging of well log measurements (white circles), the elevation datum is 1431 m (modified from Fradelizio, 2007). Overlain are the current 2D seismic survey lines in red, with x’s marking the locations of shot gathers in Figures 3.6, 6.3 and 6.4. The solid black line marks the VSP-surface survey (Gao et al., 2006), and the dashed line outlines the 3D surveys (e.g., Fradelizio et al., 2008). Red dots mark the locations of the lithology logs in Figure 3.4.
3.3. Geophysical Surveys

At a different field site elsewhere on HAFB, Young and Sun (1996, 1998) conducted ground penetrating radar (GPR) surveys to image the shallow aquifer. They successfully imaged the aquifer base, which was at roughly 9 m depth at their field site, despite difficulties associated with signal absorption due to clay content and coherent noise from remediation equipment and other metallic objects. The current site, OU-2, is also characterized by clay-rich sediment, pipes, and remediation equipment, and a somewhat deeper aquifer base, which present difficulties for effective GPR imaging.

Rice University conducted several seismic surveys at OU-2 with the purpose of mapping the paleochannel and characterizing the Provo aquifer. An ambitious acquisition program in 2000 produced 3D reflection and tomography surveys, and a 2D combined VSP-surface survey (Figure 3.5). Inversion of first arrival traveltimes in the 3D tomography survey provided an accurate 3D velocity model (Zelt et al., 2006; Azaria, 2003). A high-resolution map of the Alpine clay surface was interpreted from depth migration of the reflection survey (Fradelizio et al., 2008; Dana, 2004). Waveform tomography with the 2D VSP-surface data set produced a high-resolution velocity model that was tied to lithology at boreholes (Gao et al., 2006). Waveform tomography was also applied to 2D surface seismic data (Gao et al., 2007), which was also successful in mapping small-scale velocity variations within the aquifer, but with poorer resolution than the VSP-surface survey due to reduced seismic coverage. These experiments demonstrated the efficacy of various seismic methods for characterizing a shallow contaminated aquifer, despite extensive environmental noise due to remediation activities, vehicle traffic, jet aircraft and other military activities on the base.
Motivated by the success of previous surveys and potential benefits of full elastic imaging of the aquifer, a multicomponent seismic survey was conducted at OU-2 in 2005. Two 30 m long 2D profiles were acquired, a north-south line along and an east-west line across the paleochannel axis (Figure 3.5). The survey was conducted with three-component (3C) sources and receivers (i.e., vertical, radial, and transverse directions) resulting in a full 9C data set. Two components are the focus of this work: the vertical source-receiver component, treated as a compressional (P) wave data set, and the horizontal transverse source-receiver component, which is treated as a transverse shear (SH) wave data set. Each line consisted of 61 source and 60 receiver stations, both at 0.5 m spacing, resulting in a maximum source-receiver offset of 29.75 m. Each receiver group consisted of three geophones arranged in a Gal’perin configuration (Fradelizio, 2007; Gal’perin, 1984). For an S-wave source, a 2 lb hammer was used to horizontally strike a steel-capped wooden beam that was weighted down to improve coupling with the ground. Strikes were recorded in opposite directions and negatively stacked to attenuate incidental P-waves and boost SH-waves. The P-wave source consisted of a 12 lb hammer used to vertically strike a trailer hitch ball planted in the ground. For both sources, twelve hammer blows were stacked per source location to improve signal-noise ratio.

Comparison of the raw P- and SH-wave seismic data (Figure 3.6) indicate that both components suffer strong surface wave contamination. The signal-noise ratio of the S-wave source is somewhat worse than the P-wave source, and the SH-wave records contain strong receiver-consistent ringing that contaminates the wavefield (Fradelizio, 2007). The north-south line SH-wave component has a slightly worse signal-noise ratio.
than for the east-west line. In spite of this, previous reflection processing and depth migration indicated that the P- and SH-wave data sets could provide images of comparable quality, with mutually consistent interpretations of the Alpine clay surface (Fradelizio, 2007).

Figure 3.6:
Sample shot gathers showing the first 250 ms of the raw data records for the P-wave (a and b) and SH-wave (c and d) components from the east-west (a and c) and north-south (b and d) lines. The locations of the shot gathers are shown in Figure 3.5.
Successful full waveform tomography requires a sufficiently accurate initial velocity model to avoid cycle skipping and enable convergence (Gao, 2004). In this study, the initial model was provided by inversion of first arrival traveltimes using First Arrival Seismic Tomography (FAST), the regularized inversion method of Zelt and Barton (1998). The inversion was performed in several sequential steps. In the first step, the initial model was taken from average 1D velocities obtained in previous studies at OU-2 (Fradelizio, 2007; Gao et al., 2006, 2007). Most of these studies estimated P-wave velocity only; in these cases the initial S-wave velocity estimate was 50% of the P-wave value. The inversion results of this step for both lines were used to update average 1D background P- and S-wave velocity models for the field site as a whole (Figure 4.1). All velocity perturbation plots in this study are relative to these background profiles. A subsequent inversion step used these new 1D background velocities as initial models to produce the final traveltime tomography models.
Figure 4.1:
Average P- and S-wave 1D background velocity models at OU-2 determined from first arrival traveltime tomography using both the east-west and north-south lines. Ray coverage (see Figures 4.3 and 4.4) limits the well-constrained portion of the model to the upper 11 m.

The objective of FAST is to obtain the simplest velocity model that satisfies picked traveltimes within a specified uncertainty. This uncertainty was estimated by examining the distribution of traveltime misfit between reciprocal source-receiver pairs (Figure 4.2), which should theoretically have identical traveltimes. For all four data sets, between 84% and 89% of reciprocal pairs had traveltime misfits of 2 ms or less, thus 2 ms was deemed a suitable pick uncertainty. However, for the first inversion step (1D background estimation) the uncertainties were increased to 3 ms, as this results in a smoother model from which to estimate background velocities. It is noted that the SH-wave component on the north-south line has slightly more large misfits, consistent with the previous observation that it has the worst signal-noise ratio of the four data sets (Figure 3.6).
Figure 4.2:
Distribution of the traveltime misfit between reciprocal source-receiver pairs for each data set: the east-west line P-wave (a), the north-south line P-wave (b), the east-west line SH-wave (c), and the north-south line SH-wave (d) data sets.

The final traveltime tomography models are plotted as perturbations relative to the background velocities (Figures 4.3 and 4.4). In both lines, the P- and S-wave velocity components exhibit similar features. Low velocities in the eastern portion of the east-west line may correspond to a shallow clean sand body. Such a feature is thought to be spatially continuous throughout much of the eastern part of OU-2 based on borehole data (Fradelizio, 2007). Shallow, high-velocity anomalies may correspond to a superficial layer of highly cemented caliche. Ray coverage (Figures 4.3 and 4.4) indicates that the subsurface is fairly well sampled for depths less than about 11-12 m, but deeper regions of the velocity models are not as well constrained, nor are the edges of the model at depths greater than a few meters.
Figure 4.3:
Final traveltime tomography velocity models and ray coverage for the P- (a) and SH-wave (b) data along the east-west line. Models are plotted as perturbations relative to average 1D background velocities (Figure 4.1). For clarity, only one in five raypaths are plotted in the ray diagrams.
Figure 4.4:
Final traveltime tomography velocity models and ray coverage for the P- (a) and SH-wave (b) data along the north-south line. Models are plotted as perturbations relative to average 1D background velocities (Figure 4.1). For clarity, only one in five raypaths are plotted in the ray diagrams.
5.1. Objectives

The purpose of the synthetic waveform tomography tests is two-fold: compare behavior of the acoustic and SH-wave methods, and estimate the potential performance of waveform tomography for an imaging environment representative of the OU-2 field site. Tests were run using the same source-receiver and model geometry as the field data. The test model (Figure 5.1a) contains several circular velocity anomalies of radius 1 m (i.e., sub-wavelength size, chosen to push the limits of potential resolution), as well as an interface near the base of the model simulating the paleochannel incised in the Alpine clay layer. The ±20% velocity perturbations are superimposed on the 1D background models from traveltime tomography at OU-2 (Figure 4.1), which also served as the starting models for the waveform tomography.

