SEISMIC MONITORING AND ELASTIC FULL WAVEFORM INVERSION INVESTIGATIONS APPLIED TO THE RADIOACTIVE WASTE DISPOSAL ISSUE.

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Dedicated to my beloved parents
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ZUSAMMENFASSUNG


Nichtlineare strahlenbasierte Laufzeittomographie erlaubte eine Charakterisierung der seismischen Grobstruktur des Wirtgesteins. Bedingt durch die Geometrie der Bohrlöcher und der inhärenten Limitierungen der Laufzeittomographie, konnte keine Information bezüglich des Mikrotunnels gewonnen werden. Im Gegensatz dazu lieferten die Geophone, die im Mikrotunnel installiert waren, eine detaillierte Charakterisierung des Sättigungsprozesses. Eine integrative Interpretation der Daten in Kombination mit ausgedehnten Modellierungen ergaben, dass kurz nach


Um die im Felslabor Mont Terri gesammelten seismischen Wellenformen zu invertieren, wird ein Inversionsalgorithmus benötigt, der die Anisotropie des Opalinustons berücksichtigt. In einem ersten Schritt habe ich einen 2D elastisch und isotropen Algorithmus entwickelt. Diesen habe ich benutzt, um den Informationsgehalt von elastischen seismischen Wellen zu untersuchen. Vollständige Datensätze (Multikomponenten Quellen und Empfänger sowie Quellen- und Empfängerpositionen rund um das Untersuchungsgebiet) erlauben alle elastischen Parameter zu bestimmen. Ähnlich gut Resultate können mit Bohrloch-zu-Bohrloch Geometrien erzielt werden, wie sie typischerweise in der Bohrlochtomographie eingesetzt werden. Selbst wenn nur Einzelkomponenten Quellen eingesetzt werden

ABSTRACT

Countries worldwide are seeking solutions for the permanent removal of high-level radioactive waste (HLW) and spent nuclear fuel (SF) from the environment. Surrounding the waste with multiple engineered barriers and emplacement in deep geological repositories is widely accepted as a safe means of isolating it from the biosphere for the necessary $10^4$–$10^6$ years. As a precautionary measure, society demands that repositories be monitored for 100–300 years after they are backfilled and sealed. Effective monitoring that does not compromise the engineered and natural barriers is challenging. Seismic full-waveform tomography is a possible option. To address this issue, we have conducted extensive seismic measurements at the Mont Terri Rock Laboratory, located within a clay formation that is a potential host rock in the Swiss HLW/SF program. A scaled-down HLW/SF repository has been simulated with a 13 m long microtunnel of 1 m diameter. Initially, it was empty and then sand-filled and dry. Subsequently, it was progressively water-saturated and slightly overpressured. The monitoring system consisted of a pressure source and a hydrophone streamer located in two boreholes drilled perpendicular to the microtunnel and eight geophones equally distributed around the periphery of the microtunnel.

A non-linear anisotropic inversion of crosshole traveltimes (ray tomography) allowed the gross velocity structure of the host rock to be delineated. Due to the experiment geometry, the distances of sources and receivers from the microtunnel and the inherent limitations of traveltime tomography, this was inadequate for monitoring changes within the repository. In contrast, analysis of the seismic traces acquired using the geophones installed around the periphery of the microtunnel enabled the saturation process to be characterized in detail. An integrated interpretation of the data in combination with extensive numerical modeling suggested that after injecting the water, the clay material within the microtunnel’s excavation damage/disturbed zone (EDZ) first spalled rapidly, then it began to swell and self-sealing of the EDZ started. It was possible to characterize this change in physical properties of the EDZ by using traveltimes of the geophone data. My numerical simulations, using full knowledge of
the host rock, the microtunnel and its EDZ properties, show that with sensors installed as close to the repository as regulations allow, should allow one to be able to observe even changes in traveltimes, and thus infer changes in the repository condition.

Higher resolution images could be obtained by inverting waveforms rather than only traveltimes. But full-waveform inversion will only be able to resolve the changes occurring in the repository if the changes in the recorded data due to changed physical properties (i.e., water saturation) are not overwhelmed by recording variations. I found that a P-wave sparker source is highly repeatable up to frequencies of 3–4 kHz for propagation distances up to tens of meters involved in repository-scale monitoring. Hydrophone repeatability is limited by variable hydrophone-borehole coupling conditions, but firmly grouted geophones within the tunnels yield consistent recordings. Three kinds of coherent noise contaminate the data: (1) mechanically induced electrical effects in the hydrophone chains; (2) high currents in the sparker cable, which cause it to oscillate radially as a line source; and (3) tube waves. My investigations outline a quantitative methodology to assess data-quality requirements for successful monitoring.

To invert the data collected at Mont Terri, one needs an elastic full-waveform inversion algorithm that takes into account the anisotropy of the Opalinus clay host rock. As a first step, I developed a 2D elastic isotropic inversion algorithm that I used in a synthetic study to explore the information content offered by elastic waveform data. Comprehensive data sets that include recordings based on multicomponent (directed) sources and multicomponent (vector) receivers that fully surround the area of interest allow all elastic parameters to be reliably recovered. Similarly good results can be achieved using the more commonly employed crosshole configurations. If only single source components (e.g., those oriented perpendicular to the borehole walls) are used, there is still no significant degradation of the quality of the tomographic images. Likewise, crosshole experiments that include pressure sources and multicomponent receivers still allow P- and S-wave velocities to be recovered, but such data sets contain virtually no information about the density. Finally, seismic data collected with omni-directional pressure sources and pressure receivers contain information about P- and S-wave velocities, but there are pronounced trade-offs between these parameters. This was demonstrated through formal model-resolution analyses. From my study, I conclude that seismic data recorded with pressure sources and two-component receivers offer the best compromise between acquisition efficiency and data-
information content. This finding was exploited in a model study, in which the feasibility of non-intrusive seismic monitoring of high-level radioactive waste repositories was tested. My results indicate that sources fired along boreholes on either side of the repository and receivers suitably placed around the repository would allow water saturation processes to be characterized reliably.

Following the successful implementation of elastic isotropic waveform inversion, I have extended the algorithm to the anisotropic case with a vertical symmetry axis. My initial calculations showed that inversion for anisotropic model parameters is more complicated. Even for the most favorable source - receiver types and coverage, I observed trade-offs between the different elastic parameters.
CHAPTER 1

INTRODUCTION

1.1 PREAMBLE

Geophysical survey techniques allow the non-invasive mapping and characterization of the subsurface. Such techniques have been applied to a wide variety of problems and on a wide variety of scales, from the near-surface to the Earth’s deep interior. For example, seismic waves from earthquakes and large explosions have been used to image the mantle and core of the earth (e.g., Kennett and Bunge, 2008) as well as to elucidate the fine structure of the crust and upper mantle (e.g., Shearer, 2009). Complementary information about crustal structure has been inferred from satellite magnetic observations (e.g., Stockmann et al., 2009) as well as from gravity, resistivity and magnetotelluric investigations. On a smaller scale, seismic and electrical/electromagnetic imaging techniques have been successfully applied to oil and gas exploration and reservoir characterization (e.g., Claerbout, 1985; Sheriff and Geldart, 1985), the search for metallic minerals (e.g., Eaton et al., 2003), aquifer delineation (e.g., Walbrecker et al., 2011), and investigations of archeological structures (e.g., Casas et al., 2010). At the finest scale, inverse scattering techniques are used in materials testing to provide useful information about material cracking and defects in bridge decks, buildings and other man-made structures (e.g., Rose 1999). Considering the successful application of geophysical techniques in various areas of earth and engineering science, it is worth investigating their potential uses and abilities in the solution of the radioactive waste disposal issue. Here, the main concern is with geological disposal in deep repositories and the need to remotely monitor the site, to check for any leakage or changes in repository conditions over time.

In recent years, there has been an upsurge in interest and capability to perform time-lapse geophysical monitoring experiments (primarily seismic), or so-called 4D seismics (e.g., Li, 2003). Most applications have been for oil and gas production, to
sense depletion of producing fields and to monitor secondary recovery operations. CO2 sequestration efforts and earthquake hazard assessment have also prompted interest in conducting repeat seismic surveys with the objective of delineating minor temporal changes in the target area. It is natural to explore whether such techniques could be useful for buried nuclear waste repository surveillance.

1.2 RADIOACTIVE WASTE: ITS ORIGIN AND CLASSIFICATION

It was World War II that accelerated research on nuclear physics and first demonstrated the power of nuclear energy. Since that time, humanity has been able to harness nuclear energy for peaceful purposes, with the first nuclear power plant built in 1954 at Obninsk in the Soviet Union. Despite the many advantages of nuclear energy for electricity generation, there are also some significant concerns. One of the most important drawbacks is the production of radioactive waste, which must be dealt with or disposed of in an appropriate fashion. The amount of waste comes not only from nuclear power stations but also from industrial, medical and mining activities, as well as military sources.

There are several ways to classify radioactive waste. In what follows, I will discuss the approach used by the International Atomic Energy Agency (IAEA 1994, 2009a). Their classification is mainly according to the long term safety of waste management. The six recognized categories are exempt waste (EW), very short lived waste (VSLW), very low level waste (VLLW), low level waste (LLW), intermediate level waste (ILW) and high level waste (HLW). Brief definitions follow:

- EW is the waste that meets clearance criteria and no regulatory control is needed for radiation protection purposes;
- VSLW contains primarily radionuclides with very short half-lives; it can be stored for up to a few years to allow sufficient time to decay, leading to a reclassification as EW, and thus be cleared from regulatory control;
- VLLW does not need high level isolation and containment and can be disposed of in near-surface landfill type sites;
- LLW has a limited amount of long lived radionuclides present and requires robust isolation and containment for up to a few hundred years; it can be disposed of in engineered near-surface sites;
ILW has more long lived radionuclides than LLW, hence it requires a greater degree of isolation and containment; near-surface facilities are not applicable for disposal of ILW - it needs to be disposed of at depths of tens of meters;

HLW has a high activity concentration which, by radioactive decay, produces a significant amount of heat; it also contains a large amount of long lived radionuclides; spent fuel (SF) is also considered as radioactive waste by some countries and in this case can be classified as HLW; burial at depths of several hundreds meters and greater in stable geological formations is required for HLW disposal.

The above classification is mainly according to the activities and the half-lives of the radionuclides, and there is not a clear-cut separation between the different classes. Moreover, due to the criteria used, waste classification is not fixed and depends on the condition of the waste, such that at different points in time different classifications could be assigned to the same waste package. This is simply due to the decrease of the waste-package radioactivity over time. The different waste classes, along with the proposed disposal options, are summarized in Table 1.1.

<table>
<thead>
<tr>
<th>Waste class</th>
<th>Containment/control period</th>
<th>Disposal option</th>
</tr>
</thead>
<tbody>
<tr>
<td>EW</td>
<td>Not required</td>
<td>Not required</td>
</tr>
<tr>
<td>VSLW</td>
<td>Up to few years containment</td>
<td>Temporary storage</td>
</tr>
<tr>
<td>VLLW</td>
<td>Sufficiently long institutional control</td>
<td>Near-surface landfill</td>
</tr>
<tr>
<td>LLW</td>
<td>Up to a few hundred years containment</td>
<td>0 – 30 m deep engineered near-surface disposal</td>
</tr>
<tr>
<td>ILW</td>
<td>Often expected repository evolution scenario is required</td>
<td>From few tens to few hundreds of meters underground disposal</td>
</tr>
<tr>
<td>HLW</td>
<td>$10^6$ years of isolation period; 50-100 year after closure monitoring</td>
<td>Several hundreds of meters underground disposal</td>
</tr>
</tbody>
</table>

Table 1.1: Different waste classes and options for their disposal

References used in Table 1.1. IAEA, 2006, 2008, 2009a, 2009b; OECD, 2008a, 2008b, 2008c; Kintisch, 2009; Chapman and McCombie, 2003; Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2001, 2006; Canvel, 2006; DEFRA, 2008; Appendix D.
1.3 RADIOACTIVE WASTE: SUITABLE GEOLOGICAL REPOSITORIES

Due to their dangerous character, it is very important that both ILW and HLW do not escape into the biosphere. Hence, candidate underground repositories for ILW and HLW must meet particularly strict criteria which take into account increased temperatures due to radioactive decay and include such aspects as (i) the hydraulic and transport properties of the host rock, (ii) the hydro-mechanical properties of the host rock and overlying sediments, and (iii) the long-term behavior of the waste canisters, engineered barriers and the host rock. Clearly, the choice of the host rock is very important. It will also have an influence on further repository planning, such as the design of the repository, the choice and the design of the engineered barriers, and the monitoring possibilities.

Subsurface geology is highly variable from region to region, and not every country has the same types of geological rock units present and/or in the most convenient localities. As a consequence, it is impossible to have a globally agreed repository model; each country should choose the type of geological formation and develop its own repository concept. Moreover, at this stage, it is also very important to take into consideration the concerns of local communities and the general public, and to have their support. Already, several countries have gone back to the drawing board in order to incorporate demands from the general public in the planning process (e.g., UK and Canada (Witherspoon and Bodvarsson, 2006; Canvel 2006; UK DBERR, 2008; OECD, 2008b, 2008c; DEFRA, 2008)).

The choice of the host rock is incomplete unless it can be shown that sufficient volumes of exploitable rock are available. The exploitability criteria depend on the specific repository design and include such factors as lithological heterogeneities, degree of fracturing, presence of fault zones, etc. Accordingly, regional scale geophysical surveys (and supporting geological information) are required to identify the regions where the rock is available and is in a suitable condition. These surveys include aeromagnetic, ground-based magnetic, gravity, magnetotelluric, seismic refraction and seismic reflection investigations. Seismic experiments are particularly useful. They can yield accurate information about the thickness of the geological zone of interest and the extent of existing fractures, joints and other rock defects (e.g., Green and Mair, 1983; Birkhäuser et al., 2001; Juhlin and Stephans, 2006). Deep boreholes can also be used to calibrate and further improve the models of underground structures.
Various rock types have been considered as the host rock for geological repositories. The most favored candidates include granite, different types of clay, salt and sedimentary rock. One of the proposed clay types in Europe is Opalinus clay, which is of Mesozoic Aalenian age (~170 ma), and occurs as a strongly anisotropic claystone formation. It has extremely low hydraulic conductivity and good self sealing and retention properties, which makes it a favorable host rock for SF, HLW and ILW repositories. In Germany, Switzerland, and France, layers of Opalinus clay can be found either outcropping or deeply buried. In Switzerland, 2D and 3D seismic surveys have shown that Opalinus clay can be found in certain localities at a suitable repository depth of 400-900 m below the surface, where it has a thickness of 100-120 m (Birkhäuser et al., 2001; Appendix D). Moreover, the seismic experiments suggest that this clay layer has been subject to only low levels of horizontal tectonic stress since its deposition, implying few faults and other defects.

Figure 1.1 shows a sketch of the Swiss concept for possible SF, HLW and ILW repositories that uses Opalinus clay as the host rock. The repository is a system of parallel tunnels lying in the horizontal plane. It is accessible through the main access
tunnel (decline) or from the vertical shaft. All waste types will have four layers of barrier. SF and HLW are first vitrified and then put into a metal container. These containers are placed in a 2.5 m diameter tunnel on top of bentonite bricks and the tunnel is backfilled with compacted bentonite granulate and then sealed. The final barrier is the Opalinus clay itself. The ILW is solidified in a matrix and enclosed in drums. Several drums are then placed in a concrete canister and filled with cement. Afterwards, several of these canisters are put together in a large cavern that is then backfilled with a special mortar. Similar to HLW/SF, Opalinus clay constitutes the final barrier for the waste.

1.4 THE MONT TERRI UNDERGROUND ROCK LABORATORY (FELSLABOR MONT TERRI, FMT)

Before any radioactive waste is deposited in the Opalinus clay host rock it is important to study the behavior of the rock under realistic conditions. Fortunately, Opalinus clay outcrops in the Swiss Jura Mountains where an underground rock laboratory FMT has been constructed. The geological cross-section of the region around the laboratory is shown in Figure 1.2. The test site comprises several tunnels excavated from the escape gallery of a motorway tunnel. It has been the focus of experiments by numerous radioactive waste agencies (Bossart and Thury, 2007). Nevertheless, FMT is only a laboratory and no radioactive waste will be actually deposited there. It is used in the present study for seismic monitoring experiments.

1.5 MONITORING POSSIBILITIES

After the waste is placed in the repository, it is very important to be able to monitor the state of the repository. This monitoring must be non-intrusive in order to prevent the creation of possible escape paths for the radioactive elements. There are numerous non-intrusive monitoring techniques available (a compilation is given in Appendix C). After the closure of the repository, one would expect none or only very minor changes in the far field of the repository (i.e. >20 m distance from the repository). Hence, possible far-field changes are an indicator of unexpected strong changes in the repository state (i.e., its physico-chemical condition). Changes in surface topography (e.g., anomalous uplift or subsidence) and surface/near-surface conditions can be monitored with repeat surface-, airborne- and satellite-based geodetic and interferometric/photogrammetric measurements. On the other hand,
changes in magnetic, electrical, radiometric and density properties can be monitored with repeat airborne- and satellite-based geophysical observations (e.g., magnetic, electromagnetic, radiometric, gravimetric). The changes can occur not only in the physical condition but also in the chemical properties of the subsurface. Variations in the groundwater-table level and in the groundwater and gas chemistry can be monitored by means of repeat sampling of borehole fluids.

But most changes likely to occur within the repository are expected to be quite subtle and restricted to its near field (i.e. the HLW/SF and tunnel/shaft excavation damaged/disturbed zones (EDZ)). One option to monitor changes in the near field is continuous passive surface and borehole seismic - acoustic recording. This will allow detection and localization of macro- and micro-seismicity from acoustic emissions, and can provide information about time-lapse changes in seismic, mechanical, hydraulic and stress/pressure properties. However, the emitted energy from the acoustic emissions is expected to be rather low with very rare higher energy events. Thus, this kind of passive monitoring would require that the sensors be placed within
close vicinity to the area of interest, and might not be allowed by regulations. An alternative is to perform repeat surface-to-hole, crosshole and/or tunnel-to-hole geophysical measurements (e.g., seismic, electrical, electromagnetic, radar). This would allow monitoring of time-lapse changes in the seismic and electrical properties. The resolution of DC geoelectric imaging is too low, whereas the high electrical conductivity of clay would pose a problem for effective use of ground-penetrating radar. Hence seismic monitoring is the most promising technique. Since our goal is to have a high resolution image of the repository, full-waveform inversion of seismic data is needed.

1.6 SEISMIC INVERSION

Seismic imaging can be broadly categorized into two classes: (i) reflector imaging using back-scattered (reflected) signals to map the geometry of the various geological discontinuities, and (ii) tomographic imaging using all transmitted, refracted and reflected signals to determine the distribution of elastic properties in the subsurface. Reflection imaging has been in existence for nearly 100 years and very sophisticated migration and other advanced data processing procedures have been developed by the oil industry for mapping structures (e.g., formation boundaries, anticlines, faults) as well as stratigraphy (e.g., lithology, pinchouts, reefs). Seismic tomography technology is comparatively more recent (last 30 years) and includes both traveltime inversion (kinematic imaging), which uses just first arrival times (or other picked seismic phases), and full-waveform inversion (dynamic imaging), which uses the entire seismograms. Tomographic techniques invert the equations of physics (elastodynamics in this case) to obtain subsurface properties directly from seismic observations. The key parameters are the wavespeeds ($V_p$ and $V_s$) and attenuation factors ($Q_p$ and $Q_s$) for the P- and S-waves, which relate not only to the rock type but also the rock condition (porosity, cementation, fracturing, texture, fluid content, etc.).

The seismic waves used in the reconstruction can be either generated by stress release (e.g., earthquakes, deep heat mining) or by controlled sources such as explosions, weight drops, mechanical impacts and electrical discharges. In the former case, we do not have information about the source location; hence one of the main inversion goals is to find the source location. In the latter case, the source position (and sometimes the waveform itself) is known and so the primary emphasis is on obtaining the velocity (and attenuation) structure of the region of interest.
The resolution of tomographic images depends on the geometry of the experiment and the amount of information used in the inversion. The early seismic inversion applications used only traveltimes of first arrivals (e.g., Peterson, 1985), as mentioned earlier. This allows one to reconstruct primarily just the P-wave velocity. However, traveltimes are less sensitive to low velocities (e.g., Wielandt, 1987). Moreover, the image resolution with traveltime inversion is rather low. Starting from the 1980s, substantial research was concentrated toward inversion of the full recorded waveforms (e.g., Tarantola, 1984; Pratt and Worthington 1990). Figure 1.3 compares the results of traveltime inversion and full-waveform inversion (FWI) for 2D acoustic wave propagation. As expected, there is a significant improvement in the reconstructed image quality using the entire waveform. However, this improvement comes at the cost of heavy computations and careful system calibration, as indicated earlier.

In real world problems, seismic waves propagate through 3D elastic media. In many geological situations there is also a clearly expressed seismic anisotropy (or directional dependence in the wavespeed), either of intrinsic form due to platy minerals and the rock fabric, or of a structural form (pseudo-anisotropy) due to the present of layering and fracturing. In yet other complex situations, the rock is viscoelastic and/or poroelastic and such behavior should ideally be taken into account. However, solution of even the perfectly elastic full 3D problem is computationally extremely expensive and not feasible with the currently available computer resources.
To overcome this difficulty, several approximations can be made. The early FWI applications commonly used the acoustic approximation, which treats the medium as a fluid (P-waves only, no S-waves) and furthermore restricted attention to solving just 2D problems (e.g., Pratt and Shipp, 1999; Hicks and Pratt, 2001; Gao et al., 2006; Operto et al., 2006; Hu et al., 2009, 2011).

Two-dimensional modeling (and inversion) is a good approximation in many cases where the geology is unchanging in one direction (the strike direction y) and the seismic line is oriented perpendicular to this direction. However, the point sources used in practice are replaced mathematically by line sources, which extend infinitely in the strike direction. This gives rise to waves that spread cylindrically rather than spherically, and so it is difficult to match the observations with the synthetically calculated data. To overcome the line source issue, one can perform 2.5D modeling. This uses a point (3D) source on a 2D model. The so-called 2.5D solution is obtained by performing a spatial Fourier transform of the 3D governing equation in the y direction of symmetry. This gives rise to essentially a 2D problem to be solved for each wavenumber. The final solution is obtained by inverse Fourier transforming (summing) the wavenumber spectra. Computationally, the solution of the 2.5D problem does not require significantly more memory than the 2D problem. However, it requires that the calculations be repeated 50-200 times (for the different wavenumbers), and the wavenumber sampling strategy is complicated by the presence of pole-like behavior (sudden disruptions in the spectra) when working in the frequency domain. Optimizing the choice of wavenumbers is a topic of ongoing research.

With steady progress in computational power over the last decade and a reduction in the price of CPUs and memory, 3D acoustic FWI became feasible in recent years (e.g., Ben-Hadj-Ali et al., 2008; Vigh and Starr, 2008; Abubakar et al., 2011). Although the acoustic approximation can provide reasonable images for some problems, especially marine surface reflection surveying involving a pressure source and pressure receivers, several researchers have shown that inversion under the acoustic approximation has only limited applicability (e.g., Barnes and Charara, 2008; Marelli et al., 2011). It is especially problematic when directed sources are used, which generate strong shear waves when mode conversion is prominent (at larger angles of incidence on boundaries), and when recording on directional sensors. Thus, many problems require that full elastic inversion be performed.
Although limited shot gather 2D elastic FWIs were carried out as early as 1987 (Mora, 1987), they were so computationally demanding for the then available computers that the technique was not pursued. In a similar fashion to 3D acoustic FWI, the computational boom of this century has made 2D elastic FWI not only feasible but popular. Unfortunately, 3D elastic FWI is still out of reach. In 2D elastic FWI, most of the research has been concentrated on oil and gas exploration, hence, surface-based or ocean-bottom experimental data have been used (Shipp and Singh, 2002; Choi et al., 2008a, 2008b; Sears et al., 2008, 2010; Brossier et al., 2009; Lee et al., 2010; Maeda et al., 2011). Nevertheless, crosshole elastic inversion results also have been reported (Barnes et al., 2008). Some of the above-mentioned elastic inversions also include anisotropy (Lee et al., 2010; Barnes et al., 2008) in their solutions. As for the acoustic problem, the elastic problem can also be cast as a 2.5D problem.

In performing full-waveform inversions, one must specify, in addition to the dimension (2D, 2.5D, 3D) and type of problem (e.g., acoustic vs. elastic, anisotropic, etc), whether the solution is to be performed in the time domain or in the frequency domain. There is also considerable choice as to the type of forward modeling algorithm and the type of inverse solution algorithm to use. In the geophysical literature, there are a wide variety of options and combinations.

Solutions in the time domain do not have very large computer memory requirements, and it is much easier to identify (and separate) the various seismic phases in this domain. However, to calculate seismograms for multiple sources in the time domain, one has to repeat the calculations as many times as there are number of sources. The alternative is to solve the problem in the frequency domain. In this case, the required memory can be very large. However, solution for any additional source positions comes at practically no cost once the system matrix has been determined and inverted, each new source just requires a matrix-vector multiplication.

The choice of computational domain finally defines the partial differential equations (PDE) that have to be solved. There are several numerical methods to solve PDEs. The most widely used methods are the finite-difference method (FDM) and the finite-element method (FEM). Others include the spectral-element and boundary-element methods. The FDM approximates the derivative terms in the governing PDE’s by finite-difference operators, whereas the FEM uses the weak form of solution of the governing equation (Variational principle or Galerkin method) and
approximates the solution by means of an integral approach. Both methods lead to a linear system of equations that must be solved for the unknown displacements (and/or stresses) in the medium. The choice of the method also depends on the problem at hand.

Finally, one has to choose the inversion algorithm. One option is to use the conjugate gradient (CG) method, which uses back-propagation to compute the gradient of the misfit function. Alternative approaches are Gauss-Newton (GN) or full Newton (FN) methods, where one has to explicitly calculate the Fréchet derivatives and invert for the approximate or full Hessian matrices, respectively. GN and FN are computationally more demanding than gradient-based methods, but they converge faster and are more flexible in terms of introducing constraints and regularization. The number of parameters that one can invert for is limited by the available memory and the nature of the experiment (e.g., the number and geometry of the source and receiver arrays).

1.7 THE ESDRED PROJECT

ESDRED (Engineering Studies and Demonstration of Repository Design) is an integrated technology project within the context of the 6th Framework of EURATOM (European Atomic Energy Community). The objective is to demonstrate the technical feasibility of a HLW/SF geological repository at an industrial scale. ESDRED is divided into several modules, each of which is dedicated to different aspects of the issue. A component of ESDRED Module 1 (Buffer Constructing Technology) aims to investigate and further develop the use of monitoring techniques under repository conditions. Since a key principle identified by the European Union Thematic Network Study (European Commission, 2004) on the role of monitoring states that “monitoring must be implemented in such a way as not to be detrimental to long term safety”, this monitoring should be non-intrusive. Although we have seen that the inversion of seismic data is capable of yielding high resolution images of the subsurface, the applicability of seismic inversion for realistic HLW/SF repository monitoring has yet to be demonstrated.
1.7.1 The HG-A experiment

It was decided that the most appropriate approach for applying and developing this non-intrusive seismic inversion technique would be to monitor the phases of NAGRA’s (the Swiss National Cooperative for the Disposal of Radioactive Waste) HG-A experiment at FMT. The monitoring experiments were conducted on a 40% downscaled version of an actual repository. This means that the region of interest is a 1 m diameter microtunnel and its associated EDZ (up to 1 m wide). In the HG-A experiment, to stimulate changes in the repository, the microtunnel was progressively sand filled, water-saturated, pressurized and even gas was injected. No radioactive material was used in the experiments. Throughout all phases, crosshole measurements were conducted using two deviating boreholes that enclose the microtunnel - one upward dipping and 25 m long, the other downward dipping and 29 m long. The borehole separation varies from 2 - 25 m (see Figure 1.4). Additionally, eight vertical-component geophones were attached around the inner periphery of the microtunnel when it was first excavated. Such geophone placement would not be permitted in real repositories, since it requires wires passing through the engineered barriers. The

Figure 1.4. Experimental setup at Mont Terri rock laboratory.
geophones were installed at FMT only to improve our understanding of the repository evolution through observing changes to the seismic wavefield in the immediate vicinity of the microtunnel. The original design of the experiments included a high frequency P-wave sparker pressure source to generate seismic signals within the lower borehole. These waves were recorded on a hydrophone streamer (pressure receivers) located in the upper borehole as well as by the geophones (particle velocity detectors) around the circumference of the microtunnel. To perform the experiments and to provide good coupling conditions with the host rock, it was necessary to have both source and receiver boreholes water-filled.

Since the expected changes in the repositories are subtle, FWI rather than simple traveltime inversion is required. On the other hand, when microcracking or water infiltration occurs or the temperature of the material increases, the compressional and shear wave velocities and the density are likely to change. Correspondingly, these three parameters are important monitoring parameters. They also fully describe elastic wave propagation in isotropic media and, hence, can be reconstructed with elastic seismic FWI.

1.8 OBJECTIVES AND OUTLINE OF THE THESIS

The original objectives, as stated in the ESDRED project documents, defined the goals of my PhD project as follows.

1. Development of a suitable data acquisition procedure.
2. Traveltime analysis of the first arriving wave trains.
3. Initial analyses of the effects on the seismic waveforms caused by changing experimental conditions.
4. Development of an anisotropic time-domain forward modeling algorithm suitable for simulating seismic waveforms.
5. Development of an anisotropic frequency-domain 2.5D modeling algorithm suitable for tomographic waveform inversions.
6. Development of a waveform inversion algorithm that simultaneously inverts for the elastic medium parameters, source signature and variable receiver coupling.
7. Inversion of the borehole hydrophone data for determining the Opalinus Clay properties.
8. Inversion of the tunnel geophone data for determining changes within the microtunnel.

Over the four years of my PhD work, significant progress has been achieved on most of these project objectives. The thesis comprises 6 chapters and 5 appendices. I now provide an outline of each component.

In Chapter 2, I describe the experiments conducted at the Mont Terri underground rock laboratory (FMT). The data acquisition system using a source in one borehole and a hydrophone streamer in the other borehole and geophones attached on the circumference of the microtunnel appeared to be effective and provided data with high signal-to-noise ratios. Next in Chapter 2, I highlight the easily visible changes in first arrival wave polarities and in the frequency content due to water saturation of the microtunnel. I used crosshole traveltimes to characterize the background media and borehole-to-microtunnel traveltimes to characterize changes occurring in the EDZ. At the end of Chapter 2, I propose an experimental setup that should provide useful information not only from the changes in the waveforms but also from diagnostic changes in the traveltimes related to repository condition variations. This work has been submitted for publication to *Journal of Geophysical Research*.

Chapter 3 is a collaborative effort with my PhD colleague, Stefano Marelli, in an investigation of two repository concepts, one in a granitic environment (Grimsel) and one in Opalinus clay (Mont Terri). Analyses and simulations for experiments conducted in the Grimsel rock laboratory were primarily performed by Stefano and the analyses and simulations for the experiments conducted in FMT (Opalinus clay environment) were mainly done by me. For Opalinus clay, I used the velocity structure obtained in Chapter 2 to synthetically analyze expected changes in the recorded wavefields. These changes are used to set a signal repeatability threshold for the real experiments. The experimental data were then used to analyze the degree of repeatability for our equipment and the source/receiver coupling variability. Furthermore, several repeatable coherent noise trains and their possible sources are identified. This research has now been published in the journal *Geophysics* (volume 75, no 5, Q21- Q34).

In Chapter 4, I use my newly developed 2D elastic isotropic FWI algorithm to analyze information contained in different data sets. The algorithm is first used to find source and receiver types that offer the best reconstruction capabilities. It reveals
possible trade-offs between different inversion parameters. Next, I used the experimental setup suggested in Chapter 2 to check the reconstruction capabilities of FWI for the specific radioactive waste repository problem using a realistic source and receiver combination. A paper on this work has been submitted to the journal *Geophysics*.

In Chapter 5, I extend the FEM frequency-domain forward solution algorithm used in Chapter 4 to 2.5D elastic wave propagation in transversely isotropic media with a vertical axis of symmetry. This is an important step forward towards monitoring in a host rock like the Opalinus clay, which is known to be anisotropic.

In Chapter 6, I summarize my main findings, give recommendations, and provide an outlook for further research necessary to finally invert the recorded data.

In Appendix A, I describe the modifications and extensions that I had to make to Thomas Bohlen’s finite-difference time-domain isotropic elastic wave propagation code to handle the anisotropic case (transversely isotropic with a vertical axis of symmetry).

The possibility of including variable hydrophone coupling in the FWI algorithm is analyzed in Appendix B. Although the analysis is for the 2D acoustic problem, the approach can be easily transformed to 2.5D and 3D, and also for the elastic, anisotropic and viscoelastic problems. A paper on this work has been submitted to the journal *Geophysics*.

The experimental and predicted data are viewed from a different perspective in Appendix C. It shows our ability to synthetically reproduce recorded data and predict changes in traveltimes for other receiver configurations. This work has been submitted for publication to the *International Journal of Rock Mechanics and Mining Science*.

In Appendix D, the concept of the Swiss radioactive waste repository program is introduced. Details on the completed and ongoing seismic experiments conducted in Switzerland toward the final disposal of the radioactive waste are presented. A paper on this work has been published *First Break*, 28, 39-50.

Appendix E has no immediate connection with the radioactive waste disposal issue. Rather, it is a paper about 2D ultrahigh-resolution seismic reflection imaging of the Alpine Fault in New Zealand, for which I was a co-author and contributor. This research has been published in the *Journal of Geophysical Research* 114, B11306).
CHAPTER 2

Monitoring of radioactive waste - potential changes of elastic properties within a repository during water saturation

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2.1 ABSTRACT

Safe isolation of high-level radioactive waste (HLW) and spent nuclear fuel (SF) from the biosphere is a key task. Many countries consider monitoring evolving conditions of HLW/SF repository over a long period non-invasively, in order to not compromise the sealing of the repository. Seismic tomography is a possible option. We have performed extensive seismic measurements at the Mont Terri Rock Laboratory, located within a clay formation, a potential host rock in the Swiss HLW/SF program. A scaled-down HLW/SF repository has been simulated with a 13 m long microtunnel of 1 m diameter. Initially, it was sand-filled and dry. Then, it was progressively water-saturated and slightly overpressured. The monitoring system consists of a pressure source and a hydrophone streamer located in two boreholes drilled perpendicular to the microtunnel and eight geophones equally distributed around the periphery of the microtunnel. A non-linear anisotropic tomography of crosshole travel times allowed the gross velocity structure of the host rock to be delineated, but due to the experiment geometry this was inadequate for monitoring changes within the repository. In contrast, analysis of the full seismic traces acquired using geophones enabled the saturation process to be characterized in detail. An integrated interpretation of the data in combination with extensive numerical modeling suggested that after injecting the water, the clay material within the microtunnel’s excavation damage/disturbed zone (EDZ) first spalled rapidly, then it began to swell and self-sealing of the EDZ started. On the basis of our investigations, we conclude that seismic monitoring, with sensors installed as close to the repository as regulations allow, is feasible.

2.2 INTRODUCTION

There is a general consensus that greenhouse gases must be markedly reduced to limit global warming (Gore, 2006; Meinshausen et al., 2009; Nature editorial, 2009; Schmidt and Archer, 2009). Furthermore, it is expected that the price for oil and gas will increase substantially over the coming years and decades. On the other hand, it is evident that the need for energy will continue to increase in the foreseeable future (OECD Nuclear Energy Agency, 2008a). A possible solution for addressing the global warming problem and gaining greater independence from fossil fuels, while increasing energy production, is expansion of nuclear power production. However, this imposes considerable pressure to resolve the HLW/SF disposal issue (e.g., OECD
Surrounding HLW/SF with multiple engineered barriers and emplacement in deep (300 - 100 m) geological repositories is currently the preferred means of safely isolating it from the biosphere for the necessary $10^5$–$10^6$ years.

Potential host rocks for HLW/SF repositories are granite, indurated clay and salt, all of which are distinguished by low hydraulic conductivities. Identifying and choosing a suitable repository site will require extensive investigations. Once a repository is built, any preferential paths for the flow of fluids will then need to be delineated. The EDZ will be of particular interest (Thury, 2002; Bossart et al., 2004; Barton, 2006; Bastiaens et al., 2007; Blümling et al., 2007); EDZs are created whenever a significant volume of material is removed from the underground, thus creating a high stress gradient between the lithostatic pressure in the rock and the atmospheric pressure in the excavated zone. The extent of an EDZ depends on the type of host rock, the geomechanical conditions and the excavation method (Barton, 2006). It may be as small as a few centimetres or as large as several shaft/tunnel radii, and its physical properties may vary over time. In clay-rich rocks, the hydraulic conductivities of EDZs may decrease by orders of magnitude during the first few years after excavation as a result of various self-healing and self-sealing processes (Bossart et al., 2004; Bastiaens et al., 2007; Blümling et al., 2007). Water saturation plays an important role in these processes.

Methods for characterising EDZs have included the recording and analysis of microseismic and acoustic emissions (Falls and Young, 1998; Young et al., 2000; Young and Collins, 2001; Pettitt et al., 2002) and various geoelectric (Kruschwitz and Yaramanci, 2004; Gibert et al., 2006) and controlled ultrasonic ($>>$ 10 KHz) and seismic techniques (Falls and Young, 1998; Young and Collins, 2001; Schuster et al., 2001; Pettitt et al., 2002; Bastiaens et al., 2007; Damaj et al., 2007; Nicollin et al., 2008; Balland et al., 2009).

After filling and closure, the HLW/SF repositories in many countries will need to be monitored for hundreds of years. Since a monitoring system should not compromise any sealing mechanisms, non-intrusive surveying techniques will have to be employed. Geophysical methods could be a suitable for this purpose (e.g., Witherspoon and Bodvarsson, 2001, 2006). Controlled seismic techniques originally
developed to characterise EDZs have already been used to monitor their short-term evolution based on data acquired using energy sources and sensors placed inside or within a few metres of the EDZs. Because cable connections to sensors within a repository are unlikely to be allowed (they may affect the integrity of the sealing mechanisms), the question remains as to whether controlled seismic techniques based on data acquired outside the shafts/tunnels of a repository are capable of monitoring changed conditions within it.

Understanding the physical processes within a repository during water saturation and exploring the possibilities for monitoring them in a non-invasive manner were the motivations for carrying out our controlled seismic experiments at the Mont Terri Rock Laboratory in the Swiss Jura Mountains (Figure 2.1). The focus of our experiments was a sand-filled microtunnel, within which conditions potentially comparable to an evolving HLW/SF repository were simulated. We employed energy sources evenly distributed along one borehole and sensors evenly distributed along a
second borehole and around the interior of the microtunnel. The results of the recording, processing and inversion of the seismic data were complemented by extensive computational modelling.

After briefly reviewing the geology and experimental set up at the test site, we describe the water-saturation and pressurisation procedures applied to the microtunnel. We then show how crosshole traveltime tomography provides the anisotropic seismic velocities of the host Opalinus Clay and discuss the results of seismically monitoring the water saturation and pressurisation of the microtunnel. On the basis of the experimental results and computational modelling, we draw conclusions on whether and how a HLW/SF repository could be monitored in a non-invasive manner.

2.3 MONT TERRI ROCK LABORATORY AND OPALINUS CLAY

The host rock of the Mont Terri Rock Laboratory is the Opalinus Clay, an extremely low hydraulic conductivity formation of Aalenian age (~170 ma). Opalinus Clay has been identified as a potential host rock for radioactive waste in Switzerland (NAGRA, 2002a, 2002b; Witherspoon and Bodvarsson, 2006). It is found at appropriate depths of 500 - 1000 m in the Alpine foreland (Birkhäuser et al., 2001) and outcrops in the region of the Mont Terri facility (Thury and Bossart, 1999). The Mont Terri Rock Laboratory, which comprises several tunnels excavated from the escape gallery of a motorway tunnel, has been the focus of experiments by numerous radioactive waste agencies (Bossart and Thury, 2007).

Besides its low hydraulic conductivity, Opalinus Clay has the advantageous property of being self-sealing (Thury, 2002; Bossart et al., 2004; Blümling et al., 2007). The physical and chemical properties of Opalinus Clay and other relevant clay-rich formations have been determined in a variety of experiments (e.g., Bastiaens et al., 2007). Another distinguishing feature of Opalinus Clay is its high degree of elastic anisotropy, with slow and fast P-wave velocities (e.g., 2300 - 2500 and 3100 - 3300 m/s within an EDZ at the Mont Terri site; Nicollin et al., 2008).
2.4 EXPERIMENTAL CONFIGURATION

The experimental setup at the Mont Terri Rock Laboratory is sketched in Figure 2.1. A 13-m-long microtunnel with a diameter of 1.0 m, mimicking a 25 - 40 % scaled-down version of a repository, was constructed within the Opalinus Clay. Initially, the microtunnel was empty. It was then filled with sand and sealed with a megapacker system. Subsequently, the microtunnel was progressively water-saturated and slightly overpressured.

All phases of the microtunnel development were accompanied by seismic measurements. For crosshole monitoring purposes, two moderately dipping boreholes (25 and 29 m long) were drilled perpendicular to the axis of the microtunnel. During the experiments, both boreholes were water filled. Seismic energy was released sequentially in the lower downward dipping borehole at 0.25 m intervals using a sparker source. A 24-channel hydrophone chain with sensors at 1 m spacing was initially deployed and then shifted three times in the upward dipping borehole to simulate a 96 element array at 0.25 m spacing. In addition to the hydrophones, eight 100-Hz vertical-component geophones were attached at roughly equal distances around the interior of the microtunnel in the plane spanned by the two boreholes (Figure 2.1). All seismic data were recorded with a 24-bit acquisition system at a sampling interval of 0.064 or 0.032 ms.

