Seismic Velocity Characteristics of Partially Saturated Unconsolidated Sediments

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SEISMIC VELOCITY CHARACTERISTICS OF PARTIALLY SATURATED UNCONSOLIDATED SEDIMENTS

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Geology & Geophysics

by

Jie Shen
B.S., China University of Geosciences (Beijing), 2010
December 2015
ACKNOWLEDGEMENTS

Special thanks to my advisor, Dr. Juan Lorenzo, and committee member, Dr. Jeffrey Nunn and Dr. Carol Wicks, for all of their support and expertise in this endeavor. Without Dr. Lorenzo’s constant support and diligent mentorship, this dissertation never would have come to fruition. I am extremely grateful that Dr. Nunn and Dr. Wicks have offered their insightful advices throughout this research.

Very special thanks to my family and friends who made this experience easier. I am very grateful for my husband-to-be, Justin Hayles, for his love, patience, and support through the thick and thin of graduate school. I would like to thank my parents and grandparents, who encouraged me to the pursuit of a Ph.D. degree in geology and geophysics. Thank you Candice Pettijohn, a good friend and colleague, for all the help and input in school.

I would like to thank Frank Tsai and Hai Pham for their help with optimization techniques, Les Butler and Adam Brooks for their help with Labview programming, Ario Labs in Baton Rouge for their help with building our seismic acquisition system, Wanda LeBlanc and Cristina Gama for their help with XRD and grain size analysis, Rick Young and Chunyan Li for the support with facilities and the sand tank, Chris White and Clinton Wilson for valuable discussions, as well as former and current students in Dr. Lorenzo’s lab group for their help with experiments and presentations (David Smolkin, Shannon Chollett, James Crane, Ting Sun, Chennu Fan, Ali Al Dhamen, Abah Omale, Derek Goff, Rouhala Keshvardoost Jobaneh, Amir Javaheri, Martial Morrison, Abby Maxwell, and Trudy Watkins).
I would also like to thank Shell Exploration & Production Company for their support with funding for this research. Thank you for financial support from Geometrics Inc. Student Travel Grant for SAGEEP, the Donald Towse Memorial Fund awarded through an AAPG Grant-in-Aid, H. V. Anderson Scholarship, EnCana Scholarship and Imagine Resources Scholarship awarded by LSU Department of Geology and Geophysics. Special thanks to LSU Department of Geology and Geophysics, for their active support of graduate student research.
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ABSTRACT

Seismic velocity models of the near-surface (< 30 m) better explain seismic velocities when all elements of total effective stress are considered, particularly in materials with large cohesive and soil suction stress such as clays. Traditional constitutive elastic models assume interparticle and soil suction stresses are negligible. This study proposes a new methodology which corrects total effective stress in Hertz-Mindlin theory for interparticle and soil suction and calculates the elastic moduli by extending Biot-Gassmann theory to include pressure effects induced by water saturation changes and cohesion. The proposed model predicts seismic velocities that correlate well with measured field velocities from the literature.

Soil density, porosity, elastic moduli and the soil-water characteristic curve (SWCC) are important properties for soil characterization. Currently, geotechnical and laboratory tests for soil properties are costly and limited to point sampling sites. Seismic surveys can potentially provide laterally continuous soil property values that may complement geotechnical borehole tests with low cost. We propose a new method to invert for soil properties and the SWCC from seismic P- and S-wave velocity-vs.-depth profiles interpreted from shallow (< 25 m depth) unconsolidated sediments under conditions of near-full saturation (> 99%). The results from seismic soil property inversion are validated by comparison to geotechnical and laboratory results conducted independently in the same area as the seismic survey.

Knowledge of homogeneous and heterogeneous fluid-distribution patterns is important for the estimation of oil reserves, reservoir simulation, the interpretation of time-lapse seismic, and the selection of remediation techniques for groundwater
contamination. Problems exist in determining in-situ fluid-distribution patterns in unconsolidated sediments because laboratory tests on core samples may not be representative of in-situ conditions. We propose a new method to determine in-situ fluid-distribution patterns by inverting experimental seismic P- and S-wave velocities using the Hertz-Mindlin and Biot-Gassmann model with different averaging methods (Wood and Hill averages) and saturation-related assumptions. During the imbibition and drainage of shallow unconsolidated sands, we observe a non-monotonic P-wave velocity-vs.-water level relationship that is consistent with previous observations. This relationship can be explained by alternation in the size of fluid patches during wetting and drainage.
CHAPTER 1: INTRODUCTION

1.1 Problems, Objectives and Significance

1.1.1 Interparticle stresses in constitutive elastic models

Constitutive elastic models for granular materials are commonly accepted to explain observed seismic velocities in sands (Bachrach et al., 1998; Velea et al., 2000b) for shallow depths (< 30 m). However, velocity predictions may show improvement when additional sources of interparticle stresses are considered such as those caused by capillarity (Tinjum et al., 1997) and cohesivity. At shallow depth, these additional effects can be several orders of magnitude larger than the net overburden stress (Ikari and Kopf, 2011), particularly in clay-rich soils.