Three separate tests were conducted. A realistic SH-wave test used the S-wave background velocity and parameters mimicking the SH-wave field data at OU-2; i.e., the source signature, frequency range of inversion, and available offset range were all chosen to match the field data. An analogous realistic acoustic test used the P-wave background velocity and parameters mimicking the P-wave field data. The key differences between the realistic SH-wave and acoustic tests are background velocity and available offset range, which is roughly 5-30 m and 10-30 m in the SH- and P-wave cases respectively. For a fundamental comparison of the SH-wave and acoustic waveform tomography methods, an identical-parameter acoustic test was done using the exact same parameters as the SH-wave test, as well as the S-wave background velocity. Thus, the realistic
acoustic and SH-wave tests are meant to be accurate representations of the field site, whereas the identical-parameter acoustic tests is a hypothetical test case to compare SH-wave and acoustic waveform tomography algorithms under identical imaging parameters.

Figure 5.1:
Synthetic waveform tomography test models. Velocity models are plotted as perturbations relative to the appropriate 1D background velocity (Figure 4.1). Shown are the true model (a), the realistic SH-wave test result (b), the realistic acoustic test result (c), and the identical-parameter acoustic test result (d). Black lines in (b-d) mark true anomaly locations. Green lines in (a) mark the locations of horizontal profiles (Figure 5.2) through the models at depths of 2-3, 7, and 12 m. Five vertical profiles are also shown through the center of each circular anomaly, at positions of 5, 11, 15, 19, and 25 m.
Figure 5.2:
Profiles through the velocity perturbation models of Figure 5.1. Vertical profiles (a) are through the center of each circular anomaly, from left to right, at positions of 5, 11, 15, 19, and 25 m. Horizontal profiles (b) are as marked in Figure 5.1, from top to bottom, at depths of 2-3, 7, and 12 m.
5.2. Results and Discussion

Results of the synthetic tests are plotted in Figure 5.1 as velocity perturbations relative to the appropriate 1D background velocity. In addition, profiles through the various anomalies are plotted in Figure 5.2. The realistic SH-wave (Figure 5.1b) and identical-parameter acoustic (Figure 5.1d) tests exhibit similar results. However there are small differences, in particular, it appears that SH-wave inversion provides a slightly more accurate image of the shallower anomalies, whereas the acoustic inversion produces somewhat stronger responses for the deeper features (Figure 5.2). As these inversions were performed with identical parameters, differences must be due to the fundamental physics of acoustic and SH-wave propagation.

It is instructive to examine theoretical differences between acoustic and SH-wave propagation in two scenarios: reflection from a flat interface and scattering from a small, sub-wavelength size anomaly (Figure 5.3). The background velocity gradient in the synthetic tests causes strong bending of seismic raypaths, which when combined with a lack of near-offset traces ensures that the interface near the base of the model is illuminated primarily with medium to large incidence angles. In this incident angle range, the acoustic reflection coefficient is expected to be much stronger than the magnitude of the SH-wave coefficient (Figure 5.3a). Simple forward modeling based on the waveform tomography algorithm (i.e., equation 2) verified this observation (Figure 5.4). This difference may explain why the deep interface response is slightly stronger in the identical-parameter acoustic test than in the SH-wave test. Another type of interaction between seismic waves and subsurface velocity perturbations is scattering from a small inclusion. The acoustic and SH-wave scattering patterns exhibit similar
responses for direct forward or back scattering, but the theoretical SH-wave response is significantly diminished for oblique scattering at near right angles. The scattering patterns in Figure 5.3b are calculated for the ideal case of 3D far-field scattering from an infinitesimal point scatterer (Wu and Aki, 1985), which may not be sufficient for quantitative scattering strength predictions due to neglect of 2D effects, near-field terms, and the finite size of anomalies. However, differences between acoustic and SH-wave scattering in the ideal case are still useful to consider. A forward modeling test of scattering from a 1 m radius anomaly (Figure 5.5) verified expected behavior, although back-scattered wave amplitudes are decreased due to the effect of finite anomaly size, which is discussed in more detail in Appendix 2. For the imaging geometry in this study, as the depth of an anomaly increases, the scattered wavefield averaged over all source-receiver pairs shifts from predominantly forward scattering to back scattering. Thus, the total recorded SH-wave grows weaker with increasing anomaly depth at a more rapid rate than a scattered acoustic wave, resulting in the observed difference in depth sensitivity of the two techniques. Appendix 2 contains the details of this analysis.
Figure 5.3:
Theoretical reflection coefficient (a) and scattering pattern (b) for acoustic and SH-waves. Both (a) and (b) involve a +20% velocity anomaly and density calculated according to Gardner's relationship (Gardner et al., 1974), as for the synthetic waveform tomography tests. The reflection coefficient is plotted up to the critical angle of 56.4°. The scattering pattern is calculated for a plane wave incident from the left on a point scatterer (Wu and Aki, 1985); plus and minus signs indicate polarity of the scattered wave relative to the incident wave. The scattering pattern is normalized relative to the forward scattered wave amplitude.
Figure 5.4:
Modeled acoustic (a) and SH-wave (b) reflection from a flat +20% velocity interface at depth 12 m in a homogenous background velocity, the source-receiver offset range corresponds to the first source position in the SH-wave and identical-parameter acoustic synthetic waveform tomography tests. The acoustic signal gains strength with offset, while the SH-wave signal loses strength until it undergoes a polarity reversal. In this geometry, the expected SH-wave polarity shift and critical reflection at incidence angles of 42.4° and 56.4° would occur at offsets of 21.9 m and 36.2 m respectively.

Figure 5.5:
Modeled acoustic (a) and SH-wave (b) scattering from a +20% circular velocity anomaly of radius 1 m (black circle at the origin), in a homogeneous background model. The source is located to the left, at the dot. The source signature is a simple, symmetric, linear phase wavelet with a negative main lobe and positive sidelobes (e.g., Figure 5.4a). The acoustic wavefield has the same negative polarity for all scattering angles, while the SH-wave signal undergoes a polarity reversal as the scattering angle increases.
The realistic acoustic test results (Figure 5.1c) indicate that the larger P-wave background velocity significantly degrades resolution, an effect that overwhelms slight differences in scattering strength observed in the identical-parameter acoustic and SH-wave tests. Depending on depth, the P-wave background velocity is roughly 1.5-2 times larger than the S-wave velocity. Therefore, since the frequency content of the two components is similar, a factor of 1.5-2 reduction in resolution is expected for acoustic waveform tomography relative to the SH-wave version. As observed in Figures 5.1 and 5.2, the realistic acoustic inversion struggled to resolve many features in the model, particularly the anomalies at 7 m depth. While the loss of 5-10 m offsets plays some role in degradation of the image, increased velocity is the dominant factor. Overall, while it appears that SH-wave inversion does have some fundamental shortcomings compared to acoustic inversion in terms of depth sensitivity, they are slight compared to resolution degradation due to the change in background velocity when the frequency content of the data sets are similar.