2.5 SEQUENCE OF SEISMIC EXPERIMENTS

After installation of the megapacker, an initial seismic experiment was carried out (dry sand, experiment A). A second experiment was performed when the microtunnel was about 50% saturated (experiment B) and a third was performed immediately after completion of expected saturation (experiment C'). Experiments A to C' were carried out within a 24 hour period. Shortly after completing the expected saturation, pore pressures measured in nearby boreholes started decreasing (Lanyon et al., 2009), indicating that the microtunnel and its EDZ were not yet fully water saturated. Therefore, additional water was injected more or less continuously. The next seismic measurement (experiment C) was performed 8 months after the initial water injection. At that stage, the microtunnel was assumed to be fully saturated. With further injections, the microtunnel was then slightly overpressured and a final seismic experiment was conducted 12 months after initial saturation (experiment D).
2.6 ANALYSIS OF THE HYDROPHONE DATA: HOST ROCK CHARACTERIZATION

Non-intrusive seismic monitoring of a HLW/SF repository requires prior detailed knowledge about the medium in which the waste will be embedded. This type of information may be obtained by tomographically inverting the first-arrival traveltimes recorded on the hydrophones. Crosshole seismic traveltime tomography has proven to be efficient and reliable in many applications (e.g., Lehmann, 2007 and references therein).

2.6.1 Observations

The hydrophone data recorded at the Mont Terri site have been described in detail by Marelli et al., (2010; Chapter 3). They demonstrate the excellent repeatability of the sparker source and the high signal-to-noise ratios of the initial P-waves, which allow the first-arrival traveltimes to be picked to within 1 - 2 data samples. It is notable that the first-arrival traveltimes for all wavepaths do not change as conditions within the microtunnel and EDZ are varied. In contrast, the later arriving waveforms are highly variable as a result of poor coupling between the hydrophones and borehole walls (Chapter 3).

2.6.2 Anisotropic tomographic inversion

The pronounced seismic anisotropy of the Opalinus Clay (Nicollin et al., 2008) complicates the tomographic inversion of the first-arrival traveltime data recorded at Mont Terri. To minimize these effects, the borehole layout was chosen such that the anisotropy symmetry axis (perpendicular to the bedding of the Opalinus Clay) lay within the tomographic plane, thus enabling a 2D inversion to be performed. We have employed a non-linear anisotropic inversion algorithm based on a tilted transverse anisotropy model (Zhou and Greenhalgh, 2008) to invert the traveltime data. Since the hydrophone data allowed only the first arrivals to be picked reliably, only the density-normalised elastic moduli tensor elements $a_{11}$, $a_{13}$, $a_{33}$ and $a_{44}$ and the inclination angle of the symmetry axis within each model cell could be determined. Determination of the remaining fifth independent elastic modulus $a_{66}$ would require SH-wave traveltime data (Zhou and Greenhalgh, 2008).
We inverted 8884 first-arrival traveltimes of experiment A using 2156 inversion cells of dimension 0.6 x 0.6 m$^2$. The inversion parameters $a_{11}$, $a_{13}$, $a_{33}$ and $a_{44}$ are converted to P-wave velocities parallel ($v_{p}$) and perpendicular ($v_{p\perp}$) to the symmetry axis using:

$$v_{p} = \sqrt{a_{33}},$$  \hspace{1cm} (2.1)

and

$$v_{p\perp} = \sqrt{a_{44}}.$$  \hspace{1cm} (2.2)

Furthermore, the shear wave velocity $v_{sv}$, for which values parallel ($v_{sv\parallel}$) and perpendicular ($v_{sv\perp}$) to the symmetry axis are identical (e.g., Musgrave, 1970; Helbig, 1994), is determined using:

$$v_{sv\parallel} = v_{sv\perp} = \sqrt{a_{44}}.$$  \hspace{1cm} (2.3)

Figure 2.2a to 2.2c shows the resulting tomograms. Relatively low seismic velocities ~2 m from the borehole collars, apparent in all tomograms, are probably caused by the EDZ around the main access tunnel (Figure 2.1). The velocities perpendicular to the symmetry axis (Figure 2.2a) exhibit pronounced layering, likely
representing the bedding of the Opalinus Clay. Velocities parallel to the symmetry axis (Figure 2.2b) are less well resolved, being more affected by the smoothness constraints imposed during the inversions. As a consequence, the layering is less obvious in Figure 2.2b, with the tomogram representing average velocities. Similar observations can be made for the $v_{sv}$ tomogram in Figure 2.2c. Here, we find a low velocity zone of about 600 - 900 m/s near the borehole collars (main tunnel EDZ), an intermediate zone of about 1000 m/s in the central part of the tomographic plane, and higher velocities towards the ends of the boreholes. The inverted inclination angles of the symmetry axis (Figure 2.2d) all lie within a narrow interval centred around 40°. This indicates that the bedding of the Opalinus Clay is quite uniform. Average velocities $v_p$, $v_p$ and $v_{sv}$ in the tomograms of Figure 2.2a – 2.2c are 3110, 2340 and 1145 m/s, respectively. The $v_p$ estimates indicate an anisotropy of up to 33%, similar to the value determined by Nicollin et al., (2008) for an EDZ in a nearby tunnel.

The tomograms shown in Figure 2.2 are capable of revealing the gross structures of the host rock, but the signature of the microtunnel itself is not visible. Crosshole traveltime tomography is unable to resolve such a small structure at this scale of (the target-to-sensor wavepaths are too long relative to the size of the microtunnel/EDZ). Because the first-arrival traveltimes do not change (within the picking accuracy) as the experimental conditions are varied, virtually the same tomograms would result from inversions of data sets A, B, C and D.

A possible strategy for monitoring the saturation experiment could include full-waveform inversions of all recorded data. Unfortunately, the Mont Terri hydrophone data suffer from severe coupling problems, which vary between experiments and obscure the true shapes of the seismic waveforms (Chapter 3). This precludes the use of standard waveform inversion algorithms. Instead, coupled full-waveform inversions for material properties, source functions and receiver coupling factors would have to be performed. First attempts at such inversions have been successful for acoustic data (Appendix B), but more research is required before the hydrophone data can be useful for monitoring the saturation and pressurisation of the simulated repository. Accordingly, our analysis of the changing conditions within the microtunnel/EDZ will be restricted to the geophone data.
2.7 ANALYSIS OF THE GEOPHONE DATA: MONITORING THE EFFECTS
OF WATER SATURATION AND PRESSURIZATION

2.7.1 Observations

2.7.1.1 Signal waveforms

Figure 2.3 shows receiver gathers for experiments A and D and geophones G3 and G7, which are located on the ceiling and floor of the microtunnel, respectively (Figure 2.1). Both pairs of receiver gathers exhibit significant changes between the two experiments. Traces for experiment A and geophone G3 (Figure 2.3a) contain strong secondary phases approximately parallel to the first arrivals. After saturation and pressurization, these phases are markedly decreased (Figure 2.3c). Furthermore, some of the first-arrival polarities have changed between experiments A and D. Similar observations can be made for geophone G7, but they are much less pronounced (Figure 2.3b and 2.3d). The secondary phases are less prominent in experiment D (Figure 2.3d) and no changes of the first-arrival polarities are observed.
2.7.1.2 First-arrival polarities

For a more detailed analysis of the first-arrival polarity changes, the displays of the record sections are modified such that (i) positive polarities (first motion up) are shown in blue and negative polarities (downwards first motions) are shown in red, (ii) the first arrivals are approximately aligned using a velocity reduction technique \( t_{\text{red}} = t_{\text{obs}} - \frac{\text{dist}}{v_{\text{red}}} \), where \( t_{\text{obs}} \) = original traveltime, \( \text{dist} \) = source-receiver distance, \( v_{\text{red}} \) = average velocity along each ray path), (iii) only every 2\(^{nd}\) trace is displayed and (iv) only the first 2 ms of the first arriving wavetrains are shown. The resulting sections for experiments A, B, C and D and geophones G1 to G4 (only these geophones show polarity changes) are presented in Figure 2.4. Additionally, polarity diagrams for the same experiments and geophones are displayed in Figure 2.5. Here, each source-receiver pair is represented by a straight ray and color coded according to the first-arrival polarity shown in Figure 2.4.
During the course of the experiments (i.e., along rows in Figures 2.4 and 2.5), certain geophones exhibit a clear trend, with some polarities changing from first motion down (red) to first motion up (blue). It appears that the corresponding seismic waves have initially travelled around (been diffracted by) the microtunnel and hit the geophones from the top, causing downward motions. Later, the first arriving waves went directly through the microtunnel and approached the geophones from the bottom, causing upward motions. The remaining geophones 5 to 8 exhibit first motion up polarities for all experiments (not shown).

2.7.1.3 First-arrival traveltimes

The manually picked first-arrival traveltimes of the geophones are indicated in Figure 2.4 by the solid black lines. During the saturation/pressurisation experiments, we observed distinct changes of these traveltimes. For a more detailed analysis, the first-arrival traveltime curves for experiments A, B, C and D and all geophones are superimposed in Figure 2.6. All geophones show similar patterns. Traveltime differences between experiments A and B are very small, except for geophone G4, for which quite large differences are observed. Likewise, traveltimes for experiments C
and D are very similar. By comparison, there are significant offsets between the traveltime curves for experiments A/B and experiments C/D. They are relatively large for geophones G1 to G5 (0.2 - 0.4 ms) and somewhat smaller for geophones G6 to G8 (0.05 - 0.15 ms).

2.7.1.4 Transient changes

Results from experiment C' have been excluded from the first-arrival polarity and traveltime analyses, because the waveform shapes were very different from the other experiments. In particular, the first arrivals were very emergent, which made it impossible to determine polarities and traveltimes reliably.

The four times repetition of sparker ignitions required to simulate the 0.25 m hydrophone intervals (see section 2.4 "Experimental configuration") provided four suites of geophone recordings for each experimental configuration. Consequently, the geophones in the microtunnel should have recorded four times virtually the same data. This was indeed the case for experiments A, B, C and D (see Chapter 3 for a more extensive discussion about the repeatability of the Mont Terri experiments). During
experiment C’, significant changes occurred between the suites of sparker ignitions (approximately 20 minutes were required for each suite of sparker ignitions along the source borehole). This is demonstrated in Figure 2.7. Again, aligned receiver gathers are shown for geophones G1 to G4, but record sections from the individual suites of sparker ignitions are displayed along the rows of this figure (i.e., the shifts). Comparison of the individual rows reveals two remarkable features:

1. Some of the geophones exhibit measurable changes between consecutive source suites. For example, the relative amplitudes of the first-motion-up phases (blue) for geophone G3 increase steadily, whereas the relative amplitudes of the first-motion-down phases (red) for geophone G1 decrease for source positions \( l_s > 10 \text{ m} \). There are also substantial changes of the first arriving wavetrain patterns for geophone G4.

2. Compared with the traces shown in Figure 2.4, the dominant frequencies in Figure 2.7 are much lower.

Figure 2.7: Receiver gathers for the four shifts during experiment C’ and geophones G1 to G4. The traveltime reductions are the same as described in the caption to Figure 2.4.
2.7.1.5 Frequency spectra

The conspicuous decrease of dominant frequencies for experiment C' (Figure 2.7) are highlighted in Figure 2.8, which shows average frequency spectra computed for the first 3 ms of all recorded traces for each geophone and each experiment. As for the first-arrival traveltime curves of Figure 2.6, the spectra for experiments A and B are similar and those for C and D are similar. In contrast, the spectra for experiment C'
are quite different. Spectra for A/B have peaks between 1 and 2 kHz and a rapid decay of amplitudes towards higher frequencies. Amplitudes of spectra for experiment C’ are generally lower, particularly at higher frequencies. Spectra for C/D are substantially enriched at high frequencies, even above the levels of A/B. It is noteworthy that these observations are most pronounced for geophones G1 to G5 and to a lesser extent for geophones G6 to G8.

2.7.2 Interpretation

2.7.2.1 Qualitative aspects

Significant variations of receiver gather waveforms (including their amplitudes), first-arrival polarities, first-arrival traveltimes and frequency spectra together with the transient changes (experiment C’) clearly demonstrate that water saturation and pressurisation of the microtunnel have very pronounced effects on the seismic data. By jointly analysing these seismic attributes, we make an attempt to characterize the temporal evolution of the microtunnel and its EDZ.

Initially (experiment A), the sand filling the microtunnel is dry, thus exhibiting very low seismic velocities. Zimmer et al., (2007) give $v_p$ and $v_s$ values for dry sand of about 500 and 240 m/s, respectively. Microfractures within the EDZ cause a velocity decrease, but the EDZ velocities are likely higher than those of dry sand. The first arriving seismic waves from many source positions (Figure 2.1) therefore travel around the microtunnel and its EDZ and hit some of the geophones from the top (Figures 2.4 and 2.5).

During the first phase of water injection (experiment B), the water partially fills the interstitial pores in the sand and partly infiltrates the EDZ. This causes the seismic velocities within the microtunnel and EDZ to increase. Consequently, the fastest wavepaths of some source-receiver configurations now pass directly through the microtunnel and EDZ, causing some of the first-arrival polarities to change from first motion down to first motion up (Figures 2.4 and 2.5) and the traveltimes to slightly decrease (Figure 2.6).

Once sufficient water has percolated through the fractured EDZ, the Opalinus Clay begins to swell (e.g., Thury, 2002). If there is no confining pressure, swelling clay may spall, a well-known phenomenon observed in laboratory experiments (e.g., Thury, 2002). It is expected that small voids exist near the contact between the EDZ
and the sand. As a consequence, the sand does not provide sufficient confining pressure at the beginning of the wetting process, such that spalling is very likely to occur. Such a disintegration process loosens the geophone mounts, resulting in very weak coupling of the sensors to the microtunnel wall. It is well established that poor geophone coupling causes the high frequency portions of a seismic signal to be attenuated (e.g., Lamer, 1970; Drijkoningen, 2000), which explains the peculiar results of experiment C’ (Figures 2.7 and 2.8). It is perhaps surprising that such processes occur so quickly (within hours after the commencement of water injection).

The ongoing water injection further stimulates the swelling process, and at some point all voids near the EDZ/sand contact are filled. This enables a build-up of confining pressure that promotes self-sealing within the EDZ (e.g., Bastiaens et al., 2007; Blümling et al., 2007). The combination of EDZ self-sealing and the presence of a confining pressure improves the coupling of the geophones to the tunnel wall, and it is expected that the frequency content of seismic data will increase, which is indeed the case (see spectra for experiments C/D in Figure 2.8). Furthermore, the full saturation of the sand and the self-sealing of the EDZ results in increased seismic wave velocities. This is manifested in the reduced traveltimes for experiments C/D relative to those for experiments A/B (Figure 2.6). Finally, the increased velocities within the sand and EDZ result in straight fastest wavepaths through the sand fill of the tunnel and associated first motions up (Figures 2.4 and 2.5).

2.7.2.2 EDZ velocity and width

So far, our analysis has focused primarily on geophones G1 to G4, which are located on the side walls or the ceiling of the microtunnel (Figure 2.1). At these locations, the waveforms (including their amplitudes), first-arrival polarities, first-arrival traveltimes and frequency spectra are governed by the properties of both the microtunnel infill and EDZ. In contrast, changes to the first-arrival polarities and first-arrival traveltimes of the “floor geophones” G7 and G8 can only be attributed to changes in the EDZ. Accordingly, we have attempted to extract information about this zone from the corresponding traveltimes data. Using a straight ray approximation, the travelt ime difference $\Delta t$ of first arrivals between experiments A and D can be written as:

$$\Delta t = s(r) \left(1 - 1 / \beta \right) / v_P,$$

(2.4)
where $v_P$ is the inclination angle-dependent velocity of Opalinus Clay in the EDZ under dry conditions, $\beta$ is the fractional increase of this velocity caused by the presence of water, $r$ is the width of the EDZ, and $s(r)$ is the length of ray that passes through the EDZ (Figure 2.9a). By varying $\beta$ and $r$ systematically, we attempted to find an optimal combination of the two parameters that explained all observed traveltime differences between experiments A and D. As shown in Figure 2.9b, there exists a clear trade-off between $\beta$ and $r$ in minimizing the misfit, such that à priori information on one of the two parameters is required for a unique solution.

2.7.3 Verification

2.7.3.1 First-arrival polarity and first-arrival traveltime changes

We have computed synthetic traces using Bohlen's (2002) elastic finite-difference code modified by us to include the effects of anisotropy (transverse isotropy). Simulations were carried out for experiments A and D. For the background model, we employed the velocities in the tomograms of Figure 2.2. Velocities for dry and water-saturated sand were taken from the literature (Zimmer et al., 2007); $v_p = 500$ and 1900 m/s respectively, and $v_S = 240$ m/s for both states), and a plausible 1 m width and fractional decrease of velocities within the EDZ for experiment A were taken from Figure 2.9 (white dot). For experiment D, we assumed that the EDZ was completely self-sealed. The resulting $v_p$ models for dry and water-saturated / pressurised conditions are presented in Figure 2.10.
Figure 2.10: Close-up images of $v_p^\perp$ models used in our simulations for (a) a dry and (b) a water-saturated sand-filled microtunnel.

Figure 2.11: Predicted receiver gathers based on the velocity models shown in Figure 2.10. Traces are displayed in the same style as in Figure 2.4.
Synthetic traces and corresponding ray diagrams for the models in Figure 2.10 are shown in Figures 2.11 and 2.12. They are displayed in the same styles as those of the observed data in Figures 2.4 and 2.5. The matches between the observed and synthetic waveforms and polarities are not perfect, but we judge the overall agreement to be good. One notable difference is the greater number of first-motion-down polarities at short $\ell_5$ distances for geophone G1 in the observed data (Figures 2.4 and 2.5) than for the simulated data (Figures 2.11 and 2.2).

Comparisons of the first-arrival traveltimes picked on the observed and synthetic traces are shown in Figure 2.13. Most traveltime differences between experiments A and D are very similar for the observed and synthetic traces, with generally shorter traveltimes for experiment D than experiment A. As for the waveforms and polarities, the quality of the fits between the observed and synthetic traveltimes is variable. For example, the first arrivals picked from the G2 synthetic traces coincide well with the...
observed data, whereas the G3 synthetic traces show only a good match for source positions at $l_x < 15$ m. Similar patterns are observed for geophones G4 and G5.

The relatively good correspondence of the first-arrival polarities in Figures 2.4 and 2.5 with those in Figures 2.11 and 2.12 indicates that the velocity models in Figure 2.10 are good first-order approximations, but the discrepancies in Figure 2.13 are a clear indication that the assumption of a cylindrical-shaped uniform EDZ is unrealistic. The consistent traveltime advances of the synthetic traces relative to the observed traces for geophones G3 to G5 suggest the existence of a low-velocity feature near these geophones that is not included in the model of Figure 2.10. Interestingly, the discrepancies are large for experiment A and quite small for experiment D, indicating that the low-velocity feature has nearly disappeared by the stage of experiment D.

Considering the trade-offs between EDZ width and velocity (Figure 2.9b), other EDZ models could be employed for the simulations. We have repeated the computations using velocity models with EDZ widths of 0.5 m and 2.0 m (white crosses in Figure 2.9b). First-arrival polarities of synthetic traces computed with the
0.5 m wide EDZ do not match the observed polarities as well as those computed for the 1.0 m wide EDZ, but the match of the traveltimes are comparable. Simulations with a 2 m wide EDZ yield very similar polarities and traveltimes as those computed with the 1 m wide EDZ. We conclude that our seismic data provide only a minimum EDZ width estimate.

2.7.3.2 Full-waveform modeling of entire receiver gathers

Finally, the synthetic receiver gathers of Figure 2.14 can be directly compared with those of Figure 2.3. Synthetic traces generated for experiment A and geophone G3 (Figure 2.14a) contain strong secondary phases that arrive approximately 2 ms after the first arrivals. Analyses of wavefield snapshots demonstrate that the first arriving energy diffracts around the microtunnel and that the secondary phases are waves that propagate directly through the microtunnel. Because of the substantial velocity increase within the microtunnel and EDZ for experiment D, there is practically no time gap between the diffracted and direct phases. Consequently, the strong secondary phases are absent from Figure 2.14c. At least qualitatively, similar features are seen in the observed receiver gathers of Figure 2.3a and 2.3c. Phases
beyond 8 ms are more difficult to interpret. They likely represent P-to-S conversions at the microtunnel wall.

For experiment D and geophone G7, we note the occurrence of a secondary phase approximately 1 ms after the first arrivals (Figure 2.14d). Snapshot analyses identify this phase to be a reflection within the microtunnel. For experiment A (Figure 2.14b), this reflection appears much later and is obscured by the presence of shear waves and converted phases.

Although the correspondences between first-arrival polarities, first-arrival traveltimes and some later arriving phases in the synthetic and observed gathers of Figures 2.14 and 2.3 are good, there are also significant differences that require further investigations. These differences are likely due to limitations of the background velocity model and unknown complexities in the shape and physical properties of the EDZ. The velocity model could be substantially improved by adopting a full-waveform approach (see section 2.8.2).

2.8 IS NON-INTRUSIVE SEISMIC MONITORING OF A HLW/SF REPOSITORY FEASIBLE?

2.8.1 Traveltime tomography

The experiments conducted at the Mont Terri Rock Laboratory yield critical insights concerning the feasibility of non-intrusive seismic monitoring a HLW/SF repository. Results from traveltime tomography based on the hydrophone recordings (Figure 2.2) demonstrate that the traveltimes of waves with long target-to-sensor wavepaths do not contain enough information about the relatively small microtunnel for delineating temporal changes within it. This is particularly evident when a source-receiver pair at \( l_s = 14.5 \) m and \( l_r = 14.5 \) m is considered (see Figure 2.1). For this configuration (sparker source and hydrophone sensor on opposite sides of the microtunnel/EDZ), the effect of changes within the targets are expected to be most pronounced. In the absence of a microtunnel/EDZ, a straight raypath of length 15.94 m would be expected. At the other extreme, when a ray would completely avoid an EDZ of about 1.5 m outer diameter, the resulting curved raypath length would be approximately 16.21 m. Considering an average \( v_p \) velocity of about 3000 m/s, this would produce a maximum traveltime difference of 0.09 ms, which is close to the picking accuracy of our data. Clearly, subtle changes within a low-velocity
microtunnel/EDZ would not be detected. Nevertheless, traveltime tomography based on long target-to-sensor wavepaths seems to be suitable for determining the gross velocity structure between the boreholes.

Analyses of the data from the geophones located within the microtunnel indicate that water saturation and EDZ self-sealing produce significant changes of several seismic attributes (e.g., waveforms (including their amplitudes), first-arrival polarities, first-arrival traveltimes and frequency spectra), but installing seismic sensors within a HLW/SF is likely to be incompatible with the requirement of non-intrusive monitoring. A possible option could be to install wireless sensors (e.g., Akyildiz and Stuntebeck, 2006), but there are several technical problems associated with data transmission through rock and with the uninterrupted power supply for sensors over sufficiently long periods (many tens to hundreds of years) that first need to be resolved.

As an alternative, one could install geophones near the microtunnel. Using the models of Figure 2.10, we have computed synthetic traces for geophones located 1.5 m and 3.0 m from the microtunnel walls (Figure 2.15). At these distances, first-motion-up polarities were observed for all traces of experiments A and D. In contrast, there were measurable traveltime changes at both distances for the two experimental conditions. This is illustrated in Figure 2.16, in which synthetic traveltime differences between experiments A and D are plotted for geophones 0.0, 1.5 m and 3.0 m from the microtunnel walls (the values for 0.0 m distance correspond to the differences between the red and blue solid lines in Figure 2.13). Although the differences at 1.5
and 3.0 m distance are much smaller than those measured within the microtunnel, most are easily discernible with currently available instruments. Furthermore, the diameter of the microtunnel is only 25 - 40 % that of a functional HLW/SF repository tunnel. Simulations based on upscaled versions of our models suggest that first-arrival travelt ime differences up to a sizeable 0.3 ms would be generated 7.5 m from the edge of a 2.5 m diameter repository. These simulations are particularly relevant for the
Swiss HLW/SF programme, in which the long-term monitoring of a pilot repository of this diameter could involve placing sensors in boreholes approximately 7.5 m away (Bossart and Thury, 2007).
2.8.2 Full-waveform tomography

Assuming that the receiver coupling problem can be solved satisfactorily (Appendix B), full-waveform inversion of crosshole data could be a possible addition for monitoring a HLW/SF repository. Certain aspects of this concept were explored by Marelli et al., (2010; Chapter 3). Figure 2.17 shows one of their simulations for the Mont Terri site. Wavefield snapshots for simulations of a source at $l_s = 13$ m and velocity models relevant to experiments A (Figure 2.10a) and D (Figure 2.10c) are presented in Figure 2.17a and 2.17c, and differences between these snapshots amplified by a factor of two are displayed in Figure 2.17e. Changes within the repository and its EDZ produce significant differences of the wavefields, which can be captured with appropriate sensors in the receiver borehole. This is shown in the synthetic source gathers of Figure 2.17b and 2.17d and the difference source gather of Figure 2.17f.

Although changes of seismic waveforms recorded in distant boreholes appear to be measurable, they will inevitably be small. In contrast, differences between predicted and observed waveforms from the geophones in the microtunnel are substantial (Figures 2.3 and 2.14). With regard to waveform inversions, it is interesting to determine if similarly large differences to those observed in Figures 2.3 and 2.14 would also be observed using geophones 1.5 and 3.0 m from the EDZ. The predicted traces for the more distant versions of geophone G3 at 1.5 and 3.0 m are displayed for experiments A and D in Figure 2.18; evidently, substantial waveform differences would be observed at both distances.

2.8.3 Proposed monitoring strategy

Considering all the observations and simulations of this study, we propose the following monitoring strategy:

2.8.3.1 Experimental setup

An effective monitoring system might include a number of seismic source boreholes 10s of metres from a HLW/SF repository and observation boreholes at distances ranging from 10s of metres to as close to the repository as regulations would allow. Depending on the geometry of the repository, the boreholes could be either vertical, horizontal or inclined and either straight, curved or irregular. However, their
locations and geometries would have to be accurately determined. The observation boreholes would be backfilled and sealed with low permeability bentonite-sand mixtures. Backfilling would ensure good coupling of the sensors to the host rock. When the observation equipment needs to be replaced, the boreholes could be reamed out, new sensors emplaced and the boreholes refilled and resealed. The initial installation and replacement procedures would have a negligible impact on long-term repository safety.

2.8.3.2 Host rock characterization

Seismic crosshole measurements would be carried out before and after construction of the repository. An initial host rock velocity model based on first-arrival traveltime data would be refined via a coupled 3D full-waveform inversion for medium properties, source functions, receiver coupling factors and perhaps spatially varying attenuation (Appendix B).
2.8.3.3 Monitoring

Periodic monitoring would be initially based on first-arrival traveltime differences, with emphasis on recordings made near to the repository, because they are expected to exhibit the most pronounced changes. Once first-arrival traveltime changes are detected, 3D full-waveform difference inversion should be able to identify the locations of any developing problems in a non-intrusive manner.

2.9 CONCLUSIONS

By means of extensive experiments at the Mont Terri Rock Laboratory, we have explored the feasibility of monitoring a HLW/SF repository using seismic methods. A critical requirement of such investigations is that the sealing of the repository must not be compromised by the monitoring system.

Detailed knowledge of the rock hosting the HLW/SF repository would be required. We have established that crosshole traveltime tomography is capable of resolving the gross velocity structures, even in the presence of pronounced anisotropy. More refined velocity models may be obtained from crosshole full-waveform inversions, but this requires further algorithmic developments that account for variable coupling conditions within the source and receiver boreholes.

A controlled saturation experiment was monitored using geophones installed within the simulated HLW/SF repository. The results indicate that water saturation, pressurisation and associated EDZ self-sealing significantly affect several seismic data attributes (i.e., waveforms (including their amplitudes), first-arrival polarities, first-arrival traveltimes and frequency spectra). In turn, these attributes can be employed as diagnostics for characterizing the actual state within a repository and EDZ. Some of the results were verified by means of numerical modeling.

Numerical modeling was also employed to check if truly non-intrusive monitoring of the saturation and pressurization processes and EDZ self-sealing would be feasible. The results indicate that a measurable signature of these processes is expected to appear in the waveforms of crosshole data, and that substantial changes would be observed on seismic sensors placed near the HLW/SF repository.

On the basis of these findings we conclude that (i) non-intrusive seismic measurements are a feasible option for monitoring HLW/SF repositories and that (ii) such an endeavor would first require determining the seismic velocity structure of the
host rock by a combination of traveltime and full-waveform tomography, followed by a monitoring phase using seismic sensors installed near the repository.

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CHAPTER 3

Appraisal of waveform repeatability for crosshole and hole-to-tunnel seismic monitoring of radioactive waste repositories

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3.1 ABSTRACT

Countries worldwide are seeking solutions for the permanent removal of high-level radioactive waste from the environment. Surrounding the waste by multiple engineered barriers and emplacement in deep geological repositories is widely accepted as a safe means of isolating it from the biosphere for the necessary $10^5$ - $10^6$ years. As a precautionary measure, society demands that repositories be monitored for 100 - 300 years after they are backfilled and sealed. Effective monitoring that does not compromise the engineered and natural barriers is challenging. To address this issue, we investigate the viability of crosshole and hole-to-tunnel seismic methods for remotely monitoring high level radioactive waste repositories. Measurements are made at two underground rock laboratories in Switzerland, one within granitic rock and one within clay-rich sediments. Numerical simulations demonstrate that temporal changes of the monitored features (i.e., bentonite plug, excavation damage zone, sand-filled microtunnel) should produce significant changes in the seismic waveforms. Nevertheless, inversion for medium-property changes requires that true seismic waveform changes are not overwhelmed by recording variations. We find that a P-wave sparker source is highly repeatable up to frequencies of 3 - 4 kHz for propagation distances out to 10's of meters involved in repository-scale monitoring. Hydrophone repeatability is limited by incoherent high frequency noise and variable hydrophone - borehole coupling conditions, but firmly grouted geophones within the tunnels yield consistent recordings. Three kinds of coherent noise contaminate the data: (1) mechanically-induced electrical effects in the hydrophone chains, (2) high currents in the sparker cable cause it to oscillate radially as a line source, and (3) tube waves. Our investigations outline a quantitative methodology to assess data-quality requirements for successful monitoring. We suggest that full waveform seismic tomography can be used to monitor radioactive waste emplacement tunnels, provided that careful attention is paid to instrument fidelity and noise suppression.

3.2 INTRODUCTION

Geophysical investigations are primarily aimed at obtaining instantaneous subsurface images, but there is increasing interest in monitoring temporal changes by means of repeat (time-lapse) measurements. Examples include the surveillance of volcanoes (Chouet, 2003; Auger et al., 2006; Luckett et al., 2007), oil and gas fields (Bachrach et al., 2008), thawing permafrost (Hauck, 2002), hydrological sites (Binley
et al., 2002), landfills (Knödel et al., 2008), dams (Sjödahl et al., 2008), and CO$_2$ storage sites (Arts et al., 2004). Although the objectives and methodologies of these investigations are diverse, there is a common element that requires special attention: the geophysical data must be collected in a consistent fashion, such that any differences in the measurements reflect genuine subsurface medium-property changes and not varying data-acquisition conditions.

A particularly important task of high societal relevance is the monitoring of high-level radioactive waste (HLRW) repositories. Responsible disposal of HLRW is one of the most pressing environmental issues of modern times (OECD Nuclear Energy Agency, 1995, 2008a, 2008b; Witherspoon and Bodvarsson, 2001, 2006; Chapman and McCombie, 2003; Stone, 2004; Alexander and McKinley, 2007). Proposals for the long-term isolation of HLRW usually involve a combination of multiple engineered barriers and emplacement in deep geological repositories. Due to the hazards associated with HLRW, candidate repositories must meet strict criteria in relation to (i) the hydrological containment properties of the host material, (ii) any interactions between the radioactive waste canisters, engineered barriers, and host rock, (iii) the availability of “prior knowledge” about the host rock properties (e.g., lithological heterogeneities, fractures, faults), and (iv) risks associated with natural and anthropogenic hazards.

A number of research projects worldwide are directed at testing different repository concepts (Witherspoon and Bodvarsson, 2001, 2006; Chapman and McCombie, 2003; Alexander and McKinley, 2007). Many projects involve one of two types of underground facility: repository candidates like the Olkiluoto site in Finland (Vira, 2006) and the Forsmark site in Sweden (Nature News, 2009), and experimental underground laboratories like the Underground Research Laboratory in Canada (Brown et al., 1989), the HADES site in Belgium (Neerdael and Volckaert, 2001), the Meuse/Haute-Marne site in France (Delay et al., 2007), and the Grimsel and Mont Terri Rock Laboratory in Switzerland (Lieb, 1989; Thury and Bossart 1999).

Diverse seismic methods have proven to be suitable for exploring the structure and physical properties of potential host-rocks. These include 2D and 3D surface-reflection seismic imaging (Mair and Green 1981; Birkhäuser et al., 2001; Schmelzbach et al., 2007, Juhlin and Stephens, 2006), multi-azimuth and multi-offset VSP surveying (Enescu et al., 2004), crosshole seismic investigations (Vasco, 1991;
Once the relevant host rock is characterized and judged to be suitable, effective monitoring strategies need to be devised for the various stages of a repository's lifetime (i.e., pre-excavation, excavation, HLRW emplacement, backfilling and sealing, and 100 - 300 hundred years of post-closure). While there is access to the repository, there is a wide range of suitable geophysical methods for monitoring the host rock. Surveillance of the excavation damage/disturbance zone (EDZ) around a repository's shafts and tunnels is particularly important (Thury, 2002; Bossart et al., 2004; Barton, 2006; Blümling et al., 2007). The EDZ is created whenever a significant volume of material is removed from the underground, thus creating a high stress gradient between the lithostatic pressure in the rock and the atmospheric pressure in the tunnel. The extent of a damage zone depends on the type of host rock, the geomechanical conditions, and the excavation method (Barton, 2006). It may be as small as a few centimeters to as large as several shaft/tunnel radii, and its physical properties may vary over time; in argillaceous rocks, the hydraulic conductivities may decrease by orders of magnitude during the first few years after excavation as a result of various self-healing processes (Bossart et al., 2004; Blümling et al., 2007).

In addition to recording microseismic and acoustic emissions (Falls and Young, 1998; Young et al., 2000; Young and Collins, 2001; Pettitt et al., 2002), various geoelectric (Kruschwitz and Yaramanci, 2004; Gibert et al., 2006) and active ultrasonic (>> 10 KHz) seismic methods (Falls and Young, 1998; Young and Collins, 2001; Schuster et al., 2001; Pettitt et al., 2002; Bastiaens et al., 2007; Damaj et al., 2007; Nicollin et al., 2007; Balland et al., 2009) have been used to monitor the evolution of EDZs based on data acquired within shafts/tunnels or within boreholes drilled from shafts/tunnels.

In contrast to pre-closure surveillance of a high level radioactive waste repository, the opportunities for post-closure monitoring are severely limited (IAEA, 2001; Thompson and Simmons, 2003; EU, 2004; White et al., 2004; Nirex, 2005); it will not be accessible once it is backfilled and sealed and there should be no physical connections to the outside that could jeopardize the isolation capabilities of the engineered and natural barriers. As a consequence, microseismicity and active seismic methods provide unique possibilities for remotely monitoring a repository in a largely non-intrusive manner. The principal differences between these methods and those
employed from within a repository (Falls and Young, 1998; Young and Collins, 2001; Schuster et al., 2001; Pettitt et al., 2002; Bastiaens et al., 2007; Damaj et al., 2007; Nicollin et al., 2007; Balland et al., 2009) are the need to record seismic waves that have travelled over longer distances and the associated requirements to employ lower frequency sensors and (for the active methods) lower frequency more powerful energy sources.

In this contribution, we investigate active crosshole and hole-to-tunnel seismic methods as means to monitor induced changes to specially constructed features within two underground test facilities. One option for active seismic monitoring is crosshole traveltime tomography (e.g., Lehmann, 2007 and references therein). Unfortunately, traveltime-based methods will only be of limited value for monitoring a radioactive waste repository, which will have dimensions of only a few meters. Such target size is very small compared to the expected source-receiver distances which are involved (up to ten times larger) and therefore the effect of even modest changes in target velocity on simple travel times is likely to be very small. Regardless of the design of the site, it is very likely that the seismic velocities within the repository will be substantially lower than in the surrounding host rock. Therefore the first-arriving wave trains will predominantly “avoid” the repository and provide no direct or only very limited indirect information about changes associated with the state of the repository.

Although first-break arrival times may be little affected by changes within a repository, later parts of the seismic traces may provide useful information, which could be extracted using full-waveform inversion techniques. These techniques, originally proposed in the early 1980’s (Tarantola, 1984; Mora, 1987), are currently a hot research topic (Geophysical Prospecting, 2008).

A number of synthetic studies have established the utility of full-waveform inversion techniques, but the literature on their applications to real data is relatively sparse. A key limitation is the availability of high quality seismic data. Moreover, application of waveform inversion to monitoring problems, where subtle differential changes in the medium may result in very small changes in the seismic traces, requires particularly high fidelity data. Therefore, monitoring applications require high-quality and well-calibrated data acquisition systems and rigorous experimental repeatability. In particular, the source and receiver characteristics and their coupling to the host rock, as well as the recording instrumentation, should not change between repeat measurements. If unavoidable changes do occur, they must be known and properly
accounted for by applying appropriate correction/compensation procedures during the data analysis and/or inversion.

We describe a systematic investigation of seismic waveform repeatability for the purpose of monitoring potential radioactive waste repositories. Our computational code is a modified version of a readily available program (Bohlen, 2002) and our acquisition system is an assembly of commercial components. We compare results from two test sites located in different host-rock environments (i.e., granitic rock and a clay-rich formation).

After describing the experimental setup at the two locations, we present the results of numerical simulations that mimic changes within the areas of interest. These computations provide estimates of the changes in the seismic traces that can be realistically expected. We then examine the repeatability of our seismic source (sparker) and determine the frequency band over which our sensors (hydrophones in shallow-dipping water-filled boreholes and vertical-component geophones anchored within the tunnels) provide reliable responses. As a next step, we check the influence of the coupling conditions on the repeatability of the hydrophone recordings. Some findings are verified by repeating experiments with two other types of hydrophone arrays. For comparison purposes, we also perform repeat experiments using hydrophones in vertical boreholes at a third location. Finally, we discuss the influence of systematic noise (e.g., electrical effects in the hydrophone chain and sparker coaxial cable, and tube waves) that may limit the usable time windows of the seismic sections. On the basis of these investigations, we comment on the relative merits of the different types of receiver, how to combat coupling differences, and the influence of the host-rock medium on the overall seismic responses. Our main contribution is to outline a methodology for a quantitative assessment of data quality requirements for the effective monitoring of a HLRW repository using seismic measurements at repository scales, in particular for post-closure applications.

3.3 TEST SITES AND EXPERIMENTAL CONFIGURATIONS

3.3.1 Grimsel Test Site (GTS)

The Grimsel Test Site (GTS) in the central Swiss Alps (Figure 3.1) is dedicated to diverse studies associated with the storage of radioactive waste (GTS will not be used for waste disposal). Since the official opening of GTS in 1984, a wide variety of geophysical, geological, hydrogeological and rock mechanical experiments has been
conducted in the laboratory's tunnels and numerous boreholes (Lieb, 1989; Kickmaier and Thury, 2002). In addition to determining the physical properties of the crystalline rocks surrounding the underground laboratory, these investigations have provided key information on the resolving power of the various methods.

The Grimsel test site lies within the Variscan-age (~287 ma) Central Aare Granite and Grimsel Granodiorite (Müller, 1988; Keusen et al., 1989). This body has been affected by numerous intrusions, including prominent lamprophyre dikes. Physical properties of the host rock have been primarily explored using seismic methods (Blümling and Sattel, 1988; Gelbke et al., 1989; Vasco, 1991; Tura et al., 1992; Holliger and Buhnemann, 1996; Maurer and Green, 1997; Vasco et al., 1998; Schild et al., 2001). The various investigations revealed the presence and influence of numerous fractures and shear zones. Seismic P-wave velocities ranged from ~4500 to ~5500 m/s. Holliger and Buhnemann (1996) measured relatively high attenuation in the GTS host rock, with Q factors of 30 - 50, possibly associated with microfracturing.
Several European radioactive waste agencies have initiated and implemented experiments at GTS devoted to the non-intrusive monitoring of swelling bentonite. This clay is characterized by pronounced swelling and very low hydraulic conductivities when it is water-saturated (Villar et al., 2005a). As a consequence, many countries are planning to embed their radioactive waste within bentonite mixtures, regardless of the host-rock type. Any interaction of water with the clay due to infiltration is expected to seal the barrier. The advantage of a granitic host rock is that it provides sufficient confining pressure to the bentonite and a constant groundwater flux (Villar et al., 2005b; Alonso et al., 2008).

The experimental configuration at GTS is sketched in Figure 3.1. A 1-m-thick bentonite wall is assembled in layers at the end of a 3.5-m-diameter tunnel. Realistic closure of the repository is simulated with a 4-m-long low-pH shotcrete plug. Water introduced at a number of locations induces bentonite swelling under controlled conditions. The experimental region is equipped with several types of sensor that monitor a variety of parameters, including pressure, water content, temperature, deformation etc. (Seidler and Bosgiraud, 2008).

Since the swelling of bentonite is associated with substantial variations of its elastic properties (Wersin 2003; Villar, 2005a, b), non-intrusive seismic monitoring was considered a viable option. For this purpose, six gently dipping boreholes were drilled at regular intervals around the circumference of the tunnel, shotcrete plug, and bentonite mass (Figure 3.1). The length and diameter of the boreholes were 25 and 0.085 m, respectively. During each seismic measurement campaign, seismic energy was released at 0.25 m intervals along the gently dipping boreholes 3, 4, and 5. The source employed in our tests was a P-wave sparker (Rechtien et al., 1993) characterized by a nominally repeatable broad-band spectrum up to several kHz, depending on its coupling to the host rock (Lovell and Hornby, 1990).