Chapter 2 introduces a new constitutive elastic model that incorporates interparticle stresses, such as capillary pressure and cohesion, into seismic velocity prediction. This work is in review at *Journal of Environmental and Engineering Geophysics*.

An accurate velocity prediction model is important for the success of inversion for soil physical and fluid saturation properties. Velocity forward modeling and inversion for soil and fluid properties can be applied in hydrogeological studies and unconsolidated reservoir management to characterize soil and simulate groundwater flow.

1.1.2 Seismic inversion for soil properties and soil-water characteristic curve

Soil properties such as density, elastic moduli, porosity, and the soil-water characteristic curve (SWCC) can be measured directly in the laboratory (Van Genuchten, 1980), but these tests are costly and the necessary equipment may not be readily accessible. Laboratory soil property tests are performed on either core or bulk sediment
samples, which may not be representative of in-situ sediments. The borehole locations are usually distant from each other (> 100’s m), so that lateral soil characteristics between boreholes are difficult to predict.

Chapter 3 develops a new method on the inversion for seismic soil properties and SWCC from field-based P- and S-wave seismic velocity-versus-depth profiles in near-saturated unconsolidated sediments underneath the Marrero levee, Louisiana. Several computer programs are used in the completion of the seismic inversion (Appendix A). The formulas for the velocity prediction model can be found in Appendix B. The work in Chapter 3 is published in *Geophysics* (Shen et al., 2015).

The proposed method in Chapter 3 inverts for laterally continuous soil properties, stratigraphy and SWCC that may complement geotechnical borehole tests with a lower cost than traditional laboratory methods. The knowledge of soil properties, stratigraphy and SWCC are important for assessing foundation stability (Bell, 1992), and monitoring of contaminant movement and soil aeration (Terzaghi, 1996).

1.1.3 Seismic inversion for fluid-distribution patterns

Partially-saturated unconsolidated sediments potentially contain a mixture of two or more fluids that can be distributed either homogenously or heterogeneously. However, the commonly applied laboratory ultra-sonic core tests for identifying fluid distributions are costly and may not represent in-situ conditions because of the disturbance of unconsolidated samples during core transportation, and the scaling issues with translating between ultra-high frequencies commonly used in laboratory studies and lower frequencies used in the field (Cadoret et al., 1995; Toms-Stewart et al., 2009). Moreover, there is a lack of understanding of the alternation of P-wave velocity ($V_p$) between
decreasing and increasing trends when water level (WL) increases or decreases (namely non-monotonic $V_p$-WL relationship) in either field experiments (Bachrach and Nur, 1998) or laboratory experiments (Lorenzo et al., 2013; Velea et al., 2000a).

Chapter 4 develops a new seismic inversion workflow to determine in-situ fluid-distribution patterns that involves inverting experimental seismic P- and S-wave velocities using two rock-physics models with different assumptions. From inversion, we are able to explain the observed non-monotonic $V_p$-WL relationship by transitions between two velocity bounds: Wood (1941) and Hill (1963) bounds. We interpret the cause of the transition could be the change in patch size during the wetting and draining. Several computer programs are used in the completion of the seismic inversion (Appendix A). Appendices C-G give explanations of the water level experiments, moisture sensor calibration, in-situ bulk density measurements, grain size analysis, and XRD analysis in the sand tank for Chapter 4. This work has been submitted to Geophysics.

The proposed workflow in Chapter 4 has flexibility to be used to identify heterogeneous and homogeneous in-situ fluid-distribution patterns in unconsolidated reservoirs and aquifers with less cost than laboratory core tests. For oil and gas industry, fluid-distribution patterns affect the estimates of oil reserves, reservoir simulations (Dupuy and Stovas, 2014), and interpretation of time-lapse seismic during production (Calvert, 2005). For hydrogeology, determining the saturation pattern can help select an adequate remediation technique for groundwater contamination based on whether the contaminants occur in patches or are dispersed evenly (Dvorkin and Nur, 1998).
1.2 Seismological Background Concepts

The following sections explain geophysical concepts that may help clarify subsequent chapters to the non-specialist.