Other general observations may be made regarding image quality. For instance, it appears that the inversion response in the deeper half of the model is somewhat less than in the shallow portion, resulting in consistently underestimated magnitudes of deeper anomalies. On the other hand, the uppermost 2 m of the model appears somewhat susceptible to imaging artifacts, particularly in the acoustic case. This is due to nonlinearity inherent to the underlying physics and inversion algorithm when inclusions are close to source locations and/or when receivers lie in the scattering near-field of shallow inclusions (Aki and Richards, 2002). This aspect of waveform tomography has been recognized by other investigators (e.g., Ravaut et al., 2004), and is typically
addressed by partial or complete muting of shallow velocity model updates. The synthetic tests and field data inversions in this work were performed with model updates muted entirely above 0.5 m depth and ramping on to full strength at 1.5 m depth; however this may not be sufficiently conservative for the given imaging environment.

Overall, the tests indicate that SH waveform tomography has the potential to image finer features than the traditional acoustic version of the technique. However, it is noted that the synthetic tests were done in the ideal case of zero noise contamination, so inversion of the field data is not expected to match the impressive resolution of the synthetic images.
6.1. Data Pre-conditioning

Pre-processing of the field data prior to application of full waveform tomography was necessary in order to improve signal-noise ratio and eliminate aspects of the data that are not modeled by the acoustic or SH wave equation. Key pre-processing steps included: band-pass filtering, time windowing around the first arrival waveforms, muting of noisy and near-offset traces, normalizing trace amplitudes, and applying an amplitude correction. These steps are outlined below, with more details on processing parameters in Appendix 3. Band-pass filtering improved signal-noise ratio and restricted the data bandwidth to the modeled frequency range. Time windowing eliminated surface waves and other contaminating phases from the data. The near-offset traces are contaminated by surface waves even in the restricted time window, and therefore were muted. The minimum useable offset varies slightly between gathers, but is roughly 10 m and 5 m on average for the P- and SH-wave data sets respectively. Excessively noisy traces, more of an issue in the lower signal-noise ratio SH-wave data, were also muted. Trace-to-trace amplitude variations incorporate many different factors, such as geometric spreading, anelastic attenuation, and variability of receiver-ground coupling, source strength, and near-surface conditions. Rather than attempt to accurately account for all these factors, traces were individually normalized by their RMS amplitude. Finally, an amplitude correction factor proportional to the square root of time was applied to simulate the effect of 2D geometric spreading inherent to the 2D modeled wavefields.
A related issue that bears mentioning is the fact that the observed data quantity is particle velocity (either vertical or transverse), while acoustic and SH waveform tomography actually model pressure and particle displacement respectively. Previous work demonstrated that this issue is mitigated by trace normalization and the source signature estimation process, and may be safely neglected (Ravaut et al., 2004).

6.2. Waveform Tomography Strategy

Waveform tomography requires starting estimates for the velocity model and source signature. As discussed previously, the initial velocity model was obtained by inverting first arrival traveltimes in the data. Source signature updates may be calculated from the data for a given velocity model. Although the source estimation procedure assumes a precisely accurate velocity model, the initial velocity model tends to be sufficient to provide a starting source signature estimate that can be updated periodically throughout the inversion (Pratt, 1999). An initial source guess consisted of a simple two-lobed Keuper wavelet with sufficient frequency content to cover the bandwidth of the observed data (Figure 6.1), and a starting source update is calculated using the initial velocity model. Forward modeling at this stage confirms that the initial velocity model and starting source signature predict the observed first arrivals with sufficient accuracy to expect convergence of the waveform tomography.

The frequency range for inversion is chosen based on the observed data spectra (Figure 6.1), as well as by examining the data in the frequency domain to ensure strong and consistent events (e.g., Pratt, 1999; Gao et al., 2006). Several different styles of dividing the total bandwidth into groups for subsequent inversions were tested, but the
specific choice of frequency group breakdown did not have a significant impact on the final velocity models. The frequency groups that were ultimately used, listed in Table 1 for each of the four data components, were the choices that gave slightly better data misfit reduction than others. Inversion of three frequency components spaced by 4 Hz for each group proved to be ideal for all data sets with the exception of the north-south line, SH-wave component, for which four frequency components at 2 Hz spacing were used. This data component exhibited slightly worse signal-noise ratio than the others (Figure 3.6), which may explain why averaging more frequency components in each group proved beneficial.

Although the inversions were originally run over the entire frequency band detailed in Table 1, the final models were typically chosen earlier. The stopping points were determined primarily by the evolution of objective function values, or data misfit, as the frequency group increased (Figure 6.2), with consideration also for the geologic reasonableness of further velocity model updates. Although all group inversions reduced the data misfit for the frequency components under consideration (Figure 6.2, dotted line), the total misfit for all components (Figure 6.2, solid line) tended to increase after the first group, and then decrease rapidly over the next few groups before leveling off. In some cases it eventually began to increase again as the highest group inversions were attempted. The chosen final models for each component are marked in Figure 6.2 and identified in the Table 1 caption.
Figure 6.1:
Power spectra, averaged over all useable traces, for each of the four final pre-processed data sets: the east-west line P-wave (a), the north-south line P-wave (b), the east-west line SH-wave (c), and the north-south line SH-wave (d) data sets.

Table 1:
Schedule of frequency components used in each sequential frequency group for the four field data sets. The final velocity models were taken following groups 6, 7, 7, and 8 for the east-west line P-wave, north-south line P-wave, east-west line SH-wave, and north-south line SH-wave data sets, respectively.
Figure 6.2:
Data misfit (i.e., objective function) evolution, plotted at the central frequency in each inversion group. Plotted are the east-west line P-wave (a), the north-south line P-wave (b), the east-west line SH-wave (c), and the north-south line SH-wave (d) data sets. The solid line is the total RMS misfit summed over all frequency components following inversion of a given frequency group, and is plotted as a percentage of the misfit for the starting model. The dashed line is the percent reduction in RMS misfit over the course of inversion for each frequency group, considering only the frequency components in that group. Red x's mark the last frequency group inversion prior to selection of the final model for each component.

6.3. Waveform Tomography Results

In addition to judging inversion quality based on objective function reduction (Figure 6.2), it is beneficial to examine predicted seismograms in the time domain to ensure a reasonable match with the observed data. Figures 6.3 and 6.4 compare preprocessed and predicted shot gathers for the east-west and north-south lines respectively.