The seismic waves were primarily recorded by an acquisition system that included three multi-element hydrophone chains placed in gently dipping boreholes 1, 2, and 6, and a composite 24-bit dynamic range Geometrics Geode recording unit that allowed 96 individual channels to be simultaneously sampled at a timing interval of 20 μs. The three hydrophone chains were each equipped with twenty-four hydrophones spaced at 1 m intervals. These sensors were expected to provide a flat response from approximately 0.2 to 7.0 kHz. During the surveys, a 0.25 m
hydrophone spacing was synthesized by shifting the hydrophone chains by 0.25 m along the boreholes and repeating the experiments. To ensure rigidity and accurate relative positioning, the hydrophone chains were placed in PVC pipes. In addition to the hydrophone data, information from twenty-four 100-Hz vertical-component geophones rigidly mounted (cemented within small holes) to the front wall of the shotcrete plug was also recorded by the Geode system.

3.3.2 Mont Terri Rock Laboratory (Felslabor Mont Terri, FMT)

The second suite of experiments was conducted at the Mont Terri Rock Laboratory (FMT) in the Swiss Jura Mountains (Figure 3.2; FMT will not be used for HLRW disposal). Here, the host rock is the Opalinus clay formation, an extremely low permeability rock of Aalenian age (~170 ma). Opalinus clay has been identified as a potential host rock for radioactive waste in Switzerland (NAGRA, 2002a, 2002b; Witherspoon and Bodvarsson, 2006). It is found at appropriate depths between 500
and 1000 m in the Alpine foreland (Birkhäuser et al., 2001) and outcrops in the region of the FMT (Thury and Bossart, 1999). The test site comprises several tunnels excavated from the escape gallery of a motorway tunnel. As for the Grimsel site, the Mont Terri site has been the focus of experiments by numerous radioactive waste agencies (Bossart and Thury, 2007).

Besides its low permeability, Opalinus clay, like bentonite, has the advantageous property of being self-sealing (Thury, 2002; Bossart et al., 2004; Blümling et al., 2007). The physical and chemical properties of Opalinus clay and other relevant clay-rich formations have been determined in a variety of experiments (e.g., Bastiaens et al., 2007). A distinguishing feature of Opalinus clay is its high degree of elastic anisotropy, with slow and fast P-wave velocities of 2300 - 2500 and 3100 - 3300 m/s, respectively (Nicollin et al., 2008; Manukyan et al., 2008).

The experimental setup at FMT is sketched in Figure 3.2. A 13-m-long microtunnel with a diameter of 1.0 m, mimicking a 30 - 40 % scaled repository, was constructed in the Opalinus clay formation. For crosshole monitoring purposes, two moderately dipping boreholes (25 and 29 m long) were drilled perpendicular to the axis of the microtunnel. During the experiments, both boreholes were water filled. Initially, the microtunnel was empty. It was then filled with sand and sealed with a mega-packer system. Subsequently, the microtunnel was water-saturated and slightly over-pressured. As a last phase, gas will be injected (scheduled for mid 2010).

All phases of the experiment have been accompanied by seismic measurements. Seismic energy was released sequentially in the lower downward dipping borehole at 0.25 m intervals using the same sparker source as at GTS. The primary data acquisition system and recording strategy were essentially the same at both the sites; twenty-four 1-m-spaced hydrophones were progressively shifted in the upward dipping borehole to simulate 0.25 m spacing. At FMT, the temporal sampling interval was either 64 or 32 μs and two different installation procedures were employed. During the first 6 experiments, the hydrophone chain was inserted with a hook and pulley system. For the remaining experiments, the hydrophone chain was placed in a rigid PVC pipe as described for GTS. In addition to the hydrophones, eight 100-Hz vertical-component geophones were planted at roughly equal distances around the interior of the microtunnel in the plane spanned by the two boreholes (Figure 3.2).
3.4 NUMERICAL SIMULATIONS

To quantify waveform changes expected to be caused by medium changes within and around the simulated repositories at the Grimsel and Mont Terri sites, numerical modeling experiments were performed. For the sake of simplicity and computational efficiency, we restricted the simulations to two dimensions (2D). For the GTS experiment, our 2D setup would correspond to, for example, a source placed along borehole 5 and hydrophones placed along borehole 2 (Figure 3.1). At FMT, the geometry of the boreholes is essentially two-dimensional (Figure 3.2). Synthetic seismic traces were computed for GTS using a visco-elastic finite-difference time-domain modeling code described by Bohlen (2002). For FMT, synthetic seismic traces were calculated using an elastic-wave version of the same code that we modified to incorporate anisotropy, using a similar implementation to that reported by Juhlin (1995).

End-member scenarios were considered for the Grimsel site synthetic experiment: a dry and a fully water-saturated bentonite block (Table 3.1). P-wave velocities for granite were based on traveltime inversions of observed GTS data (Maurer and Green, 1997), whereas the remaining P- and S-wave velocities and densities for granite, shotcrete, and dry and wet bentonite were based on a personal communication from Peter Blümling (NAGRA). No excavation disturbance zone was included in the GTS model.

<table>
<thead>
<tr>
<th>Material</th>
<th>$V_p$ (m/s)</th>
<th>$V_s$ (m/s)</th>
<th>$\rho$ (kg/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Granite</td>
<td>5200</td>
<td>2700</td>
<td>2600</td>
</tr>
<tr>
<td>Shotcrete</td>
<td>2820</td>
<td>1810</td>
<td>2200</td>
</tr>
<tr>
<td>Bentonite (dry)</td>
<td>500</td>
<td>260</td>
<td>1400</td>
</tr>
<tr>
<td>Bentonite (saturated)</td>
<td>2000</td>
<td>500</td>
<td>1600</td>
</tr>
</tbody>
</table>

Table 3.1: Rock properties used for GTS simulations. The velocity values for granite indicate the median velocities of the model, on top of which 5% stochastic fluctuations (3m correlation length in both directions) were added.

<table>
<thead>
<tr>
<th>Material</th>
<th>$V_p$ (m/s)</th>
<th>$V_s$ (m/s)</th>
<th>$\rho$ (kg/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Opalinus clay</td>
<td>3110</td>
<td>2340</td>
<td>2500</td>
</tr>
<tr>
<td>Sand (dry)</td>
<td>500</td>
<td>240</td>
<td>1855</td>
</tr>
<tr>
<td>Sand (saturated)</td>
<td>1900</td>
<td>240</td>
<td>2155</td>
</tr>
</tbody>
</table>

Table 3.2: Rock properties used for FMT simulations. The two values for the Opalinus clay indicate the $V_p$ velocities parallel and perpendicular to the axis of isotropy.
For the FMT experiment, we modeled a sand-filled microtunnel that was either
dry or water-saturated (Table 3.2). Elastic parameters for the Opalinus clay were
derived from an anisotropic traveltime inversion of observed FMT data (Manukyan et
al., 2008), and its density was taken from NAGRA (2002b). The properties of dry and
wet sand were estimated from the literature (Zimmer et al., 2007). We included an
excavation disturbance zone in the FMT model with dry/water-saturated velocities
decreasing linearly from normal Opalinus clay values at a radius of 1.5 m to 60/72 %
of normal values at the surface of the microtunnel. On the basis of seismic sections
recorded at the two test sites, we chose Ricker-wavelet sources with center
frequencies of 3 and 2 kHz for GTS and FMT, respectively. These correspond to
dominant P-wavelengths of ~1.73, ~0.94, ~0.17 and ~0.67 m for granite, shotcrete,
and dry and wet bentonite, and 1.17 - 1.55 m for Opalinus clay and ~0.25 and ~0.95 m
for dry and wet sand.

Figure 3.3 shows the results for a selected shot position at each site. Wavefield
snapshots at a time t = 3.6 ms for the dry and wet bentonite scenarios at GTS are
presented in Figure 3.3a and 3.3b, and simulated seismic sections for a hydrophone in
borehole 2 are displayed in Figure 3.3d and 3.3e. Corresponding diagrams for the dry
and wet sand scenarios at FMT are given in Figure 3.3h and 3.3i (t = 7.4 ms) and 3.3k
and 3.3l. Differences between the dry and the water-saturated scenarios at the two
sites, magnified by a factor 2, are displayed in Figure 3.3c, 3.3f, 3.3j, and 3.3m.

The snapshots and seismic sections clearly illustrate that the simulated
repositories at both test sites cause a large amount of scattering. It is also noteworthy
that a substantial part of the seismic energy is reflected from or near the simulated
repository boundaries, demonstrating that useful information is contained not only in
the transmitted but also in the reflected wavefields. This is especially important at
GTS, where information in measurement planes not intersecting the repository can be
collected. Differences in the seismic traces occur along most of the length of the
receiver boreholes, indicating that the boreholes should extend well outside the
monitored regions for optimum results.

To gain further insight with regard to the data accuracy required for performing
reliable waveform inversions, changes in the seismic traces simulated for the dry and
wet conditions need to be quantified. A suitable tool for this task is cross-correlation.
Unless specified otherwise, we have used 5 ms time windows starting at the first break
of each trace for computing the normalized cross-correlation coefficients of simulated
and observed seismic traces. As shown in the synthetic seismic sections (Figure 3.3), this time window includes most of the relevant information for the Grimsel and Mont Terri sites.

Zero-lag cross-correlation coefficients for traces in Figure 3.3d/3.3e and 3.3k/3.3l are plotted in Figure 3.3g and 3.3n, respectively. The coefficients range from 0.75 - 1.0 for GTS traces, whereas larger variations of 0.1 - 1.0 are observed for the FMT traces. Analyses using other shot positions yielded similar results.
These variations of cross-correlation coefficient are caused by changes in the seismic contrast between the anomalous features (i.e., bentonite plug, EDZ, and microtunnel) and the surrounding host rock. The anomalous features have lower velocities than the host rock at both sites, so waves passing through them are somewhat delayed. At GTS, the bentonite has a significant contrast with the granite, both when dry (1:10.4; Table 3.1) and when fully saturated (1:2.6). Hence, the early part of the recorded wavefield is expected to be dominated by waves diffracted around the anomalous feature in both dry and water-saturated conditions, and little affected by the target zone itself (Figure 3.3g). When the microtunnel is filled with dry sand at FMT, the velocity ratio with normal Opalinus clay is considerable (average of 1:5.5). In contrast, the velocity ratio is quite small (average of 1:1.4) for water-saturated sand conditions. As a consequence, the transmitted seismic paths through the FMT microtunnel are expected to affect the early part of the recorded wavefield in the water-saturated scenario, but not when the sand is dry. This is clearly borne out in the cross-correlation plot (Figure 3.3n).

Success or failure of waveform-based inversion relies on its capability to exploit the waveform differences shown in Figure 3.3f and 3.3m. This requires data accuracy and repeatability to be significantly better than these differences. The cross-correlation coefficients plotted in Figure 3.3g and 3.3n indicate that this is a challenging task. In particular, for GTS it will be necessary to generate highly repeatable seismic sections, such that small variations of the source signal and/or the receiver coupling would result in cross-correlation coefficients of 0.95 or better for repeat experiments under the same conditions. Furthermore, the 2D simulations shown in Figure 3.3a – 3.3g tend to overestimate the effects of the swelling bentonite. In a realistic 3D configuration, the overall magnitude of the waveform perturbations would probably be smaller, making the monitoring task even more challenging.

Based on the results of synthetic experiments (e.g., Figure 3.3), we conclude that repeatability of “identical” equipment should yield cross-correlation coefficients of better than 0.95 over a wide frequency band. It was with this goal that we conducted the various experiments at GTS and FMT.

We also ran a much smaller set of numerical simulations using a realistic three-dimensional GTS model, in order to assess the 3-D effect of out-of plane refractions. The resulting seismograms can be split into two distinct components, namely the first-arriving waves refracted around the low-velocity repository, and waves scattered by
this anomaly. Our simulations show that the first arriving wavefield is virtually unaffected by changes in the repository, whereas changes in the later portions of the seismograms are significant and quantitatively similar to the 2D case. Therefore, only these later parts can be exploited for monitoring. Nevertheless, most of the conclusions obtained from the 2D simulations also hold for realistic 3D structures, but stricter requirements on the repeatability of the later phases may need to be imposed in the 3-D case, where the seismic signatures are more complicated.

3.5 REPEATABILITY TESTS

Repeatability of seismic experiments is governed by several factors, including the:

- source signal,
- coupling of the source to the medium,
- coupling of the receiver to the medium, and
- fidelity of the receiver and acquisition system.

To study the effects of these different factors, extensive tests were performed at the Grimseland Mont Terri sites. The GTS experiments were conducted when the bentonite block was partially saturated and the FMT experiments were conducted during a phase of slight over-pressurization of the microtunnel (the actual state of the simulated repositories is not critical for the repeatability tests).

3.5.1 Source and geophone coupling

For this set of experiments, we consider a single source position at a distance of 13.5 m in borehole 5 at GTS and a single source position at a distance of 18 m at FMT, and firmly grouted vertical-component geophones at the front of the shotcrete plug (GTS) and within the microtunnel (FMT). Ten repeat shots at exactly the same locations were fired consecutively and compared (Figure 3.4a and 3.4b). To quantify the repeatability, the 10 traces at each site were stacked to form a master trace and cross-correlation coefficients between the master trace and the individual traces were computed. Here, the entire traces were cross-correlated in order to include the later phases in the traces recorded at GTS (Figure 3.4a). The resulting cross-correlation coefficients demonstrate excellent repeatability of the source signal and geophone
recordings; the average of the cross-correlation coefficients shown at the bottom of each trace is >0.99.

The dominant lower frequency phases visible in the later portions of the GTS traces are probably the result of resonances around the shotcrete plug, but for our purposes it is only important to note that the GTS signals also include significant high-frequency energy up to ~3 kHz (see summed amplitude spectra of the individual traces represented by the red curve Figure 3.4c). The FMT signals have significant energy up to ~4 kHz (Figure 3.4d).

To estimate repeatability of the seismic traces as a function of frequency, coherence spectra were computed. The coherence spectrum $C(f)$ is defined as

$$C(f) = \frac{S^2(f)}{A_1(f) A_2(f)},$$

where $f$ is frequency and $S$ is the cross-spectrum between two time series with power spectra $A_1$ and $A_2$. Values of $C(f)$ lie between zero (no repeatability) and one (perfect repeatability).
repeatability). Coherence is not computed for frequencies that have amplitudes less than 5% of the maximum amplitudes.

The averaged coherence spectra over all 45 (10 x 9/2) combinations of the 10 traces from GTS and the 10 traces from FMT are shown by the blue lines in Figure 3.4c and 3.4d. These figures indicate that the sparker source produces highly repeatable signals that are consistently recorded by the firmly attached geophones over a wide frequency band. After removal and reinsertion of the sparker in the boreholes, the experiments were repeated. The results were essentially identical. We conclude that the sparker source and firmly attached geophones produce the required repeatability for high-precision seismic monitoring.

3.5.2 Hydrophone coupling in dipping boreholes

In the next step, we consider the same shots as in Figure 3.4, but analyze the responses of typical hydrophones at a distance of 9 m in borehole 5 at GTS and at a distance of 23.5 m at FMT. The unfiltered traces are displayed in Figure 3.5a and 3.5b.

Compared to the excellent repeatability of the geophone recordings (Figure 3.4a and 3.4b), the cross-correlation coefficients for the hydrophone data in the moderately dipping hydrophone boreholes are substantially inferior for the GTS data (average cross-correlation coefficient of ~0.92) and slightly inferior for the FMT data (average of ~0.99). These lower values are primarily caused by energetic, but largely incoherent high-frequency signals. It is notable that there is no clear amplitude decay towards higher frequencies in the GTS spectrum of Figure 3.5c.

The averaged coherency spectra in Figure 3.5c and 3.5d (blue lines) show uniformly high values over the frequency range 0.5 - 3.0 kHz for GTS and 0.5 - 4.0 kHz for FMT. Figure 3.5e and 3.5f show the corresponding 0.5 - 3.0 kHz and 0.5 - 4.0 kHz bandpass filtered traces together with the cross-correlation coefficients based on recomputed master traces. The corresponding, recomputed frequency and coherence spectra are given in Figures 3.5g and 3.5h. For the bandpass-filtered traces, the average cross-correlation coefficients are ~0.99 for GTS and >0.99 for FMT, which we judge to be adequate for monitoring purposes. On the basis of these observations, seismic traces shown in subsequent figures were bandpass filtered using the frequency ranges indicated, unless otherwise specified.
Coupling of the hydrophones to the host rock was further investigated via two simple experiments at each site. Initially, the hydrophone chains were installed in the observational boreholes and the sparker was fired at several positions within the source boreholes. Then, the hydrophone chains were removed, disassembled, reassembled, and reinserted to the same nominal positions. With these experiments, we wished to determine to what extent very small changes in hydrophone position

Figure 3.5: (a) to (d) are the same as Figure 4 (a-d), but for hydrophones at each site. (e) to (h) are the same as (a) to (d), but the traces have been bandpass filtered (corner frequencies of 0.5-3 kHz for GTS and 0.5-4 kHz for FMT). Coherence curves are truncated above the lowest frequencies for which the amplitudes are less than 5% of the respective maximum amplitudes.
(i.e., variations of at most ~1.0 cm) and seating in the boreholes affected the waveform shapes. At both test sites we observed significant changes in the waveforms (Figure 3.6a and 3.6b) due to the coupling differences associated with small variations of hydrophone position and seating on the floor of the borehole. The corresponding zero-lag cross-correlation coefficients between traces recorded using the original and reinserted hydrophones (Figure 3.6c and 3.6d) quantified the differences in Figure 3.6a and 3.6b. The coefficients ranged from 0.2-0.8 for Grimsel and from negative values to 0.8 for Mont Terri, all of which were clearly unacceptably low. Much improved cross-correlation coefficients (Figure 3.6g and 3.6h) were obtained by
limiting the lengths of correlated traces to the first cycle immediately after the first break (Figure 3.6e and 3.6f).

An analogous experiment was later conducted at a third location (unrelated to GTS and FMT) using the same source and receiver assemblies in vertical boreholes. We employed the same insertion/extraction/reinsertion procedure as we employed for the GTS and FMT experiments. Cross-correlations between seismic traces before and after reinsertion were much higher for the vertical-borehole experiments (average cross-correlation coefficient of ~0.9) than for the dipping hole experiments, but still the coupling effects were significant. The cross-correlation coefficients for repeat shots were also much higher, with an average value of ~0.99.

We now compare seismic traces recorded by sensors adjacent to each other. Figure 3.7a presents recordings from a shot fired in borehole 5 and recorded in borehole 2 at distances from 12.5-14.25 m at GTS, and Figure 3.7b displays traces recorded at distances from 3.25-5.0 m at FMT. For optimum visual comparison, the first breaks of the traces are in each case aligned. Since the 0.25 m receiver spacing was achieved by shifting the 1 m spaced hydrophones repeatedly in increments of 0.25 m, the first four traces in each of Figure 3.7a and 3.7b were recorded with the same hydrophone and the last four traces were recorded by an adjacent hydrophone. In most of the experiments the hydrophones were moved together with the PVC pipe. As a consequence, the positions and coupling conditions of the hydrophones within the pipe were not expected to change, but small variations of the recordings may have been due to changes of the geology along the boreholes and minor changes of the overall wavepaths. Cross-correlation coefficients for adjacent traces (numbers at the

Figure 3.7: Effect of hydrophone chain shifting and different hydrophone transfer functions at (a) GTS and (b) FMT. The eight traces in each diagram are a subset of shot gathers recorded using two hydrophone elements separated by 1 m, but shifted three times by 0.25 m. The numbers between the traces are cross-correlation coefficients of adjacent traces. Note the relatively high coefficients (≥0.48) for adjacent traces of the same hydrophone and low coefficients (≤0.24) for adjacent traces of different hydrophones.
bottom of the traces in Figure 3.7a and 3.7b) for the first four and last four traces range from 0.53 to 0.88; these differences are likely due to changing geological conditions. In contrast, cross-correlation coefficients between traces 4 and 5, corresponding to two different hydrophones, are only 0.17-0.24. This indicates that the individual hydrophones have different responses and/or that this is again the result of the significant effects of slightly different sensor position and seating. From our observations it is not possible to separate these two effects.

As the last step of our hydrophone coupling investigation, we have compared selected source and receiver gathers from GTS and FMT (Figures 3.8a, 3.8d, 3.9a, and 3.9d). At both test sites, receiver gathers (Figures 3.8d and 3.9d) exhibit much higher spatial continuity than source gathers (Figures 3.8a and 3.9a). This is further evidence that source characteristics and source coupling are very consistent, whereas hydrophone characteristics and/or hydrophone coupling are highly variable.

Figure 3.8: (a)-(c) Shot gathers and (d)-(f) receiver gathers recorded at GTS using different hydrophone chains at shot distance 13 m and receiver distance 13 m. (a) and (d) A hydrophone chain data; (b) and (e) B hydrophone chain data; (c) and (f) C hydrophone chain data.
3.5.3 Hydrophone chain comparisons

The large variations of hydrophone coupling and/or hydrophone responses motivated us to determine if comparable results would be obtained using other types of hydrophone chains. We have compared our hydrophone chain (referred to as A) with two additional hydrophone chains having different designs (referred to as B and C), and, thus, different coupling properties. The three tested hydrophone chains have comparable nominal individual hydrophone frequency responses, but the single sensors are assembled within the streamer following different concepts: hydrophones in chain A have individual metal casings connected via takeouts to the main signal cable, while chains B and C mount the sensors “in-line”, encased in a plastic shielding. Furthermore, hydrophone chains A and B have built-in pre-amplifiers (active), whereas hydrophone chain C does not (passive).

Examples of shot and receiver gathers recorded using the different hydrophone chains at Grimsel and Mont Terri are shown in Figures 3.8 and 3.9, respectively. As for the A traces, events on the B and C receiver gathers (Figures 3.8e, and 3.8f and 3.9e, and 3.9f) are much more continuous than on the B and C source gathers (Figures
3.8b and 3.8c and 3.9b and 3.9c). It is noteworthy that the variability of traces in the B source gathers is even more pronounced than in the A source gathers. By comparison, the B receiver gathers show a high degree of spatial continuity of the different seismic phases. On the basis of these comparisons, we conclude that the pronounced variations in the recordings caused by different coupling conditions and/or hydrophone responses is a common feature of all hydrophone chains and not a particular problem of the A hydrophone chains employed in our experiments.

3.6 SYSTEMATIC NOISE

Several rather unusual phases are evident on many of our GTS and FMT seismic sections. Typical examples are shown for GTS data in Figure 3.10. A horizontal band of weak energy (highlighted by the blue box) appears to start on all traces at practically the same time as the earliest arrival on the source gather of Figure 3.10a. Amplitude normalization results in this phase appearing to be most prominent in traces with relatively long source-receiver offsets. Inductive effects within the hydrophone cable due to vibrations produced by the earliest seismic waves striking the cable are the most likely source of this phase (Figure 3.11a). In contrast, the horizontally aligned weak phase (highlighted by the red box) in the receiver gather of Figure 3.10b cannot be explained by such point sources. Instead, it appears to be generated within the coaxial sparker cable, which behaves as an approximate monochromatic line source along the borehole as a result of the very high current flow at the onset of capacitor discharge (Figure 3.11b). The sudden surge in current subjects the cable to a strong radial force that acts almost simultaneously over its entire length, thereby causing an expansion pulse.
At later times, two prominent phases appear in all seismic sections. These phases with linear or nearly linear moveouts are shown in the GTS receiver gather of Figure 3.12a. They are related to tube waves that strike the ends of the source borehole (Figure 3.12b; Cheng and Toksoz, 1981; Meredith et al., 1993). Conversion of tube-waves to radiating P-waves at the end of the borehole creates the faster phase (green lines in Figure 3.12b), whereas conversion of tube-waves that have travelled to and from the end of the borehole to radiating P-wave energy at the sparker casing generates the slower phase (red lines in Figure 3.12b; the predicted traveltimes for these phases are shown by the green and red lines in Figure 3.12a).

The examples shown in Figures 3.10 and 3.12 are extracted from GTS data, but similar phases, though somewhat weaker, are seen in the FMT data. The occurrence of
these additional phases has consequences for waveform inversions. They either have to be incorporated in the forward modeling or removed (suppressed) by appropriate data processing prior to waveform inversion.

3.7 DISCUSSION

Keeping the coupling conditions of the sensors constant is highly desirable for successful full-waveform inversions. Even when the sensors are fixed in place, the effects of locally varying coupling conditions on the seismic traces cannot be neglected. These effects can be accommodated by assuming that they are unknowns to be determined during the full-waveform inversion process. The procedures are comparable to those used to invert for source signatures (e.g., Ernst et al., 2007). Maurer and Musil (2004) demonstrated that variable coupling conditions for both sources and receivers can be included in ray-based amplitude inversions. We expect that similarly good results can eventually be achieved for full-waveform inversions, albeit more complicated.

Comparison of data recorded in the granitic rock at the Grimsel test site and in the clay formation at the Mont Terri site reveals common features and some notable differences. The most important difference is the more prominent high frequency incoherent noise at GTS. A data set collected within vertical boreholes at another hard-rock site also contains substantial levels of high frequency incoherent noise. We do not know the exact origin of this noise. Preliminary modeling suggests that it may be generated by the sparker tool itself, acting as a resonant secondary source which is highly sensitive to its position and seating in the source borehole. The different behavior at GTS and FMT is probably related to i) different impedance contrasts between the borehole water and the host rock, producing different energy transmission efficiencies, and ii) different frequency-dependent attenuation in the hard and soft rock.

High frequency noise could also be due to ubiquitous microfractures in crystalline host rocks. Such fracture systems could react unpredictably to the stresses applied by the source pulse. The presence of ubiquitous microfractures at GTS would also explain the relatively low Q values found by Holliger and Buhnemann (1996).

Modeling shows that increasing water saturation within the bentonite plug, the excavation disturbance zone, and the microtunnel will produce measurable changes to the seismic waveforms. The changes should be larger at the FMT soft-rock site than at
the GTS hard-rock site because of differences in contrast between the two host rocks and the monitored features. Furthermore, soft-rock environments are more likely to experience larger changes over time. Whether such changes can be observed in practice will depend on the magnitude of change being appreciably larger than uncertainties associated with noise and receiver coupling variations. Noise was higher and hydrophone coupling problems were more severe at the hard-rock site, further complicating the ability to sense small changes in the target region.

Preliminary analyses of traces recorded under different saturation conditions (not presented here) indicate that time-lapse inversion of waveforms is a viable option for sensing the state of the target features, at least for the Mont Terri soft-rock site. However, care needs to be exercised to ensure that source and receiver coupling differences between experiments are minimized and properly accounted for in the data processing and/or inversion. This paper has outlined a systematic methodology for quantitatively assessing whether the data quality and repeatability are sufficient for effective full-waveform monitoring to take place.

3.8 CONCLUSIONS

Our repeatability tests at the Grimsel and Mont Terri sites lead to the following principal conclusions.

- Numerical simulations demonstrate that realistic changes in a high level radioactive waste repository (such as fluid saturation of the bentonite fill and damage zone) can produce significant changes in seismic data (waveforms) recorded outside of the volume of interest. Such changes can be detected provided data quality meets strict requirements in terms of repeatability, reliability and bandwidth; comparison of traces recorded during repeat experiments under the same source, receiver, and site conditions should yield cross-correlation coefficients of > 0.95, and the meaningful frequency bandwidth content should be at least 2 - 3 kHz.

- Seismic contrasts between the host rocks and target features play a major role in determining the level of detectable change in recorded seismic traces. Somewhat paradoxically, changes to relatively low host-rock-target contrasts (e.g., FMT) can induce larger changes to the seismic waveforms than changes to much higher host-rock-target contrasts (e.g., GTS). High contrasts that
would typically occur at a hard-rock repository may be particularly challenging for any monitoring endeavor.

- The seismic sparker source (i) is highly repeatable for frequencies up to 5 kHz, (ii) is not susceptible to coupling problems, and (iii) provides significant energy in a frequency band of several kHz.

- Repeatability of hydrophone recordings is limited by the occurrence of incoherent high-frequency noise. Application of appropriate bandpass filters reduces the effects of this noise and results in higher cross-correlation coefficients between repeat traces, but it also restricts the usable frequency band available for full-waveform inversions.

- The coupling of hydrophones to the host rock has a major effect on the transfer function of the acquisition system. Minor variations in hydrophone positioning and seating result in substantial changes of the seismic sections. This finding has been verified by using three different types of hydrophone chains.

- Hydrophone coupling effects are more severe in gently dipping boreholes than in vertical ones. This difference is probably due to complex coupling of hydrophones in the former case (hydrophone - water - rock plus hydrophone - rock or hydrophone - PVC pipe - rock) and relatively straightforward coupling in the latter case (hydrophone - water - rock).

- Comparison of different detector types (hydrophone chains and firmly anchored geophones) demonstrates that:
  
  i. geophones that can be firmly anchored to the host rock show much better repeatability than removable hydrophones;
  
  ii. the frequency response of geophones is narrower than hydrophones, especially when mounted on complex engineered structures (e.g., the shotcrete plug at GTS);
  
  iii. retrievability of firmly anchored geophones is reduced with respect to mobile hydrophone chains, thus resulting in reduced longevity of the receiver assembly;
iv. Hydrophones only allow scalar pressure data to be recorded, whereas a variety of other sensors (e.g., multicomponent accelerometers or geophones) provide full vector-field information.

- Seismic energy generated by a sparker source and detected by a hydrophone chain is contaminated with several types of systematic noise that originate from (i) mechanically-induced electric effects in the hydrophone chain cables, (ii) high currents running in the sparker cable, thereby acting as a secondary line source, and (iii) tube waves that travel along the source borehole and are converted to body waves at the end of the borehole and at the casing of the sparker tool.

Results of our modeling investigations indicate that crosshole and hole-to-tunnel seismic methods are likely to provide useful information for the remote monitoring of high level radioactive waste repositories over repository-scale distances. The monitoring boreholes and tunnels need not intersect the repositories, but the closer they approach the repositories the higher the resolution and reliability of information provided by the seismic data. Our field tests demonstrate the utility of the sparker energy source and the repeatability of full waveforms recorded by the rigidly anchored geophones. Although the first arrivals and the initial one to two pulse cycles on the hydrophone-supplied waveforms are also consistent, the latter parts of these waveforms are less predictable.

A seismic system suitable for the remote monitoring of radioactive waste repositories over periods up to 100-300 years will need to have energy sources and sensors that can be well coupled to the host rock and at the same time periodically updated. The sparker in a water-saturated borehole is one possibility for the energy source. For the sensors, one possibility would be to attach multicomponent sensors to rigid frames that are inserted into the boreholes. An appropriate cement would be pumped into the boreholes. Once the cement hardens, the sensors would be firmly attached to the host rock. The borehole would have to be reamed out to replace the sensors. Alternative options could involve using a suitably modified version of a landstreamer equipped with multicomponent geophones or accelerometers (Van der Veen and Green, 1998; Van der Veen et al., 2001). Such a detector could allow for good retrievability in both dry and wet boreholes/tunnels, but coupling efficiency and stability in dipping boreholes would have to be assessed. From surface seismic
experience we do not favor such an approach. In our opinion, given the strict requirements in terms of detector coupling and retrievability, a new detector assembly design has to be developed in accordance with the specific repository structure.

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CHAPTER 4

Exploitation of data information content in elastic waveform inversions

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4.1 ABSTRACT

Elastic waveform inversions have the potential to provide detailed subsurface images of the elastic parameters (P- and S- wave velocities and density), but acquisition of suitable data sets and their inversion are non-trivial tasks. We explore the information content offered by elastic waveform data by means of a 2D synthetic study. Comprehensive data sets that include recordings based on multicomponent (directed) sources and multicomponent (vector) receivers that fully surround the area of interest allow all elastic parameters to be reliably recovered. Results that are almost as good can be achieved using the more commonly employed crosshole configuration. If only single source components (e.g., those oriented perpendicular to the borehole walls) are used, then there is no significant degradation of the quality of the tomographic images. Crosshole experiments that include pressure sources and multicomponent receivers still allow P- and S- wave velocities to be recovered, but such data sets contain virtually no information about the density. Finally, seismic data collected with omni-directional pressure sources and pressure receivers contain information about P- and S- wave velocities, but there are pronounced trade-offs between these parameters. This is demonstrated through formal model-resolution analyses. From our study, we conclude that seismic data recorded with pressure sources and two-component receivers offer the best compromise between acquisition efficiency and data-information content. This finding is exploited in a model study, in which the feasibility of non-intrusive seismic monitoring of high-level radioactive waste repositories is tested. Our results indicate that sources fired along boreholes either side of the repository and receivers suitably placed around the repository allow water saturation processes to be reliably characterized.

4.2 INTRODUCTION

Seismic waveform inversions are a powerful means for constructing high resolution subsurface images. These techniques were first presented in the time domain (e.g., Tarantola, 1984). Later, they were also formulated in the frequency domain (e.g., Pratt and Worthington 1990). During the past few years, the popularity of seismic waveform inversions has increased enormously, as reflected in a large number of publications, including special issues of journals (Geophysical Prospecting 2008, Geophysics 2009) and conference proceedings (e.g., EAGE 2010, SEG, 2010, EGU 2011).
There is an ongoing debate in the geophysical literature as to whether time- or frequency-domain inversions are the preferred option. Advantages of time-domain inversions include the memory efficient implementation of the forward problem (e.g., Bohlen, 2002) and the fact that the original data (i.e., the seismic sections) are considered, which makes phase identification possible and data preprocessing (e.g., time windowing) more straightforward. Frequency-domain forward modeling is typically formulated as a matrix inverse problem $Au = x$, where the system matrix $A$ characterizes the material properties, vector $u$ represents the unknown displacement or pressure field, and vector $x$ describes the source characteristics (e.g., Pratt, 1999). Direct matrix solvers (e.g., Schenk et al., 2002) allow such systems of equations to be solved very efficiently for many sources $x$, that is, the solutions for a suite of source positions can be obtained swiftly because once $A^{-1}$ (e.g., by the LU factorization of $A$) is obtained, it can be multiplied with the different source vectors (e.g., Pratt, 1999). This advantage comes at the expense of large memory and run time requirements for calculating the inverse of $A$ or an appropriate representation thereof. Another advantage of frequency-domain inversions is that only a few judiciously chosen frequencies are typically required for obtaining results that are comparable to those that include all frequencies contained in the waveforms (e.g., Sirgue and Pratt, 2004; Maurer et al., 2009).

Most time- and frequency-domain seismic waveform inversion studies employ the acoustic approximation, and in most cases only 2D problems are considered (e.g., Pratt and Shipp, 1999; Hicks and Pratt, 2001; Gao et al., 2006; Operto et al., 2006; Hu et al., 2009, 2011). Only recently have researchers started to investigate the 3D acoustic problem (e.g., Ben-Hadj-Ali et al., 2008; Vigh and Starr, 2008; Abubakar et al., 2011) and in some cases even pseudo-anisotropic full waveform inversion of surface seismic data. Unfortunately, they can only use frequencies up to 10-20 Hz, and the pseudo-anisotropic inversions entail acoustic approximations in transversely isotropic media, which do not fully honor the wave physics. The low frequency limit is imposed by the 3D modeling requirements, which sacrifices much of the available data bandwidth.

Several studies have highlighted the limited applicability of the acoustic approximation for seismic waveform inversion problems (e.g., Barnes and Charara, 2009). Interestingly, early waveform inversion studies were performed with elastic forward operators (Mora, 1987), but the heavy computational costs rendered this
approach impractical at the time. During the past decade, elastic waveform inversions experienced a revival, stimulated by the availability of enhanced computing power. Most elastic studies found in the literature have been devoted to surface-based or ocean-bottom experiments (Shipp and Singh, 2002; Choi et al., 2008a, 2008b; Sears et al., 2008; Brossier et al., 2009; Sears et al., 2010; Lee et al., 2010; Maeda et al., 2011), but some crosshole studies have been reported (Barnes et al., 2008). A handful of recent conference papers have also appeared that treat full waveform inversion in 2D VTI (anisotropic) media (Barnes and Charara, 2010; Gholami et al., 2010; Plessix and Rynja, 2010). To date, no 3D elastic-waveform inversion results have been published, but it is expected that reports of such studies will appear within the next few years.

The advantages of elastic versus acoustic waveform inversions are twofold. First, acoustic inversions of elastic data are prone to artifacts, because of the systematic discrepancies between the observed and predicted data (Barnes and Charara, 2009). Even for pressure sources, the observed data contain mode-converted S-waves that are not accounted for in the simulated data. The problem can be partially alleviated through the use of pressure receivers (equivalent to the divergence of the displacement vector, thus strongly favoring P-waves) and by considering only those portions of the seismic traces that are less affected by elastic (shear wave) effects. However, some systematic inconsistencies may persist, and surgical muting of the “contaminated” portions of the seismic traces can cause the information content of the seismic data to be considerably reduced.

We focus here on the second, and, in our view, even more important advantage of elastic waveform inversions. It is the capability of elastic inversions to extract information on all elastic parameters (bulk- and shear moduli and density), which will be highly beneficial for a wide range of applications from civil engineering to whole earth studies. Although this conceptual advantage of elastic waveform inversions is well understood, there are no published studies on the information content of elastic waveform data. In particular, it is unclear how different source-receiver layouts and different source and receiver types/orientations affect the quality of the tomographic images. In an attempt to fill this gap, we investigate systematically the resolving power of elastic waveform transmission tomography experiments.

After a brief introduction to our implementation of forward modeling and inversion, we examine the imaging capability of four-sided versus crosshole source-receiver geometries. Next, we describe the performance of different source- and
receiver types (directed versus omni-directional), where we highlight potential trade-offs between individual elastic properties, which can degrade the quality of the tomograms. Finally, we present our findings for the experimental design of a seismic study of a simulated (scaled down) high-level radioactive waste repository, where we demonstrate that appropriately designed elastic waveform inversion experiments could be useful for the non-invasive monitoring of changes within an actual repository.

Because of the aforementioned advantages of frequency-domain waveform inversions, we have chosen to perform all inversions in the frequency domain, but some of the results are verified using time-domain forward modeling. Accordingly, we expect that all our findings can be transferred in a straightforward manner to time-domain inversions.

4.3 2D FORWARD MODELING AND INVERSION

Frequency-domain elastic waveform inversions require the forward modeling problem for \( u_{ik}^j \) to be solved, where the Fourier transformed displacement \( u \) at receiver \( j \) generated by a source at \( i \) is computed as a function (\( g \)) of the source and receiver properties \( s_i^j \) and \( r_i^j \) (position coordinates, directivity and coupling factors), the angular frequency \( \omega \), and the medium distributions of P- and S-wave velocities \( V_p \) and \( V_S \), and density \( \rho \). The indices \( k \) and \( l \) indicate the orientation of the source excitation and the receiver component (in Cartesian coordinates \( x \) or \( z \) in the following), respectively. For simplicity, we consider only the 2D problem, in which material properties only change in the \( x \)- and \( z \)-directions and a line source along the third direction (\( y \) or \( x_2 \)) is implicit. Using the above indexing scheme, the frequency-domain 2D equation of motion for an isotropic elastic medium can be written as (Aki and Richards 2009):

\[
\begin{align*}
0 &= \rho \omega^2 u_{ikx}^j + \rho \partial_x \left[ V_p^2 \partial_x u_{ikx}^j + \left( V_p^2 - 2V_S^2 \right) \partial_x u_{ikz}^j \right] + \rho V_S^2 \partial_x \left[ \partial_x u_{ikx}^j + \partial_x u_{ikz}^j + F_k^j \delta_{kx} \right], \\
0 &= \rho \omega^2 u_{ikz}^j + \rho V_S^2 \partial_z \left[ \partial_z u_{ikx}^j + \partial_z u_{ikz}^j \right] + \rho \partial_z \left[ \left( V_p^2 - 2V_S^2 \right) \partial_z u_{ikx}^j + V_S^2 \partial_z u_{ikz}^j + F_k^j \delta_{kz} \right],
\end{align*}
\]

(4.1)

where \( \partial_{x,z} \) is the partial derivative with respect to \( x \) or \( z \), \( F_k^j(\omega) \) is the source spectrum, and \( \delta \) is the Kronecker delta (either 1 or zero, depending on whether the subscripts are equal or not).
We solve equation 4.1 using a finite-element approach that is similar to that described by Min et al., (2003). As boundary conditions, we implement perfectly matched layers, which were introduced for electromagnetic waves (Berenger, 1994) and subsequently modified and adapted to a wide range of other wave-propagation modeling problems (de Hoop et al., 2007). In our implementation, we follow the formulations given by Zheng and Huang (2002) and Basu and Chopra (2003).

To solve the resulting system of finite-element equations, we employ an LU decomposition-based direct-matrix solver, which preserves the sparseness of the LU factors (Schenk et al., 2002). This ameliorates to some extent the increased memory consumption of direct matrix solvers, but the memory requirements are still substantially higher than those of iterative solvers.