For the east-west line, the acoustic inversion provides a good match to the observed P-wave data set, particularly in predicting the emergence of a faster refracted phase at around 20 m offset. The SH-wave inversion also provides a decent match to the noisier
SH-wave data set, including a change in moveout slope at roughly 17 m offset. The quality of the match is slightly worse for the noisier north-south line, although the acoustic inversion predicts the observed data fairly accurately over the limited range of usable offset. The fit to the SH-wave data is also quite good considering the larger amount of noise observed in this component, in particular a change in moveout slope at roughly 15 m offset is accurately recovered. These seismic sections also illustrate a fundamental difference between the P- and SH-wave data in terms of usable offset range. While the SH-wave data tended to permit the use of shorter offsets, the lower signal-noise ratio of the SH source caused a greater fraction of the long-offset traces to be deemed too noisy for use and muted.

Figure 6.3:
Sample shot gathers of pre-processed observed data (a and c) and seismograms predicted by waveform tomography (b and d), for the P- (a and b) and SH-wave (c and d) data sets from the east-west line. The data are shown with reversed polarity to emphasize features in the waveforms. The location of the shot gather is shown in Figure 3.5.
Figure 6.4:
Sample shot gathers of pre-processed observed data (a and c) and seismograms predicted by waveform tomography (b and d), for the P- (a and b) and SH-wave (c and d) data sets from the north-south line. The data are shown with reversed polarity to emphasize features in the waveforms. The location of the shot gather is shown in Figure 3.5.

The final waveform tomography velocity models are plotted in Figures 6.5 and 6.6 for the east-west and north-south lines, respectively. The models are plotted both in terms of absolute velocity as well as perturbations relative to 1D average background velocities (Figure 4.1). Note the rather large velocity perturbations, which range up to about 60% in small regions of many of the models. While it is possible that the inversion is over-estimating anomaly magnitudes, these results are consistent with previous studies at OU-2 that observed extreme lateral velocity variation due to lithologic heterogeneity in the Provo Formation, particularly in the vadose zone (Fradelizio et al., 2008; Gao et al., 2006, 2007; Zelt et al., 2006). In general, the SH-wave components appear to give better shallow resolution than the P-wave components, particularly for the east-west line.
Image quality appears to be better for the east-west line than for the north-south line, consistent with a higher signal-noise ratio. The east-west line P- and SH-wave velocity models are qualitatively consistent with each other, exhibiting common features such as a general dip to the east of velocity contours in the western part of the line and generally lower velocities on average for the eastern part of the line than the western. This last observation is also consistent with the traveltime tomography results (Figure 4.3). Key differences between the P- and SH-wave velocity models are primarily in small-scale features at depths of less than 3-4 m in the model. Synthetic tests discussed previously indicated that the SH-wave inversion might be slightly better than the acoustic inversion at imaging the shallowest part of the model, suggesting that these small-scale features may be true features unresolved by the acoustic inversion. However, the synthetic tests also demonstrated that waveform tomography is sometimes susceptible to near-surface instability, so interpretation of the shallowest features should be done cautiously. Overall, the consistency of features observed in the P- and SH-wave traveltime and waveform tomography models, as well as the good match between observed and predicted data, suggest that the waveform tomography results for the east-west line are fairly robust and accurate.

The north-south line velocity models exhibit much less consistency between the P- and SH-wave velocity models. Some features are consistent however: high shallow velocities at both ends of the line bracket lower near-surface velocities in the middle of the line, and the deep middle portion of the line appears to be characterized by lower velocities. These observations are also consistent with the traveltime tomography models (Figure 4.4). While the north-south line images are of lesser quality, some features that
show qualitative consistency between the P- and SH-wave traveltime and waveform
tomography models are probably trustworthy.
Figure 6.5:
Final waveform tomography models for the acoustic (a and c) and SH-wave (b and d) inversions on the east-west line. Models are plotted as absolute velocities (a and b) and perturbations relative to the appropriate 1D background velocity (c and d). Solid black lines on the perturbation maps indicate the depth of the Alpine clay interface estimated from well measurements (Figure 3.5). Dashed lines emphasize interpretations discussed in the text.
Figure 6.6:
Final waveform tomography models for the acoustic (a and c) and SH-wave (b and d) inversions on the north-south line. Models are plotted as absolute velocities (a and b) and perturbations relative to the appropriate 1D background velocity (c and d). Solid black lines on the perturbation maps indicate the depth of the Alpine clay interface estimated from well measurements (Figure 3.5). Dashed lines emphasize interpretations discussed in the text.
Rigorous interpretation is difficult without well control and petrophysical data to correlate with seismic observations. However, a preliminary interpretation of the velocity models in Figures 6.5 and 6.6 is based on the premise that dry unconsolidated sand and gravel exhibit lower velocity than clay-rich sediment, and highly water-saturated sediment will have significantly increased P-wave velocity and neutral to low S-wave velocity (Bachrach and Nur, 1998). Additional interpretative power is gained by the availability of both P- and S-wave velocity models. Features that are common to both components are likely lithology related; whereas high P-wave velocity associated with a small low S-wave velocity anomaly may be caused by fluid saturation. Interpretations can be checked for consistency with results from previous studies at OU-2 (e.g., Fradelizio, 2007; Gao et al., 2006; Figure 7.1), enhancing the robustness of many of the conclusions here.
Figure 7.1:
The final velocity model (a) from a previous VSP-surface survey at the study site, which approximately coincides with the southern two thirds of the north-south line in the current study (Figure 3.5). Also shown is the velocity difference from the 1D average of the model (b), and a geologic interpretation of the model (c), based on the lithology logs at either end of the line (from Gao et al., 2006).
The dominant feature in the east-west line is a large low-velocity anomaly in the eastern half of the line. Borehole observations suggest the existence of a shallow, clean sand body in the eastern part of OU-2 (Fradelizio, 2007); the low-velocity anomaly is interpreted as this sand body. The vertical offset in the sand body at a position of about 20 m may be depositional or erosional in nature, or it may be due to small-scale slumping observed in the area (Dana, 2004). A sand body such as this can play a key role in subsurface fluid transport if it is continuous, but vertical offsets like the one observed have the potential to weaken the continuity and transport capability of the sand body. Higher velocities to the west and overlying the sand in the middle of the model are thought to be sediments richer in clay content. A thin low-velocity anomaly extending from the main sand body up towards the surface at the western end of the model is observed in both components, although it is weak in the P-wave velocity model. This may be a thin extension of the sand interbedded between clays. In general, velocity contours for both components dip to the east in the western part of the line and to the west in the eastern part of the line, which parallels the expected shape of the paleochannel. Unfortunately, it appears the model sensitivity is probably not sufficient at depth to see the interface itself, except possibly at the edges of the line.

Gao et al. (2006) applied waveform tomography to a combined VSP-surface data set that approximately coincided with the southern 21 m of the north-south line (Figures 3.5 and 7.1). Lithology logs at either end of the line and good seismic wave coverage provided by down-hole receivers enabled extensive lithologic interpretation in their work, much of which was correlated in a subsequent surface seismic study (Gao et al., 2007). Several of the features observed by Gao et al. (2006, 2007) are also seen in this work and
guide the following interpretations. Their northern lithology log is nearly coincident with
the north-south line at a position of roughly 21 m, and exhibits heterogeneous sand,
gravel, and clay in the upper 3 m of the subsurface, overlying more homogenous clay-
rich sediment from 3-12.5 m depth. Gao et al. (2006) interpreted a low-velocity anomaly
at 1-4 m depth extending from a position of about 10 m to 21 m as this sand and gravel
body. A complex low-velocity anomaly overlying a more homogenous region is
observed in both components in this study, and is interpreted in the same way. To the
south of 10 m, the observed low-velocity anomaly of Gao et al. (2006) dips sharply down
to lower depths of 4-6 m. This deeper part of the anomaly is not as well imaged in this
work, and in the P-component it appears to be cut off from the shallow part by a north-
dipping high-velocity anomaly. Gao et al. (2006) observed a low-velocity finger
sandwiched by higher velocities dipping down to the north at a position of roughly 15-19
m and depth of 6-9 m. This feature is also seen in the P-component of the north-south
line, albeit shifted and tilted slightly, which is probably due to different seismic coverage
in the two surveys. These observations suggest that coarse-grained, high-permeability
features in the aquifer, identified as low-velocity anomalies, may be isolated from one
another, with significant hydrogeologic implications for fluid transport continuity
throughout the aquifer. However, thin permeable stringers, observed in both lines, have
the potential to provide permeable pathways if they connect to other high-permeability
bodies.

We observe a region of high P-wave velocity and neutral to low S-wave velocity
in the Provo Formation at the southern end of the north-south line, where Gao et al.
(2006) observed high velocities that they associated with clay-rich sediment detected in
the southern lithology log. A similar feature is seen at the western edge of the east-west line below the estimated Alpine clay surface, and might be indicative of Alpine clay. These observations suggest that some fine-grained Provo and Alpine clays may retain significant water saturation as a capillary fringe above the average water table. This velocity signature may also have potential for future use as a lithology indicator.

Several observations are common to all four velocity models. Both lines exhibit thin high-velocity layers at the surface, particularly in the S-wave velocity models. This feature is interpreted as a highly cemented superficial caliche layer overlying the unconsolidated sediment of the Provo Formation, and is also observed in previous work (Gao et al., 2006, Fradelizio, 2007). In general, the upper 6-8 m of the velocity models are very complex and heterogeneous, whereas deeper regions are typically more homogenous. This is probably caused at least partially by decreased inversion sensitivity and resolution at depth; however, it is noted that lithology logs from the paleochannel further north exhibit a great deal of heterogeneity and high clay content in the upper 6 m of the Provo Formation, but relatively continuous sand and gravel in the lower part of the aquifer (Figure 3.4). The VSP-surface survey (Gao et al., 2006), which should have better sensitivity at depth than the current survey, also found much less velocity heterogeneity deeper in the model. Therefore, this aspect of the velocity models may accurately reflect geology characteristic of the Provo Formation, in which case the majority of intra-aquifer DNAPL traps might tend to be shallow and lie above the average water table, making them less of a regional contamination hazard.
CHAPTER 8
DISCUSSION OF WAVEFORM TOMOGRAPHY MODELS

The synthetic waveform tomography tests succeeded in imaging velocity features down to the base of the model with reasonable accuracy, albeit with somewhat reduced sensitivity. Unfortunately, the field data inversions do not appear to have similar sensitivity to the deeper parts of the model. The inversions performed in this study are intended primarily as a proof-of-concept for SH waveform tomography, and thus were done fairly simply, without making use of more elaborate waveform tomography techniques that may be able to extend model sensitivity to greater depth. Many of these techniques have been successfully applied to acoustic waveform tomography in the past, and may be readily extended to the SH-wave method, which would be necessary if the base of the aquifer were to be imaged by waveform tomography using the current data. One simple way to achieve better depth penetration is to follow each standard frequency group inversion with a second inversion for which the velocity model updates are boosted with depth (Brenders and Pratt, 2007). Another technique is to update the model using a more sophisticated Gauss-Newton method rather than the gradient method used in this study. This involves multiplying the gradient by some approximation to the inverse Hessian matrix rather than a simple scalar step length (Pratt et al., 1998), which preconditions the model updates to account for the variable illumination with depth that is inherent to surface seismic acquisition. This approach has been successfully applied with the acoustic approximation to improve characterization of deeper parts of the model (Ravaut et al., 2004; Operto et al., 2006).
Many applications of waveform tomography invert first arrivals only, however model sensitivity at depth can be improved by inverting later phases as well, leading to more elaborate inversion techniques. Examples include designing a multi-step inversion process to sequentially fit various phases in the data, spatially weighting the model updates in an appropriate manner at each step (Chironi et al., 2006), and combining inversions for a low-wavenumber background model with high-wavenumber inversions of reflected events (Hicks and Pratt, 2001). This type of approach must be done cautiously with single-component data, as the acoustic wave equation is unable to predict complicated phases that occur later in the record, such as mode-converted waves. On the other hand, SH-wave data lends itself to inversion of a longer coda, as the entire record is ideally free of contaminating phases.

Inversion of a longer SH-wave coda was attempted in this study, but the Love wave phase, although predictable with the SH wave equation, has a much larger amplitude than other events and tended to dominate the inversion. This resulted in even more bias of model updates to near-surface features. Muting of the Love wave phase and inversion of the later scattered wavefield was then attempted, but the inversion was plagued by cycle skipping in the scattered wavefield, leading to instability in deep regions of the models. This suggests that the initial velocity model provided by first arrival traveltime tomography was insufficiently constrained below the region sampled by first arrival rays. Studies that apply waveform tomography to longer coda tend to also use more elaborate traveltime inversion methods that consider several events rather than first arrivals alone. Such a method seems to be necessary in this case if waveform tomography is to be applied to a longer coda.
Another interesting focus of future research could be the incorporation of the separate acoustic and SH-wave methods into a single joint waveform tomography method. This approach could then attempt to find a single, elastic subsurface model by inverting both data components at once. It may also be possible to develop a fully elastic version of waveform tomography that could correctly model the P-SV system, and therefore use both vertical and horizontal radial data components in the inversion as well.

Aside from extending the inversion technique, modification of the survey acquisition design could also enable greater depth sensitivity in the inverted models. First and foremost, the use of longer source-receiver offsets would be valuable. For waveform tomography, long offsets are vital to constrain low-wavenumber velocity variation (Ravaut et al., 2004), and they also provide deeper sampling while still using first arrivals. However, the longer offsets in the current SH-wave data sets already struggled with excessive noise, so a survey with increased offset would probably also require higher signal-noise ratio, at least for the SH-wave components. The S-wave source could provide an improved signal-noise ratio simply by stacking more shots at each source position, or by upgrading to a more efficient, and expensive, vibratory-style source.

Despite limited inversion sensitivity at depth, acoustic and SH waveform tomography provided accurate, high-resolution models of subsurface P- and S-wave velocity, and enabled robust interpretation of lithology within the shallow part of the Provo aquifer. Limitations could be mitigated with further extension of more elaborate waveform tomography techniques to SH-waves, or modification of the survey design.
CHAPTER 9
SUMMARY AND CONCLUSIONS

This study explores the development of an SH-wave version of frequency-domain, full waveform tomography, an advanced seismic inversion technique previously applied only to single-component data under an acoustic approximation. The work is focused on the specific application of characterizing a shallow, contaminated, groundwater aquifer at Hill Air Force Base, Utah. This is a problem for which the intrinsic benefits of SH-waves, namely smaller wavelength and relative independence from pore fluid effects, are expected to be particularly beneficial.