For the solution of the inverse problem, we use an iterative Gauss-Newton algorithm, which has some significant advantages for waveform inversion problems (Pratt et al., 1998). For example, it allows measures of the goodness of the inversion (e.g., the model-resolution matrix) to be computed. This is essential for the experimental design part of our study. The iterative Gauss-Newton inversion algorithm can be written as:

\[
\mathbf{m}^{n+1} = (\mathbf{J}^T \mathbf{J} + \alpha^2 \mathbf{I} + \beta^2 \mathbf{L}^T \mathbf{L})^{-1} \left\{ \mathbf{J}^T \left[ \left( \mathbf{d}^{\text{obs}} - \mathbf{d}^{\text{pred}} \right) + \mathbf{J} \mathbf{m}^{n} \right] + \alpha^2 \mathbf{I} \mathbf{m}^{n} \right\},
\]

(4.2)

where the model parameter vector \( \mathbf{m}^{n} \) includes the wave-propagation velocities \( V_P \) and \( V_S \), and density \( \rho \), and \( n \) is the iteration number (i.e., \( \mathbf{m}^{0} \) represents the initial model). The continuous subsurface parameters \( V_P(x, z), V_S(x, z) \), and \( \rho(x, z) \) are discretized on \( Q \) rectangular cells. The \( \alpha^2 \mathbf{I} \) term imposes regularization constraints in the form of damping (\( \mathbf{I} = \text{identity matrix} \) and \( \alpha^2 = \text{scaling factor} \)), whereas \( \beta^2 \mathbf{L}^T \mathbf{L} \) governs the smoothing to be applied (\( \mathbf{L} = \text{Laplacian smoothing operator} \), \( \beta^2 = \text{scaling factor} \)). The vectors \( \mathbf{d}^{\text{obs}} \) and \( \mathbf{d}^{\text{pred}} \) are the observed and predicted (modeled) displacements \( u_{ij} \). The quantity \( \mathbf{J} \) appearing in equation 4.2 is the Jacobian matrix. Its individual elements are the partial derivatives or sensitivities of the data with respect to the model parameters, given by:

\[
J_{pq} = \frac{\partial d_{pq}^{\text{pred}}}{\partial m_q^n},
\]

(4.3)

where \( p = 1 \ldots P \), the number of data points, and \( q = 1 \ldots Q \), the number of model parameters.
The displacements \( u_{il}^{\|} \) are formally rewritten as:

\[
u_{il}^{\|} = F_k^{\|}(\omega) \ s_i(\omega) \ r_j(\omega) \ G_{il}^{\|}(\omega, x, z), \tag{4.4}
\]

where \( G_{il}^{\|}(\omega, x, z) \) is the Green’s tensor for the elastic problem in the frequency domain, and for this equation \( s_i(\omega) \) is the source coupling factor and \( r_j(\omega) \) is the receiver coupling factor (there is no summation over repeat indices). Although the source and receiver coupling factors can have a significant influence on the waveforms (Appendix B), for the sake of simplicity they are assumed to be unity in this study, and thus they are omitted in the following equations.

In contrast to the method of back-propagated residuals (e.g., Tarantola, 2005), where the partial derivatives that constitute the Jacobian matrix never have to be formed explicitly, the Gauss-Newton algorithm (equation 4.2) requires them to be computed. Zhou and Greenhalgh (2010) provide explicit expressions for the elastic sensitivities, which after transforming from the Lamé elastic parameters to \( V_P, V_S, \) and \( \rho \) can be written for the 2D case as:

\[
\begin{align*}
\frac{\partial u_{il}^{\|}}{\partial V_p} &= -2\rho V_p \ F_k^{\|}(\omega) \int_{\Omega} \frac{\partial G_{il}^{\alpha\bar{\alpha}}}{\partial x_a} \frac{\partial G_{il}^{\beta\bar{\beta}}}{\partial x_b} \\
\frac{\partial u_{il}^{\|}}{\partial V_S} &= 2\rho V_S F_k^{\|}(\omega) \int_{\Omega} \left\{ 2 \frac{\partial G_{il}^{\alpha\bar{\alpha}}}{\partial x_a} \frac{\partial G_{il}^{\beta\bar{\beta}}}{\partial x_b} \left[ \frac{\partial G_{il}^{\alpha\bar{\alpha}}}{\partial x_a} \frac{\partial G_{il}^{\beta\bar{\beta}}}{\partial x_a} + \frac{\partial G_{il}^{\alpha\bar{\alpha}}}{\partial x_b} \frac{\partial G_{il}^{\beta\bar{\beta}}}{\partial x_b} \right] \right\}, \\
\frac{\partial u_{il}^{\|}}{\partial \rho} &= F_k^{\|}(\omega) \int_{\Omega} \left\{ \omega^2 \ G_{il}^{\alpha\bar{\alpha}} G_{il}^{\beta\bar{\beta}} - (V_p^2 - 2V_S^2) \frac{\partial G_{il}^{\alpha\bar{\alpha}}}{\partial x_a} \frac{\partial G_{il}^{\beta\bar{\beta}}}{\partial x_b} - \rho^2 \left[ \frac{\partial G_{il}^{\alpha\bar{\alpha}}}{\partial x_b} \frac{\partial G_{il}^{\beta\bar{\beta}}}{\partial x_a} + \frac{\partial G_{il}^{\alpha\bar{\alpha}}}{\partial x_a} \frac{\partial G_{il}^{\beta\bar{\beta}}}{\partial x_b} \right] \right\},
\end{align*}
\]  

(4.5)

where \( a \) and \( b \) take on the values 1 and 3 and the Einstein summation convention is used only for \( a \) and \( b \) in the above expression. The quantity \( \Omega \) stands for a particular point in the domain over which the integration is performed for each cell (\( \Omega \)). As outlined in Appendix 4.A, these integrations can be carried out analytically, but \( G \) and its derivatives must be computed numerically.

Substantial differences in the average sensitivities with respect to \( V_P, V_S, \) and \( \rho \) can degrade the condition number of the Hessian matrix \( J^T J \) (e.g., Press et al., 1992), which may cause the Gauss-Newton update formula in equation 4.2 to be unstable. Therefore, it is advantageous to apply matrix scaling to \( J \) (Smith, 1976). Instead of scaling each individual column such that \( \|J_p\| = 1 \), which may “inflate” very small
sensitivities of poorly resolved cells, we have applied sub-Jacobian matrix scaling to each type of parameter, such that the norms of all columns related to $V_P$ have the same value as the norms of the columns related to $V_S$ and $\rho$.

Equations 4.1 to 4.5 describe the theoretical basis for forward modeling and inversion of vectorial displacements $u_{ij}$. The formulation can be converted to omnidirectional measured pressure fields generated by directional forces or by omnidirectional pressure sources. This is discussed in more detail in Appendix 4.B.

4.4 INFORMATION CONTENT OF ELASTIC WAVEFORM DATA

For our initial investigation of the information content offered by elastic waveform data, we employ the elastic model displayed in Figure 4.1. It consists of two cross-shaped anomalous bodies having higher and lower $V_P$, $V_S$, and $\rho$ values relative to the background. Furthermore, the model includes an elongated low-velocity/low-density feature intended to represent a fracture zone. To mimic a realistic scenario, we superimposed 10% stochastic fluctuations with correlation lengths of 5 m in the horizontal direction and 2 m in the vertical direction on the respective background values.

Synthetic waveform data were generated using a finite-element frequency-domain modeling algorithm based on equation 4.1, but it is important to note that this choice is not critical. Comparisons with a finite-difference time-domain algorithm (Bohlen, 2002) provided very similar results. As the data space, we considered nine frequencies equally spaced between 300 and 1500 Hz. This required a forward modeling grid of $0.05 \times 0.05 \text{ m}$ cells. A total of nearly 190,000 such cells were used to represent the model in Figure 4.1. Source amplitudes usually vary as a function of
frequency. In our numerical experiments, we scaled the source amplitudes so that all frequencies had similar values across the employed spectral band. There already exist studies on the information content of seismic data as a function of the frequencies chosen (e.g., Maurer et al., 2009). Therefore, we kept the frequencies fixed and included all frequencies in all numerical experiments.

For the inversions, we merged the forward cells to form larger inversion units of $0.30 \times 0.30 \text{ m}$, which resulted in a total of $3 \times 5,220 = 15,660$ unknowns. For the initial models, we used homogeneous $V_p$, $V_s$, and $\rho$ values set to the average of the true structures shown in Figure 4.1. To avoid trapping in local minima, we started the inversions with only the lowest frequency and subsequently added higher frequencies until all nine frequencies were included. As shown in equation 4.2, to stabilize further the inversions, damping and smoothing constraints were applied. For each set of inverted frequencies, the algorithm started with relatively high damping and smoothing that gradually decreased as the iterations proceeded. To ensure convergence, we performed a relatively large number of 51 Gauss-Newton iteration steps, whereby the last 20 iterations included all 9 frequencies.

To assess the information content offered by each data set, we considered not only the quality of the resulting tomograms, but also the formal model-resolution matrix defined as (e.g., Menke, 1989):

$$ R = (J^T J + \alpha^2 I + \beta^2 L^T L)^{-1} J^T J. $$

(4.6)

It relates the estimated model parameters ($m^{est}$) to the true model parameters ($m^{true}$):

$$ m^{est} \approx R m^{true}. $$

(4.7)

Of particular interest are the diagonal elements of $R$, which are measures of the resolution of the model estimate. Diagonal elements close to zero indicate poorly resolved model parameters, whereas values close to one indicate well resolved model parameters. Since the magnitudes of the diagonal elements depend on the amount of regularization supplied, it is difficult to compare diagonal elements of the resolution matrix for different experimental setups. The matrix scaling, applied to equalize the sensitivities of $V_p$, $V_s$, and $\rho$, also affects the magnitudes of the model-resolution matrix entries. Therefore, only relative changes within a particular tomogram will be considered.
4.4.1 Four-sided experiment, all source and receiver components

As a proxy for the full information content of an elastic waveform data set (comprehensive data set), we considered a deployment in which there are 32 source and 32 receiver positions at 2m spacing along the four edges of the test model (Figure 4.2a-c). Furthermore, we assumed that seismic waves were excited with $x$- and $z$-directed forces at all positions and that all remaining positions (for each source firing) were occupied with receivers recording $x$- and $z$-components of the resulting displacement fields. This resulted in $9 \times 4 \times 32 \times 31/2 = 17,856$ complex frequency data points (excluding reciprocal configurations).

The tomograms in Figure 4.2a and b demonstrate that a comprehensive data set has the potential to recover fully the $V_P$ and the $V_S$ velocity structures. Even some of the stochastic features are imaged. The shapes of the density structures are also recovered (Figure 4.2c), but the contrast magnitudes are underestimated. Plots of the model-resolution diagonal elements in Figure 4.2d-f, indicate that the resolution is best near the source and receiver positions and, except for the lower velocity/density
anomalous structures, decreases towards the center of the models. This is similar to patterns found for acoustic waveform inversion experiments (Maurer et al., 2009), but it is different from results from ray-based traveltime tomography, in which the resolution is best in the center of the models (having the highest number of crossing raypaths). All resolution patterns in Figures 4.2d-f have relatively high values in areas where the seismic velocities are low. This can be explained by the smaller wavelengths (for a given frequency) in such features, which is expected to increase the model resolution. Conversely, model resolution within high-velocity bodies is low.

### 4.4.2 Two-sided experiment, all source and receiver components

In seismic field experiments, it is rarely possible to place sources and receivers all around the region of interest, but it is common to encompass the area of investigation with two boreholes and perform crosshole experiments. Compared to the 4-sided experiment in Figure 4.2, we reduce the source and receiver spacing for our crosshole experiments from 2.0 m to 0.5 m and densify the borehole occupation. This results in 41 source positions in one borehole and 41 receiver positions in the other, yielding $9 \times 4 \times 41 \times 41 = 60,516$ complex frequency data points.
Although the number of data points is increased by more than a factor of three, the quality of the resulting tomographic images in Figure 4.3a-c is slightly lower than those in Figure 4.2a-c, primarily due to the reduced angular coverage of the target. The $V_S$ tomogram is comparable to its comprehensive (4-sided) counterpart, but the $V_P$ and the density tomograms are somewhat inferior. In particular, the high velocity cross is not so well imaged.

The patterns of model-resolution diagonal elements in Figure 4.3d-f are also comparable to those in Figure 4.2d-f, but as expected, they show decreased values at the top and the bottom of the tomograms, where no sources and receivers are placed in the 2-sided experiment.

### 4.4.3 Two-sided experiment, x-directed sources, x- and z-directed receivers

Implementing multicomponent sources in a borehole is complicated and might require different source types for each component. This is not only very laborious from an acquisition point of view, but it can also lead to complex inversion strategies due to the difference in the source characteristics. Therefore, we restrict the next set of experiments to sources oriented perpendicular to the borehole axis.
Results from an inversion experiment with 41 $x$-directed sources and 41 two-component receivers (30,258 data points) are shown in Figure 4.4. The tomograms are very similar to those in Figure 4.3. Calculations with only $z$-directed sources and two-component receivers result in very similar images (not shown) to those displayed in Figure 4.4. It seems that application of an extra source component increases the experimental costs without yielding significant add-on information.

4.4.4 Two-sided experiment, pressure sources, $x$- and $z$-directed receivers

Directed borehole sources are generally quite arduous to operate, because they have to be clamped to the borehole walls. In contrast, pressure sources (e.g., small explosive charges, sparkers or piezo-electric sources) that achieve coupling to the borehole walls through the borehole fluid, allow much faster data acquisition. To a first approximation, pressure signals in boreholes can be considered as isotropic (omni-directional) pressure sources. Although pressure sources predominantly generate P-wave energy, the resulting seismic traces contain information on the S-wave velocity structure as a result of mode conversions at seismic discontinuities.
Inversion results for pressure sources and two-component receivers (30,258 data points) are shown in Figure 4.5. The $V_P$ and $V_S$ velocities are still well recovered, although there are clearly more artifacts in the tomograms and the edges of the crosses appear to be somewhat blurred. Considering the nature of the source, the quality of the S-wave velocity image is surprisingly good. These findings are supported by the corresponding model-resolution plots in Figure 4.5d-e. Seismic data generated with a pressure source seem to contain very little information about the densities; only a hint of structure is evident in Figure 4.5e.

### 4.4.5 Two-sided experiment, pressure sources, pressure receivers

The most efficient acquisition mode for seismic crosshole tomography includes a pressure source and hydrophones (omni-directional scalar pressure sensors) for receiving the signals. The hydrophones do not need to be clamped to the borehole walls, and many hydrophones in the form of an array can be operated simultaneously in a single streamer. The hydrophones essentially measure the cubical dilatation, or divergence of the vector displacement, thus strongly favoring P over S waves.

![Figure 4.6: As for Figure 4.2, but for a 2-sided configuration using pressure sources and pressure receivers.](image)
Intuitively, one would expect that such a setup should produce reasonable \( V_P \) images, but that \( V_S \) and \( \rho \) characteristics would be unresolved. The resulting tomograms from a pressure source and pressure receiver experiment (15,129 data points) are shown in Figure 4.6. The \( V_P \) tomogram in Figure 4.6a is rather blurred and clearly of much lower quality than equivalent tomograms in Figures 4.2 to 4.5. The \( V_S \) tomogram (Figure 4.6b) indicates the presence of the two crosses, but the signs of the anomalies are reversed! No features are distinguished in the density tomogram (Figure 4.6c), which contains artifacts in the vicinity of the two boreholes.

It would be no surprise to the vast majority of practitioners that P-wave images are better than S-wave images when using a P-wave source and P-wave receiver. The surprise is the similarity of the model-resolution diagrams. Clearly, our reliance on the diagonal elements of the resolution matrix as the sole indicator of resolution is inadequate for this example.

Additional insights into the unexpected model-resolution results are provided by the selected sensitivity patterns in Figure 4.7, computed for a source-receiver pair located approximately at the midway positions of the two boreholes. The \( V_P \) and \( V_S \) sensitivities have similar shapes and similar magnitudes. This explains the similarities of the model-resolution plots in Figure 4.6d and e, but not the differences in the quality of tomographic images in Figure 4.6a and b. The shape and low magnitudes of the density sensitivities in Figure 4.7c explain the model-resolution pattern and the tomographic image in Figure 4.6f and c. The generally low sensitivities are “boosted” by the matrix scaling applied to the Jacobian matrix (see 2D forward modeling and inversion section), and the increased sensitivity values in the “outer space” artificially

![Figure 4.7: Sensitivities for a 600 Hz pressure source in the left borehole and a single pressure receiver in the right borehole, both at 13 m depth. Sensitivities are computed for the true model. a), b), and c) Real parts of the sensitivities for \( V_P \), \( V_S \), and \( \rho \), respectively.](image-url)
enhance the model resolution in these regions (Figure 4.6f). As a consequence, the pronounced artifacts in Figure 4.6c are created. This illustrates a potential disadvantage of matrix scaling.

To understand the different qualities of the $V_P$ and $V_S$ tomograms in Figure 4.6a and b, it is necessary to consider not only the diagonal elements but the full model-resolution matrix. In Figure 4.8a, we display the full model-resolution matrix in the form of a sparse matrix plot. The black dots represent all diagonal elements and those off-diagonal elements with an absolute value larger than 50% of the corresponding diagonal element from the same row of the matrix. Since the model-resolution matrix is to a first order symmetric, a column-wise comparison would have led to a similar image.

The model vector $\mathbf{m}$ is set up such that it includes the $V_P$ values first, followed by the $V_S$ and $\rho$ entries. Accordingly, the model-resolution matrix can be subdivided into 9 sub-matrices, as indicated schematically in Figure 4.8a. Large off-diagonal elements indicate the presence of parameter trade-offs, such that the corresponding parameters cannot be resolved independently. For example, $V_P$ velocities for a given cell are expected to trade-off with $V_P$ velocities of adjacent cells. Similarly $V_S$ and $\rho$ for a given cell trade off with their counterparts in neighboring cells (i.e., the $V_S - V_S$ and $\rho - \rho$ sub-matrix entries). This explains the large off-diagonal values very near the main diagonal (this gives the main diagonal its blurred character). In addition, there

Figure 4.8. Full-model-resolution matrix shown in sparse matrix format. In addition to the diagonal elements only those values higher than 50% of the diagonal element of the same row are shown. Sub-matrices representing trade-offs between $V_P$, and $V_S$ are highlighted in blue. a) 2-sided pressure source and pressure receiver experiment. b) 2-sided pressure source and two-component receiver experiment.
are pronounced sub-diagonal entries for the sub-matrices $V_P - V_S$, $V_P - \rho$, $V_S - \rho$. Of particular interest are the off-diagonal elements that relate $V_P$ and $V_S$ velocities (i.e., those along the sub-diagonal lines highlighted by the blue boxes in Figure 4.8a). This indicates that “pressure source – pressure receiver” data cannot fully resolve these two parameters independently. Clearly, the resolving power for $V_P$ velocities is higher than that for $V_S$ velocities. The strong trade-offs in Figure 4.8a cause the $V_S$ tomogram in Figure 4.6b to act as a “garbage can”, such that any discrepancies between the true and inverted $V_P$ parameters are projected into the $V_S$ tomogram. For comparison, Figure 4.8b shows the corresponding model-resolution plot for the pressure source - multicomponent receiver experiment (Figure 4.5). Here, only marginal trade-offs between $V_P$ and $V_S$ are observed, and the associated inverted images have the correct relative magnitudes.

4.5 CASE STUDY: FEASIBILITY OF NON-INTRUSIVE MONITORING OF HIGH-LEVEL RADIOACTIVE WASTE AND SPENT FUEL (HLW/SF) REPOSITORIES USING ELASTIC WAVEFORM INVERSIONS

4.5.1 Background information

Our simulated inversions suggest that a combination of pressure sources and multicomponent receivers provide the most favorable benefit/cost ratio for full-waveform inversion experiments involving crosshole elastic data. We now consider these findings for an experimental design study devoted to a radioactive waste monitoring problem.

The ability to monitor potentially changing conditions within a high-level radioactive waste - spent fuel (HLW/SF) repository and its surroundings is likely to be a key prerequisite for public acceptance of a radioactive waste disposal program. Since the integrity of the seals of a HLW/SF repository should not be affected in any way by the monitoring system, wired in-situ sensors are not an option (IAEA, 2001). Non-intrusive monitoring with seismic tomography has been identified as a possible solution (e.g., Appendix D). At the Mont Terri rock laboratory located in western Switzerland, a HLW/SF repository has been simulated (at reduced scale) with a 1-m-diameter microtunnel (Chapter 2 and 3). Two inclined boreholes have been drilled perpendicular to the microtunnel axis. Between these boreholes, extensive seismic crosshole measurements have been performed.
The microtunnel was first filled with dry sand. Later, it was progressively water saturated and slightly overpressured. This process was monitored via several seismic measurement campaigns (Chapter 2). Analyses of the seismic data revealed that changes within the microtunnel and its surrounding excavation disturbed/damage zone (EDZ) have a clearly measurable effect on the seismic data. Manukyan et al., (2011; Chapter 2) also performed numerical simulations for identifying suitable seismic monitoring configurations that provide important information without affecting safety regulations concerning the repository seals. For detailed information on the host rock, they concluded that crosshole waveform inversions should be employed prior to the construction of the repository. Repeated crosshole measurements after construction of the repository then have the capability to identify changes of the elastic properties, but the expected variations are likely to be quite small. Accordingly, they suggested placing additional sensors as close to the repository as regulations would allow. These sensors would allow changes within the repository and its EDZ to be monitored.

### 4.5.2 Microtunnel model and experimental configuration

The conclusions of Manukyan et al., (2011; Chapter 2) are based on traveltime analyses and full-wavefield modeling. Here, we test their proposed experimental configuration using elastic waveform inversions of the simulated data. For this purpose, we consider three different scenarios at Mont Terri, namely:

(i) before excavation of the microtunnel,
(ii) after the microtunnel is filled with dry sand,
(iii) after water saturation of the sand-filled microtunnel.

At stage (i), only the unaltered host rock needs to be considered. This is a clay formation (Opalinus clay) with pronounced seismic anisotropy (Nicollin et al., 2008; Chapter 2). Developments of elastic-waveform inversion codes that incorporate anisotropy are currently underway; they were not available for this study. Consequently, we restrict our analysis to an isotropic elastic medium that mimics the Opalinus clay as close as the isotropic assumption allows. The assumed host rock structure is depicted in Figure 4.9a-c. It has average $V_p$, $V_s$, and $\rho$ values of approximately 2800 m/s, 1200 m/s, and 2500 kg/m$^3$. Ten percent stochastic
Figure 4.9: Models used to generate observed data for all 3 repository scenarios. a), b), and c) True $V_P$, $V_S$, and $\rho$ values before repository excavation. Black box and the black circles are the monitoring region and locations of receivers employed for the monitoring. d), e) and f) Values for a dry repository including a 1-m-diameter microtunnel and 1-m-wide EDZ. g), h), and i) Values after water saturation. j) - o) Close-ups of the black boxes in d) - i) with different color scales.
fluctuations with a preferential dipping orientation intended to represent a tilted layered medium are added to the background values. The elastic parameters and structural features are inferred from traveltime tomography (Chapter 2) and geological considerations (Lanyon et al., 2009).

For the dry sand scenario (ii), $V_P$, $V_S$, and $\rho$ were chosen to be 1100 m/s, 600 m/s, and 1855 kg/m$^3$ (Zimmer et al., 2007). Chapter 2 determined a trade-off between the radial extent and velocity decrease of the EDZ, such that a 1-m-wide EDZ with an average 10% velocity reduction (relative to the unaltered host rock) was a good approximation. Since we had no information concerning the density reduction in the EDZ, the respective $\rho$ values were left unchanged; because the pressure source-multicomponent receiver experiments were not sensitive to density variations (Figure 4.5), this simplification was not critical. The resulting velocity and density models for this scenario (ii) are shown in Figure 4.9d-f.

Experimental results in Manukyan et al., (2011; Chapter 2) indicate that full water saturation leads to healing of the EDZ. Therefore, for the EDZ of scenario (iii) we use elastic parameters of the unaltered host rock (i.e., full healing). For the water-saturated infill material, $V_P$, $V_S$, and $\rho$ are taken to be 1900 m/s, 600 m/s, and 2155 kg/m$^3$ (Figures 4.9g-i).

According to our findings in the previous sections and suggestions made by Manukyan et al., (2011; Chapter 2), we have simulated an initial host-rock characterization experiment in which we have placed 29 pressure sources in a downward-inclined lower borehole, 24 two-component receivers in an upward-inclined upper borehole, and 8 two-component receivers equally spaced around the microtunnel at a constant distance of 3.5 m (Figure 4.9a and j). The receivers in the borehole were oriented parallel and perpendicular to the borehole axis, whereas those around the microtunnel were oriented horizontally and vertically. Source and receiver spacings within the boreholes were 1 m. In the host rock characterization part of our simulations, we did not use data from the receivers distributed around the microtunnel (Figure 4.9j). We solved the forward problem using a $0.06 \times 0.06$ m grid cell size and merged 49 of these grids to form each $0.42 \times 0.42$ m inversion grid cell. This resulted in a total of $3 \times 5,609 = 16,827$ unknowns. Our data space included 9 frequencies resulting in $9 \times 2 \times 24 \times 29 = 12,528$ data points. The frequencies were equally spaced.
between 300 and 700 Hz. This frequency range was consistently employed for all experiments. Unfortunately, we were unable to consider higher frequencies, because the low velocities of dry sand would have resulted in very short wavelengths that would have required a very dense spatial sampling of the forward modeling grid that is currently well beyond our computational resources.

4.5.3 Determining the background (pre-excavation) model

Figure 4.10 shows the inversion results for the background model with no tunnel present. The \( V_p \) velocities are well imaged, whereas only low values of \( V_s \) close to the borehole collars are delineated. As expected from earlier test results (e.g., Figures 4.5c and 4.6c), the density structure remains virtually unresolved.

To check the reliability of the tomograms, we computed synthetic seismic traces for the true elastic parameters (Figure 4.9a-c) and the inverted models (Figures 4.10). The seismic traces were computed using a finite-difference time-domain code (Bohlen, 2002) with a 2 kHz center-frequency Ricker wavelet, which is close to the source pulse observed at Mont Terri (Chapter 3). Since we have only matched frequencies up to 700 Hz in the waveform inversion, the seismic traces were correspondingly low-pass filtered (Figure 4.11). There is very good agreement between the seismic sections computed using the true and inverted models. As an independent test, we additionally simulated seismic sections for the 8 two-component receivers located around the microtunnel (Figure 4.9j). Figure 4.12 demonstrates that seismic sections computed using the true and inverted models at these locations also match well.
4.5.4 Monitoring the microtunnel

For the monitoring phase of the numerical experiments, pressure sources at 1 m intervals were placed in both boreholes and seismic waves were simulated at the 8 two-component receivers located around the microtunnel (Figure 4.9d). This resulted in \(9 \times 8 \times 2 \times (24 + 29) = 7,632\) complex frequency data points. Since we expected changes to occur only in the close vicinity of the tunnel, we calculated the forward solution over the whole domain, but restricted the inversion domain to an 8 x 8 m box centered on the microtunnel (black rectangle in Figure 4.9a). As initial models for the inversions involving the microtunnel, we used the velocity and density distributions determined for the background model (Figure 4.10). For the solution of the forward

---

Figure 4.11: For pre-excavation conditions, comparisons of seismic sections for the true and inverted models using a pressure source in the lower borehole and receivers oriented perpendicular to the axis of the upper borehole. The simulations were carried out using a 2 kHz Ricker wavelet source and subsequent low pass filtering (700 Hz corner frequency). The true and inverted seismic traces practically overlap.

Figure 4.12: For pre-excavation conditions, comparisons of seismic sections for true and inverted models using a pressure source located at 12 m distance in the lower borehole (see Figure 4.9a) and 8 vertical-component receivers located 3.5 m from the microtunnel center (see Figure 4.9j). The simulations were carried out using a 2 kHz Ricker wavelet source and subsequent low pass filtering (700 Hz corner frequency). There is good agreement between the true and inverted seismic traces.
problem we used the same 0.06 x 0.06 m grid. However, for inversion we merged only 4 forward cells to form a 0.12 x 0.12 m grid, leading to 3 x 4,489 = 13,467 unknowns.

Figure 4.13a shows a comparison of seismic sections for the same source-receiver configuration used to generate Figure 4.12, but for the true models of the dry
and water-saturated microtunnel (Figure 4.9d-i). The seismic traces for the two scenarios exhibit clear differences, thereby indicating that they contain information about the changes from dry to water-saturated conditions. These differences are observed in signals from all source positions (e.g., Figure 4.13b).

The inversion results for the dry and water-saturated conditions are shown in Figures 4.14. The $V_p$ tomograms in Figure 4.14a and d are close to the true models in Figure 4.9j and m. The match of the $V_S$ tomograms is slightly inferior, but the inverted tomograms clearly indicate that changes have occurred around the repository. The density tomograms also show anomalous values in the area of the microtunnel, but they are not indicative of significant changes. Seismic sections simulated for the true and inverted models are very similar (e.g., Figure 4.15).

Finally, we investigate how well the tomograms in Figures 4.14 are capable of explaining the higher frequencies that are not included into the inversions. For this purpose, we show again seismic sections computed for the true and inverted models, but this time without low-pass filtering (Figure 4.16). Most features in the early parts of the sections match well, but there are significant discrepancies in the later parts of the traces. These later quite prominent phases observed in the seismic sections computed for the true models (blue traces in Figure 4.16) are the result of multiple reflections within the microtunnel. The boundaries that caused these reflections are rather blurred in the inverted models (Figure 4.14). As a result, these later phases could not be reproduced by the corresponding seismic sections (red traces in Figure 4.16) due to the absence of the higher frequencies. We consider this observation to be
more encouraging than disappointing: once computer resources allow the addition of higher frequencies in our inversion scheme, then the quality of the tomograms are expected to improve. In particular, it should be possible to image more accurately the discontinuities at the microtunnel boundaries.

4.6 DISCUSSION

Our investigations have demonstrated that several source-receiver configurations provide sufficient information for imaging small-scale features with crosshole waveform tomography. It is also noteworthy that our inversion results do not seem to depend strongly on the initial models. In fact, in all the simulations shown in Figures 4.2 to 4.6, we started with homogeneous models, and for the waste repository study inverted values of the unaltered host rock were used.

The discrepancies between the unfiltered seismic traces computed with the true and inverted Mont Terri models (Figure 4.16) indicate that elastic waveform inversion may be capable of delineating sharp discontinuities once higher frequencies are included. To take advantage of this feature, it may be useful to modify the smoothness constraints in the Gauss-Newton algorithm, such that an $L_1$ norm regularization would be applied. Several studies have demonstrated that $L_1$ norm regularization better reconstructs model edges (e.g., Theune, 2010). This could be implemented using the approach proposed by Farquharson and Oldenburg (1998).

An important finding of our study concerns the trade-offs between the inverted $V_p$ and $V_S$ velocities (Figure 4.6). We expect this to be even more severe for anisotropic inversions. This was also indicated in the study by Gholami et al., (2010).
We suggest performing analyses similar to those presented in this paper, but for the more challenging anisotropic case.

4.7 CONCLUSIONS

We have used a novel 2D elastic full-waveform frequency-domain inversion algorithm that employs finite-element forward modeling with a direct-matrix solver and explicit expressions for the sensitivities contained in the Jacobian matrix. This allows Gauss-Newton inversions to be computed in a very efficient manner, but this advantage comes at the expense of increased memory requirements. Our numerical experiments clearly demonstrate that under ideal conditions (e.g., multicomponent sources and multicomponent receivers placed all around the area of interest and low noise environments), high quality images for $V_P$, $V_S$ and $\rho$ can be obtained. Analyses of the diagonal elements of the model-resolution matrix indicate that even crosshole pressure source - pressure receiver data sets contain information about both $V_P$ and $V_S$ velocities, but tomographic inversions and consideration of the full model-resolution matrix indicate that these two parameters cannot be resolved independently for such data sets. For a more advanced scenario, in which pressure sources are placed in one borehole and two-component receivers are placed in another borehole, satisfactory $V_P$ and $V_S$ tomograms can be derived, but the density structure remains unresolved.

The finding that pressure source - multicomponent receiver experiments lead to satisfactory tomographic images has been exploited in a design study for monitoring high-level radioactive waste. Our results indicate that such non-intrusive monitoring experiments are indeed capable of characterizing a repository and its surroundings by means of full-waveform elastic inversion. Further work is required to fully implement an anisotropic elastic inversion code, which would be more appropriate for the actual rock conditions at the Mont Terri simulated nuclear waste repository field site.

4.8 ACKNOWLEDGEMENTS

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APPENDIX 4.A: SENSITIVITY INTEGRATIONS

The integrands in equation 4.5 describe point sensitivities. For the inversion, the sensitivities of cells having finite dimensions need to be computed. For the 2D constant-block parameterization, we consider rectangles of dimension $\Delta x \times \Delta z$. Using the simplified assumption that the Green’s functions vary linearly within each block, finite-element shape functions can be used to evaluate the integrals (Zhou and Greenhalgh 1999). The Green’s function at an arbitrary point $\hat{\Omega}$ within a block can be expressed as:

$$G_{\hat{k}l}^{\hat{e}} = \sum_{e=1}^{4} N_{e}(\hat{\Omega})G_{\hat{k}l}^{\hat{e}}, \quad (4.A-1)$$

where the sum runs over the 4 corner points $\hat{\Omega}_e$ and the shape functions $N_e$ are given by:

$$N_e = \frac{1}{4}(1 + \xi_x)(1 + \eta_e), \quad (4.A-2)$$

The natural coordinates $\xi$ and $\eta$, which transform from the actual co-ordinates $x$, $z$ to the unit square, are defined as:

$$\xi = \frac{2}{\Delta x} (x - x_{\text{center}}),$$
$$\eta = \frac{2}{\Delta z} (z - z_{\text{center}}), \quad (4.A-3)$$

and $(x_{\text{center}}, z_{\text{center}})$ is the center of the block (Figure 4.A-1). The corner points $\xi_e$, and $\eta_e$ are at (-1, -1), (1, -1), (1, 1), (-1, 1).

Integration of the sensitivities over a block involves computing integrals of the form:

$$\int \int_{-1 \leq \xi \leq 1, -1 \leq \eta \leq 1} N_e N_f^{\text{source}} d\xi d\eta \quad (e, f = 1...4),$$
$$\int \int_{-1 \leq \xi \leq 1, -1 \leq \eta \leq 1} \frac{\partial N_e^{\text{source}}}{\partial \xi_i} \frac{\partial N_f^{\text{receiver}}}{\partial \xi_j} d\xi d\eta \quad (i, j = 1, 2; e, f = 1...4), \quad (4.A-4)$$
$$\int \int_{-1 \leq \xi \leq 1, -1 \leq \eta \leq 1} N_e \frac{\partial N_f^{\text{receiver}}}{\partial \xi_i} d\xi d\eta \quad (i = 1, 2; e, f = 1...4).$$

These integrals can be evaluated analytically:

$$\int \int_{-1 \leq \xi \leq 1, -1 \leq \eta \leq 1} N_e N_f^{\text{receiver}} d\xi d\eta = \frac{1}{36} (3 + \xi_x\xi_y)(3 + \eta_x\eta_y) = \Psi_{ij}^{(l)}. \quad (4.A-5)$$

The expressions for the spatial derivatives with respect to $x$ and $z$ are:
Hence, the sensitivities for each cell can be written as:

\[
\frac{\partial u_{ij}^q}{\partial V_p} = -2\rho V_p f(\omega) \sum_{e,f=1}^{4} G^{(\delta)}_{ks_a} G^{(\delta)}_{bs_b} \Psi_{eijab}^{(2)},
\]

\[
\frac{\partial u_{ij}^q}{\partial V_s} = 2\rho V_s f(\omega) \left\{ 2 \sum_{e,f=1}^{4} G^{(\delta)}_{ks_a} G^{(\delta)}_{bs_b} \Psi_{eijab}^{(2)} - \left[ \sum_{e,f=1}^{4} G^{(\delta)}_{ks_a} G^{(\delta)}_{bs_b} \Psi_{eijab}^{(2)} + \sum_{e,f=1}^{4} G^{(\delta)}_{ks_a} G^{(\delta)}_{bs_b} \Psi_{eijab}^{(2)} \right] \right\},
\]

(4.A-7)

\[
\frac{\partial u_{ij}^q}{\partial \rho} = f(\omega) \left\{ \omega^2 \sum_{e,f=1}^{4} G^{(\delta)}_{ks_a} G^{(\delta)}_{bs_b} \Psi_{eijab}^{(1)} - (V_p^2 - 2V_s^2) \sum_{e,f=1}^{4} G^{(\delta)}_{ks_a} G^{(\delta)}_{bs_b} \Psi_{eijab}^{(2)} \right\}.
\]

The \( \Psi^{(1)} \) and \( \Psi^{(2)} \) factors depend on the indices \( a \) and \( b \). They only have to be calculated once.
APPENDIX 4.B: PRESSURE SOURCES AND PRESSURE RECEIVERS

For 2D elastic isotropic wave propagation, a pressure source can be formulated as an increase in the diagonal components of the stress tensor:

\[
\sigma_{xx} = \sigma_{zz} = -p . \tag{4.B-1}
\]

If \( G^x_{il} \) and \( G^z_{il} \) are the solutions of equation 4.1 for \( x \)- and \( z \)-directed sources located at position \( i \), then the solution for a pressure source at the same location is given by:

\[
G^p_{il} = \frac{\partial G^x_{il}}{\partial x_i} + \frac{\partial G^z_{il}}{\partial z_i} , \tag{4.B-2}
\]

where \( x_i \) and \( z_i \) are the Cartesian coordinates of the source and the subscript \( p \) indicates a pressure source.

Similarly, for each location in space at any point in time, the pressure can be calculated from the stress tensor as:

\[
p = -\frac{\sigma_{xx} + \sigma_{zz}}{2}. \tag{4.B-3}
\]

In the isotropic elastic case, the diagonal elements of the stress tensor can be written as:

\[
\sigma_{xx} = \rho V_p^2 \frac{\partial u_x}{\partial x} + \rho \left( V_p^2 - 2V_s^2 \right) \frac{\partial u_z}{\partial z} ,
\]

\[
\sigma_{zz} = \rho \left( V_p^2 - 2V_s^2 \right) \frac{\partial u_x}{\partial z} + \rho V_p^2 \frac{\partial u_z}{\partial z} . \tag{4.B-4}
\]

Hence, if \( G^x_{kj} \) and \( G^z_{kj} \) are the \( x \)- and \( z \)-directed displacements at location \( j \) (for an impulsive source) then the pressure at the same location is given by:

\[
G^p_{jk} = -\rho \left( V_p^2 - V_s^2 \right) \left( \frac{\partial G^x_{kj}}{\partial x_j} + \frac{\partial G^z_{kj}}{\partial z_j} \right) . \tag{4.B-5}
\]

Applying equations 4.B-2 and 4.B-5 to equation 4.5 will not change the form of equation 4.5 but rather increase its applicability for \( k \) and \( l \) to assume \( x \), \( z \) and \( p \) values.

Similarly, in equation 4.A-7, \( k \) and \( l \) can take on values \( x \), \( z \), and \( p \).
CHAPTER 5

Elastic wave modeling (and inversion) in vertically transversely isotropic media
5.1 INTRODUCTION

In Chapter 4, I considered the reconstruction capabilities of seismic waveform inversion in the context of radioactive waste repository imaging. The medium was assumed to be elastic and isotropic. However, Opalinus clay, the preferred repository host rock in Switzerland, is seismically anisotropic. This needs to be taken into account in the inversion. To a first approximation, Opalinus clay can be represented as a transversely isotropic (TI) solid. This is one of the simplest classes of anisotropy. It is rather prevalent in nature. In TI media, there is a single axis of symmetry. In the plane perpendicular to this axis, there is no directional dependence in the wavespeed. Such planes might coincide with the platy fabric of the rock, the bedding plane, the fracture plane or the joint orientation. For waves travelling in all directions other than in this plane, there is a directional dependence in the wavespeed. Five elastic constants are required to characterize a TI medium.

In this chapter, I extend the modeling (and inversion) analysis for TI media having a vertical axis of symmetry. The extension to arbitrary tilt angles of the symmetry axis can be achieved through coordinate rotations. Moreover, the real data involves point sources having 3D wavefield characteristics (as opposed to line sources assumed in 2D modeling) and so this has to be taken into account in the inversion of field data.