Section 2 discussed the underlying theory of waveform tomography, and how the method can be extended to SH-wave data. Next, background of the field site puts the imaging objectives of this study in the broader framework of previous studies and relevant near-surface geologic characteristics. Section 4 dealt with the application of traveltime tomography to the field data, a vital first step before waveform tomography can be attempted. Next, the behavior of acoustic and SH waveform tomography was compared using synthetic tests characteristic of the field data. Section 6 covered application of waveform tomography to the OU-2 data, and discussed the quality of the results and trustworthiness of features in the resultant models. Finally, the waveform tomography velocity models were interpreted within the framework of previous OU-2 studies in section 7, and section 8 discussed shortcomings of the results and possible mitigating steps for the future.
Synthetic tests demonstrated the effect of scattering physics on acoustic and SH-wave imaging, and also illustrated, together with the field data, how smaller S-wave velocities can provide significantly improved resolution. Unfortunately, the depth sensitivity of the models was limited by the survey geometry and inversion approach used; however there are several steps that could be taken in the future to mitigate this issue.

The combination of P- and S-wave velocity information helped constrain interpretation of lithologic and water-saturation features at the field site, several of which have potentially significant hydrogeologic implications for the Provo aquifer. A relatively extensive clean sand body was identified in the eastern part of the site, but it exhibits a vertical offset that may inhibit continuity and fluid transport. The aquifer is thought to contain multiple high-permeability bodies that may or may not be in communication with one another. Aquifer heterogeneity appears to be concentrated in the upper 6 m of the subsurface, suggesting that intra-aquifer DNAPL traps may be more likely to occur in the shallower part of the aquifer, above the average water table. Therefore, they may not present as much of a regional contamination hazard.

In closing, while SH-wave surveys are often subject to increased technical difficulties compared to traditional single-component acquisition, SH waveform tomography can be a valuable imaging tool to improve resolution and provide additional subsurface information, particularly with extension of more elaborate waveform tomography techniques to the SH-wave method.
LIST OF REFERENCES


APPENDIX 1

FORWARD MODELING AND INVERSION EQUATIONS

In this appendix, explicit forms of the forward modeling and gradient calculations, equations 2 and 5, are derived for the acoustic and SH wave equations.

Equation A1 is a general frequency-domain wave equation that is applicable to both acoustic and SH-waves, obtained by taking the Fourier transform of the time-domain acoustic and SH wave equations, equations 1a and 1b, for a wavefield with time dependence as $e^{-i\omega t}$:

$$\omega^2 a u + \nabla \cdot (b \nabla u) = f(x, \omega), \quad (A1)$$

$$a = 1/m; \quad b = 1/\rho \quad \text{(acoustic)},$$

$$a = \rho; \quad b = m \quad \text{(SH)},$$

$$m = \rho c^2,$$

where the wavefield variable $u(x, \omega)$ is pressure and displacement in the acoustic and SH-wave cases respectively. The elastic parameters $a$ and $b$ have different definitions for the acoustic and SH-wave cases, and depend on density, $\rho$, and a generalized modulus $m$ that is calculated from the specified density and seismic velocity, $c$. In the acoustic and SH-wave cases $m$ corresponds to the Lame parameters $\lambda$ and $\mu$ respectively, or equivalently bulk and shear modulus. Taking a finite-difference approximation to equation A1 results in matrix equation 2. Entries in the impedance matrix $S$ are calculated using a 9-point finite-difference star (Jo et al., 1996; Stekl and Pratt, 1998), as shown in equation A2:
\[
f(iz,ix) = be \cdot u(iz,ix) + ad \cdot u(iz-1,ix-1) + aa \cdot u(iz,ix-1) + \ldots \text{etc},
\]
(A2a)

\[
be = C \omega^2 a(iz,ix) + \frac{A}{2d^2} [4b(iz,ix) + b(iz,ix-1) + b(iz,ix + 1) + b(iz - 1,ix) + b(iz + 1,ix)] \ldots
\]
\[
\ldots - \frac{B}{4d^2} [4b(iz,ix) + b(iz-1,ix-1) + b(iz + 1,ix - 1) + b(iz - 1,ix + 1) + b(iz + 1,ix + 1)],
\]

\[
aa = D \omega^2 a(iz,ix-1) + \frac{A}{2d^2} [b(iz,ix) + b(iz,ix-1)],
\]
\[
ad = E \omega^2 a(iz-1,ix-1) + \frac{B}{4d^2} [b(iz,ix) + b(iz-1,ix-1)],
\]

weighting constants: \(A = 0.5461\), \(B = 0.4539\), \((A + B = 1)\)
\(C = 0.6248\), \(D = 0.0938\), \(E = 0\), \((C + 4D + 4E = 1)\) (A2b)

where \(a\) and \(b\) are the elastic constants and \(d = dx = dz\) is the model grid spacing. The equations for the other side and corner entries are analogous to the equations for \(aa\) and \(ad\). Equation A2a implies that in the row of \(S\) corresponding to point \((iz,ix)\), entry \(be\) is placed in the column corresponding to \((iz,ix)\), \(ad\) is placed in column \((iz-1,ix-1)\), etc. Substituting the definition of elastic parameters \(a\) and \(b\) specific to the acoustic or SH-wave case gives the appropriate impedance matrix for that wave equation.

To obtain explicit equations for the objective function gradient (and thus the model update), it is necessary to differentiate the impedance matrix \(S\) with respect to the seismic velocity at an arbitrary node \((iz,ix)\), the result is referred to as the derivative matrix for the point \((iz,ix)\). Equation A3 gives the form of the velocity model update; it is similar to a combination of equations 4 and 5 for the model parameter update and
gradient calculation, but specific to a model parameterization consisting of seismic velocity at each subsurface node:

\[
c(iz,ix)^{(k+1)} = c(iz,ix)^{(k)} - \alpha^{(k)} \Re \left\{ u^t \left[ \frac{\partial S^t}{\partial c(iz,ix)} \right] b \right\},
\]

(A3)

where \( b \) is the back-propagated wavefield obtained by applying the inverse impedance matrix to the data residuals (see equation 5).

The entries in \( S \) are defined in terms of the elastic parameters \( a \) and \( b \), not velocity, so begin by expanding the derivative matrix according to the chain rule:

\[
\frac{\partial S^t}{\partial c(iz,ix)} = \frac{\partial S^t}{\partial a(iz,ix)} \frac{\partial a(iz,ix)}{\partial c} + \frac{\partial S^t}{\partial b(iz,ix)} \frac{\partial b(iz,ix)}{\partial c} = S_a(iz,ix) \frac{\partial a(iz,ix)}{\partial c} + S_b(iz,ix) \frac{\partial b(iz,ix)}{\partial c},
\]

(A4)

where \( S_a(iz,ix) \) and \( S_b(iz,ix) \) denote the derivatives of the transpose of the impedance matrix with respect to \( a(iz,ix) \) and \( b(iz,ix) \) respectively, and are specific to a particular node \((iz,ix)\). This is not to be confused with individual rows and columns in \( S \), \( S_a \), and \( S_b \), which each also correspond to a node in the subsurface. The partial derivatives of \( a \) and \( b \) with respect to velocity are calculated from the definitions in equation A1, setting density proportional to the fourth root of velocity (Gardner et al., 1974):

\[
\frac{\partial a}{\partial c} (iz,ix) = \frac{-2}{\rho(iz,ix)c^3(iz,ix)}, \quad \frac{\partial b}{\partial c} (iz,ix) = \frac{-1}{4\rho(iz,ix)c(iz,ix)} \quad \text{(acoustic),}
\]

\[
\frac{\partial a}{\partial c} (iz,ix) = \frac{\rho(iz,ix)}{4c(iz,ix)}, \quad \frac{\partial b}{\partial c} (iz,ix) = \frac{2\rho(iz,ix)c(iz,ix)}{4\rho(iz,ix)c(iz,ix)} \quad \text{(SH).}
\]

(A5)

The matrices \( S_a \) and \( S_b \) are calculated from the definition of the impedance matrix in equation A2, but to simplify the calculation a 5-point finite-difference star is assumed (i.e., set weighting constants \( A=C=1 \) and \( B=D=E=0 \)). While this slightly changes the value of the model update, it is a minor effect and has little impact on the final inversion.
result after multiple iterations. In the following, $S_a$ and $S_b$ are given for a specific node $(iz,ix)$, and rows and columns in matrices $S$, $S_a$, and $S_b$ are identified with the node that they correspond to, e.g., $(iz,ix)$, $(iz-1,ix)$, etc.

Referring to the forward modeling equation, equation A2, there is only one entry in $S$ that contains $a(iz,ix)$ for a specific point $(iz,ix)$, and that is the row and column both corresponding to that point. Therefore, $S_a$ has only one non-zero entry, and the entry in $S_a(iz,ix)$ at row $p$, column $q$, is given by:

$$[S_a(iz,ix)]_{p,q} = \begin{cases} \omega^2, & p = q = (iz,ix) \\ 0, & \text{otherwise.} \end{cases} \quad (A6)$$

Referring again to equation A2, the entries in $S$ that contain $b(iz,ix)$ for a specific point are identified and the derivatives calculated to give the nonzero entries in $S_b(iz,ix)$ shown in equation A7:

$$S_b(iz,ix) = \frac{1}{2d^2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \\ 1 & -4 & 1 & 1 \\ 1 & -1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \text{row } (iz,ix-1) \\ \text{row } (iz-1,ix) \\ \text{row } (iz,ix) \\ \text{row } (iz+1,ix) \\ \text{row } (iz,ix+1) \end{bmatrix} \quad (A7)$$

The negative entries on the diagonal come from the $b$ factors in the definition of $be$ (see equation A2), the positive entries in row and column $(iz,ix)$ arise from the first and second $b$ factor, respectively in the $aa$ definition (with similar terms from equations for $cc$, $dd$, and $ff$ as well).

Finally, define $ga(iz,ix)$ and $gb(iz,ix)$ as the scalar values that are obtained by multiplying the wavefield vectors $u$ and $b$ through the matrices $S_a(iz,ix)$ and $S_b(iz,ix)$ respectively (see equations A3 and A4). The model update for a specific iteration is then given by equation A8:
\[ \delta c(iz, ix) = -\alpha \text{Re} \left\{ ga(iz, ix) \frac{\partial a}{\partial c} (iz, ix) + gb(iz, ix) \frac{\partial b}{\partial c} (iz, ix) \right\}, \]  

where the derivatives of \( a \) and \( b \) with respect to velocity \( c \) are given in equation A5 for the acoustic and SH-wave cases, and is the only difference in the equation for the two methods. Constant density is a common assumption that allows one to neglect the density contribution to the overall velocity model update. This amounts to dropping the \( gb \) term in the acoustic case and the \( ga \) term in the SH-wave case.
APPENDIX 2
ACOUSTIC AND SH-WAVE SCATTERING

This appendix is an in-depth discussion of differences between acoustic and SH-wave scattering, including the effect of finite-size anomalies and the impact of anomaly depth on scattering angle coverage, and hence average observed scattered signal strength. It is based on 3D, fully elastic scattering equations derived in Wu and Aki (1985).

Acoustic scattering is considered by setting the shear modulus to zero in the P-P scattering equation (Wu and Aki, 1985). The 2D SH-wave scattering equation is obtained by restricting S-S scattering to the transverse (y) component of waves traveling in the incident (x-z) plane. The acoustic and SH-wave scattered displacement fields that result from a plane wave of angular frequency \( \omega \) and unit amplitude incident on an inclusion at the origin at time zero are given by equations A9:

\[
\begin{align}
 u_A(r, \theta, t) &= \frac{\omega^2 V}{4\pi \alpha_0^2} \left( \delta \rho \cos \theta - \delta \lambda \right) \frac{e^{-i\omega(t-r/\alpha_0)}}{r}, \\
 u_{sh}(r, \theta, t) &= \frac{\omega^2 V}{4\pi \beta_0^2} \left( \delta \rho - \delta \mu \cos \theta \right) \frac{e^{-i\omega(t-r/\beta_0)}}{r},
\end{align}
\]

where \( V \) is the volume of the inclusion described by average density and Lame parameter perturbations \( \delta \rho, \delta \lambda, \) and \( \delta \mu, \) which are assumed to be small relative to background values \( \rho_0, \lambda_0, \) and \( \mu_0. \) Acoustic and S-wave background velocities are specified by \( \alpha_0 \) and \( \beta_0, \) \( r \) is distance from the anomaly, and the scattering angle is \( \theta \) (defined so that direct forward transmission is \( \theta = 0^\circ \) and direct back scattering is \( \theta = 180^\circ \)). While the two equations are similar, in the acoustic case the modulus contribution is isotropic whereas in the SH-wave case the density contribution is the isotropic term. This study assumes a
Gardner's equation relationship between density and velocity (Gardner et al., 1974), in which density is proportional to the fourth root of velocity. This implies that the modulus term is significantly larger than the density term. Therefore, acoustic scattering is predominantly isotropic, but SH-wave scattering depends strongly on the cosine of the scattering angle, which results in small scattered wave magnitudes for oblique scattering at near right angles (Figure 5.3b).

The theoretical scattering patterns, equations A9, are predicated on two significant assumptions: near-field effects are negligible and the illuminating wavelength is sufficiently large to treat the inclusion as a point (i.e., ignore phase differences between waves scattered from different parts of the inclusion). Figure 5.5 suggests that, for the imaging environment under consideration in this work, the first assumption is generally valid while finite anomaly effects (i.e., Mie scattering) should be accounted for. The scattering equations, equations A9a and A9b, may be modified (Wu and Aki, 1985) for a spherical inclusion of non-negligible size by replacing the inclusion volume $V$ with the volume factor in equation A10, which takes the same form for both the acoustic and SH-wave cases:

$$\Theta(\theta) = \frac{4\pi a^3}{\left(\frac{\omega a}{c_0} \sin\frac{\theta}{2}\right)^2} \left[ \sin\left(2\frac{\omega a}{c_0} \sin\frac{\theta}{2}\right) - \cos\left(2\frac{\omega a}{c_0} \sin\frac{\theta}{2}\right) \right]. \quad (A10)$$

where $a$ is the radius of the inclusion and $c_0$ is the background velocity (either acoustic or S-wave). For an inclusion radius of 1 m (as in the synthetic waveform tomography tests) and typical frequencies under consideration in this study, the volume factor reaches a maximum of $V$ in the forward direction ($\theta = 0^\circ$) and has a frequency-dependent minimum in the back-scattered direction ($\theta = 180^\circ$). The observed scattered wave amplitudes in a
simple modeling test (Figure 5.5) can be fit to the scattering pattern equations A9 and A10 for a suitable choice of frequency. Using 57 Hz, close to the dominant frequency (roughly 55 Hz), gives a close fit between the calculated scattered wave amplitudes and the modeled data (Figure A.1). Based on the quality of this fit, it is reasonable to use theoretical acoustic and SH-wave scattering equations to explain observations from the synthetic waveform tomography tests.