5.2. GOVERNING EQUATIONS

The 3D elastic equation of motion in the time-space domain can be written as (Aki and Richards, 1980):

$$\rho \ddot{u}_i - C_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} = F_i, \quad (5.1)$$

where $i, j, k$ and $l$ take on the values 1, 2 and 3 ($x_1, x_2$ and $x_3$ correspond to $x, y$ and $z$ in Cartesian coordinates), $\rho$ is the density, $u_i$ is the $i$-th component of the displacement vector, $C_{ijkl}$ is the elasticity modulus tensor, and $F_i$ is the $i$-th component of the external force. By performing a temporal Fourier transform, one can obtain the 3D elastic equation of motion in the frequency-space domain:

$$-\rho \omega^2 \tilde{u}_i - C_{ijkl} \frac{\partial^2 \tilde{u}_k}{\partial x_j \partial x_l} = \tilde{F}_i, \quad (5.2)$$

where $\tilde{A}(\omega, x, y, z)$ is the temporal Fourier transform of $A(t, x, y, z)$:
\[
\bar{A}(\omega, x, y, z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(t, x, y, z) e^{-i\omega t} \, dt,
\]
\[
A(t, x, y, z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \bar{A}(\omega, x, y, z) e^{i\omega t} \, d\omega.
\]

Because of the symmetry in the 3 x 3 x 3 x 3 elastic modulus tensor \(C_{ijkl}\), one can use reduced Voigt notation and write it as a 6 x 6 matrix in \(C_{\alpha\beta}\) form:

\[
\begin{array}{cccccc}
i j & or & kl & : & 11 & 22 & 33 & 32 = 23 & 31 = 13 & 12 = 21 \\
\downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow
\end{array}
\]

\(\alpha\beta 1 2 3 4 5 6\). (5.4)

In the most general anisotropic medium, \(C\) has 21 independent components. In the vertically transversely isotropic (VTI) media, this reduces to just 5 independent coefficients (\(C_{11}, C_{13}, C_{33}, C_{44},\) and \(C_{66}\)) that can be written as:

\[
C = \begin{bmatrix}
C_{11} & (C_{11} - 2C_{66}) & C_{13} \\
(C_{11} - 2C_{66}) & C_{11} & C_{13} \\
C_{13} & C_{13} & C_{33} \\
C_{44} & & & C_{44} \\
& & & & C_{66}
\end{bmatrix}.
\]

(5.5)

Taking into account equation 5.5, the equation of motion 5.2 can be written as:

\[
0 = \rho \omega^2 \bar{u}_x + \partial_x \left[ C_{11} \partial_x \bar{u}_x + (C_{11} - 2C_{66}) \partial_y \bar{u}_y + C_{13} \partial_z \bar{u}_z \right] \\
+ \partial_y \left[ C_{66} \partial_y \bar{u}_y + C_{66} \partial_y \bar{u}_x \right] \\
+ \partial_z \left[ C_{44} \partial_z \bar{u}_z + C_{44} \partial_z \bar{u}_x \right] + \bar{f}_x,
\]

(5.6)

\[
0 = \rho \omega^2 \bar{u}_y + \partial_x \left[ C_{66} \partial_x \bar{u}_x + C_{66} \partial_y \bar{u}_y \right] \\
+ \partial_y \left[ (C_{11} - 2C_{66}) \partial_y \bar{u}_y + C_{11} \partial_y \bar{u}_y + C_{13} \partial_z \bar{u}_z \right] \\
+ \partial_z \left[ C_{44} \partial_z \bar{u}_z + C_{44} \partial_z \bar{u}_y \right] + \bar{f}_y,
\]

(5.7)

\[
0 = \rho \omega^2 \bar{u}_z + \partial_x \left[ C_{44} \partial_x \bar{u}_x + C_{44} \partial_z \bar{u}_z \right] \\
+ \partial_y \left[ C_{44} \partial_y \bar{u}_y + C_{44} \partial_z \bar{u}_z \right] \\
+ \partial_z \left[ C_{13} \partial_z \bar{u}_z + C_{13} \partial_y \bar{u}_y + C_{33} \partial_z \bar{u}_z \right] + \bar{f}_z,
\]

(5.8)

Since in our experiments model parameters are not expected to change along the microtunnel axis (y direction), a Fourier transform can be taken in the y direction to obtain the 2.5D equation of motion. Hence equations 5.6 - 5.8 transform into:
\[ 0 = \rho \omega^2 \ddot{\mathbf{u}}_x + \partial_x \left[ C_{11} \partial_x \ddot{\mathbf{u}}_x + ik_y \left( C_{11} - 2C_{66} \right) \ddot{\mathbf{u}}_y + C_{13} \partial_z \ddot{\mathbf{u}}_z \right] \]
\[ + ik_y \left[ C_{66} \partial_x \ddot{\mathbf{u}}_y + ik_y C_{66} \ddot{\mathbf{u}}_y \right] \]
\[ + \partial_z \left[ C_{44} \partial_z \ddot{\mathbf{u}}_z + C_{44} \partial_z \ddot{\mathbf{u}}_y \right] + \ddot{f}_x , \] (5.9)

\[ 0 = \rho \omega^2 \ddot{\mathbf{u}}_y + \partial_x \left[ C_{66} \partial_x \ddot{\mathbf{u}}_y + ik_y C_{66} \ddot{\mathbf{u}}_y \right] \]
\[ + ik_y \left[ \left( C_{11} - 2C_{66} \right) \partial_x \ddot{\mathbf{u}}_x + ik_y C_{11} \ddot{\mathbf{u}}_y + C_{13} \partial_z \ddot{\mathbf{u}}_z \right] \]
\[ + \partial_z \left[ ik_y C_{44} \ddot{\mathbf{u}}_y + C_{44} \partial_z \ddot{\mathbf{u}}_y \right] + \ddot{f}_y , \] (5.10)

\[ 0 = \rho \omega^2 \ddot{\mathbf{u}}_z + \partial_x \left[ C_{44} \partial_x \ddot{\mathbf{u}}_z + C_{44} \partial_z \ddot{\mathbf{u}}_y \right] \]
\[ + ik_y \left[ ik_y C_{44} \ddot{\mathbf{u}}_y + C_{44} \partial_z \ddot{\mathbf{u}}_y \right] \]
\[ + \partial_z \left[ C_{13} \partial_z \ddot{\mathbf{u}}_z + ik_y C_{13} \ddot{\mathbf{u}}_y + C_{33} \partial_z \ddot{\mathbf{u}}_z \right] + \ddot{f}_z , \] (5.11)

where \( \ddot{A}(\omega, x, k_y, z) \) is the double (temporal and spatial) Fourier transform of \( A(t, x, y, z) \):

\[ \ddot{A}(\omega, x, k_y, z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(t, x, y, z) e^{-ik_y y} dy, \] (5.12)

\[ \ddot{A}(\omega, x, y, z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \ddot{A}(\omega, x, k_y, z) e^{ik_y y} dk_y. \]

5.3 WAVE PROPAGATION IN VTI MEDIA: FEM IMPLEMENTATION

5.3.1. Formulation

Equations 5.9 - 5.11 can be solved using the finite-element method. Below, I follow the approach described in Latzel (2010) for solving the partial differential equations. I start with equation 5.9, multiply it with an arbitrary weighting function \( W_j(x, z) \) and integrate over the domain \( \Omega \) in the \( x - z \) plane. This leads to:

\[ 0 = \int_{\Omega} \left[ W_j \rho \omega^2 \ddot{\mathbf{u}}_x + W_j \ddot{f}_x \right] d\Omega \]
\[ + \int_{\Omega} \left[ W_j \partial_x \left[ C_{11} \partial_x \ddot{\mathbf{u}}_x + ik_y \left( C_{11} - 2C_{66} \right) \ddot{\mathbf{u}}_y + C_{13} \partial_z \ddot{\mathbf{u}}_z \right] \right] d\Omega \]
\[ + \int_{\Omega} \left[ \left( C_{66} \partial_x \ddot{\mathbf{u}}_y + ik_y C_{66} \ddot{\mathbf{u}}_y \right) \right] d\Omega \]
\[ + \int_{\Omega} \left[ \partial_z \left[ C_{44} \partial_z \ddot{\mathbf{u}}_z + C_{44} \partial_z \ddot{\mathbf{u}}_y \right] \right] d\Omega. \] (5.13)

After integrating by parts one obtains:
\[
0 = \int_{\Omega} \left\{ W_j \rho_0 \omega^2 \bar{\mathbf{u}}_x + W_j \bar{f}_x \right\} d\Omega \\
+ \int_{\Omega} \left\{ -\partial_x W_j \left[ C_{11} \partial_x \bar{\mathbf{u}}_x + ik_y \left( C_{11} - 2C_{66} \right) \bar{\mathbf{u}}_y + C_{13} \partial_z \bar{\mathbf{u}}_z \right] \right\} d\Omega \\
+ \int_{\Omega} \left\{ ik_y W_j \left[ C_{66} \partial_y \bar{\mathbf{u}}_y + ik_y C_{66} \bar{\mathbf{u}}_x \right] \right\} d\Omega \\
+ \int_{\Omega} \left\{ -\partial_y W_j \left[ C_{44} \partial_y \bar{\mathbf{u}}_y + C_{44} \partial_z \bar{\mathbf{u}}_z \right] \right\} d\Omega \\
+ \oint_{\Gamma} \left\{ W_j \left[ C_{11} \partial_x \bar{\mathbf{u}}_x + ik_y \left( C_{11} - 2C_{66} \right) \bar{\mathbf{u}}_y + C_{13} \partial_z \bar{\mathbf{u}}_z \right] \right\} n_x d\Gamma \\
+ \oint_{\Gamma} \left\{ W_j \left[ C_{44} \partial_y \bar{\mathbf{u}}_y + C_{44} \partial_z \bar{\mathbf{u}}_z \right] \right\} n_y d\Gamma,
\]

where \( \Gamma = \partial \Omega \) is the boundary of \( \Omega \). In the following, \( \Omega = [x_1, x_2] \times [z_1, z_2] \subset \mathbb{R}^2 \) denotes the area of one element in the FEM mesh (Figure 5.1). I denote:

\[
I_1^x = \int_{\Omega} \left\{ W_j \rho_0 \omega^2 \bar{\mathbf{u}}_x + W_j \bar{f}_x \right\} d\Omega,
\]

\[
I_2^x = \int_{\Omega} \left\{ -\partial_x W_j \left[ C_{11} \partial_x \bar{\mathbf{u}}_x + ik_y \left( C_{11} - 2C_{66} \right) \bar{\mathbf{u}}_y + C_{13} \partial_z \bar{\mathbf{u}}_z \right] \right\} d\Omega \\
+ \int_{\Omega} \left\{ ik_y W_j \left[ C_{66} \partial_y \bar{\mathbf{u}}_y + ik_y C_{66} \bar{\mathbf{u}}_x \right] \right\} d\Omega \\
+ \int_{\Omega} \left\{ -\partial_y W_j \left[ C_{44} \partial_y \bar{\mathbf{u}}_y + C_{44} \partial_z \bar{\mathbf{u}}_z \right] \right\} d\Omega,
\]
\[ I_j^* = \oint_\Gamma \left[ C_{1j} \partial_x \bar{u}_x + \partial_y \left( C_{1j} - 2C_{66} \right) \bar{u}_y + C_{1j} \partial_z \bar{u}_z \right] n_z \, d\Gamma \]
\[ + \oint_\Gamma \left[ C_{4j} \partial_x \bar{u}_x + C_{4j} \partial_z \bar{u}_z \right] n_z \, d\Gamma. \]  

(5.17)

The surface integral \( I_j^* \) will either cancel on assemblages of adjacent elements or will vanish over the boundary of the domain through the use of Neumann boundary conditions (viz., zero value for the derivative of the quantity with respect to the boundary normal direction).

To derive the matrix formulation, I approximate the solution wavefield by means of linear shape functions:

\[ \bar{u}_I = \sum_k \bar{u}_I^K \left( k_j \right) N_K \left( x, z \right). \]  

(5.18)

For the weighting functions \( N_j \), one can use the Galerkin approach \( W_j = N_j \). This leads to:

\[ I_1^* = \sum_k \bar{u}_I^K \int_{\Omega} N_j \rho N_K d\Omega + \int_{\Omega} N_j \bar{f}_I d\Omega, \]  

(5.19)

\[ I_2^* = \sum_k \bar{u}_I^K \int_{\Omega} \left( -\partial_x N_j C_{1j} \partial_x N_K - \partial_y N_j C_{4j} \partial_z N_K \right) d\Omega \]
\[ + \sum_k \bar{u}_I^K \int_{\Omega} \left( -\partial_z N_j C_{1j} \partial_x N_K + \partial_y N_j C_{4j} \partial_z N_K \right) d\Omega \]  

(5.20)

Likewise, by repeating the same steps for equation 5.10 and 5.11, I finally arrive at the matrix equation solution in the following form

\[ \omega^2 M U + K U + F = 0, \]  

(5.21)

where I used rectangular elements (Figure 5.1):

\[ U = \begin{bmatrix} \bar{u}_x \\ \bar{u}_z \\ \bar{u}_y \end{bmatrix} \quad \text{with} \quad \bar{u}_I = \begin{bmatrix} \bar{u}_I^x \\ \bar{u}_I^z \\ \bar{u}_I^y \end{bmatrix} \]  

(5.22)

and the shape function matrix \( N \):
The mass matrix \( M \) has the form:

\[
M = \begin{bmatrix}
M_{xx} & 0 & 0 \\
0 & M_{zz} & 0 \\
0 & 0 & M_{yy}
\end{bmatrix}
\]

with \( M_{ii} = \begin{bmatrix} M_{Iii} & M_{Jii} & M_{Kii} & M_{Lii} \\ M_{Iii} & M_{Jii} & M_{Kii} & M_{Lii} \\ M_{Kii} & M_{Kii} & M_{Kii} & M_{Kii} \\ M_{Lii} & M_{Lii} & M_{Lii} & M_{Lii} \end{bmatrix}, \tag{5.24}
\]

and the stiffness matrix \( K \) is given by

\[
K = \begin{bmatrix}
K_{xx} & K_{xz} & K_{xz} \\
K_{zx} & K_{zz} & K_{zy} \\
K_{xy} & K_{yz} & K_{yy}
\end{bmatrix}
\]

with \( K_{ij} = \begin{bmatrix} K_{Iij} & K_{Jij} & K_{Kij} & K_{Lij} \\ K_{Iij} & K_{Jij} & K_{Kij} & K_{Lij} \\ K_{Kij} & K_{Kij} & K_{Kij} & K_{Kij} \\ K_{Lij} & K_{Lij} & K_{Lij} & K_{Lij} \end{bmatrix}. \tag{5.25}
\]

For constant values of \( C_{ij} \) within each element, these parameters can be taken out of the integrals for calculating the elements of the \( M \) and \( K \) matrices. Hence, one only needs to calculate nine different integrals:

\[
\int N_t^2 N_b d\Omega, \quad \int \partial_x N_t N_b d\Omega, \quad \int N_t \partial_x N_b d\Omega, \quad \int N_t \partial_z N_b d\Omega, \quad \int \partial_x N_t \partial_x N_b d\Omega, \quad \int \partial_x N_t \partial_z N_b d\Omega, \quad \int \partial_z N_t \partial_x N_b d\Omega, \quad \int \partial_z N_t \partial_z N_b d\Omega, \quad \int \partial_z N_t \partial_z N_b d\Omega
\]

and \( \int N_t \partial_\xi N_b d\Omega \) for these integrations, it is convenient to define local coordinates \((\xi, \eta)\) (Figure 5.1). The relationship between the global and local coordinates for an element with its lower left corner at \((x_1, z_1)\) and its upper right corner at \((x_2, z_2)\) is:

\[
\xi = \frac{x - x_m}{\Delta x}, \quad \eta = \frac{z - z_m}{\Delta z}, \tag{5.26}
\]

where \( x_m = \frac{1}{2}(x_1 + x_2) \) and \( z_m = \frac{1}{2}(z_1 + z_2) \) are the coordinates of the midpoint and \( \Delta x = (x_2 - x_1) \) and \( \Delta z = (z_2 - z_1) \) are the side lengths of the element. For the derivatives and the volume element from equation 5.26, we obtain:
\[ \frac{\partial s}{\Delta x} = \frac{2}{\Delta x} \frac{\partial \xi}{\eta}, \]  
(5.27)

\[ \frac{\partial z}{\Delta z} = \frac{2}{\Delta z} \frac{\partial \eta}{\xi}, \]  
(5.28)

\[ d\Omega = dx dz = \frac{\Delta x \Delta z}{4} d\xi d\eta. \]  
(5.29)

Using linear shape functions, we have:

\[ N_i = \frac{1}{4} (1 - \xi)(1 + \eta), \]

\[ N_j = \frac{1}{4} (1 + \xi)(1 + \eta), \]

\[ N_K = \frac{1}{4} (1 + \xi)(1 - \eta), \]

\[ N_L = \frac{1}{4} (1 - \xi)(1 - \eta), \]  
(5.30)

where the subscripts refer to the nodes of the element (Figure 5.1). From the choice of shape function, the values of the necessary integrals can be computed as:

\[ I_{s0}^{AB} := \int N_i N_j d\Omega = \begin{bmatrix} 4 & 2 & 2 & 1 \\ 2 & 4 & 1 & 2 \\ 2 & 1 & 4 & 2 \\ 1 & 2 & 2 & 4 \end{bmatrix} \frac{\Delta x \Delta z}{36}, \]  
(5.31)

\[ I_{s0}^{AB} := \int \frac{\partial s}{\Delta x} N_i N_j d\Omega = \begin{bmatrix} -2 & -1 & -2 & -1 \\ -1 & -2 & -1 & -2 \\ 2 & 1 & 2 & 1 \\ 1 & 2 & 1 & 2 \end{bmatrix} \frac{\Delta z}{12}, \]  
(5.32)

\[ I_{s0}^{AB} := \int N_i \frac{\partial z}{\Delta z} N_j d\Omega = \begin{bmatrix} -2 & -1 & 2 & 1 \\ -1 & -2 & 1 & 2 \\ -2 & -1 & 2 & 1 \\ -1 & -2 & 1 & 2 \end{bmatrix} \frac{\Delta z}{12}, \]  
(5.33)

\[ I_{s0}^{AB} := \int \frac{\partial s}{\Delta x} N_i N_j d\Omega = \begin{bmatrix} -2 & -2 & -1 & -1 \\ 2 & 2 & 1 & 1 \\ -1 & -1 & -2 & -2 \\ 1 & 1 & 2 & 2 \end{bmatrix} \frac{\Delta x}{12}, \]  
(5.34)

\[ I_{s0}^{AB} := \int \frac{\partial z}{\Delta z} N_i N_j d\Omega = \begin{bmatrix} -2 & 2 & -1 & 1 \\ -2 & 2 & -1 & 1 \\ -1 & 1 & -2 & 2 \\ -1 & 1 & -2 & 2 \end{bmatrix} \frac{\Delta x}{12}, \]  
(5.35)
where the pair of lower indices mean derivatives with respect to \(x, z\) or no derivatives for \(N_A\) and \(N_B\), respectively with \(A,B \in \{I,J,K,L\}\). The following matrix notation is used:

\[
\begin{bmatrix}
  II & IJ & IK & IL \\
  JI & JJ & JK & JL \\
  KI & KJ & KK & KL \\
  LI & LJ & LK & LL \\
\end{bmatrix}
\]

These integrals allow the mass and stiffness matrices to be written in a compact form:

\[
M_{JKxx} = M_{JKyy} = M_{JKzz} = I_{00}^J K, \\
K_{JKxx} = -C_{11} I_{xx}^{J} - k_2^2 C_{66} I_{00}^{JK} - C_{44} I_{zz}^{JK}, \\
K_{JKyy} = -ik_y (C_{11} - 2C_{66}) I_{x0}^{JK} + ik_y C_{66} I_{0x}^{JK}, \\
K_{JKzz} = -C_{13} I_{xz}^{JK} - C_{44} I_{xz}^{JK}, \\
K_{JKxy} = -ik_x C_{66} I_{x0}^{JK} + ik_y (C_{11} - 2C_{66}) I_{0x}^{JK}, \\
K_{JKyz} = -C_{66} I_{xz}^{JK} - k_2^2 C_{11} I_{00}^{JK} - C_{44} I_{zz}^{JK}, \\
K_{JKzx} = ik_x C_{13} I_{0x}^{JK} - ik_y C_{44} I_{20}^{JK}, \\
K_{JKzy} = -C_{44} I_{xz}^{JK} - C_{13} I_{xz}^{JK}, \\
K_{JKzy} = ik_x C_{44} I_{0x}^{JK} - ik_y C_{13} I_{0x}^{JK}, \\
K_{JKzz} = -C_{44} I_{xx}^{JK} - k_2^2 C_{44} I_{00}^{JK} - C_{33} I_{zz}^{JK}.
\]
5.3.2 Perfectly matched layer boundary conditions

A similar derivation can also be followed for the boundary layer (or perfectly matched layer, PML). In the PML, I follow the formulations given by Zheng and Huag (2002) and Basu and Chopra (2003) and use the following complex coordinate stretching approach:

\[ \bar{x}_i = \int_0^{x_i} \varepsilon_i(s) \, ds, \quad i = x, z, \quad (5.42) \]

where \( \varepsilon_i = 1 \) at the boundary of the computational domain and there is no coordinate stretching in the \( y \) direction. Following Latzel (2010), I use linear stretching for the PMLs:

\[ \varepsilon_x = 1 - i(\alpha_x + \beta_x \xi), \]
\[ \varepsilon_z = 1 - i(\alpha_z + \beta_z \eta). \quad (5.43) \]

From equation 5.42, I obtain:

\[ \frac{d}{d\bar{x}_i} = \frac{1}{\varepsilon_i} \frac{d}{dx_i}, \quad i = x, z. \quad (5.44) \]

Hence, for elements in the PML layer, equations 5.9 - 5.11 become:

\[ 0 = \rho \omega^2 \varepsilon_x \varepsilon_z \bar{u}_y + \partial_x \left[ \frac{\varepsilon_x}{\varepsilon_z} C_{11} \partial_x \bar{u}_x + ik_y \varepsilon_x \left( C_{11} - 2C_{66} \right) \bar{u}_y + C_{13} \bar{u}_z \right] \]
\[ + ik_y \left[ \varepsilon_x C_{66} \partial_y \bar{u}_y + ik_y \varepsilon_x C_{66} \bar{u}_x \right] \]
\[ + \partial_z \left[ C_{44} \partial_z \bar{u}_z + \frac{\varepsilon_x}{\varepsilon_z} C_{44} \bar{u}_x \right] + \varepsilon_x \varepsilon_z \bar{f}_y, \quad (5.45) \]

\[ 0 = \varepsilon_x \varepsilon_z \rho \omega^2 \bar{u}_y + \partial_x \left[ \frac{\varepsilon_x}{\varepsilon_z} C_{66} \partial_x \bar{u}_y + ik_y \varepsilon_x C_{66} \bar{u}_x \right] \]
\[ + ik_y \left[ \varepsilon_x \left( C_{11} - 2C_{66} \right) \partial_y \bar{u}_y + ik_y \varepsilon_x \bar{u}_y + \varepsilon_x C_{13} \bar{u}_z \right] \]
\[ + \partial_z \left[ ik_y \varepsilon_x C_{44} \partial_z \bar{u}_z + \frac{\varepsilon_x}{\varepsilon_z} C_{44} \partial_z \bar{u}_x \right] + \varepsilon_x \varepsilon_z \bar{f}_y, \quad (5.46) \]

\[ 0 = \varepsilon_x \varepsilon_z \rho \omega^2 \bar{u}_y + \partial_x \left[ \frac{\varepsilon_x}{\varepsilon_z} C_{44} \partial_x \bar{u}_z + C_{44} \partial_z \bar{u}_x \right] \]
\[ + ik_y \left[ ik_y \varepsilon_x \varepsilon_z C_{44} \bar{u}_y + \varepsilon_x C_{44} \partial_z \bar{u}_x \right] \]
\[ + \partial_z \left[ C_{13} \partial_z \bar{u}_z + ik_y C_{13} \bar{u}_y + \frac{\varepsilon_x}{\varepsilon_z} C_{33} \partial_z \bar{u}_x \right] + \varepsilon_x \varepsilon_z \bar{f}_y, \quad (5.47) \]
Following the same steps as for equations 5.9 - 5.11, we obtain for the modified equations 5.45 - 5.47 the expressions:

$$
\tilde{M}_{jkxx} = \tilde{M}_{jkxy} = \tilde{M}_{jkzz} = \rho \tilde{t}_{00}^{AB},
$$

(5.48)

$$
K_{jkxx} = -C_{11} \tilde{t}_{jk}^{xx} - k_1^2 C_{66} \tilde{t}_{jk}^{xx} - C_{44} \tilde{t}_{jk}^{zz},
$$

$$
K_{jkxy} = -i k_y \left( C_{11} - 2 C_{66} \right) \tilde{t}_{jk}^{xy} + i k_y C_{66} \tilde{t}_{jk}^{xy},
$$

$$
K_{jkzz} = -C_{13} \tilde{t}_{jk}^{zz} - C_{44} \tilde{t}_{jk}^{zz},
$$

(5.49)

$$
K_{jkyy} = -i k_y C_{44} \tilde{t}_{jk}^{yy} + i k_y \left( C_{11} - 2 C_{66} \right) \tilde{t}_{jk}^{yy},
$$

$$
K_{jkyy} = -C_{44} \tilde{t}_{jk}^{yy} - C_{33} \tilde{t}_{jk}^{yy},
$$

where $\tilde{t}_{jk}^{AB}$ are defined as follows

$$
\tilde{t}_{00}^{AB} := \int \varepsilon \varepsilon_s N_A N_B d\Omega,
$$

(5.50)

$$
\tilde{t}_{x0}^{AB} := \int \varepsilon_x \partial_x N_A N_B d\Omega,
$$

(5.51)

$$
\tilde{t}_{0x}^{AB} := \int \varepsilon_x N_x \partial_x N_B d\Omega,
$$

(5.52)

$$
\tilde{t}_{z0}^{AB} := \int \varepsilon_z \partial_z N_A N_B d\Omega,
$$

(5.53)

$$
\tilde{t}_{0z}^{AB} := \int \varepsilon_z N_z \partial_z N_B d\Omega,
$$

(5.54)

$$
\tilde{t}_{xx}^{AB} := \int \frac{E_x}{E_x} \partial_x N_A \partial_x N_B d\Omega,
$$

(5.55)

$$
\tilde{t}_{zz}^{AB} := \int \frac{E_z}{E_z} \partial_z N_A \partial_z N_B d\Omega,
$$

(5.56)

$$
\tilde{t}_{xz}^{AB} := \int \partial_x N_x \partial_x N_B d\Omega = I_{xz}^{AB},
$$

(5.57)

$$
\tilde{I}_{xz}^{AB} := \int \partial_z N_z \partial_z N_B d\Omega = I_{xz}^{AB}.
$$

(5.58)

Taking into account 5.26, 5.30 and 5.43, one can integrate 5.50 - 5.56 to give:

$$
\tilde{I}_{00}^{AB} = \frac{\Delta x \Delta z}{4} \left[ \left( 1 - i \alpha_x \right) \left( 1 - i \alpha_x \right) \int N_A N_B d\xi d\eta - i \beta_x \left( 1 - i \alpha_x \right) \int \xi N_A N_B d\xi d\eta 
\right.
\left. -i \beta_x \left( 1 - i \alpha_x \right) \int \eta N_A N_B d\xi d\eta - \beta_x \beta_x \int \xi \eta N_A N_B d\xi d\eta \right],
$$

(5.59)
\[ \bar{I}^{AB}_{x_0} = \frac{\Delta x}{2} \left[ (1 - i\alpha_z) \int \partial_{\bar{z}} N_A N_B d\bar{z} d\bar{\eta} - i\beta_z \int \eta \partial_{\bar{z}} N_A N_B d\bar{z} d\bar{\eta} \right], \]  
\[ (5.60) \]

\[ \bar{I}^{AB}_{0x} = \frac{\Delta x}{2} \left[ (1 - i\alpha_x) \int N_A \partial_x N_B d\xi d\eta - i\beta_x \int \eta N_A \partial_x N_B d\xi d\eta \right], \]  
\[ (5.61) \]

\[ \bar{I}^{AB}_{z0} = \frac{\Delta x}{2} \left[ (1 - i\alpha_z) \int N_A \partial_z N_B d\xi d\eta - i\beta_z \int \xi N_A \partial_z N_B d\xi d\eta \right], \]  
\[ (5.62) \]

\[ \bar{I}^{AB}_{\bar{z}x} = \frac{\Delta x}{2} \left[ (1 - i\alpha_x) \int N_A \partial_{\bar{z}} N_B d\bar{z} d\bar{\eta} - i\beta_x \int \bar{\eta} \partial_{\bar{z}} N_A N_B d\bar{z} d\bar{\eta} \right], \]  
\[ (5.63) \]

\[ \bar{I}^{AB}_{\bar{x}z} = \frac{\Delta x}{2} \left[ (1 - i\alpha_z) \int \bar{\xi} N_A \partial_{\bar{z}} N_B d\bar{\xi} d\bar{\eta} - i\beta_z \int \bar{\eta} \partial_{\bar{z}} N_A N_B d\bar{\xi} d\bar{\eta} \right], \]  
\[ (5.64) \]

\[ \bar{I}^{AB}_{\bar{x}\bar{z}} = \frac{\Delta x}{2} \left[ (1 - i\alpha_z) \int \bar{\xi} N_A \partial_{\bar{z}} N_B d\bar{\xi} d\bar{\eta} - i\beta_z \int \bar{\eta} \partial_{\bar{z}} N_A N_B d\bar{\xi} d\bar{\eta} \right], \]  
\[ (5.65) \]

where

\[ G^i = \begin{cases} 
\frac{\operatorname{arctan}(\alpha_i + \beta_i) - \operatorname{arctan}(\alpha_i - \beta_i)}{\beta_i} + i\beta_i \frac{\log \left( \frac{(\alpha_i + \beta_i)^2 + 1}{(\alpha_i - \beta_i)^2 + 1} \right)}{2\beta_i^2} & \beta_i \neq 0 \\
2 & \beta_i = 0
\end{cases} \]
\[ (5.66) \]

The resulting integrals have the following values:

\[ J^{AB}_{00} := \int N_A N_B d\xi d\eta = \frac{1}{9} \begin{bmatrix} 4 & 2 & 2 & 1 \\ 2 & 4 & 1 & 2 \\ 2 & 1 & 4 & 2 \\ 1 & 2 & 2 & 4 \end{bmatrix}, \]  
\[ (5.67) \]

\[ J^{\bar{z}AB}_{\bar{z}0} := \int \xi N_A N_B d\bar{\xi} d\bar{\eta} = \frac{1}{9} \begin{bmatrix} -2 & -1 & 0 & 0 \\ -1 & -2 & 0 & 0 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix}, \]  
\[ (5.68) \]

\[ J^{\bar{x}AB}_{\bar{x}0} := \int \bar{\xi} N_A N_B d\bar{\xi} d\bar{\eta} = \frac{1}{9} \begin{bmatrix} -2 & 0 & -1 & 0 \\ 0 & 2 & 0 & 1 \\ -1 & 0 & -2 & 0 \\ 0 & 1 & 0 & 2 \end{bmatrix}, \]  
\[ (5.69) \]
\[ J_{00}^{\xi_0} := \int \xi N A N \xi d \xi N = \frac{1}{9} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad (5.70) \]

\[ J_{00}^{\xi} := \int \xi N A N \xi d \xi N = \frac{1}{6} \begin{bmatrix} -2 & -1 & -2 & -1 \\ -1 & -2 & -1 & -2 \\ 2 & 1 & 2 & 1 \\ 1 & 2 & 1 & 2 \end{bmatrix}, \quad (5.71) \]

\[ J_{00}^{\eta} := \int \eta N A N \eta d \eta N = \frac{1}{6} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & -1 \\ -1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}, \quad (5.72) \]

\[ J_{00}^{\eta} := \int N A \xi^2 N \xi d \xi N = \frac{1}{6} \begin{bmatrix} -2 & -1 & 2 & 1 \\ -1 & -2 & 1 & 2 \\ -2 & -1 & 2 & 1 \\ -1 & -2 & 1 & 2 \end{bmatrix}, \quad (5.73) \]

\[ J_{00}^{\eta} := \int \eta N A \xi^2 N \xi d \xi N = \frac{1}{6} \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}, \quad (5.74) \]

\[ J_{00}^{\eta} := \int \xi N A \xi N d \xi N = \frac{1}{6} \begin{bmatrix} -2 & -2 & -1 & -1 \\ 2 & 2 & 1 & 1 \\ -1 & -1 & -2 & -2 \\ 1 & 1 & 2 & 2 \end{bmatrix}, \quad (5.75) \]

\[ J_{00}^{\xi_0} := \int \xi N A \xi N \eta d \xi N = \frac{1}{6} \begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad (5.76) \]

\[ J_{00}^{\xi_0} := \int \xi \eta N A N \xi d \xi N = \frac{1}{6} \begin{bmatrix} -2 & 2 & -1 & 1 \\ -2 & 2 & -1 & 1 \\ -1 & 1 & -2 & 2 \\ -1 & 1 & -2 & 2 \end{bmatrix}, \quad (5.77) \]
\[ J_{\eta \bar{\eta}}^{eAB} = \int \xi N_{\xi, \eta} N_{\bar{\eta}} d\xi d\eta = \frac{1}{6} \begin{bmatrix} 1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & -1 & 1 \end{bmatrix}, \] (5.78)

\[ \int_{-1}^{1} \partial_{\xi} N_{\xi, \eta} N_{\bar{\eta}} d\eta = \frac{1}{12} \begin{bmatrix} 2 & 1 & -2 & -1 \\ 1 & 2 & -1 & -2 \\ -2 & -1 & 2 & 1 \\ -1 & -2 & 1 & 2 \end{bmatrix}, \] (5.79)

\[ \int_{-1}^{1} \eta \partial_{\xi} N_{\xi, \eta} N_{\bar{\eta}} d\eta = \frac{1}{12} \begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}, \] (5.80)

\[ \int_{-1}^{1} \partial_{\eta} N_{\xi, \eta} N_{\bar{\eta}} d\xi = \frac{1}{12} \begin{bmatrix} 2 & -2 & 1 & -1 \\ -2 & 2 & -1 & 1 \\ 1 & -1 & 2 & -2 \\ -1 & 1 & -2 & 2 \end{bmatrix}, \] (5.81)

\[ \int_{-1}^{1} \xi \partial_{\eta} N_{\xi, \eta} N_{\bar{\eta}} d\xi = \frac{1}{12} \begin{bmatrix} -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}. \] (5.82)

### 5.4 NUMERICAL VERIFICATION

As a first test, the individual elements of the elasticity tensor were chosen such that they represent an isotropic medium. In this case

\[ C_{11} = C_{33} = \rho V_{p}^2, \]
\[ C_{44} = C_{66} = \rho V_{s}^2, \] (5.83)
\[ C_{13} = \rho V_{p}^2 - 2 \rho V_{s}^2. \]

Then, comparisons with the truly isotropic code described in Latzel (2010) were performed. There was a good match of the two solutions (not shown). Next, comparisons with an analytic solution for a 3D anisotropic full space (Vavrycuk, 2007) were performed. This comparison is possible since the displacement \( u(\omega) \) can be written as:

\[ u(\omega) = s(\omega) G(\omega), \] (5.84)
where $\omega$ is the frequency, $s(\omega)$ is the source spectrum and $G(\omega)$ is Green’s function.

The analytic solutions for the frequency-domain components of the Green’s tensor in the special case of VTI media where
\[ C_{11} = C_{33}, \]
\[ C_{13} = C_{11} - 2C_{44}, \]
(5.85)
can be written as
\[
G_{ij}(x, y, z, \omega) = \frac{1}{4\pi \rho} \sqrt{\frac{a_{11}}{a_{44}}} \frac{g_{i}^{(1)} g_{j}^{(3)}}{R^2} \left[ \frac{1}{i\omega} \right] \left[ \exp\left( i\omega \tau^{(1)} \right) - \exp\left( i\omega \tau^{(2)} \right) \right] \\
+ \frac{g_{k}^{(1)} g_{l}^{(1)} - \delta_{kl}}{4\pi \rho r} \left[ \frac{1}{a_{11}} \exp\left( i\omega \tau^{(1)} \right) \left[ \left( \frac{-1}{i\omega \tau^{(1)}} \right)^2 + \left( \frac{-1}{i\omega \tau^{(1)}} \right)^2 \right] \right] \\
- \frac{1}{a_{44}} \exp\left( i\omega \tau^{(2)} \right) \left[ \left( \frac{-1}{i\omega \tau^{(3)}} \right)^2 + \left( \frac{-1}{i\omega \tau^{(3)}} \right)^2 \right] \right] \\
+ \frac{1}{4\pi \rho} \left\{ \frac{g_{k}^{(1)} g_{l}^{(1)} \exp(i\omega \tau^{(1)})}{\sqrt{a_{11}^{(1)}} \tau^{(1)}} + \frac{g_{k}^{(2)} g_{l}^{(2)} \exp(i\omega \tau^{(2)})}{\sqrt{a_{44}^{(2)}} \tau^{(2)}} \right\} \\
+ \frac{g_{k}^{(3)} g_{l}^{(3)} \exp(i\omega \tau^{(3)})}{a_{66} \sqrt{a_{44}^{(3)}} \tau^{(3)}},
\]
(5.86)

where
\[
a_{ij} = \frac{C_{ij}}{\rho} \quad \text{(5.87)}
\]
are the density normalized elastic parameters,
\[
\tau^{(1)} = \frac{r}{\sqrt{a_{11}}}, \quad \tau^{(2)} = \frac{r}{\sqrt{a_{44}}}, \quad \text{and} \quad \tau^{(3)} = \frac{r}{\sqrt{a_{66}}} \sqrt{N_{1}^{2} + N_{2}^{2} + \frac{a_{66}}{a_{44}} N_{3}^{2}},
\]
(5.88)
are the travel times, and
\[
g^{(1)} = \begin{bmatrix} N_{1} \\ N_{2} \\ N_{3} \end{bmatrix}, \quad g^{(2)} = \frac{1}{\sqrt{N_{1}^{2} + N_{2}^{2}}} \begin{bmatrix} -N_{1}N_{3} \\ -N_{2}N_{3} \\ N_{1}^{2} + N_{2}^{2} \end{bmatrix}, \quad g^{(3)} = \frac{1}{\sqrt{N_{1}^{2} + N_{2}^{2}}} \begin{bmatrix} -N_{3} \\ 0 \end{bmatrix}
\]
(5.89)
are the polarization vectors. In the above, \( r \) is the distance of the observation point from the source, \( R = \sqrt{x^2 + y^2} \) is the distance of the observation point from the symmetry axis and \( N = x/r \) is the ray direction.

For comparing the 3D analytic expression with my FEM solution, a 2D to 2.5D transformation had to be carried out by integrating over 113 equally distributed wavenumbers \( k_y \), whereby wavenumbers near singularities in the \( k_y \) spectrum were avoided.

Results are shown in Figure 5.2. Horizontal and vertical cross sections through the slices in Figure 5.2 are shown in Figures 5.3 and 5.4. There is a good match between the analytic and numerical solutions inside the domain of interest. Small differences are most likely the result of the 2.5D integration, which is not yet optimized.
5.5 2D ANISOTROPIC WAVEFORM INVERSION – FIRST RESULTS

As soon as the forward problem is solved, one can implement a Gauss-Newton inversion algorithm similar to that presented in Chapter 4. This can be conveniently achieved using explicit expressions for the sensitivities given by Zhou and Greenhalgh (2010). Here, I present preliminary results using my anisotropic full-waveform inversion scheme. For the true model, I have chosen one that is very similar to that depicted in Figure 4.1, but a VTI parameterization (additional elastic constants) was considered. The corresponding values for $C_{11}$, $C_{13}$, $C_{33}$, and $C_{44}$ are shown in Figure 5.5. They correspond to a 30% difference between the maximum (horizontal direction) and minimum (vertical direction) of the P-wavespeeds (density was assumed to be homogeneous at 2500 kg/m³). The same 4-sided vectorial source-receiver configurations considered for computing the tomograms in Figure 4.2 were
also employed for the anisotropic inversion. Moreover, the same spatial discretizations of the forward and inversion grids were used and the same frequency schedule as for the isotropic inversions was followed.

Waveform inversions were performed in which the cross anomalies existed in just one of the parameters $C_{11}$, $C_{13}$, $C_{33}$, and $C_{44}$ at a time, the remaining ones being held fixed as homogeneous distributions. The starting models in each case were the true background values. Results for the four separate experiments in which just one elastic constant was varied are shown in Figure 5.6. For each inversion, I obtained very good reconstructions of the anomalies. Results for anomalies in all of the parameters and a simultaneous inversion in which each parameter was allowed to vary are shown in Figure 5.7. The recovered parameters $C_{11}$, $C_{33}$ and $C_{44}$ all reveal the anomalous bodies quite well, although their magnitudes are underestimated. The best result is obtained for $C_{44}$. The $C_{13}$ tomogram exhibits a reversal in relative magnitude for the two anomalies, with the bottom cross appearing lower in elasticity than the top cross, when in fact the opposite is true. This is likely the result of parameter trade-offs similar to those observed for the isotropic case with crosshole configurations and pressure sources and pressure receivers (see section 4.3.5). In the anisotropic case,
such problems are exacerbated; they even occur for the four-sided experiment in which all possible source-receiver directions are involved (comparable results for the isotropic case are shown in Figure 4.6). This is a clear indication that the anisotropic inversion problem is more underdetermined, more difficult and more ambiguous. Clearly, further research is required to properly account for the resulting trade-offs.
Figure 5.7: Four-parameter simultaneous waveform inversion results for a 4-sided configuration using two-component sources and two-component receivers. White lines delineate the true model boundaries (see Figure 5.5).
6. CONCLUSIONS AND OUTLOOK

The initial seismic experiments carried out at the Mont Terri underground rock laboratory (FMT) were designed to remotely image any physical changes in the microtunnel from just two boreholes drilled into a strongly anisotropic host rock. The main goal of my PhD project was to use this experimental configuration to assess the capabilities and limitations of the seismic tomography technique as a means of effectively monitoring possible changes within radioactive waste repositories. To achieve these goals, I performed in-mine crosshole seismic experiments of a simulated scaled-down repository at FMT. The experiments were conducted using a pressure (sparker) source and pressure receivers (hydrophones). The borehole fluid was expected to provide good source and receiver coupling, which would be essential in sensing subtle elastic changes in the microtunnel. Placement of additional geophones around the microtunnel perimeter was opportunistic, providing additional data to analyze.

In the course of my PhD investigations, significant progress was achieved in four main areas:

1. understanding and characterizing processes occurring in the simulated repository due to changing water saturation conditions;
2. analyzing the recorded data sets regarding their signal fidelity, waveform repeatability and the presence of systematic and other forms of noise that might obscure subtle changes taking place in the repository;
3. determining information content for isotropic elastic waveform inversions;
4. taking the first steps towards performing anisotropic elastic waveform inversions.

6.1 UNDERSTANDING WATER SATURATION EFFECTS

To achieve the goals of my research, I first conducted several crosshole and tunnel-to-hole experiments on a sand-filled tunnel subjected to different degrees of water saturation and pressurization levels. The recorded data show that for the Opalinus clay host rock, the “active” region is not just the microtunnel itself, but also
the EDZ that surrounds it. When water comes into contact with clay, complex interactions begin, having both short and long term effects.

Immediately after the sand becomes fully water saturated, the frequency content of the seismograms recorded by the geophones decreases significantly (loss of high frequencies). This means that the first effect of the water-clay interaction is a weakening of the clay, causing the geophone anchors to become more loosely coupled. Moreover, the time lapse seismograms recorded by the geophones show progressive changes in the traveltimes and polarities of the first arriving wave, indicating that the clay in the EDZ stays active and changes its properties for some time after water saturation.

In contrast to these short term changes of the clay in the EDZ, the long term changes due to water saturation result in clay hardening. When the water penetrates the EDZ, it leads to swelling of the clay and a consequent increase of seismic wave velocities in the EDZ. This is readily seen in the changing traveltimes of the geophone records. Moreover, the frequency content of the geophone data increases, with a return of higher frequencies in response to improved coupling.

The spalling of clay is a significant, albeit unwanted phenomenon in the repositories. It is expected to happen only in the early stages of water seepage into the repository. Such spalling is not expected to be a problem in practice, because the actual repository will be filled with a bentonite and sand mixture that should support the clay. At the later stages of water infiltration, the saturated clay will heal and improve the overall sealing of the repository.

I used traveltimes of geophone data to characterize the EDZ and traveltimes of hydrophone data to determine the gross velocity structure of the host rock. With this velocity information, I simulated a full scale experiment (i.e., a 2.5 m diameter microtunnel). The simulations indicate that the water saturation process would generate traveltime differences up to 0.3 ms at geophones located as close to the repository as regulations would allow (i.e., a distance of 7.5 m from the microtunnel walls). This is more than half the period of the dominant signal recorded at FMT and can be easily detected. It significantly increases our expectations of waveform inversion to sense changes in the repositories.
6.2 SIGNAL REPEATABILITY

Although crosshole first arrival traveltimes (at the distances involved relative to the tunnel diameter) alone do not convey any useful information about the microtunnel, the full seismograms contain diagnostic information about its state. In order to extract this information, one needs to perform full-waveform inversions. However, to invert the full waveforms it is necessary to have highly repeatable signals. For monitoring purposes, the repeatability of the recorded seismograms should be much higher than the expected (time-dependent) changes due to variations in the physical properties of the microtunnel fill material between the different (time-lapse) experiments. The 2D full wavefield simulations that I carried out show that despite the small size of the microtunnel, there are significant changes in the waveforms for most source-receiver pairs. Repeat field experiments under stable tunnel conditions at FMT show that the source generates a very repeatable signal. Geophone recordings of these signals are also very repeatable. Whenever the hydrophone streamer is moved or reinserted into the borehole, its coupling to the host rock varies, leading to pronounced differences in the recorded seismic sections. Experiments using two other hydrophone streamers of different design show that the variable coupling issue is present for all of them. Fortunately, Maurer et al. (2011) demonstrate that variable coupling can be accommodated as an unknown transfer function to be resolved along with the medium properties in a full-waveform inversion scheme (see Appendix B). Nevertheless, high repeatability of the signals recorded with the geophones on the microtunnel walls and the significance of directional information provided by multi-component sensors (as opposed to omni-directional hydrophones) prompted us to install an array of grouted three-component geophones in the upper borehole.

Firmly fixed geophones would allow one to not only invert for the material properties, but also to perform differential tomography and invert for changes in the material properties. The choice of geophone type and their cementation in the upper borehole was investigated within the scope of a Masters thesis project (Cornée, 2010). Within the first week after cementation, an increase in the high frequency content and a slight decrease in the first arrival traveltimes were observed (Figure 6.1). This indicated that the cement had hardened to a sufficient degree, leading to improvements in geophone coupling and hence the quality of the recorded data.
Even if the recorded signal is highly repeatable, it can still contain systematic noise that contaminates the signals of interest. It is very important to identify this noise, such that it can either be removed before the inversion (by appropriate processing) or incorporated in the forward modeling part of the inversion such that there is consistency between the observed and synthesized data. During the course of the experiments, three types of systematic noise were identified. They are generated by (1) the source cable, (2) the receiver cable and (3) tube waves within the source borehole. It should be remarked that accurate modeling of such noise events would require very dense spatial discretisation (finer than the borehole radius), which would be extremely computationally expensive.

6.3 DATA INFORMATION CONTENT ANALYSIS FOR ISOTROPIC ELASTIC WAVEFORM INVERSION

A significant part of my research was devoted to the development of a frequency-domain seismic full-waveform inversion algorithm. My inversion algorithm employs finite-element forward modeling using a direct matrix solver and explicit expressions for the sensitivities contained in the Jacobian matrix. This allows Gauss-Newton inversions to be computed in a very efficient manner, but this advantage comes at the expense of increased memory requirements. My numerical experiments clearly demonstrate that under ideal conditions (e.g., multi-component (directed) sources and multi-component (vector) receivers placed all around the area.
of interest and low noise conditions), high quality images of $V_P$, $V_S$ and $\rho$ can be obtained. Analyses of the diagonal elements of the model resolution matrix indicate that even crosshole pressure source - pressure receiver data sets contain information about both $V_P$ and $V_S$ velocities, but tomographic inversions and consideration of the full model resolution matrix indicate that these two parameters cannot be completely resolved independently. For a scenario in which pressure sources are placed in one borehole and two-component receivers are placed in another borehole, satisfactory $V_P$ and $V_S$ tomograms can be derived, but the density structure remains unresolved.

The finding that pressure source - multi-component receiver experiments lead to satisfactory tomographic images has been exploited in a design study for monitoring high-level radioactive waste using the experimental setup suggested in section 6.1. These results indicate that such non-intrusive monitoring experiments are indeed capable of characterizing a repository and its surroundings by means of full-waveform elastic inversion.

6.4 ANISOTROPIC WAVEFORM INVERSION

The next step towards inversion of recorded data is an extension of the code to the anisotropic case. I have made the necessary developments and modifications of the 2D elastic waveform inversion algorithm to handle the vertically transversely isotropic (VTI) case. This is the simplest class of anisotropy, but is rather widespread in nature. The more general case, as occurs at Mont Terri, is a TI medium with a tilted axis of symmetry. My initial inversion attempts show that even for the optimum 2-component source and 2-component receiver configuration, there is a trade-off between the different elastic parameters. Hence for the VTI case (and by implication, the tilted TI case), modified inversion strategies are required.

6.5 OUTLOOK

Although significant steps have been made towards inversion of seismic crosshole data sets, important issues remain to be resolved before one can invert the data collected at Mont Terri. In particular, 2.5D anisotropic waveform inversion (project goal 5, see section 1.8), which was only partly achieved, needs to be further developed. Some progress in the direction of 2.5D modeling, wavenumber sampling and the validity of 3D to 2D data conversion is being made by Masters student
Ludwig Auer. Until such time as the 2.5D inversion algorithm is developed and tested, it will not be possible to invert the data recorded at FMT (project goals 7 and 8 in section 1.8). Below, I outline the remaining open questions and provide some possible strategies to tackle them.

- **Tilted axis of symmetry**
  
  Opalinus clay at FMT is characterized by a transversely isotropic medium with a tilted symmetry axis (TTI). Hence, both the forward and the inverse problems have to take this into account.

  **Possible solution**
  
  If the direction of the symmetry axis does not change significantly within the domain of interest, then a simple coordinate transformation can be applied and only a relatively simple VTI problem has to be solved. If there are substantial changes in the symmetry direction within the inversion domain, then a full TTI problem would need to be solved. My initial calculations for TTI media showed instabilities in the perfectly matching layer (PML) boundary conditions. Thus, further work is required to check and modify the PMLs if true TTI modeling is required.

- **Parameter trade-offs during waveform inversions**
  
  The incorporation of anisotropy in seismic inversion requires an increase in the number of parameter types to be resolved at each spatial position. For VTI inversions in 2D media, one has to invert for five different parameter types (4 elastic constants and density), which would increase to six (5 elastic constants and density) for the 2.5D problem. For the TTI case, the angle defining the direction of the symmetry axis also has to be estimated. Since the number of inversion parameters defines the size of the Hessian matrix, the computational requirements for anisotropic inversions will be significantly higher than for isotropic inversions. Moreover, I have already shown the existence of trade-offs between the different parameters. The trade-off is not so strong in the isotropic inversion case (it appears only for pressure source – pressure receiver configurations). In contrast, for the VTI case trade-offs are observed even when using combined horizontal- and vertical-component sources and combined horizontal- and vertical-component receivers placed around all four sides of the domain of interest.
**Possible solution**

One way to overcome these trade-offs is a separation of the inversion parameters into two or more groups, each group containing only “compatible” parameters. Then, one full inversion step would consist of a few sub-steps, each of which would update only a single set of parameter types. This inversion strategy will also reduce the size of the Hessian matrix for each inversion sub-step and hence the memory requirements. The only drawback would be an increase in the computational time for each of the iterations.

- **Wavenumber sampling**

  Once the 2D anisotropic forward modeling problem is fully solved, one can proceed to the solution of the 2.5D problem. Since the 2.5D problem can be viewed as the solution of multiple 2D problems (one for each wavenumber), the computational time is proportional to the number of the wavenumbers. In the frequency domain, the wavenumber spectra are highly oscillatory. The oscillation frequency is not constant, but depends on the source-receiver distance and the wavenumber itself, increasing with higher values. Hence, it is necessary to employ a good (not necessarily equally spaced) wavenumber sampling strategy. Additionally, one has to take into account the existence of poles or sudden disruptions in the wavenumber spectra.

  **Possible solution**

  One way to avoid these poles or singularities is to use complex frequencies (e.g. Phinney, 1965; Bouchon, 1979, 2003; Mueller, 1985; Mallick and Frazer, 1987). This approach will move the poles away from the real wavenumber axis, allowing integration along the real axis (inverse Fourier transform with respect to wavenumber) and synthesis of the frequency-domain wavefield. Moreover, complex frequencies could be used to time-window the recorded seismic sections. This time-windowing would allow one to eliminate unwanted arrivals, such as tube waves.

- **Higher frequencies**

  With a solution in hand for the 2.5D anisotropic inversion problem, it should be possible to invert the Mont Terri recorded data. Please note that for the 2D isotropic inversions of the simulated radioactive waste repository presented in Chapter 4, I used frequencies up to only 700 Hz. In contrast, the repeatable signals at FMT contain
useful information in frequencies up to 4000 Hz. To take advantage of this additional information would necessitate an increase in the frequencies used in the inversion process, which in turn would require a decrease in the grid spacing and a consequent increase in the size of the matrices to be inverted.

Possible solution

To solve this issue, one can either use a machine with much greater memory or change the forward solution from a direct matrix solver to a less memory intensive iterative solver.

- Structural 3D effects

Although the experiment is symmetric along the microtunnel axis, the geological structure may be somewhat asymmetric due to heterogeneities.

Possible solution

In similar fashion to tube wave suppression, out-of-plane reflections may be eliminated from the 2.5D inversion process by appropriate time-windowing. However, removing the out-of-plane arrivals could lead to a significant reduction in the amount of useful data. Using a 3D code (e.g., Bohlen, 2002), synthetic data sets for anomalies of various contrasts and at different distances from the $y=0$ plane could be generated. Inversions of these data sets with the 2.5D code would allow one to assess the applicability limits of the 2.5D inversion algorithm.

- Inversion of noisy data

In Chapters 4 and 5 I inverted noise-free data. In the real data world, noise (both random and systematic) is always present.

Possible solution

Inversion of noisy data can provide reasonable reconstructions of subsurface properties. Barnes et al. (2008) showed that with a signal-to-noise ratio (SNR) of 4, it was possible to determine a very good image. The SNR for the data collected at Mont Terri varies, but depending on the source and receiver distances it is generally greater than 30. Hence, I expect very good tomograms from inversions of the Mont Terri data sets.
APPENDIX A

Finite-difference time-domain implementation of seismic wave propagation in vertically transversely isotropic media
The 2D elastic equation of motion in vertically transversely isotropic (VTI) media in the space-time domain can be written as

$$\rho \frac{\partial v_i}{\partial t} = \frac{\partial \sigma_{ij}}{\partial x_j} + f_j, \quad i, j = x, z,$$  \hspace{1cm} (A1)

where $x_j$ indicates the two spatial directions $(x, z)$, $\rho$ is the density, $v$ is the particle velocity, $f$ is the external body force and $\sigma$ is the stress tensor. For the VTI case, in which $z$ is the symmetry axis direction, the stress components can be related to the particle velocity components through the following expressions

$$\frac{\partial \sigma_{xx}}{\partial t} = C_{11} \partial_x v_x + C_{13} \partial_z v_z,$$  \hspace{1cm} (A2)

$$\frac{\partial \sigma_{xz}}{\partial t} = C_{13} \partial_x v_x + C_{33} \partial_z v_z,$$  \hspace{1cm} (A3)

$$\frac{\partial \sigma_{zz}}{\partial t} = \frac{\partial \sigma_{zz}}{\partial t} = C_{44} \partial_x v_x + C_{44} \partial_z v_z.$$  \hspace{1cm} (A4)

where $C_{11}, C_{33}, C_{44}, C_{13}$ are the four independent components of the elasticity tensor $C$.

To approximate the spatial partial derivatives I follow the approach used by Bohlen (2002), who defined the variables on a staggered grid (Figure A.1) and employed fourth-order forward and backward operators $D_x^+$ and $D_x^-$, respectively (Levander, 1988)

$$\frac{\partial g(x)}{\partial x} \Bigg|_{(i+1/2)h} \approx D_x^+ [g(i)] = \frac{1}{24h} \left[ -g(i+2) + 27(g(i+1) - g(i)) + g(i-1) \right]$$  \hspace{1cm} (A5)

$$\frac{\partial g(x)}{\partial x} \Bigg|_{(i-1/2)h} \approx D_x^- [g(i)] = \frac{1}{24h} \left[ -g(i+1) + 27(g(i) - g(i-1)) + g(i-2) \right]$$  \hspace{1cm} (A6)

The $D_x^+$ and $D_x^-$ operators approximate the partial derivatives of an arbitrary continuous function $g(x)$ at $i^+ = (i + 1/2)h$ and $i^- = (i - 1/2)h$, respectively, where $h$ is the distance between two grid points.

The temporal partial derivatives of an arbitrary continuous function $g(x)$ are approximated by the Crank-Nicholson scheme:

$$\frac{\partial g(x,z,t)}{\partial t} \bigg|_{(i,k,\Delta t)} \approx \frac{g^{n+}(i,k) - g^{n-}(i,k)}{\Delta t}$$  \hspace{1cm} (A7)
where \( i, k, n \) are indices for the two spatial directions \((x, z)\) and time \( t\), respectively. Here \( \Delta t \) is the time step.

By applying these operators to the partial differential equations (A1) – (A4), one obtains the following explicit FD scheme:

\[
v_x^n (i^+, k) = v_x^{n-1} (i^+, k) + \frac{\Delta t}{\rho(i^+, k)} \left\{ D_x^+ \left[ \sigma_{xx}^n (i, k) \right] + D_z^+ \left[ \sigma_{xz}^n (i^+, k^+) \right] + f_x^n (i^+, k) \right\} \tag{A8}
\]

\[
v_z^n (i, k^+) = v_z^n (i, k^+) + \frac{\Delta t}{\rho(i, k^+)} \left\{ D_x^- \left[ \sigma_{xz}^n (i^+, k^+) \right] + D_z^- \left[ \sigma_{zz}^n (i, k) \right] + f_z^n (i, k^+) \right\} \tag{A9}
\]

\[
\sigma_{xx}^n (i, k) = \sigma_{xx}^{n-1} (i, k) + \Delta t \left\{ C_{11} (i, k) D_x^- \left[ v_x^n (i^+, k) \right] + C_{13} (i, k) D_z^- \left[ v_x^n (i, k^+) \right] \right\} \tag{A10}
\]

\[
\sigma_{zz}^n (i, k) = \sigma_{zz}^{n-1} (i, k) + \Delta t \left\{ C_{13} (i, k) D_x^- \left[ v_x^n (i^+, k) \right] + C_{33} (i, k) D_z^- \left[ v_z^n (i, k^+) \right] \right\} \tag{A11}
\]

\[
\sigma_{xz}^n (i^+, k^+) = \sigma_{xz}^{n-1} (i^+, k^+) + \Delta t \left\{ C_{43} (i^+, k^+) D_x^+ \left[ v_x^n (i^+, k^+) \right] + C_{44} (i^+, k^+) D_z^+ \left[ v_z^n (i^+, k^+) \right] \right\} \tag{A12}
\]

in which a staggered temporal grid is used, with the displacements defined on the nodes of the temporal grid and the stresses at the midpoints.
APPENDIX B

Receiver-coupling effects in seismic waveform inversions

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B.1 ABSTRACT

Seismic waveform inversion offers opportunities for detailed characterization of the subsurface. However, its full potential can only be exploited when any systematic source and receiver effects are either carefully avoided or appropriately accounted for during the inversions. Repeated crosshole measurements in the Mont Terri (Switzerland) underground laboratory have revealed that receiver coupling may significantly affect the seismic waveforms. More seriously, coupling conditions may vary during the course of a monitoring experiment. To address this problem, we have developed a novel scheme that estimates medium properties, frequency-dependent source functions, and frequency-dependent receiver-coupling factors. We demonstrate the efficacy of the new scheme via a 2D numerical acoustic crosshole experiment in which realistic receiver-coupling factors are incorporated. Because determination of medium parameters and estimation of source functions and receiver-coupling factors are largely separated, the method can be easily adapted to any other waveform inversion problem, including elastic, anisotropic, 2.5D, or 3D situations.

B.2 INTRODUCTION

Geophysical tomography is a powerful and versatile tool for a wide range of imaging problems in the earth sciences. Wavefield techniques, such as the seismic and ground-penetrating radar methods, have proven to be particularly useful in diverse applications that range over many different length scales from whole earth investigations to laboratory testing.

A common feature of these methods is that observable data \( d \) can be represented in the general form:

\[
d_{ij} = s_i \otimes G_{ij} \otimes r_j, \tag{B.1}
\]

where \( s_i \) represents properties of source \( i \), the Green’s function \( G_{ij} \) characterizes wave propagation between source \( i \) and receiver \( j \), and \( r_j \) includes the properties of receiver \( j \) and its immediate environment. The generic operator \( \otimes \) may either represent convolution (time-domain waveform analyses), multiplication (frequency-domain waveform analyses or ray-based amplitude tomography), or addition (traveltime analyses).

In many applications, it is assumed that two of the three quantities on the right side of equation B.1 are at least approximately known. As an example, well-
established earth models and previously determined properties of receivers are used in earthquake source studies (e.g., Ferreira and Woodhouse, 2006). Likewise, reliable information on time delays specific to certain source and/or receiver locations is a stringent prerequisite in crosshole traveltime tomography (e.g., Lehmann, 2007, and references therein).

Nevertheless, there is often clear evidence that insufficient a priori knowledge exists for more than one quantity on the right side of equation B.1. For instance, simultaneous inversions for earthquake hypocentral parameters and layered earth models require corrections that account for traveltime anomalies caused by near-surface structures beneath the seismic stations (e.g., Kissling, 1988; Maurer and Kradolfer, 1996; Bijwaard and Spakman, 2000). Moreover, correction terms have also been used to account for velocity anomalies in the vicinity of the earthquakes themselves (e.g., Hearn and Clayton, 1986). Comparable techniques in other geophysical subdisciplines include estimating residual static corrections in seismic reflection processing (e.g., Yilmaz and Doherty, 2001) and determining static shifts in magnetotelluric analyses (e.g., Jones, 1988). The importance of properly accounting for source and receiver effects has also been recognized in crosshole radar tomography. For example, initial tomographic inversions of crosshole radar amplitude data acquired within an alpine rock glacier yielded unreasonable results (Maurer and Musil, 2004). Interpretable subsurface images were only obtained after incorporating amplitude correction factors for each transmitter and receiver in the inversion process.

In recent years, substantial effort has been made to extend seismic and ground-penetrating radar traveltime and amplitude tomography to full-waveform inversions. Although these techniques were proposed more than 20 years ago (e.g., Tarantola, 1986; Mora, 1987), they only became popular quite recently (e.g., Plessix, 2008; Buske et al., 2009). The early algorithms were formulated in the time domain, but it was soon recognized that frequency-domain inversion algorithms offer several advantages (e.g., Ikelle et al., 1986; Pratt, 1999; Zhou and Greenhalgh, 2003); with spectral amplitudes and phases from only a few well chosen frequencies, tomographic images comparable to their time-domain counterparts can be obtained at substantially lower computational costs (e.g., Sirgue and Pratt, 2004; Maurer et al., 2009). Frequency-domain approaches are particularly useful for iterative inversion schemes. Furthermore, they benefit from the fact that most seismic and ground-penetrating
radar data are band limited, such that only a small number of frequencies is required for characterizing large parts of entire waveforms.

The recent literature includes numerous synthetic waveform inversion studies, but only a few applications to real data have been reported (e.g., Vigh and Starr, 2008; Plessix et al., 2010; Sirgue et al., 2010). This is likely due to several systematic effects that require further research. First, most synthetic waveform inversions are restricted to two dimensions, but the 3D radiation characteristics of seismic sources usually requires at least a 2.5D problem to be solved (e.g., Zhou and Greenhalgh, 2006). Second, source characteristics are generally unknown. For surface-based seismic data sets, source signatures can be estimated from receiver traces located close to the sources (notwithstanding the differences between near-field and far-field wavefield characteristics), but in crosshole applications this is not possible. To address this issue, a number of researchers describe algorithms that include the unknown source function in the inversion process (e.g., Zhou et al., 1997; Pratt, 1999; Greenhalgh and Zhou, 2004; Ernst et al., 2007). All such approaches assume a common source function for all source positions. Although this seems to be generally justified, because a seismic source is expected to be highly repeatable, the coupling conditions to the medium of interest may vary according to position (e.g., breakouts in the borehole wall may affect the source signature in crosshole investigations). Third, coupling effects could influence the receiver characteristics. Whereas the need to invert for generally unknown source functions is well understood, it is usually assumed that transfer functions and receiver-coupling conditions can be ignored. Since seismic receivers are typically selected to provide a flat response in the frequency band of interest, this assumption may appear to be reasonable. But we have evidence that receiver-to-ground coupling conditions may markedly influence the recordings. Most seriously, the coupling behavior may vary during the course of a monitoring program.

An important feature of full-waveform inversions is their ability to exploit subtle changes in the data for the detailed imaging of subsurface structures. This advantage will be lost when waveforms are significantly influenced by source or receiver-coupling effects. Such effects may preclude waveform inversion algorithms from being employed.

We begin this contribution by demonstrating that source and receiver-coupling effects in seismic crosshole data acquired in an underground rock laboratory are substantial. Then, a simple method for computing appropriate spectral correction
factors as part of a frequency-domain waveform inversion scheme is introduced. The performance of the new algorithm is demonstrated using a synthetic 2D acoustic data set.

B.3 SOURCE AND RECEIVER-COUPLING EFFECTS IN CROSSHOLE SEISMIC INVESTIGATIONS

To demonstrate the important effects of source and receiver coupling, we consider a well-controlled seismic crosshole experiment conducted at the Mont Terri rock laboratory located in the Swiss Jura Mountains. The host rock is the Opalinus clay formation, which has an extremely low permeability. It has been identified as a potential host rock for the disposal of high-level radioactive waste in Switzerland because of its swelling and self-sealing properties when subjected to water infiltration (e.g., Bossart and Thury, 2007). A distinguishing feature of Opalinus clay is its high degree of elastic anisotropy (e.g., Nicollin et al., 2008), with slow and fast P-wave velocities of about 2500 and 3300 m/s, respectively.

Figure B.1: Acquisition geometry of the Mont Terri crosshole seismic experiment. Source and receiver boreholes were drilled from the sidewall of the main access tunnel. The microtunnel, represented by the green circle, is perpendicular to the tomographic plane defined by the source and receiver boreholes.
The experimental setup at the Mont Terri rock laboratory is sketched in Figure B.1. It represents a scaled-down version (smaller by a factor of 2.5 - 6.0) of a high-level radioactive waste repository and possible monitoring scheme. A 1-m-diameter microtunnel intended to mimic the repository was drilled 13 m into the Opalinus clay host rock. Two inclined boreholes (25 and 29 m long) were drilled perpendicular to the axis of the microtunnel for crosshole monitoring purposes.

A high frequency sparker was employed as the source, and the seismic waves were detected by a 24-channel hydrophone chain with 1 m receiver spacing. Source spacing was 0.25 m and a receiver spacing of 0.25 m was simulated by shifting the hydrophone chain in 0.25 m increments and repeating all sources. More details on this experiment can be found in Chapter 3.

Figure B.2 shows examples of source and receiver gathers for a source at a distance of 15 m in the lower borehole and a receiver at 15 m in the upper borehole. Substantial changes in source-gather waveforms are observed within a few milliseconds of the first breaks (Figure B.2a). These changes are either the result of...
geological heterogeneity or they are caused by variable receiver-coupling conditions. In contrast, the receiver gather is distinguished by generally uniform signals within the same time window (Figure B.2b), thereby indicating that the high-frequency sparker source produces a repeatable signal and that source coupling conditions do not vary significantly along the source borehole.

By means of a reverse experiment, in which the sparker source was fired in the upper borehole and the hydrophone chain was placed in the lower borehole, we sought to determine if geological heterogeneity or variable receiver coupling caused the strong variations observed in Figure B.2a. The resulting source gathers again showed large variations and the receiver gathers were again quite uniform (not shown), thereby indicating that variable receiver coupling was the dominant factor.

The significance of variable receiver coupling was further demonstrated via a hydrophone chain reinsertion experiment. For this, a source position at about 15 m horizontal distance was occupied and the hydrophone chain was placed in the upper borehole. After recording traces using this deployment (blue traces in Figure B.3), the hydrophone chain was removed and immediately reinserted at the same position to
within 1 - 2 cm. Subsequently, the source position was reoccupied to within 1 - 2 cm, the sparker ignited again, and a new suite of traces recorded (red traces in Figure B.3). First breaks of the two suites of traces match to within a sample interval (0.032 ms), but the overall waveform shapes differ markedly. The elastic parameters within the area of interest did not change between the two experiments, and extensive tests have demonstrated that the repeatability of the seismic source was very good (Figure B.2 and Chapter 3). Accordingly, only variable receiver coupling could have produced these astonishingly large differences, which are most likely caused by minor changes in the seating/orientation of the hydrophones on the borehole wall. It is noteworthy that we have also observed similar (although smaller) effects in data obtained using a hydrophone chain hanging freely in vertically-oriented boreholes.

Variable receiver coupling does not normally create problems for traveltime inversions, but differences in later parts of the waveforms will be detrimental for waveform inversions. This is particularly critical for monitoring experiments, such as those being performed in the Mont Terri laboratory (Figure B.1). Changes within the microtunnel are expected to generate waveform anomalies that are much smaller than the differences between the traces in Figure B.3 (Chapter 3).

**B.4 SIMULTANEOUS ESTIMATION OF MEDIUM PROPERTIES, SOURCE FUNCTIONS, AND RECEIVER-COUPLING FACTORS**

A possible option to account for variable coupling is to estimate coupling properties as part of the waveform inversion scheme. Although coupling properties may be influenced by non-linear effects, we judge that the phenomenon can be reasonably well approximated with a linear receiver-coupling term. This is the same assumption typically made for source estimation (e.g., Pratt, 1999). According to equation B.1, observed and predicted frequency-domain data $d^{ob}$ and $d^{pred}$ can be written as the product:

$$d^{ob}_j(\omega) = s_j(\omega) \cdot G_j(m, \omega) \cdot r_j(\omega),$$

(B.2)

where $\omega$ is frequency and the vector $m$ contains the medium properties (e.g., P-wave velocities for the acoustic case, which would be the true values for the observed data but the estimated values for the current model for the predicted data). The quantities $d^{ob}_j$, $s_j$, $G_j$ and $r_j$ are complex numbers, different for each frequency. Here, we assume that the sources exhibit an isotropic radiation pattern. Likewise, the receivers are
assumed to have no azimuthal dependency. To invert for medium properties alone, an iterative Gauss-Newton-type algorithm can be employed (e.g., Pratt et al., 1998):

$$ \mathbf{m}^{\text{est}} = (\mathbf{J}^\mathsf{T} \mathbf{J} + \lambda^2 \mathbf{I} + \gamma^2 \mathbf{L})^{-1} \mathbf{J}^\mathsf{T} \left[ \left( \mathbf{d}^{\text{obs}} - \mathbf{d}^{\text{pred}} \right) + \mathbf{J} \mathbf{m}^{\text{est}} + \lambda^2 \mathbf{m}^{\text{est}} \right], $$

where the superscript \( \text{est} \) indicates estimated (inverted) quantities. \( \mathbf{J} \) is the Jacobian matrix that includes partial derivatives of the data with respect to the model parameters, \( \mathbf{I} \) is the identity matrix, and \( \mathbf{L} \) is a Laplacian smoothing operator. The parameters \( \lambda \) and \( \gamma \) control the amount of damping and smoothing to be applied.

One way to account for unknown source functions and receiver-coupling factors would be to include them in the inversion as additional model parameters. This would require the vector \( \mathbf{m} \) to be augmented with \( ns \times n\omega \) source functions and \( nr \times n\omega \) receiver-coupling factors, where \( ns, nr, \) and \( n\omega \) are the number of sources, receivers, and frequencies. The partial derivatives with which the Jacobian matrix would have to be augmented for source and receiver terms would be:

$$ \frac{\partial d_{ij}}{\partial s_i} = G_{ij} \cdot r_j \quad \text{and} \quad \frac{\partial d_{ij}}{\partial r_j} = G_{ij} \cdot s_i. $$

Equations B.4 indicate the non-linearity of the problem (i.e., the partial derivatives for the source functions depend on the receiver coupling, and vice versa). In combination with the generally pronounced non-linearity of the waveform inversion problem (e.g., Mulder and Plessix, 2008), joint inversion for all parameters simultaneously is unlikely to provide stable results. Indeed, we have implemented such an algorithm and verified this assertion. Furthermore, the size of the Hessian matrix \( \mathbf{J}^\mathsf{T} \mathbf{J} \) is substantially increased when several frequencies and a large number of source and receiver terms are included.

To resolve this issue, we have designed and implemented a robust source-function and receiver-coupling estimation scheme that is outlined schematically in Figure B.4. Initially, receiver-coupling factors \( r_{ij}^{\text{est}} \) are set to 1.0 and the Green’s functions \( G_{ij} \) are calculated using initial estimates of the medium parameters (e.g., homogeneous values throughout the model). A first computation of \( s_{ij}^{\text{est}} \) is then performed using:

$$ s_{ij}^{\text{est}}(\omega) = \text{mean} \left( \frac{d_{ij}^{\text{obs}}(\omega)}{G_{ij}(\omega) \cdot r_{ij}^{\text{est}}(\omega)} \right) $$

Subsequently, \( r_{ij}^{\text{est}} \) is determined using
Figure B.4 Flowchart of our source function and receiver-coupling factor estimation procedure as part of an iterative waveform inversion scheme. The various parameters are defined in the text.
A potential problem that may arise during the evaluation of equations B.5 and B.6 concerns values of $G_{ij}(\omega)$ that are close to zero. Such values need to be eliminated prior to the application of the mean() operators. Equations B.5 and B.6 are evaluated repeatedly until convergence is achieved (typically after 3 - 5 iterations). Then, the predicted data $\mathbf{d}^{\text{pred}}$ can be computed using equation B.2. A new estimate of $\mathbf{m}^{\text{est}}$ is obtained by minimizing the discrepancies between $\mathbf{d}^{\text{obs}}$ and $\mathbf{d}^{\text{pred}}$ using the Gauss-Newton update given by equation B.3. As outlined in Figure B.4, the entire procedure is repeated until updates of $\mathbf{m}^{\text{est}}$ become negligibly small and/or the root-mean-square differences between $\mathbf{d}^{\text{obs}}$ and $\mathbf{d}^{\text{pred}}$ are below a prescribed error level (typically after 10 - 15 iterations).

The computation of the mean values in equations B.5 and B.6 is equivalent to a least-squares (L2 norm) inversion for the parameters $s_i^{\text{est}}$ and $r_j^{\text{est}}$. One could obtain a more robust L1 norm estimate (e.g., Rice and White, 1964) by simply replacing the mean() by the median() operator in equations B.5 and B.6.

**B.5 SYNTHETIC EXAMPLE**

Inversion of the field data acquired at the Mont Terri rock laboratory (Figures B.1 to B.3) requires that a 2.5D anisotropic elastic waveform inversion algorithm be applied. Such algorithms are currently under development. As a consequence, we are not yet able to invert the field data. Instead, we demonstrate the performance of our algorithm using simulated 2D acoustic (constant density) data that includes realistic coupling factors based on the field data reported above. It is important to note that the methodology summarized in Figure B.4 can be transferred in a straightforward manner to anisotropic elastic waveform inversion problems once appropriate algorithms, computer codes, and computer resources are available. It is only the Green’s functions $G_{ij}$ that would have to be modified.

The experimental configuration for the simulations is shown in Figure B.5. It includes 26 sources and 26 receivers distributed along two boreholes within a medium that contains high (+500 m/s) and low (-500 m/s) cross-shaped velocity anomalies embedded in a homogeneous background of 2000 m/s. The source is a Ricker wavelet with a 1500 Hz center frequency. Figure B.6a shows the resulting seismic traces for a
source position 18 m along the source borehole. These traces are generated using a frequency-domain finite-element code (Maurer, et al., 2009). The blue traces represent the simulations using the heterogeneous model in Figure B.5, whereas the black traces are obtained for a homogeneous 2000 m/s model. Differences between the blue and black traces represent information on the anomalous structures contained in the seismic data.

For the computation of the traces shown in Figure B.6a, no receiver-coupling effects were included (i.e., $r_j(\omega)=1.0$). To simulate realistic receiver-coupling conditions, we convolve representative receiver-coupling effects contained in the observed data (Figure B.3) with the synthetic traces (Figure B.6a) for the heterogeneous model in Figure B.5. We assume that the changes of the coupling
conditions between the two experiments of Figure B.3 are a reasonable proxy for the overall coupling conditions, but it is important to note that the overall coupling effect must be inherently larger than its changes. For computing the contamination caused by variable receiver-coupling conditions, we Fourier transformed 26 randomly selected trace pairs generated during the reinsertion experiment (note, that only every fourth trace of this experiment is shown in Figure B.3). Then, divisions of the corresponding frequency spectra were performed, whereby an appropriate white noise level was introduced to prevent instabilities in the presence of small denominators. To ensure causality of the contaminated traces, imaginary parts of the resulting ratios
were replaced by Hilbert transforms of the corresponding real parts (e.g., Bracewell, 2000). Inverse Fourier transformation of the resulting coefficients into the time domain yielded 26 time series \( \hat{r}_j(t) \) that represent changes in the receiver-coupling conditions. Subsequently, all traces simulated for the \( j \)th receiver (\( j = 1 \ldots 26 \)) were convolved with \( \hat{r}_j(t) \). The resultant contaminated traces shown in Figure 6b (red) exhibit considerable variations that far exceed the signatures associated with the cross-shaped anomalies.

For the inversion of the synthetic data, we started with a homogeneous velocity model (2000 m/s) and three low frequencies (200, 300, and 400 Hz), and then progressively added frequencies up to 2000 Hz. For the final iteration steps, only 8 frequencies were employed, such that the data space included \( 8 \times 26 \times 26 \times 2 = 10,816 \) data points (real and imaginary parts of the complex valued data \( d_{ij}(\omega) \) were treated as separate data). The velocity model comprised 14,000 inversion cells, and \( 8 \times (26 + 26) = 416 \) source functions and receiver-coupling factors needed to be estimated.

Velocity tomograms based on three waveform-inversion scenarios are presented in Figure B.7. For Figure B.7a, the known synthetic source function (only one source function was used to generate the synthetic data) and receiver-coupling factors are employed in equation 2 (i.e., equations B.5 and B.6 are not required). The two crosses are well resolved in this tomogram. For Figure B.7b, the known synthetic receiver-coupling factors are used in equation B.2 (i.e., equation B.6 is not required), but "unknown" source functions (multiple source functions are allowed in the inversion
process) are determined using equation B.5. Although there are minor artifacts along the source and receiver boreholes, the two crosses are again well resolved. Finally, P-wave velocities, "unknown" source functions, and "unknown" receiver-coupling factors are determined during the computation of the tomogram in Figure B.7c, the quality of which is comparable to that in Figure B.7a and b. Waveform inversion of the synthetic data without prior knowledge of the receiver-coupling factors and without taking them into account fails to produce a meaningful tomogram (not shown).

The tomograms in Figure B.7 are based on inversions using 8 frequencies. With knowledge of the recovered velocity structure (i.e., knowledge of the Green’s functions $G_{ij}$), source functions and receiver-coupling factors can be estimated for a full-range of frequencies using equations B.5 and B.6. This allows us to compute predicted traces via equation B.2 and an inverse Fourier transform. Figure B.8 shows a comparison of original traces (red) and predicted traces using the velocity model in Figure B.7c (blue trace) and a source 18 m along the source borehole. The agreement is excellent.
B.6 DISCUSSION

The reinsertion experiment at the Mont Terri underground laboratory (Figure B.3) revealed that receiver-coupling problems can be severe. Although the Mont Terri example probably represents an extreme case, similar effects are likely to influence most seismic data. For example, we have observed significant changes in traces acquired during reinsertion experiments in vertical boreholes. Even when an experiment is perfectly repeatable (e.g., when seismometers are firmly grouted in the boreholes), coupling is expected to be an issue (recall that overall coupling effects are expected to be larger than their changes).

It will be interesting to investigate receiver-coupling effects in waveform inversions of surface-based seismic data. Various authors have emphasized problems associated with variable geophone coupling (e.g., Krohn, 1984; Drijkoningen, 2000; van Vossen and Trampert, 2007). For near-surface applications, incorporation of variable geophone coupling may be particularly important for successful waveform inversions.

Equations B.5 and B.6 yield source functions and receiver-coupling factors by determining systematic effects in the data that are common for all recordings based on a particular source or a particular receiver position. It is possible that these source functions and receiver-coupling factors are not only influenced by conditions at the sources and receivers, but also by other systematic effects. For example, application of the acoustic approximation for inverting-elastic wave data or ignoring significant anelasticity are expected to produce such systematic effects. Since one is primarily interested in the material properties contained in the Green’s function $G$, the inevitable trade-offs between the different contributions are not a serious concern.

Finally, we would like to emphasize an important limitation of our procedure for estimating simple source functions and receiver-coupling factors. We have implicitly assumed that the source and receiver radiation patterns are known and correctly reproduced by the forward modeling algorithm. It is possible that source functions and receiver-coupling factors exhibit angular variations that are generally unknown and, thus, cannot be accurately modeled. A possible option for addressing this problem would be to form groups of receivers or sources that lie within similar azimuth/inclination ranges with respect to particular sources or receivers, respectively. This would decrease the degree of over determinacy, such that the mean values computed in equations B.5 and B.6 become statistically less well constrained. It would
be necessary to appraise the severity of angular variations and data quality jointly in order to determine optimum group sizes that represent reasonable compromises between angular resolution and data redundancy.

**B.7 CONCLUSIONS**

A variety of field experiments have indicated that receiver-coupling effects can be significant, probably distorting waveform inversions in a major way. Our scheme for estimating unknown source functions and unknown receiver-coupling factors provides a powerful tool for addressing this problem. The scheme has been applied to 2D synthetic acoustic data, but conceptually the methodology can be extended in a relatively straightforward fashion to 2.5D and 3D elastic, visco-elastic, and anisotropic media; the scheme for estimating the source function and receiver-coupling factors is only weakly linked to the tomographic inversion algorithm.

Computation of the source functions and receiver-coupling factors is efficient, requiring an insignificant amount of computing time compared to that required to calculate predicted waveforms, sensitivities, and Gauss-Newton inversion steps. Consequently, such an estimation scheme, or variant thereof, could be included in every waveform inversion procedure.

**B.8 ACKNOWLEDGMENTS**

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APPENDIX C

Can deep radioactive waste repositories be remotely monitored?

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C.1 ABSTRACT

Expansion of nuclear power generation may be an option to curb humanity's carbon output and associated influence on global warming and simultaneously contributes to long-term energy security. But such an expansion is unlikely unless society is convinced that projected volumes of high level radioactive waste and spent nuclear fuel can be securely and permanently removed from the biosphere. A key element in gaining the public's trust requires demonstrating that radioactive waste sealed in deep geological repositories can be remotely monitored and safely retrieved should the need arise. Our investigations show that crosshole and tunnel-to-hole seismic surveying, similar in principle to computer-aided tomography used in medicine, has the potential to monitor deep radioactive waste repositories non-intrusively.

C.2 INTRODUCTION

Climate change and the quest for dependable energy sources are near the top of many national agendas. It is generally agreed that anthropogenic greenhouse gases must be reduced to limit global warming (Pachauri and Reisinger, 2007), and the OECD estimates that the worldwide demand for energy will more than double by 2050 (OECD, 2008a). A growing number of influential analysts, organizations, and governments conclude that the solution to these problems requires an appropriate mix of enhanced sustainable energy sources together with a substantial increase in nuclear power (OECD, 2008a; Lovelock, 2006; Mackay, 2008; UK DBERR, 2008). Consequently, countries worldwide are considering renewing or expanding their nuclear power capabilities or building their first nuclear plants (OECD, 2008a; UK DBERR, 2008; Nature news, 2008, 2009a, 2009b; Kintisch, 2009; IAEA, 2008). According to the OECD (OECD, 2008a), the number of nuclear plants will likely increase from 439 in 2008 to 580-1400 by 2050, depending on society's views on nuclear power.

Despite the renewed enthusiasm for nuclear power in some quarters, there continues to be reluctance amongst the general public, primarily because of the perceived problem of high level radioactive waste (HLW) and spent nuclear fuel (SF) (OECD, 2008a; UK DBERR, 2008; IAEA, 2008; Chapman and McCombie, 2003; Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2001, 2006). Yet, most researchers involved in HLW/SF investigations judge that engineered
containment combined with deep burial in geological formations would allow HLW/SF to be isolated from the environment for the $10^6$ yrs necessary to make it effectively harmless (OECD, 2008a, 2008b, 2008c; Kintisch, 2009; IAEA, 2006, 2008; Chapman and McCombie, 2003; Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2001, 2006; Canvel, 2006; DEFRA, 2008). The engineered barriers include the reprocessing waste in an insoluble matrix or the actual fuel rods, corrosion-resistant containers, and a bedding/backfill of highly impermeable clay. Potential geological formations are granite, tuff, indurated clay or salt.