Figure A.1:
Comparison of predicted (lines) and observed (circles) scattering patterns from modeling acoustic (a) and SH-wave (b) scattering from a +20% circular velocity anomaly of radius 1 m (see Figure 5.5). The amplitudes are normalized to a value of one for the direct forward scattered wave. A correction factor (Wu and Aki, 1985) for the inclusion’s finite size based on a frequency of 57 Hz was included in the predicted scattering patterns in order to fit the observed data.

To examine the impact of these scattering radiation patterns on the ability of waveform tomography to image various parts of the model, it is useful to consider how scattering angle coverage depends on anomaly depth. For the same parameters used in the realistic SH-wave and identical-parameter acoustic synthetic tests, the distribution of observed scattering angles for all source-receiver pairs is computed and plotted for an
anomaly at several depths in the middle of the seismic line (Figure A.2a). Increasing the anomaly depth shifts the scattering angle distribution from predominantly forward scattering to predominantly back scattering. As the fraction of traces that record oblique scattering increases, the average SH-wave response diminishes. To quantify this effect, the average scattered wave magnitude (including the Mie effect) recorded at all traces is computed for a series of scattering angle distributions at various anomaly depths (Figure A.2b). While both acoustic and SH-wave scattering strength decrease as anomaly depth increases due to the common Mie scattering effect (equation A10), the average SH-wave scattering strength decreases at a faster rate due to the additional effect of inherent angle-dependence in the ideal SH-wave scattering equation (equation A9b). Therefore, for the offset range and background velocity model in the current study, it is reasonable to infer that fundamental scattering physics will tend to bias waveform tomography imaging towards shallow features, and will affect SH-wave imaging to a greater degree than acoustic imaging.
Figure A.2:
Scattering angle coverage varies with anomaly depth. The anomaly is located in the middle of a seismic line with the same geometry as the synthetic SH waveform tomography test. Histograms (a) show the changes in scattering angle distribution with increasing anomaly depths of 2, 7, and 12 m. The histograms consider the scattering angle calculated for every useable trace in the data set. The acoustic and SH-wave average scattering strength is calculated for several such distributions and plotted versus anomaly depth (b). The scattering amplitude is normalized to the forward scattered amplitude as in Figures 5.3(b), 5.5, and A.1. The SH-wave scattering strength decreases at a faster rate than the acoustic scattering strength as anomaly depth increases.
APPENDIX 3
DATA PRE-PROCESSING FOR WAVEFORM TOMOGRAPHY

This appendix lists the steps performed and parameters used for pre-processing of the P- and SH-wave data sets prior to waveform tomography. Several of the processing steps are discussed in more detail in Fradelizio (2007), particularly the SH-wave predictive deconvolution. Justification for the overall pre-processing flow is discussed in Section 6.1.

P-wave data sets:

1. Vector rotation:
   Rotate the Gal'perin coordinate system used for acquisition (Fradelizio, 2007; Gal’perin, 1984) into vertical, radial, and transverse components, and extract the vertical component.

2. Load field site geometry to trace headers.

3. Restrict trace length:
   Trim the original 1000 ms record to 250 ms to be consistent with the chosen frequency spacing of 4 Hz for waveform tomography modeling and inversion. All important aspects of the data used in this study occur well within this window.

4. Band-pass filter:
   Apply a zero-phase Butterworth filter with 15-120 Hz pass-band. The filter has a 48 dB/octave slope at both ends of the pass-band.

5. Trace windowing:
Apply a surgical mute to extract the first arrival in the data; the window is roughly 30-40 ms long, with 5 ms tapers at both ends.

6. Band-pass filter:
Re-apply the filter from step 4 to smooth any windowing effects.

7. Trace killing:
Mute noisy and near-offset traces that do not have a sufficiently long first arrival waveform uncontaminated by Rayleigh waves (i.e., less than roughly 10 m offset).

8. Trace equalization:
Normalize each individual trace by its RMS amplitude.

9. Amplitude scaling:
Amplitudes are corrected with a square root of time factor to mimic 2D geometric spreading inherent to wavefield modeling.

**SH-wave data sets:**

1. Vector rotation:
Rotate the Gal'perin coordinate system used for acquisition (Fradelizio, 2007; Gal'perin, 1984) into vertical, radial, and transverse components, and extract the transverse component.

2. Stack opposing strikes:
Negatively stack strokes with opposing polarity to attenuate incidental P-waves generated by the S-wave source and enhance SH-wave components. Trace pairs that are misaligned by more than 5 ms (as determined from cross-correlation) are muted. Roughly 6% and 8% of the traces in the east-west and north-south lines respectively are muted, again
suggesting that the SH-wave component is slightly noisier for the north-south line than
the east-west line (see Sections 3.3, 4, and 6.2).

3. Load field site geometry to trace headers.

4. Restrict trace length:
Trim the original 1000 ms record to 250 ms to be consistent with the chosen frequency
spacing of 4 Hz for waveform tomography modeling and inversion. All important
aspects of the data used in this study occur well within this window.

5. Band-pass filter:
Apply a zero-phase Butterworth filter with 10-120 Hz pass-band. The filter has a 12
dB/octave slope at both ends of the pass-band.

6. Trace windowing:
Apply a surgical mute to extract the first arrival in the data; the window is roughly 30-40
ms long, with 5 ms tapers at both ends.

7. Band-pass filter:
Apply a zero-phase Butterworth filter with 15-100 Hz pass-band. The filter has a 36
dB/octave slope at both ends of the pass-band.

8. Predictive deconvolution:
Design and apply a predictive deconvolution to receiver gathers to remove receiver
consistent ringing from the data (Fradelizio, 2007). The deconvolution used an operator
length of 54 ms and prediction lag of 12 ms.

9. Band-pass filter:
Apply a zero-phase Butterworth filter with 10-100 Hz pass-band. The filter has a 48
dB/octave slope at both ends of the pass-band.
10. Trace windowing:
Re-apply window gates from step 5.

11. Band-pass filter:
Re-apply the filter from step 9 to smooth any windowing effects.

12. Trace killing:
Mute noisy and near-offset traces that do not have a sufficiently long first arrival waveform uncontaminated by Love waves (i.e., less than roughly 5-6 m offset).

13. Trace equalization:
Normalize each individual trace by its RMS amplitude.

14. Amplitude scaling:
Amplitudes are corrected with a square root of time factor to mimic 2D geometric spreading inherent to wavefield modeling.