Although there is consensus that the permanent disposal of HLW/SF is technically tractable, the majority of countries have yet to identify appropriate sites for their repositories (OECD, 2008a, 2008b, 2008c; Kintisch, 2009; IAEA, 2006, 2008; Chapman and McCombie, 2003; Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2001, 2006; Canvel, 2006; DEFRA, 2008). This has largely been the result of critical errors in public relations and failures in the political approval and licensing procedures. Until recently, disposal strategies were based on rigid schemes established during the early days of nuclear power: (a) develop the technologies, (b) identify the repository site, (c) inform the public, (d) excavate the repository and create the engineered barriers, (e) emplace the waste, and (f) backfill and seal all points of access to the repository. It was assumed that post-closure monitoring would not be required and that the HLW/SF would not be retrievable once the repository was closed. Of the active civilian HLW/SF programmes, only Finland (OECD, 2008a; Kintisch, 2009; Witherspoon and Bodvarsson, 2001, 2006) has proceeded to stage (d). Indeed, several countries have been told to go back to the drawing board and include demands from the general public in the planning process (e.g., UK and Canada [UK DBERR, 2008; Witherspoon and Bodvarsson, 2006; OECD, 2008b, 2008c; DEFRA, 2008]).

As a result of these setbacks, fundamental new strategies are being developed by some countries (IAEA, 2008; Chapman and McCombie, 2003; Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2001, 2006; Canvel, 2006; OECD, 2008b, 2008c, 2008d; DEFRA, 2008; NWMO, 2009; NUMO, 2004). Principal elements of these strategies variously include (i) involving the public in siting the repositories, (ii) flexible staged HLW/SF programmes that can be adapted to account for new knowledge and improved technologies, (iii) pilot repositories, and (iv) enabling long-term retrievability and monitoring, including an extensive period of
post-closure monitoring. Except for post-closure monitoring, these new procedures are relatively straightforward once funding is approved.

Although the long-term safety of well-designed repositories should be assured without the need for post-closure surveillance (Chapman and McCombie, 2003; Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2001, 2006; Canvel, 2006; OECD, 2008b, 2008c; IAEA, 2006; DEFRA, 2008), the general public and other stakeholders are demanding post-closure monitoring for up to several hundred years to assure societal confidence and acceptance of HLW/SF disposal concepts (Chapman and McCombie, 2003; Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2006; OECD, 2004; IAEA, 2001; EU, 2004; Thompson and Simmons 2003; White et al., 2004; Torata et al., 2005). Accordingly, most countries with HLW/SF programmes now include the possibility of post-closure monitoring. However, compared to the broad range of instruments capable of providing high resolution information on evolving conditions within open repositories, there are few options for monitoring backfilled and sealed ones (Chapman and McCombie, 2003; Alexander and McKinley, 2007; OECD, 2004; IAEA, 2001; EU, 2004; Thompson and Simmons 2003; White et al., 2004; Torata et al., 2005).

One key constraint on post-closure surveillance is that the monitoring systems should not impair a repository's engineered and natural rock barriers. This precludes systems that require hard physical connections to a repository's interior. Furthermore, a repository's 500-1000 m depth and the expected small 2-6 m diameters of its shafts/tunnels limit the utility of non-borehole methods; surface-, airborne-, and satellite-based systems will only supply information on far-field variations created by any changes within a repository (table C.S1). In contrast, sensors inside a repository or in nearby boreholes that respond to waves travelling through a repository have a chance of providing detailed knowledge of changing conditions within the repository near field, defined to include the HLW/SF, engineered barriers, and inevitable excavation damaged/disturbed zones (EDZs) that surround a repository's shafts/tunnels. EDZs are generated whenever voluminous rock is removed from the subsurface, in many cases irrespective of the excavation method (Barton, 2007). Since EDZs may extend from the shaft/tunnel walls for distances up to several times the shaft/tunnel radius and their hydraulic conductivities evolve with time, they may be critical elements in the long-term safety of a repository (Bossart et al., 2004; Bossart and Thury, 2007; Bastiaens et al., 2007; Blümling, 2007).
Except for reviews of relevant geoscience methods (IAEA, 2001; EU, 2004; Thompson and Simmons 2003; White et al., 2004; Torata et al., 2005), surprisingly little research has been conducted on the feasibility of post-closure remote surveillance as a means of monitoring the long-term performance of closed HLW/SF repositories. As an initial step, we have investigated the suitability of high frequency crosshole and tunnel-to-hole seismic methods for this purpose. Changes to seismic wave properties could be diagnostic of enhanced water saturation, gas generation due to corrosion of the HLW/SF containers (Alexander and McKinley, 2007; Witherspoon and Bodvarsson, 2006; White et al., 2004), thermal expansion or other swelling of the waste and/or barriers, and changes to the mechanical, hydraulic, and stress/pressure conditions.

C.3 CROSSHOLE AND TUNNEL-TO-HOLE SEISMIC SURVEYS

Many crosshole and tunnel-to-hole seismic methods were developed during the concept verification phases of HLW/SF disposal programmes (Wong et al., 1983; Maurer and Green, 1997; Hayles et al., 1999). They have since been used to map lithologies and structures in areas of geological interest to these programmes and employed widely in other investigations. Ultrasonic (i.e. frequencies >20 kHz) versions of these methods have been used to study EDZs with energy sources and sensors placed inside or within a few metres of the EDZs (Bastiaens et al., 2007; Pettitt et al., 2002; Nicollin et al., 2008). But can similar methods detect changes within the near field of a repository using equipment placed outside the shafts/tunnels?

Our crosshole and tunnel-to-hole seismic experiments were conducted inside the Mont Terri underground rock laboratory, an international research facility within the low permeability Opalinus Clay formation of northern Switzerland (Figure C.1a). This same formation at a greater depth is a primary candidate to host Switzerland's HLW/SF repository. To create conditions expected in a repository, a 1 m diameter microtunnel (simulating a 25-40% downscaled repository tunnel) extending for 13 m was constructed in the Opalinus Clay and filled with dry sand. The sand and EDZ were progressively saturated with water and finally overpressured to 600 kPa, changing conditions intended to resemble the expected evolution of a sealed repository.

Part of our monitoring system was located in two water-filled boreholes (Figure
For each experiment, a high frequency P-wave sparker ignited at 113 locations equally spaced along the source borehole generated seismic waves detected by 96 hydrophones equally spaced along the receiver borehole and by 8 vertical 100 Hz geophones cemented equally spaced around the inside of the microtunnel. We report here selected results of 4 experiments for varying microtunnel/EDZ conditions: (A) dry, (B) 50% water-saturated, (C) fully water-saturated, and (D) pressurised water-saturated. Water saturation and pressurization are expected to increase the P-wave velocities (Zimmer et al., 2007).

Seismic traces generated at all hydrophones from all sources demonstrate the excellent repeatability of the sparker source and the high signal-to-noise ratios of the first-arrival P-waves (Chapter 3). First-break traveltimes (FBTs) can be picked to
within 1-2 data samples (0.032-0.064 ms), whereby the first-break is the earliest discernible signal on a trace. Since the Opalinus Clay is both heterogeneous and anisotropic (Nicollin et al., 2008), an anisotropic code (Zhou and Greenhalgh, 2008) was used to tomographically invert the FBTs. Figure C.2 shows the P-wave velocities obtained by inverting 8884 hydrophone FBTs picked on experiment A data. A high degree of anisotropy is clear from the different velocities perpendicular (Figure C.2a) and parallel (Figure C.2b) to the ~41° inclined symmetry axis. The quasi-layered maximum P-wave velocities mimic the Opalinus Clay bedding.

The hydrophone FBTs for experiments A to D vary by no more than a sample interval. Accordingly, essentially the same P-wave velocity images are derived from all hydrophone FBT data sets. There is no evidence for the microtunnel or associated EDZ in Figure C.2, because FBT tomography based on seismic signals with dominant 2 m wavelengths and long target-sensor raypaths will not resolve such small structures (Figure C.1). However, observed variations in the waveform character as water saturation and pressure increase and companion waveform simulations (Chapter 3) suggest that the microtunnel/EDZ and changes therein could be resolved by employing full-waveform strategies to invert the hydrophone data. Elastic full-waveform inversion that provides estimates of anisotropic velocities, source wavelets, and correction factors for variable source and receiver coupling is challenging (Chapter 3), but we expect to develop the necessary algorithms within the next 2 years.

Clear evidence that increasing water-saturation and pressure within the microtunnel/EDZ affects the transmitted seismic waves is contained in seismic traces generated at the geophones fixed to the microtunnel walls (Figure C.3). We
concentrate here on seismic sections G1-G4, for which the polarities of some first-arrival waveforms flip between experiments A/B and experiments C/D. In addition to the polarity flips, the first-arrival amplitudes and the general character of the seismic sections are noticeably different for the two pairs of experiments (compare seismic sections in the left columns with those in the right columns of Figure C.3), and the FBTs of the C/D traces are earlier than those of the equivalent A/B traces by up to a sizeable 0.35 ms.

C.4 SIMULATIONS AND INTERPRETATION

To understand the substantial changes in the seismic sections that result from soaking and pressurising the microtunnel/EDZ, we have used a finite-difference modeling code to simulate seismic waves passing through plausible models for conditions prevailing during experiments A and D (Figure C.4a and b). The background medium for both models was based on the P-wave velocities of Figure
C.2 and associated S-wave velocities derived by the anisotropic tomographic inversion process (Zhou and Greenhalgh, 2008). For the dry conditions of experiment A, P- and S-wave velocities of 500 and 240 m/s were assigned to the microtunnel sand (Zimmer, et al., 2007) and velocities within the EDZ were increased linearly from 80% of background values at the microtunnel wall to background values 1 m away. For the water-saturated and pressurised conditions of experiment D, P- and S-wave velocities of 1900 and 240 m/s were assigned to the microtunnel sand and velocities within the EDZ were set to background values. Figure C.4c shows synthetic seismic sections based on these two models. Although the match between the observed (left and right columns of Figure C.3) and synthetic (Figure C.4c) sections is imperfect, the
models correctly predict polarity flips, first-arrival amplitude variations, changes in the character of the seismic sections and marked decreases in the FBTs (Figure C.5) as conditions within the microtunnel/EDZ evolve. Discrepancies between the observed and synthetic sections are likely due to shortcomings of the background velocity model and unknown complexities in the shape and physical properties of the EDZ. Nevertheless, the models and synthetic seismic sections, together with snapshots of the simulated waves travelling through the models (not shown here), provide a basis for interpreting the observed data.

Our simulations demonstrate that many first-arrival waveforms are the superposition of waves that have travelled through the microtunnel with waves diffracted around it. The velocity discontinuity and velocity gradient discontinuity at the inner and outer EDZ boundaries are sources of diffracted waves. Waves travelling
directly through the microtunnel strike the vertical geophones from below (positive polarities), whereas the diffracted waves strike them from below or above (negative polarities for the latter case) according to the source-receiver geometries. Superposition of waves with kinematic and dynamic properties dependent on the changing velocities explains the polarity flips and first-arrival amplitude variations. By water saturating the microtunnel/EDZ, the velocity of the direct wave and one of the diffracted waves increases, with the highest increase being for the direct wave. These velocity increases change the reverberation conditions within the microtunnel/EDZ, which influence the general waveform characteristics, and decrease the FBTs.

**C.5 MONITORING POSSIBILITIES**

FBTs recorded along the receiver borehole (Figure C.1) allow the broad-scale anisotropic velocity structure between the two boreholes to be determined, but not the detailed structures and their time variations in the vicinity of the microtunnel/EDZ. In contrast, large FBT variations recorded on the microtunnel walls are evidence for changing physical conditions in this critical region. Because sensors may not be allowed within a closed repository, we need to determine the range of distances from the microtunnel over which FBT variations can be discerned. For the dry and pressurised water-saturated models of Figure C.4a and b, we have computed FBT differences for sensors placed along the microtunnel walls (i.e. the differences between the solid blue and red lines in Figure C.5) and at various distances from the microtunnel. Figure C.6 shows that FBT differences up to 0.1 ms would be detected 3 m from the microtunnel wall as a result of the changing hydrological conditions. Simulations based on 2.5 times upscaled versions of the models suggest that FBT differences up to 0.3 ms would be detected 7.5 m from a 2.5 m diameter repository. Once FBT differences are observed, tomographic inversion of elastic-wave fields recorded at various locations around the repository should eventually allow the detailed physical property changes to be resolved.

**C.6 DISCUSSION AND CONCLUSIONS**

Our experimental results suggest that crosshole and tunnel-to-hole seismic surveys would detect the effects of sizeable water-saturation and pressure variations within a backfilled and sealed underground HLW/SF repository. Computer
simulations demonstrate that such changes within a realistic repository would generate substantial waveform variations in seismic data recorded 10s of meters from the repository boundaries. These changes would also trigger distinct FBT variations at sensors placed within 5-10 m of a repository, which would be grounds for alerting authorities to potential problems within the repository or EDZ. This suggestion is realistic, at least for Switzerland, where observation boreholes are provisionally planned to be located ~2.5 m from the walls of a 2.5 m diameter pilot repository (Bossart and Thury, 2007).

An effective monitoring system might comprise a number of seismic source boreholes 10s of meters from a repository and a series of observation boreholes alongside the repository shafts/tunnels. The observation boreholes could be backfilled and sealed with low permeability bentonite-sand mixtures. When sensors need to be

Figure C.6: Predicted traveltime differences between experiments A and D for geophones G1-G4 (blue symbols) and geophones located radially 1.5 m (green symbols) and 3.0 m (red symbols) from the microtunnel edge. Vertical bars - ± one sample interval.
replaced, inexpensive drilling technologies would allow the boreholes to be safely reamed out. After installing new sensors, the boreholes could be backfilled and sealed again. The initial installation and replacement procedures would have a negligible impact on long-term repository safety. With a suitably designed network of sources and receivers and 3-D full-elastic-waveform inversion codes that account for anisotropy, it should be possible to pin-point the locations of any developing problems in a non-intrusive manner.

Regardless of whether or not one considers nuclear power as essential for resolving humanity's long-term energy needs and at the same time contributing to reducing greenhouse gases, the problem of existing and growing volumes of HLW/SF needs to be addressed. With growing terrorist activity worldwide, the security risks associated with the current practice of storing HLW/SF at the surface is increasing. The results of our preliminary studies suggest that crosshole and tunnel-to-hole seismic techniques will allow deep geological repositories to be monitored remotely and effectively.

C.7 ACKNOWLEDGEMENTS

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APPENDIX D

Geophysics applied to nuclear waste disposal investigations in Switzerland

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D.1 ABSTRACT

Numerous scientists are involved in the Swiss research programmes to develop safe solutions for the long-term disposal of high-level radioactive waste. Geophysics plays an important role in these programmes with respect to site characterisation and the development of monitoring techniques. Two seismic projects are highlighted in this report, one with the objective of site characterisation that was successfully completed some years ago (Marchant et al., 2005) and one on monitoring techniques and underground small-scale characterisation that is ongoing. A comprehensive 3D seismic reflection data set acquired in Northern Switzerland has provided detailed images of gently dipping but relatively undisturbed sedimentary layers, some of which are suitable host formations for radioactive waste repositories. Crosshole and hole-to-tunnel tomographic seismic techniques for monitoring the development of a repository with radioactive waste during the observational phase are being developed and tested in two Swiss underground research laboratories, one located within crystalline rock and one situated within a massive and mainly homogeneous marine claystone (Opalinus Clay).

D.2 INTRODUCTION

Safe disposal of radioactive waste is an important environmental issue of today’s society that profits from the use of energy by nuclear power production. Proposals for the long-term disposal of high-level radioactive waste (HLW) and Spent Fuel (SF) usually involve a combination of multiple engineered barriers and disposal in deep geologic repositories (natural barrier). Candidate repositories must meet strict criteria defined within different laws and regulations from the authorities. Important parameters and processes that need to be evaluated include beside others: (i) the hydraulic and transport properties of the host rock, (ii) hydro-mechanical properties of the host rock and the overlying sediments, (iii) repository induced processes (e.g. thermo-hydro-mechanical processes), (iv) long-term behaviour of waste canisters, engineered barriers and host rock.

Exploration programmes to identify suitable host rocks and potential repository sites have been undertaken in countries worldwide. Many of these programmes have involved seismic surveys for investigating the local geological and structural conditions (e.g. Green and Mair, 1983; Brocher et al., 1998; Birkhäuser et al., 2001;
Juhlin and Stephens, 2006). In addition, relatively deep underground research laboratories have been used to evaluate investigation methods and tools, obtain host rock properties under relevant conditions, conduct large-scale experiments under repository-like conditions and test waste management concepts (e.g. Brown et al., 1989; Lieb, 1989; NEA, 2001; Delay et al., 2007; Bossart and Thury, 2007).

In this contribution, we provide a brief review of selected Swiss geophysical investigations associated with HLW disposal projects. Many of these investigations have either been initiated, conducted or managed by Nagra, the Swiss National Cooperative for the Disposal of Radioactive Waste. The first geophysical reconnaissance campaigns in the 1980's were aimed at assessing the Variscan-age crystalline basement as a host rock for a HLW repository in Northern Switzerland (Thury et al. 1994). They included aeromagnetic, ground-based magnetic, gravity, magnetotelluric and seismic refraction and reflection surveys (Figure D.1). Seven
deep (1306 to 2482 m) boreholes were drilled to calibrate the geophysical site investigations and to provide in situ host rock parameters.

In the early 1990s the focus shifted from crystalline basement in the early 1990s to the Jurassic-age Opalinus Clay formation, primarily because of the latter's homogeneity, extremely low hydraulic conductivity, favourable self-sealing and retention properties and good exploration prospects. A second campaign of regional 2D seismic surveys was carried out to improve the understanding of the structure of the Mesozoic sediments in the prospect area of North-Eastern Switzerland. Based on these data, a 50 km² region in Northern Switzerland (Zürcher Weinland) was selected as an area in which to evaluate the three pillars of the feasibility study: siting, engineering and safety feasibility of a potential HLW repository in Opalinus Clay (Nagra 2002). High-resolution seismic imaging of the Mesozoic sedimentary strata, which included a large 3D seismic reflection data set, and information from an 8th dedicated borehole (the 1007 m deep borehole at Benken, Figure D.1) provided together with the findings from the underground research laboratory Mont Terri important input to this evaluation.

In parallel with the surface and borehole investigations in the 1980ies and 90ies, two underground research laboratories were constructed within Switzerland (Figure D.1). The Grimsel Test Site (GTS) in the central Swiss Alps provides opportunities to study various phenomena under repository-like conditions in a granitic environment (Lieb, 1989; Kickmaier and McKinley, 1997), whereas the international underground research laboratory Mont Terri in the Swiss Jura is appropriate for investigating conditions in a clay-rich sedimentary formation (Bossart and Thury, 2007).

D.3 CONCEPT OF DEEP GEOLOGICAL DISPOSAL OF HIGH-LEVEL RADIOACTIVE WASTE

In agreement with internationally established principles for waste management (e.g. IAEA 1995), Swiss law requires the disposal of radioactive waste in deep geological repositories, following the principle of a staged closure. This principle requires a distinct monitoring period of about 50 to 100 years before the decision on final closure of the repository. Long-term safety of the repository must be ensured through a system of multiple passive and natural barriers. It is mandatory that the
Repository is passively safe after closure. Monitoring is only required to demonstrate that time-dependent processes stay within given ranges and that the observations of the system are according to expectations. Therefore, it is important that monitoring installations do not negatively influence the passive safety of the repository (e.g. by providing preferential transport pathways). The time period for which compliance with the national and international safety criteria has to be demonstrated is $10^6$ years.

Figure D.2 illustrates a possible layout of a repository for the three radioactive waste types: spent fuel (SF), vitrified high-level waste (HLW) from the reprocessing of spent fuel and long-lived intermediate-level waste (ILW). In each case, the principal components of the multi-barrier system are: i) waste form, ii) canister or container, iii) buffer or backfill, and iv) deep underground disposal in the host rock. In the proposed Swiss repository concept (Nagra, 2002), thick-walled carbon steel canisters (or containers with alternative materials) containing SF and/or HLW will be emplaced coaxially within a system of parallel emplacement tunnels (Figure D.2). ILW packages will be put in concrete containers that are also placed in tunnels. The tunnels for the SF and/or HLW will be backfilled with highly compacted bentonite.
that will form a buffer around the canisters, whereas the tunnels for the ILW will be backfilled with mortar.

A pilot facility consisting of several short emplacement tunnels and an observation tunnel will be constructed along the same principles and with the same materials as the main facility. Here, a representative amount of radioactive waste will be disposed. The pilot facility, which has to be hydraulically separated from the main repository, will be designed to permit adequate monitoring of the performance of the engineered and natural barriers.

**D.4 REGIONAL INVESTIGATIONS**

After the acceptance of the general feasibility of a repository for HLW by the Swiss authorities, a program was set up to evaluate potential sites to host the repository. This procedure follows strictly the requirements set up in a sectoral plan enforced by the Swiss government. In a staged approach potential host formations and sites all over Switzerland were selected following a structured and traceable approach. It turned out that Northern Switzerland became the focus of Nagra’s investigations for a HLW repository for a number of reasons, including its:

- relative tectonic stability (including favourable uplift and erosion rates),
- low levels of seismic activity,
- comparatively subdued topography,
- simple layered geology, and
- adequate host rock formations at a suitable depth range.

Northern Switzerland has a low uplift rate of about 0.1 mm/year and a correspondingly low erosion rate. Candidate rocks can be reached using conventional mining or civil engineering technologies in this general region.

The primary objectives of the early regional surveys were to determine the depths, structures and lithologies of the crystalline basement and overlying Mesozoic and Cenozoic sediments (Figure D.3). Of particular importance was the information supplied by Nagra seismic reflection surveys and deep boreholes and the results of
reprocessing and reinterpreting previous seismic reflection and borehole data acquired for hydrocarbon exploration and academic research.

The various seismic reflection profiles provide good quality images of the strata down to depths of about 1 km in the target area and confirm that the Mesozoic and Cenozoic sedimentary formations are good targets for seismic exploration (Figure D.4). In contrast, it is generally difficult to image structures that underlie these formations. Examples are the exploration of Permo-Carboniferous deposits that appear to form deep troughs within the Variscan-age crystalline basement. Interpretations of early refraction and gravity data had suggested their existence, which was later confirmed by observations in several deep boreholes, but even modern seismic reflection data provided only limited information on the lateral extent of this Permo-Carboniferous trough system (Marchant et al, 2005).

Figure D.3: Simplified tectonic map of northern Switzerland showing the location of Nagra seismic profiles, the 3D seismic survey area and deep boreholes.
Analysis of the regional 2D seismic profiles acquired in 1991/92 has indicated that the Opalinus Clay formation in northernmost Switzerland occurs over a depth range suitable for a HLW repository (400 - 900 m below surface; Figure D.4). Furthermore, the relatively uninterrupted nature of reflections from its upper and lower boundaries suggests that it has been subjected to only low levels of horizontal tectonic stress since the sediments were deposited. Based on safety-related geological considerations, this area of Switzerland was selected for local investigations, including a comprehensive 3D seismic campaign acquired in 1996/97 (Birkhäuser et al., 2001) and an additional borehole drilled in 1998/99 at Benken (Nagra, 2001).

D.5.1 Design and data acquisition

In a moderately populated and intensively farmed area, conducting an extensive 3D seismic field campaign requires substantial advance planning. Model calculations
were carried out to define field parameters for optimum imaging of the sedimentary rocks over the desired depth range (Table D.1). A combination of air photographs and digital plans of infrastructure provided input for planning the permitting and the data acquisition (Figure D.5a). It was possible to deploy practically all geophones with only minor deviations from the planned receiver lines. The majority of source points were situated in open fields and areas along small roads, such that most could be accomplished within 10 m in-line and 30 m cross-line of the planned positions (Kuhn & Graf, 1996).

Source points were excluded in the vicinity of sensitive buildings and infrastructure (e.g. underground cables, pipes and drainage systems). Both explosives and Vibroseis were used for the sources. Depending on the ground conditions and the required safety distances from sensitive infrastructure, explosive charges of either 200 g or 600 g were placed in shot holes of variable configurations and lengths (Table D.2). The use of Vibroseis was restricted to roads and sufficiently stable paths. To avoid structural damage to buildings, conventional non-linear sweeps were replaced.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Survey size</td>
<td>~50 km2</td>
</tr>
<tr>
<td>Target depth</td>
<td>250 m - 1200 m</td>
</tr>
<tr>
<td>Geophone type</td>
<td>SM4U, 10 Hz</td>
</tr>
<tr>
<td>Source type</td>
<td>Explosives &amp; Vibroseis</td>
</tr>
<tr>
<td>Active channels</td>
<td>480</td>
</tr>
<tr>
<td>Active geophone lines</td>
<td>8</td>
</tr>
<tr>
<td>Line spacing (source and geophone lines)</td>
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</tr>
<tr>
<td>Station spacing (sources and geophones)</td>
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<td>15 m x 15 m</td>
</tr>
<tr>
<td>Nominal fold</td>
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</tr>
<tr>
<td>Sampling rate</td>
<td>2 ms</td>
</tr>
<tr>
<td>Record length</td>
<td>4000 ms</td>
</tr>
</tbody>
</table>

Table D.1: Field parameters for the 3D seismic survey
by random sweeps in critical built-up areas. In addition to the reflection seismic data, up-hole recordings were carried out at 17 positions within the survey area in order to calibrate the seismic velocities of the unconsolidated overburden for the calculation of static corrections.

The three month field campaign was carried out during winter to minimise the impact on agricultural production. Cooperation with the local population proved to be very constructive. Thanks to the overall acceptance, 98.4% of the ~9,000 planned

<table>
<thead>
<tr>
<th>Source type</th>
<th>Description</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Explosives</td>
<td>200 g charges in three 2.5 m deep boreholes</td>
<td>47.9%</td>
</tr>
<tr>
<td></td>
<td>600 g charges in a 6-12 m deep borehole</td>
<td>29.5%</td>
</tr>
<tr>
<td>Vibroseis</td>
<td>10 – 100 Hz, 12 s non-linear sweep</td>
<td>15.7%</td>
</tr>
<tr>
<td></td>
<td>10 – 100 Hz, 24 s random sweep</td>
<td>6.9%</td>
</tr>
</tbody>
</table>

Table D.2: Source parameters and statistics
source points could be recorded. The nominal CDP fold of 20 was reached for almost the entire survey area (Figure D.5b).

D.5.2 Data processing

The data processing focused on imaging the shallow to moderately deep target rock formations (Table D.3). Special attention was given to obtaining seismic traces with optimally balanced frequency spectra. Despite very different source signals (i.e. different size explosive charges in holes of varying length plus Vibroseis; Table D.2) and highly variable coupling conditions, careful application of surface-consistent amplitude balancing and surface consistent deconvolution yielded traces with uniform
spectral characteristics ready for subsequent processing. The useful frequencies after these steps were mostly in the 10 - 85 Hz range.

After the issues of varying source signal and ground static corrections were resolved, the next step in processing was the correct spatial positioning of the reflection signals, at that time solved with dip move out (DMO) corrections calculated before velocity analysis and normal move-out corrections, muting, stacking and a 3D finite-difference migration. The DMO operator had to be re-designed to allow handling the reflections at shallow levels. A carefully applied 3D FX deconvolution after migration considerably improved the image quality. In order to preserve a maximum of the high frequencies recorded from the target horizons, which generally dip at 3 to 6° throughout the area, a CDP-dependant bandpass filter was applied at the end. After this processing, a coherency cube was derived from the amplitude dataset.

**D.5.3 Interpretation**

Using a seedline grid, the boundaries of the sedimentary formations were traced semi-automatically throughout the 3D seismic volume and thereafter, attribute analyses were carried out (Figures D.6 and D.7). The predicted thickness of the Opalinus Clay formation based on 2D profiles (Naef & Birkhäuser, 1996) is confirmed to be 100 - 120 m. This simple observation is one of the most important results of the 3D seismic survey as it confirms the Opalinus Clay to be prospective in the area for potentially hosting a repository for radioactive waste.

Figure D.6 demonstrates that the Opalinus Clay formation is seismically significantly more transparent than both the overlying Malm marl and the underlying Lias formation. Faults intersecting the Opalinus Clay formation with heaves of only around 10 metres can be resolved directly from the amplitude data. Only the bordering, northwest - southeast trending Neuhausen fault, well known from earlier 2D-seismic data, penetrates the entire overburden and much of the Mesozoic section (N in Figures D.6 and D.7).

Small scale irregularities seen from attribute analysis of the uppermost Keuper marker horizon (TSt in Figure D.7d) are noteworthy, particularly in the southwestern part of the survey area. Deformation of the reflectors decreases significantly in an upward direction from the uppermost Keuper to the base of the Opalinus Clay (Figure
D.7c). Above this horizon, no small-scale fragmentation is discernable within the 3D seismic volume (Figure D.7a and D.7b).

The enlargement in Figure 6 reveals one of the few faults that slightly offsets the largely undisturbed bedding of the Opalinus Clay. Using attribute analysis it is possible to identify a sequence of such faults. Together, they form an en-echelon pattern that defines the Wildensbuch flexure (W in Figure D.7), an east-west trending feature that merges with the Neuhausen fault (N in Figure D.7) at Wildensbuch. These local transtensional structures extend some distance into the overlying Malm marl (Figure D.7a). Their maximum observed vertical displacement at the level of the Opalinus Clay is ~17 m. The interpretation of the 3D seismic data confirms the conclusions of previous regional geological analyses that included...
information from extensive 2D seismic surveys: the Opalinus Clay formation has resided beneath the Zürcher Weinland in a practically undisturbed state since it was deposited some 180 Ma ago.

The 1007 m deep Benken borehole was drilled after the 3D seismic survey was completed. It provided the means to acquire geological and geophysical data that complemented the 3D survey results. In particular, lithological, sonic and density logs were collected within the borehole and a walkaway vertical-seismic profile (VSP) survey was conducted. The VSP survey involved sensors down the borehole and sources at the surface. Figure D.8 demonstrates excellent correlations between a synthetic seismogram derived from the borehole sonic and density logs, the processed VSP section and the corresponding cross-section extracted from the 3D data volume.
These correlations allow the borehole lithological information to be reliably extrapolated in all directions on the basis of the 3D seismic data.

**D.6 MONITORING BASED ON RESEARCH IN THE SWISS UNDERGROUND RESEARCH LABORATORIES**

Once the site for a high-level radioactive waste repository has been chosen, it should be relatively straightforward to design strategies for monitoring its construction and operational performance. Some countries are also considering a monitoring period after waste emplacement, which will be much more difficult because data transmission from the backfilled repository to the open repository observation tunnels will be severely restricted or even prohibited as soon as construction and operation tunnels have been backfilled and sealed. Clearly, monitoring systems must not compromise the integrity of the engineered and natural
rock barriers. As a consequence, remote monitoring systems or data acquisition with wireless data transmission systems will be preferred. But there are very few remote-monitoring techniques capable of providing the required resolution. For example, the expected 400 - 900 m depth of the repository and the small 2 - 6 m diameters of its shafts and tunnels will seriously limit the utility of all surface-, airborne- or satellite-based geophysical techniques. Fortunately, crosshole or hole-to-tunnel tomographic seismic methods may provide the means to track changing conditions within the waste, the engineered barriers and the excavation disturbed zones (EDZs) that surround the repository's shafts and tunnels. Variations in seismic wave properties could be diagnostic of (i) changes in pore water pressure, (ii) gas pressure built-up by corrosion of the waste containers, (iii) thermal expansion or swelling of the engineered and natural barriers, and (iv) changes to the mechanical, hydraulic and stress conditions.

To address the issue of repository monitoring, a number of international research groups have been conducting experiments in Switzerland's two underground research laboratories at Grimsel (GTS) and Mont Terri (Figure D.1). We highlight here two ongoing studies, both of which include tomographic seismic experiments. One suite of experiments concerns the remote monitoring of bentonite layers within GTS. Regardless of the host formation to be used for a repository, many countries are planning to surround their high-level radioactive waste with a bentonite buffer, primarily because of its extremely low hydraulic conductivity and its favourable self-sealing and sorption properties. The second suite of experiments involves the remote surveillance of a sand-filled microtunnel and surrounding EDZ under various water-saturation and pressure conditions at Mont Terri. Since EDZs may extend considerable distances from the tunnels or shafts (up to twice their radii) and their potentially enhanced hydraulic conductivities, they may form preferential flow-paths along tunnels and thus enhance potential transport of radionuclides out of the repository. Experiments at both sites are ongoing, such that the results described below are preliminary.

**D.6.1 Experimental configurations**

Sketches of the experimental configurations at GTS and Mont Terri are presented in Figures D.9 and D.10. For both suites of experiments, a sparker energy
source and multi-element hydrophone chains (located in water-filled boreholes) and 100 Hz vertical-component geophones (attached to the tunnel wall) are employed.

At GTS, the layers of bentonite form a 1-m-thick wall wedged at the end of a 3.5 m diameter tunnel by a 4 m long shotcrete plug. Swelling of the bentonite induced by injecting water at a number of locations is expected to be accompanied by substantial variations of its elastic properties. To test this concept, tomographic seismic experiments are being conducted in six gently dipping 25 m long boreholes located at regular intervals around the circumference of the tunnel, shotcrete plug and bentonite wall (Figure D.9). During each measurement campaign, energy from the P-wave sparker is released at 0.25 m intervals along boreholes 3, 4 and 5 and recorded by an acquisition system that includes hydrophones at 0.25 m intervals along boreholes 1, 2 and 6 and twenty-five geophones rigidly mounted to the front wall of the shotcrete plug (Chapter 3).

At Mont Terri, a 13 m long sand-filled microtunnel with a diameter of approximately 1.0 m (Figure D.10) is intended to mimic a 30 - 40 % scaled emplacement tunnel within the Opalinus Clay formation. During successive experiments, the microtunnel is progressively water-saturated, over pressured and
eventually injected with gas. To monitor the expected changes to the seismic properties of the sand-filled tunnel and EDZ, energy from the P-wave sparker is released at 0.25 m intervals along the 29 m long borehole S and recorded by an acquisition system that includes hydrophones at 0.25 m intervals along the 25 m long borehole R and eight geophones mounted at roughly equal distances around the interior of the microtunnel (Chapter 3). The two boreholes and geophones are located within a common plane perpendicular to the microtunnel axis.

### D.6.2 Computational simulations

To provide a basis for interpreting the recorded data, wavefields and synthetic seismic sections for models that represent completely dry and fully water-saturated conditions at the two sites have been computed (D.Figure 11). Bohlen's (2002) visco-elastic finite-difference time-domain modelling code, modified by the ETH group to
include the effects of significant anisotropy at the Mont Terri site, was used for the 2-
D computations. Ricker-wavelet sources based on the recorded data had centre
frequencies of 3 and 2 kHz for the GTS and Mont Terri computations. Granite,
shotcrete, dry bentonite and water-saturated bentonite in the GTS model are assigned
P-wave velocities of 5.2, 2.8, 0.5 and 2.0 km/s, respectively. Opalinus Clay in the
Mont Terri model had maximum and minimum velocities of 3.1 and 2.3 km/s and an
EDZ with dry/water-saturated velocities decreasing linearly from 100 % of normal
values at 1.5 m radius to 60/72 % at the surface of the microtunnel. The dry and
water-saturated sand had velocities of 0.5 and 1.9 km/s. The rationale for these
velocities and related physical properties is given by Marelli et al. (2010, Chapter 3).
For the simulations, a source was located at 13.5 m in borehole 5 and hydrophones
along borehole 2 in the GTS model (Figure D.9) and a source was placed at 13 m in
borehole S and hydrophones along borehole R in the Mont Terri model (Figure D.10).
Results of the computational studies, including those shown in Figure D.11, predict that first-arrival traveltime variations resulting from the changing water-saturation conditions within the respective target structures (bentonite at GTS; sand-filled microtunnel and EDZ at Mont Terri) are unlikely to yield significantly different traveltime tomograms; first-arrival traveltimes at the hydrophones are practically invariant. At both sites, seismic velocities within the target structures are uniformly lower than those of the host formations for both dry and water-saturated conditions. As a consequence, direct waves passing through the target structures travel much slower than waves diffracted around them, such that at moderate to far distances (e.g. at the hydrophones) the first arrivals are diffracted waves that are little affected by the changing conditions within the target structures. The situation is somewhat different for distances closer to or within the target structures (e.g. at the geophones in Mont Terri), in that the direct and diffracted waves arrive at similar times. For example, systematically different first-arrival polarities in the Mont Terri simulations indicate that the earliest phases at some geophones are direct waves and at others they are diffracted waves.

Wavefield snapshots and hydrophone sections in Figure D.11 reveal marked changes in the characteristics of later arriving phases for the dry and water-saturated conditions. Many of these phases are reflections and diffractions from the boundaries of the target structures and energy resonating within them. These changes, which are highlighted in the difference wavefield plots (Figure D.11c and D.11i) and difference hydrophone sections (Figure D.11f and D.11l), may be the basis for monitoring the internal conditions of the target structures. Indeed, the simple observation of significantly changing waveform characteristics would be grounds for additional investigations or perhaps remedial actions. It would be even better if we could extract information on the changing velocities from the later arriving phases.

D.6.3 Crosshole hydrophone data

Marelli et al. (2010, Chapter 3) have presented preliminary results of studies at both sites (e.g. Figure D.12 from GTS). They demonstrated that the sparker energy source produced consistent signals rich in frequencies up to ~5 kHz out to distances greater than 25 m. Although the hydrophone recordings contained reliable and repeatable first-arrival pulses, the signals were contaminated with incoherent high frequency noise and the effects of variable hydrophone-to-rock coupling conditions.
The events between the first arrivals and the oblique green line in the hydrophone recordings of Figure D.12 are a combination of reflections and diffractions of the type represented in the synthetic sections of Figure D.11 modulated by the effects of varying hydrophone-to-rock coupling conditions. Obviously, it is going to be necessary to account for variable hydrophone-to-rock coupling conditions in any attempt to invert the crosshole hydrophone data using full-waveform techniques.

Strong events indicated by the green and red lines in Figure D.12 (and other parallel events) are various types of tube wave (Cheng and Toksoz, 1981). Conversion of tube-waves to radiating P-waves at the end of the source borehole creates the faster phase indicated by green lines in Figure D.12b, whereas conversion of tube-waves that have travelled to and from the end of the borehole to radiating P-wave energy at the sparker casing generates the slower phase indicated by red lines.

D.6.4 Hole-to-tunnel geophone data

Typical geophone sections recorded within the microtunnel at Mont Terri are presented in Figure D.13. The signal-to-noise ratios of the geophone sections at both
sites are generally much higher than those of the hydrophone sections. Sections recorded at geophone G15 near the base of the tunnel under dry conditions and water-saturated and pressurised conditions are shown in Figure D.13a and D.13d, respectively. Those recorded at geophone G7 near the top of the tunnel under the same conditions are displayed in Figure D.13b and D.13e.

The change from dry to water-saturated and pressurised conditions resulted in changes to the first-arrival traveltimes and character of subsequent events at all geophones. Water saturation and pressurisation caused the first waves to arrive ~0.1 ms earlier on the lower geophones (using the white line at 2.5 ms as a guide, compare the first arrivals at G15 in Figure D.13a and D.13d). Since the first arriving waves only travelled through the host rock and EDZ before encountering the lower geophones, this decrease in traveltime must have been caused by increased velocities within the EDZ (Manukyan et al., 2008).

As predicted by the modelling studies, a noticeable feature of geophone recordings from the upper parts of the microtunnel is the systematic variation in polarity of the first arrivals, with negative polarities being generated by sources in the first ~7 m of the source borehole in Figure D.13b and D.13e and positive polarities...
elsewhere. The boundary between negative and positive polarities varies according to the water-saturation conditions, but happens to be the same for the two end-member states for the particular geophone recordings shown in Figure D.13. The explanation for the varying polarities sketched in Figure D.13c is based on the results of the synthetic computations. First arrivals from most source positions are waves that have travelled directly through the EDZ and microtunnel and cause the geophone to register upwards motion, whereas the first arrivals from the first ~7 m of the source borehole are diffracted waves that have travelled around the outer part of the EDZ, imparting downward motion to the geophone. In the upper parts of the microtunnel, the decreases in first-arrival traveltimes that result from water-saturation and pressurisation vary between 0.2 and 0.4 ms (use the white line at 3.0 ms in Figure D.13b and D.13e as a guide for estimating the differences in the earliest first arrivals).

D.7 DISCUSSION AND CONCLUSIONS

Switzerland-based researchers were the first to employ state-of-the-art 3D seismic reflection surveying techniques in a programme associated with radioactive waste disposal. The information provided by the high-resolution images allowed to evaluate the depth and thickness of the Opalinus Clay formation, confirm its low degree of deformation and prove the absence of larger tectonic structures in the target area. As a consequence, 3D seismic surveying will likely play a key role in Switzerland's search for the final site of its HLW repository.

With regard to the project concerned with monitoring of repositories, full-waveform inversion schemes are going to be needed to extract important information from events recorded after the first arrivals in the hydrophone and geophone data sets. A primary goal of current research is to produce full-waveform inversion codes that provide high-resolution images of relatively small targets embedded within large rock masses by accounting for (i) the presence of the boreholes, (ii) significant anisotropy of the host media and (iii) variable hydrophone-to-rock coupling conditions. For example, Maurer et al. (2010, Appendix B) have recently developed a full-waveform acoustic inversion scheme that estimates medium properties as well as frequency-dependent source functions and frequency-dependent hydrophone-rock coupling factors. They have successfully tested this scheme on synthetic acoustic data contaminated with systematic coupling effects that have the same statistical characteristics as the GTS hydrophone data. Once an elastic-wave version of this code
is completed, it will be applied to the recorded various data sets. A second research goal, which will involve a combination of field and computational studies, will be to determine how far the seismic sensors can be placed from an emplacement tunnels and still record variations in first-arrival traveltimes due to significant changes within the repository.

D.8 ACKNOWLEDGEMENTS

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APPENDIX E

Ultra-high-resolution seismic imaging of the Alpine Fault, New Zealand

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E.1 ABSTRACT

High-resolution seismic reflection surveys across active fault zones are capable of supplying key structural information required for assessments of seismic hazard and risk. We have recorded a 360-m-long ultra-high-resolution seismic reflection profile across the Alpine Fault in New Zealand. The Alpine Fault, a rare continental transform that juxtaposes major tectonic plates, is capable of generating large (M > 7.5) damaging earthquakes. Our seismic profile across a northern section of the fault targets fault-zone structures in Holocene to late Pleistocene sediments and underlying Triassic and Paleozoic basement units from 3.5 - 150 m depth. Since ultra-shallow seismic data are strongly influenced by near-surface heterogeneity and source-generated noise, an innovative processing sequence and non-standard processing parameters are required to produce detailed information on the complex alluvial, glaciofluvial and glaciolacustrine sediments and shallow- to steep-dipping fault-related features. We present high-quality images of structures and deformation within the fault zone that extend and complement interpretations based on shallow paleoseismic and ground-penetrating radar studies. Our images demonstrate that the Alpine Fault dips 75° - 80° to the southeast through the Quaternary sediments, and there is evidence that it continues to dip steeply between the shallow basement units. We interpret characteristic curved basement surfaces on either side of the Alpine Fault and deformation in the footwall as consequences of normal drag generated by the reverse-slip components of displacement on the fault. The fault dip and apparent ~35 m vertical offset of the late-Pleistocene erosional basement surface across the Alpine Fault yield a provisional dip-slip rate of 2.0 ± 0.6 mm/yr. The more significant dextral-slip rate cannot be determined from our seismic profile.

E.2 INTRODUCTION

Knowledge of fault-zone structure in the shallow subsurface is important for understanding seismic hazard and risk. Key physical properties of potentially active faults are usually determined or inferred from surface outcrops, geomorphology, shallow boreholes, and/or trenches. High-resolution geophysical imaging at greater depths can extend and enhance interpretations of fault-zone structure and behavior.

There are only a few examples worldwide of continental transform faults juxtaposing major tectonic plates, the most notable being the San Andreas and Alpine faults. The Alpine Fault is a large transpressional strike-slip fault that accommodates
much of the ~36 mm/yr relative plate motion across the South Island of New Zealand. Although surface rupture of the fault has not been recorded in the ~200 years of European settlement, paleoseismic evidence suggests the fault is likely to rupture in large events (M > 7.5), posing a considerable seismic hazard in the region (Sutherland, et al., 2007).

At our survey site along the northern section of the Alpine Fault (Figure E.1), the fault trace emerges from dense bush and mountainous terrain to cross an open, relatively flat area known as Calf Paddock. Abandoned late Quaternary river terraces and stream channels formed by the Maruia River are offset vertically and horizontally across the main trace of the fault (Wellman, 1952), indicating ongoing displacement. Paleoseismic trenching suggests the last surface rupture at Calf Paddock occurred between 1530 and 1700 A.D. (Yetton, 2002). Extensive 3D ground-penetrating radar (GPR) surveys (McClymont, et al., 2008; McClymont et al., 2009) delineate multiple fault strands in shallow Quaternary gravels, and a borehole and seismic refraction profiles (Garrick and Hatherton, 1974) provide limited constraints on fault geometry to basement depth. Detailed shallow geophysical imaging to the level of the basement and deeper has not previously been undertaken at Calf Paddock or elsewhere along the Alpine Fault.

Imaging of shallow features presents general challenges for seismic processing that are amplified when the targets are complexly deformed structures associated with active fault zones (e.g. Pratt et al., 1998; McBride and Nelson, 2001; Improta and Bruno, 2007). Specific problems related to fault zones within unconsolidated sediments and underlying basement include (1) high degrees of near-surface heterogeneity (e.g., large lateral variations in near-surface velocity and weathered-layer thickness) that require the careful computation and application of static corrections; (2) the presence of substantial source-generated noise (e.g., ground roll, guided phases, and multiple reflections); and (3) difficulties in imaging steeply dipping and/or severely deformed structures within and about the fault zone.

Steeply dipping faults inferred from abrupt terminations or offsets of sedimentary reflections may be difficult to trace through less reflective basement unless reflections from the actual fault planes are recorded. However, there are only a few examples of reflections being recorded from steeply dipping strike-slip fault planes (Lemiszki and Brown, 1988; Adam et al., 1992; Stern and McBride, 1998; Hole et al., 2001; Okaya, et al., 2007).
We have acquired ultra-high-resolution seismic reflection data targeting shallow deformation structures in the Alpine Fault zone down to and beyond basement depth. With careful processing and interpretation we have addressed many of the problems inherent in the high-resolution seismic imaging of active faults. Our final high-quality seismic images have provided constraints on key physical properties of the shallow fault zone at Calf Paddock.

After describing the geological setting and seismic data acquisition, we outline our processing strategies with emphasis on the calculation and application of corrections for near-surface velocity heterogeneity and enhancement of very shallow reflections. Stacked and migrated sections then reveal conspicuous offsets in basement reflections and ambiguous moderately steep-dipping (~50°) energy near the projected location of the fault zone within the basement. We use a finite-element modeling approach to investigate the origin of the moderately steep-dipping energy in Appendix E.A. Finally, we discuss the significance of these features and present a provisional geological interpretation of the migrated seismic section.

E.3 THE ALPINE FAULT

E.3.1 Variation in slip rates

The Alpine Fault marks the boundary between the Australian and Pacific plates through the South Island of New Zealand (Figure E.1a). It is a major transpressive dextral fault that accommodates approximately two-thirds of the relative plate motion (Sutherland, et al., 2006; Norris and Cooper, 2007). Basement terranes are laterally offset >470 km across the fault, and a smaller but important component of convergence is responsible for rapid uplift of the Southern Alps. Maximum dextral and dip-slip rates of ~25 mm/yr and 10 mm/yr occur along the central section of the fault (Berryman, et al., 1992; Norris and Cooper, 2000). To the north, relative plate motion is increasingly taken up by younger strike-slip faults of the Marlborough Fault zone (MFZ in Figure E.1a), such that the estimated slip on the Alpine Fault decreases north of the intersection with the Hope Fault to ~10 mm/yr (dextral) and ~6 mm/yr (dip-slip) (Norris and Cooper, 2000; Langridge and Berryman, 2005). Further north at our survey site, the slip rates are likely to have decreased further, though this has not been quantified.
Figure E.1: (a) Pre-Cenozoic basement terranes of the South Island of New Zealand (following classification of Bradshaw, 1989) are offset by ~470 km along the Alpine Fault (black line). Much of the relative motion between the Australian and Pacific plates (DeMets, et al., 1994) in the north of the Island is taken up along the Alpine Fault and the Marlborough Fault Zone (MFZ). Continuations of the plate boundary offshore are marked by dashed lines. The yellow star indicates the location of our Calf Paddock study site. (b) Sketch of the local geology in the vicinity of the study area adapted from Mabin (1983) and Nathan et al. (2002). (c) Aerial photograph of Calf Paddock showing the location of the seismic profile, borehole, and paleoseismic trench. Also shown are the Alpine Fault (AF, solid line where there is a visible surface scarp) and overlapping en-echelon fault strands (SF) with no surface expression (McClymont, et al., 2009).
E.3.2 Variations in fault character

Much of the Alpine Fault appears as a simple linear trace striking 055° on satellite photos (Berryman, et al., 1992). It is inferred to have a moderate to steep southeasterly dip through the upper crust (Norris and Cooper, 2007); reflections at ~20 – 30 km depth on regional-scale seismic reflection profiles east of the Alpine Fault have been interpreted as defining a fault plane dipping ~50° to the east (Davey, et al., 1995; Kleffmann, et al., 1998; Okaya, et al., 2007). At shallower depths, oblique slip is accommodated through more complex fault structures. In the central section of the Alpine Fault, the surface trace follows a zigzag pattern of alternating predominantly strike-slip and predominantly thrust sections on a scale of 1 - 10 km (Norris and Cooper, 1995). Steeply dipping narrow fault zones are inferred along the strike-slip sections, whereas relatively shallow fault dips have been observed at outcrops of the thrust sections. Further north towards our study site, the fault trace appears roughly linear with small scale en-echelon step-overs (Berryman, et al., 1992), suggesting that oblique slip is accommodated differently in this region. Additional detailed imaging of the near-surface fault zone at Calf Paddock to elucidate questions of fault dip and geometry as well as the nature of near-surface faulting is therefore of interest.

E.3.3 Local geology

At Calf Paddock (Figure E.1b), the Alpine Fault is distinguished by a ~2-m-high linear fault scarp that cuts across a sequence of abandoned terraces of the Maruia River. The constituent glaciofluvial valley sediments date from periods of late-Pleistocene aggradation that followed phases of advance and retreat of the Maruia Glacier (Suggate, 1965; Mabin, 1983). During the last phase of ice advance (i.e. the end of the late-Pleistocene Otira Glaciation, c. 22 - 14 ka), the glacier flowed from the southeast dividing into two lobes on either side of Marble Hill (Figure E.1b; Mabin, 1983). Basement southeast of the fault is Triassic-age Alpine schist, whereas that to the northwest is locally variable with Paleozoic-age marble outcropping close to our seismic profile (Nathan, et al., 2002).

Paleoseismic trenches 60 - 80 m to the northeast of our seismic profile on the youngest river terrace intercept a narrow zone of variably dipping (40 - 90°) faults within the upper 1 - 2 m of gravels (Yetton, 2002). Such gravels are either exposed at the surface or covered by a thin layer of undisturbed topsoil. GPR surveys at Calf
Paddock reveal a narrow fault zone dipping steeply to the southeast at ~80° to a depth of ~15 m (McClymont, et al., 2008; McClymont, et al., 2009). Notable changes in GPR reflection geometry are observed across the main strand of the fault. Additional changes in reflection characteristics ~30 m on either side of the main trace are interpreted as secondary left-stepping en-echelon fault strands and associated deformation. GPR data allow one of these secondary fault strands to be mapped to within 30 m of our seismic profile (SF in Figure E.1c). The relationships between the main fault and secondary faults below the sediment cover are unknown.

Garrick and Hatherton (1974) describe the results of seismic refraction surveying along lines perpendicular and oblique to the fault. They also present information from a borehole 39 m southeast of the fault trace (Figure E.1c) that penetrated 26 m of gravels and underlying basement schist to a depth of 83 m. The borehole revealed zones of shearing and a steeply dipping fault within the schist, but it did not reach the Alpine Fault itself. Interpolating from the surface scarp to the basement offset (inferred from the refraction profiles) and the base of the borehole led them to estimate a minimum average fault dip of ~65° at this location.

The strong change in lithological and seismic properties at the sediment-basement contact observed in the borehole and refraction data correlate well with the strongest reflections in our data. We interpret this contact to represent an unconformity formed by glacial erosion during the late Pleistocene. Subsequent offset and deformation of this important marker surface is highlighted in our seismic images.

E.4 ULTRA-HIGH-RESOLUTION SEISMIC DATA ACQUISITION

Our ultra-high-resolution seismic data were acquired along a line oriented perpendicular to the surface fault scarp, approximately 10 m northeast of a fault-monitoring concrete wall that acts as a large strain gauge\(^1\). Acquisition parameters (Table E.1) were chosen to provide highly detailed images of the fault zone from the near-surface through the Quaternary sediments and basement to depths of ~150 m. A 5 kg-hammer source (six blows against a steel plate) located every 1 m along the profile provided adequate depth penetration and a broad frequency bandwidth of reflection energy. Stacking seismic signals generated by the hammer blows increased

\(^1\) Evison's Wall, erected at the site in the 1960s, is now a well known New Zealand landmark.
the signal-to-ambient-noise ratio and reduced the relative strength of the recorded steel-plate ‘bounce’ at traveltimes >100 ms.

Data were recorded on a 240-channel 24-bit Geometrics Geode acquisition system. Receivers (single vertical 30-Hz geophones) spaced at 0.5 m intervals were offset from the sources by ~0.5 m to the southwest. Roll-along was achieved by moving 48 receivers at a time. The resulting 360-m-long profile has a fold of up to 60 with a common-midpoint-spacing of 0.25 m.

**E.5 SEISMIC DATA PROCESSING**

Careful processing (Table E.2) was required to produce meaningful images of the Alpine Fault and adjacent regions. Although the individual processes in Table E.2 are relatively standard tools in deep exploration seismology, it was necessary to adapt the processing flow and parameters to address the specific problems of our complex shallow data set. To ensure that all critical events were preserved and that artificial reflections were not created, it was essential to follow the results of the testing and processing on representative common-source and common-midpoint (CMP) gathers and

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source</td>
<td>5 kg hammer (6 stacked blows)</td>
</tr>
<tr>
<td>Geophone frequency</td>
<td>30 Hz</td>
</tr>
<tr>
<td>Receiver spacing</td>
<td>0.5 m</td>
</tr>
<tr>
<td>Source spacing</td>
<td>1 m</td>
</tr>
<tr>
<td>Lateral offset of source</td>
<td>0.5 m</td>
</tr>
<tr>
<td>CMP spacing</td>
<td>0.25 m</td>
</tr>
<tr>
<td>Fold</td>
<td>~60</td>
</tr>
<tr>
<td>Source-receiver offset range</td>
<td>typically 0.5– 60 m</td>
</tr>
<tr>
<td>Active channels</td>
<td>240</td>
</tr>
<tr>
<td>Line length</td>
<td>360 m</td>
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<tr>
<td>Record length</td>
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</tr>
<tr>
<td>Sample rate</td>
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</tr>
</tbody>
</table>

Table E.1: Data Acquisition Parameters
stacks of the data (Steeples et al., 1997; Büker et al., 1998b). Such an approach was especially important in our attempts to image ultra-shallow (<10 m depth) structures (Schmelzbach et al., 2005). Each process was eventually applied on the basis of demonstrated clear overall improvement of the unmigrated and migrated images. We present (i) the results of our general processing sequence, (ii) a near-surface tomographic velocity model that helps us devise an appropriate strategy for determining static corrections, and (iii) the output of an alternative processing sequence designed to enhance the shallowest reflections from the Quaternary sediments.
E.5.1 Pre-stack processing

Raw source gathers (e.g., Figure E.2a) are dominated by low-frequency (<140 Hz, peak frequency ~50 Hz) ground roll and higher frequency air waves. In many source gathers, strong low-frequency guided phases are also present, representing trapped energy within the near-surface low-velocity layer (e.g., Robertsson et al., 1996). Strong reflections are visible only within the optimum reflection windows. Spectral analysis shows that reflections generally have a broad bandwidth of up to 600 Hz with a peak frequency of ~150 Hz. As a consequence, they can be separated in the frequency domain from the ground roll and guided phases to a large degree. Spectral whitening in the range 100 - 600/500 Hz successfully removes much of the coherent noise and sharpens the reflections (Figure E.2b). A time-variant spectral whitening scheme is adopted, in which the maximum frequency is reduced with increasing traveltime to avoid amplifying high-frequency noise with depth (Table E.2).
Large static shifts in the data were caused by topographic relief (up to 5 m; our shallowest targets are only 3.5 m below the surface at some locations) and strong lateral variations in the properties of the near-surface weathering layer. After applying refraction-static corrections, which are discussed in some detail in the next section, we accounted for small residual-static shifts using a method that maximizes the CMP stack power within selected windows and chosen source-receiver-offset ranges (Ronen and Claerbout, 1985). Strict quality control and testing of the residual-static solutions were necessary; clearly erroneous values were identified and removed. A first pass of residual-static computation and application (source/receiver corrections <0.6 ms) was followed by renewed velocity analyses and a second residual-static calculation (corrections <0.3 ms). Application of surface-consistent refraction- and residual-static corrections markedly enhanced the coherency and stacking power of reflections (Figure E.2c).

Airwave attenuation, mild F-K filtering, and a top mute reduced remaining coherent noise (Figure E.2d) before stacking. The F-K filter was designed to pass coherent events with apparent velocities >350 m/s, thus attenuating residual surface-wave energy while enhancing the coherency of reflections. This filter was most effective in the source domain, because the close trace spacing (0.5 m) allowed filtering of higher frequencies without introducing artifacts due to aliasing.

**E.5.2 Refraction tomogram and computation of refraction-static corrections**

First-arrival traveltimes in source gathers (e.g., Figure E.3a) provide evidence for considerable velocity contrasts and lateral variations in the near-surface weathering layer. By modeling this layer via a tomographic inversion of first arrivals, we demonstrate that a simple 2-layer velocity model for refraction-static calculations is appropriate. We show that failing to adequately correct for near-surface velocity variations can lead to erroneous stacking of reflections.

A semi-automated picking algorithm was used to estimate first-arrival traveltimes on all source gathers. Subsequent minor manual corrections were necessary for near and long offsets and noisy traces. In general, errors in picks were estimated to be <1.5 ms. Errors may have been greater at near offsets, where direct arrivals and airwaves overlapped to some degree.

We employed a tomographic algorithm based on a fast finite-difference Eikonal solver for calculating 2-D raypaths and traveltimes and a least-squares scheme for the
inversion (Lanz et al., 1998). Our simple 1-D starting model had a velocity of 100 m/s at zero-depth that increased linearly to 2200 m/s at 40 m depth and a strongly reduced gradient thereafter. Weights for data (45.5%), smoothing (45.5%), and damping (9%) in the inversion process were chosen on the basis of systematic trial inversions and a qualitative trade-off analysis of model complexity and root-mean square (RMS) deviation between the observed and model-predicted traveltimes. An RMS deviation of 1.3 ms was obtained after 15 iterations; this deviation is close to the <1.5 ms first-break picking errors. Model-predicted traveltimes in Figure E.3a closely match the picked values at most offsets. Some overestimation of the velocity occurs for near-offset traces, where the inversion struggles to fit the strong near-surface velocity gradient.

Tests show that the results of the inversion are robust, with the main features of the velocity tomogram in Figure E.3c being relatively insensitive to the choice of starting model and regularization parameters. For the processing of the seismic
reflection data, the near-surface low-velocity layer (shown by the blue to yellow colors in Figure E.3c) is the most important feature in the velocity tomogram. Large source and receiver static shifts of up to 3 ms result from its changing velocity and thickness; a combination of simple elevation and residual static corrections do not correct for such shifts.

A two-layer refraction-static velocity model appears to be appropriate for our data (Figure E.3c). We use weathering layer velocities estimated from the direct arrivals along the length of the line and initial smoothed refractor velocities to determine refractor depth and source and receiver delay times through iterative inversion (based on Lawton, 1989). The resulting simplified refraction-static velocity model reflects the main features imaged in the velocity tomogram (Figure E.3c). Source and receiver refraction-static corrections to an intermediate datum above the topography are then calculated using a replacement velocity of 1730 m/s. Application of the computed static corrections (Figure E.3d) to source gathers substantially reduces the distortion of phases across the fault (compare traces marked by green arrows in Figure E.3b with the equivalent traces in Figure E.3a).

E.5.3 Application of refraction- and residual-static corrections

The combination of refraction- and residual-static corrections improves the coherency of stacked reflections and reduces stacking artifacts due to non-hyperbolic reflection moveout. Severe static problems are apparent in CMPs centered above the thickest part of the low-velocity layer (distances 60 - 105 m in Figure E.3c). In the example CMP supergather of Figure E.4a, the strong reflection C1 is obscured at near offsets by surface-wave energy. At offsets >30 m, the reflection is distorted by progressive thinning of the low-velocity layer, such that maximum stacking power occurs along an incorrect hyperbolic path and the reflection appears discontinuous when stacked (Figure E.4b). Correction of near-surface effects using the combined refraction- and residual-static corrections improves the coherency in the CMP domain (Figure E.4c) and eliminates the artificial discontinuity of reflection C1 in the stack (Figure E.4d). In cases such as this, underestimating the effects of near-surface lateral velocity variations when calculating static corrections would lead to structural misinterpretations.
E.5.4 Velocity analysis and post-stack processing

Stacking velocities (Figure E.5) were determined from careful analyses of constant-velocity stacks and semblance plots. Velocities ranged from 1580 - 1700 m/s for the deeper Quaternary sediments (A and B units) to 1750 – 2500 m/s for the dipping sediment-basement interface (C reflections) and deeper features. Where events had conflicting dips (e.g., B and C2 at 95 – 110 ms; Figure E.5b), compromise velocities were chosen from the constant-velocity stacks to image the most important structural features. Application of dip-moveout corrections to this data set did not improve the imaging of all events with conflicting dips, and even weakened some strongly dipping deeper features (e.g. diffractions).

F-X deconvolution (Canales, 1984; Yilmaz, 2001) and bandpass frequency filtering enhanced the signal-to-noise ratio after stack (Figure E.6a). Phase-shift time migration using a smoothed interval-velocity field was then performed (based on Gazdag, 1978). Phase-shift migration was chosen to optimize the imaging of
moderately to steeply dipping events, though other migration schemes (including depth migration) produced similar results. Diffractions from reflection terminations were successfully collapsed in the final migrated image (compare Figures E.6a and E.6b). Finally, time-to-depth corrections using a strongly smoothed interval-velocity field were applied. Excellent agreement of the final depth-converted stack with borehole information ~39 m southeast of the fault trace was achieved by using 100% of the smoothed interval-velocity field for migration and depth conversion.

E.5.5 Enhancing shallow features with alternative processing

An alternative processing scheme (Table E.2) was designed to improve the resolution of very shallow reflections and abrupt truncations and vertical offsets of reflections caused by steeply dipping faults (compare Figure E.7 with Figure E.6b). The alternative processes included surface-consistent deconvolution, bottom mutes, and dip-moveout corrections.

Surface-consistent spiking deconvolution (Levin, 1989; Yilmaz, 2001), which replaced time-variant spectral whitening in our general processing flow, successfully enhanced shallow reflections inside the optimum reflection window; signal-to-noise ratios and reflection coherency were improved and near-surface reverberations (e.g., following C2 in Figure E.6b) were largely attenuated. Because strong surface-wave energy remained outside this window, application of a significant bottom mute to the source gathers was necessary. Consequently, deeper reflections and diffractions best
seen within the portions of source gathers affected by ground roll energy were not clearly imaged after deconvolution. Thus, spectral whitening was a more robust solution for the general processing of our data.

Dip-moveout corrections (DMO) using a dip-scan stack technique (Jakubowicz, 1990) further enhances shallow reflection coherency. DMO techniques are traditionally employed to image events with conflicting dips, determine true stacking velocities of dipping events, and reduce reflection point smear. Only shallow reflections from the Quaternary sediments (e.g., 2 and 3 in Figure E.7) are improved in this manner. In addition, DMO is principally responsible for the markedly enhanced image of the shallowest reflection (1 in Figure E.7) in our data.
Except for an offset that follows the change in topography at the Alpine Fault and an adjacent 30-m-long disrupted zone to the northwest, the ultra-shallow reflection 1 is relatively flat and continuous along the length of the profile. It originates from a discontinuity at 4.5 - 5 m depth to the northwest of the Alpine Fault (5 - 6 ms below the surface on the refraction-static-corrected section of Figure E.7; for such shallow events, the replacement velocity of 1730 m/s converts traveltime to depth) and slightly shallower at ~3.5 m (~4 ms) to the southeast. This reflection is visible as a clear hyperbolic event with a low normal-moveout (NMO) velocity of ~500 m/s in some CMP gathers (e.g., Figure E.8). Generally, imaging ultra-shallow events using standard processing schemes is problematic because of the large velocity gradients and resulting effects of NMO stretch. The dip-scan stack DMO method successfully enhanced this low-stacking-velocity reflection without adversely affecting the image of deeper reflections.

In addition to the large offset of basement reflection C₁ - C₂ at the Alpine Fault (AF in Figure E.7), prominent vertical offsets I and II are observed in the footwall basement reflection C₁ at ~45 and ~80 m distance. At location II, reflection C₁ is clearly offset ~5 ms in source gathers (arrows in Figure E.9), indicating a sharp ~5 m basement dislocation at this position. Although no clear offset is discerned in source gathers at location I, the unmigrated stack contains a conspicuous weakening and
change in dip of reflection $C_1$ at the relevant position (Figure E.6a). We conclude that there is a small fault at location II and a high probability of another at location I.
E.6 GEOLOGICAL INTERPRETATION

Our provisional interpretation of the ultra-high-resolution seismic reflection data set acquired at Calf Paddock is based on the unmigrated section in Figure E.6a and the migrated sections in Figures E.6b, E.7, and E.10.

E.6.1 Ultra-shallow seismic reflector/refractor

The depth and character of the boundary causing the ultra-shallow reflection 1 at distances of 0 - 70 m and 100 - 360 m in Figure E.7 matches the strong velocity gradient at the 1200 m/s iso-velocity line (yellow line) in the tomogram of Figure E.3c. This boundary could be the top of the groundwater table and/or a change in sediment facies. The estimated increase in velocity from 300 - 560 m/s above the boundary to more than 1700 m/s below is typical of a transition from dry to saturated sediments (Telford et al., 1990), and the proximity of the Maruia River indicates that the groundwater table must lie in the depth range of our tomogram. However, the ~5 m step across the fault scarp, which is greater and sharper than the fault expression at the surface, and the slight thickening of the low-velocity layer to the northwest
support an interpretation in terms of a sediment facies change. The contact between subhorizontally-layered Holocene fluvial sediments of the Maruia River and underlying dipping late-Pleistocene gravels is imaged in 3D GPR data at approximately the same depth as the seismic boundary (McClymont, et al., 2008; McClymont, et al., 2009; the GPR data were collected during a wetter period when the groundwater table was close to the surface, such that is was not imaged in the GPR data). Taking all observations into account, we interpret the shallow boundary at 3.5 - 5 m depth as the groundwater table that is controlled to some degree by the contact between the Holocene and Late-Pleistocene gravels. The thickening of the low-velocity layer in the footwall of the fault at distances of 60 - 100 m likely results from an accumulation of sediment in a colluvial wedge at the base of the fault scarp.

E.6.2 Interpretation of seismic units

We identify six distinct seismic units (A₁, A₂, A₃, B, C₁, C₂) on the migrated depth-converted section in Figure E.10:

- Seismic units A₁, A₂, and A₃ of strong semi-continuous reflections on either side of the fault from near the surface to as deep as ~40 m are interpreted to be late-Pleistocene gravels. Undifferentiated gravel was intersected from the near-surface to 26 m depth in the borehole southeast of the surface fault trace (Garrick and Hatherton, 1974); note the good correlation between the thickness of gravels observed in the seismic image and the borehole information (Figure E.10).

- Reflections from seismic unit A₃ appear to grade into gently dipping continuous reflections B at greater depth. We interpret seismic unit B as layered sediments from an earlier period of less turbulent deposition.

- The sediment-basement interface produces strong reflections C₁ and C₂ that are offset across the Alpine Fault and at other locations along the profile. From mapped surface outcrops (Figure E.1b), we infer that marble basement C₁ to the northwest is juxtaposed against schist basement C₂ to the southeast.

Extensive glaciation of the Maruia Valley occurred during the late-Pleistocene Otira Glaciation. This incorporated five main phases of ice advance and retreat from ~22 000 to ~14 000 years before present (Mabin, 1983; Suggate, 1990). The relatively smooth basement imaged in the seismic data is interpreted as an erosional surface that
deepened towards the former valley floor during this period. This surface has enhanced curvature in the shallow part of the section, an apparent primary vertical offset of ~35 m, and two secondary vertical offsets of ~5 m, all of which we associate with subsequent transpressive movement along the Alpine Fault (AF in Figure E.10) in the late Pleistocene and Holocene.

The valley sediments are likely to originate from periods of late-Pleistocene postglacial aggradation (Suggate, 1965; Mabin, 1983). From their gently dipping layered geometry, older sediments of seismic unit B (>50 m thickness) are likely to be glaciolacustrine in origin. Younger sediments extending to the near-surface (seismic units A1, A2, and A3) were probably deposited in glaciolacustrine fan, alluvial, and/or glaciofluvial environments. Note the marked change in reflection pattern across the Alpine Fault.

Characteristic seismic units A1, A2, and A3 are mirrored in the higher resolution 3D GPR data (McClymont, et al., 2008; McClymont, et al., 2009). Although the hanging-wall seismic reflections A3 have apparent dips of ~15° to the southeast (Figures E.7 and E.10), the 3D GPR data suggest the true dips are oblique to the profile and somewhat steeper at 20° - 35° to the southwest. McClymont et al. (2009) interpret these sediments to result from progradation of a late-Pleistocene alluvial or glaciolacustrine fan in a northeast to southwest direction. This fan likely extended across the fault and some distance further into the valley to the south-west, as suggested by the > 40 m thickness of unit A3. As a consequence, we infer the presence of similar fan sediments overlying the basement unconformity in the footwall and juxtaposed after lateral movement along the fault.

Immediately to the northwest of the Alpine Fault and extending for about 30 m, reflections of footwall seismic unit A2 have relatively low amplitudes and variable dips (Figures E.7 and E.10), whereas 3D GPR reflections at the same location are quasi-continuous and dip moderately to the northwest. By comparison, footwall seismic reflections A1 have apparent dips of <10° to the southeast (Figures E.7 and E.10), which the 3D GPR data indicate are close to true dips. Seismic units A1 and A2 are interpreted as fluvial sediments preserved in the accommodation space provided by the repeatedly downthrown side of the Alpine Fault (McClymont, et al., 2008). By implication, these sediments are younger than seismic unit A3 and may have also overlain this unit on the hanging wall before being subsequently eroded through downcutting of the Maruia River. We interpret the different dip directions of the two
units A₁ and A₂ to be a consequence of transpressive folding between the Alpine Fault (AF) and the secondary faults I and II (Figure E.10; McClymont, et al., 2009); sediments in the region represented by seismic unit A₂ are folded and tilted in a general northwest direction.

E.6.3 Geometry of the Alpine Fault at shallow depths

From our data, much of the reverse-slip along the Alpine Fault at Calf Paddock appears to be confined to a single major fault trace. Based on reflection truncations, the fault has an apparent southeasterly dip of 75° - 80° from the surface fault scarp through the Quaternary sediments to the offset basement at ~60 m depth.

The dip of the Alpine Fault within the shallow basement is not so well constrained. The moderately steep-dipping reflection package X-X’ projects to the basement offset created by the Alpine Fault in Figures E.6 and E.10. If X-X’ contains fault-plane reflections, then the fault would have a distinct listric geometry with dip decreasing from 75° - 80° within the Quaternary sediments to ~50° within the basement. The combination of steep dip within the Quaternary sediments to ~60 m depth and shallower dip within the basement is compatible with the borehole-based minimum average 65° dip from the surface to 83 m depth (Garrick and Hatherton, 1974).

There are two observations to consider before accepting such a large change in fault dip. First, although the results of finite-difference modeling presented in Appendix E.A demonstrate that X-X’ could indeed contain fault-plane reflections, they also demonstrate that X-X’ could be a simple multiple of the basement reflection C₂. Based on the geometry, amplitude, and general character of X-X’, it is not possible to distinguish between these two interpretations. Second, the gentle dips of the layered sediments represented by seismic unit B (best observed in Figure E.7) are consistent with a modest decrease in fault-plane dip with depth (Amos et al., 2007) or a modest rotation of the fault plane and entire hanging wall over time, but are difficult to reconcile with a significant shallowing of the fault plane below the sediment cover.

In the interpreted seismic section of Figure E.10, the maximum fault dip in the basement is a simple depth projection of the 75° - 80° dip observed within the Quaternary sediments, whereas the minimum fault dip is defined by the reflection package X-X’. Taking into account the gentle dips of seismic unit B, we speculate that
the Alpine Fault continues to have a relatively steep dip within the shallow basement (i.e., close to the dashed line in Figure E.10).

### E.6.4 Curvature and faulting of the basement surface

There is a notable curvature of the basement surface on either side of the Alpine Fault. This could represent the topography of the pre-faulted glacial valley, but the following observations support an interpretation of the characteristic paired convex hanging-wall curvature and concave footwall curvature in terms of normal drag generated by the dip-slip component of Alpine Fault displacement (see Figures 1 and 5 of Grasemann et al., 2005):

- strong changes in reflection characteristics in the region represented by unit A₂ (as seen in the seismic reflection and GPR data);
- the prominent faults I and II.

Transpressive forces acting in the region between the Alpine Fault and fault I would have tilted and faulted the shallow sediments, and bending of the footwall would have generated faults I and II.

Small changes in reflection dip and continuity in the hanging wall of the Alpine Fault indicate the presence of other possible subsidiary faults (e.g., dashed lines in Figure E.10). The borehole penetrates a steeply dipping crushed zone at 37.5 – 45 m depth within schist bedrock, which has been interpreted as a fault. No information is given on the dip direction of this fault, though its depth coincides with the extension of one of the possible subsidiary fault strands (see intersection of dashed line with the borehole in Figure E.10).

### E.6.5 Provisional dip-slip rate estimation

Significant apparent vertical offset of basement in the seismic profile suggests substantial fault slip since the late Pleistocene. Although quantifying dip-slip rates from vertical offsets of dated horizontal surfaces and known fault dips is clearly possible, estimates are complicated by uncertainties in age, fault dip, original topography, and true offset of the surface. Consequently, we can only provide a provisional estimate of dip-slip rate across the Alpine Fault at Calf Paddock.

We assume that the erosional basement surface dates from the Otira Glaciation (22 000 – 14 000 years ago). Given that the apparent vertical offset in basement is ~35
m and fault dip is 75 - 80 °, the apparent dip-slip rate at Calf Paddock (estimated using the average values of these parameters) is 2.0 mm/yr with a possible range of 1.6 – 2.6 mm/yr (estimated from the appropriate upper and lower bounds of these parameters). In presenting this provisional estimate, we recognize that the true vertical offset of the basement surface may differ from the apparent offset due to (i) potential topography of the surface prior to oblique slip and/or (ii) normal fault drag and distributed deformation close to the fault. Our provisional dip-slip rate of 2.0 ± 0.6 mm/yr is consistent with the inferred lower slip rates for the northern section of the Alpine Fault (Berryman, et al., 1992; Norris and Cooper, 2000).

E.7 CONCLUSIONS

We have presented ultra-high-resolution seismic reflection sections of the Alpine Fault and adjacent regions from the shallow subsurface to ~150 m depth. To obtain high-definition images over this depth range, we designed a general processing sequence that included time-variant spectral whitening, refraction- and residual-static corrections, F-K filtering, stacking-velocity analyses, post-stack signal enhancement, and migration. In applying this processing sequence we demonstrated the importance of static corrections at our Calf Paddock study site, where substantial lateral variations in near-surface physical properties exist; a combination of refraction- and residual-static corrections was necessary to account for distortions of reflections in CMP gathers and avoid generating artificial discontinuities in the stacked and migrated seismic sections. An alternative processing sequence that included surface-consistent deconvolution and dip-moveout corrections enhanced the coherency and strength of shallow reflections, in particular a prominent ultra-shallow reflection at 3.5 - 5 m depth.

Our ultra-high-resolution seismic data contain clear images of the following geological units at successively greater depths:
- a subhorizontal layer of Holocene sediments abandoned by the Maruia River;
- dipping late-Pleistocene gravel units deposited in various glaciolacustrine fan, alluvial, and glaciofluvial settings;
- subhorizontal late-Pleistocene layered sediments of probable glaciolacustrine origin (only seen in the hanging wall of the Alpine Fault);
the top of the Triassic-age Torlesse schist basement in the hanging wall of the Alpine Fault and Paleozoic-age marble basement in the footwall.

The new seismic images provide details on key properties of the Alpine Fault from the surface through the Quaternary sediments into the shallow basement, the top of which is vertically offset ~35 m across the fault in our profile. The Alpine Fault has a steep southeasterly dip of 75° - 80° through the sediments, but its dip within the basement is not so tightly constrained. A package of moderately steep-dipping quasi-continuous reflections that projects to the basement offset at the Alpine Fault may contain fault-plane reflections, indicating a listric shallowing of dip to 50° through basement. Alternatively, the fault dip through basement could be steeper, given that this package of reflections could represent a simple multiple reflection from the dipping basement surface. The subhorizontal nature of the interpreted glaciolacustrine sediments in the hanging wall favor a smaller change in fault dip with depth. Our preferred interpretation is that the Alpine Fault continues to dip relatively steeply within the shallow basement.

Fault slip appears to be accommodated predominantly on a single fault strand, though significant deformation is observed elsewhere. For example, a marked increase in curvature of the basement surface on either side of the Alpine Fault and strong deformation in the footwall sediments and basement are likely consequences of normal drag created by dip-slip displacements on the fault.

The ~35 m apparent vertical offset of basement across the Alpine Fault together with the estimated age of the eroded basement surface and measured fault dip within the Quaternary sediments yield a provisional dip-slip rate of 2.0 ± 0.6 mm/yr. This provisional dip-slip rate does not account for possible out-of-plane topography on the dated surface or normal drag on this surface close to the fault.

Our 2D ultra-high-resolution seismic reflection data supply high-quality images of the active Alpine Fault and additional information on fault geometry at depths beyond the reach of GPR surveying and trenching. These are the most vivid shallow seismic images of any continental transform fault zone. Complex fault and deformation structures in the near-surface and the dominant, but unknown recent lateral component of slip along the Alpine Fault at Calf Paddock invite the use of 3D seismic reflection studies to further elucidate and refine our interpretations of fault-zone deformation.
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APPENDIX E.A: MODERATELY STEEP-DIPPING ENERGY X-X’

The moderately steep-dipping reflection package X-X’ on the unmigrated section (Figures E.6a and E.A.1a) appears after migration as a suite of ~50° dipping events that projects upwards to the basement offset (Figure E.6b). We investigate two plausible explanations for these events. First, we show that X-X’ could contain primary reflections from a moderately steep-dipping fault plane given a plausible impedance contrast across the fault. Alternatively, X-X’ could be a simple multiple of the strong basement reflection C2.

To simulate the two possible scenarios, we have computed synthetic seismograms using Bohlen's (2002) viscoelastic finite-difference modeling code. Energy from 10 vertical sources spaced at 20 m intervals was sequentially propagated through the simple velocity models of Figures E.A.1b and E.A.1d and "recorded" on 504 hypothetical receivers spaced at 0.5 m intervals along the modeled section of the profile. After simple processing (i.e., bandpass filtering, 60 ms AGC, and velocity analyses), the synthetic CMP-sorted data were stacked. No adjustments to a datum were necessary, because static shifts in the real data (Figure E.3d) were generally small (0 ± 1.5 ms) over this section of the profile and thus had negligible effect on the observed traveltimes.

Since we were only interested in traveltime simulations of primary and multiple P-wave arrivals (the optimum >2400 m/s stacking velocity of X-X’ was much greater than that of the primary reflection C2, precluding X-X’ from being a reflected S wave or P-to-S converted phase), we used (i) a low Qs value of 3 to attenuate S-wave energy, (ii) an artificially high weathering-layer velocity to avoid numerous near-surface reverberations, and (iii) a relatively short 50 ms AGC to equalize the amplitudes of the simulated fault-plane reflection and basement multiple in the two stacked sections.

The resultant synthetic stacked sections in Figures E.A.1c and E.A.1e demonstrate that both models are capable of explaining X-X’. A substantial impedance contrast would be required to generate fault-plane reflections. Seismic refraction studies at Calf Paddock (Garrick and Hatherton, 1974) indicate a velocity contrast between marble (~5000 m/s) on the northwest side of the Alpine Fault and schist (~4000 m/s) on the southeast side. Moreover, fault gouge and highly deformed rock within the fault zone are expected to have anomalously low velocities (Mooney and Ginzburg, 1986), and strong weathering of the more vulnerable schist may
Figure E.A.1: Synthetic modeling of moderately steep-dipping energy that projects to the surface trace of the Alpine Fault. (a) Unmigrated section (as in Figure E.6a) highlighting the moderately steep-dipping energy X-X’. (b) Simple fault-plane P-wave velocity model 1 used in the finite difference modeling. S-wave velocities and densities used in the modeling are defined by the experimentally determined P wave velocities using standard relationships. (c) Resulting stacked synthetic section showing modeled events. (d) and (e) As for (b) and (c), but with model 2 (i.e., uniform velocity across the fault). The multiple of the basement reflection is now clearly seen. Blue shading represents positive pulse polarity.
increase velocity contrasts at shallow depths close to the fault. Generally, a surface multiple would be observed at double the traveltime of a primary reflection on an unmigrated stack. However, our computations demonstrate that a dipping boundary produces a multiple at less than double the traveltime (see also Telford, et al., 1990).

Based on the kinematic and dynamic characteristics of X-X’, it is not possible to distinguish between the two explanations. Fortunately, other information contained in the seismic reflection sections (i.e., the gently dipping package of layered reflections B) help resolve this dilemma.
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Curriculum Vitae

PERSONAL
Born on June 22, 1984.
Armenian citizen.

EDUCATION
2006 – 2011 Ph.D. in Geophysics, Institute of Geophysics, ETH Zurich, Zurich, Switzerland.
2004 – 2006 M.Sc. in Physics (summa cum laude), Department of Solar Energy and Environmental Physics, Ben-Gurion University of the Negev, Sede Boqer, Israel.
1999 – 2003 B.Sc. in Physics, Department of Physics, Yerevan State University, Yerevan, Armenia.

HONORS AND AWARDS
2005 The Bona Terra Foundation Prize for Excellence in Desert Studies, Ben-Gurion University of the Negev, Sede Boqer, Israel
2004 Full scholarship for Master’s degree, Ben-Gurion University of the Negev, Sede Boqer, Israel
1999 Second Prize, Third inter-high school Olympiad in Mathematics, Yerevan, Armenia
1998 Second Prize, Republic Olympiad in Mathematics, Yerevan, Armenia
1998 Third Prize and Special Prize, Regional Olympiad in Informatics, Yerevan, Armenia

IT SKILLS
Programming Languages: C /C++, Matlab, Pascal
Visualization Software/Toolkits: ParaView, MayaVi
Versioning Tools: TortoiseSVN
Operating Systems: Windows, Linux

LANGUAGES
Armenian – native speaker
English – fluent
Russian – fluent
German – basic