1.2.1 Seismic reflection and refraction arrivals

Seismic reflections can be used to locate the boundary between two materials with different acoustic impedance. When compressional (P) and Shear (S) waves interact with a boundary with a large enough acoustic impedance (product of velocity and density) contrast, the energy will be partitioned into reflected and refracted waves following Snell’s law. We can estimate seismic velocities in each subsurface layer by modeling the arrival times of refraction arrivals in offset-travel time plots using forward ray-tracing.

1.2.2 Seismic velocity

The study of seismic P- and S-wave velocities yields information about the subsurface because wave propagation relates to elastic properties and density of the propagating media (equations 1.1 and 1.2):

\[ V_P = \sqrt{\frac{K + \frac{4}{3}\mu}{\rho}} \]  \hspace{1cm} (1.1)

\[ V_S = \sqrt{\frac{\mu}{\rho}} \]  \hspace{1cm} (1.2)

where \( V_P \) is the compressional wave velocity, \( V_S \) is the shear wave velocity, \( K \) is bulk modulus, \( \mu \) is shear modulus, and \( \rho \) is density. The shear modulus can also be estimated if an S-wave travels through a rock with a known density (equation 1.3):

\[ \mu = V_S^2 \rho \]  \hspace{1cm} (1.3)
1.2.3 Total effective stress

Total effective stress in unsaturated unconsolidated sand are distinct from those in hard rocks (Fredlund, 1993). In hard rocks at depth, total effective stress is simplified to net overburden stress (difference between overburden stress and pore pressure). In shallow unconsolidated unsaturated soil, interparticle stresses, such as those caused by capillarity (Tinjum et al., 1997) and cohesivity, can be several orders of magnitude larger than net overburden stress (Ikari and Kopf, 2011), particularly in clay. For the accurate prediction of velocity, the definition of total effective stress is composed of four terms:

\[ P = (\sigma_T - u_a) + \sigma'_S + \sigma_{CO} \]  

where \( \sigma_T \) is the total external stress, \( u_a \) is pore-pressure, \( \sigma'_S \) is soil suction stress (Lu and Likos, 2006), and \( \sigma_{CO} \) is apparent tensile stress at the saturated state caused by cohesive or physiochemical forces (Bishop et al., 1960). Physiochemical forces are local forces arising from individual contributions from van der Waals attractions, electrical double layer repulsion, and chemical cementation effects (Lu and Likos, 2006).

The commonly accepted Hertz-Mindlin theory (Hertz, 1882; Mindlin, 1949) estimates shear and bulk moduli of the dry granular matrix from grain elasticity, porosity, grain contact geometry, and effective stress at the grain contacts (Mavko et al., 2009):

\[ K_m = \frac{3 C^2 (1-\phi)^2 G_0^2}{18\pi^2 (1-\nu)^2} P \]  
\[ G_m = \frac{5-4\nu}{5(2-\nu)} \frac{3 C^2 (1-\phi)^2 G_0^2}{2\pi^2 (1-\nu)^2} P \]

where \( C \) is grain coordination number, \( G_0 \) is the grain shear modulus, \( \nu \) is the grain Poisson’s ratio, \( K_m \) is the bulk modulus of the skeletal matrix, \( G_m \) is the shear modulus of the skeletal matrix, and \( P \) is the effective stress at the grain contacts. In this version of
Hertz-Mindlin model, \( P^{1/3} \) is proportional to matrix elasticity and \( P^{1/6} \) is proportional to seismic velocity (equations 1.1, 1.2, 1.5, and 1.6).

### 1.2.4 Capillary pressure

Capillary pressure (or matric suction) is one component in total effective stress and equal to the stress difference at the air-water interface. At equilibrium, capillary pressure around a capillary tube is balanced by the weight of the water column pulled up by surface tension (Fredlund and Rahardjo, 1993). Traditional capillary pressure estimations assume a medium with a constant pore size \((r)\) and no layering. In the equilibrium state, the capillary pressure is equal to the weight of the water column rising in the pore space (Fredlund and Rahardjo, 1993):

\[
(u_a - u_w) = \rho_w g h_c = \frac{2\gamma \cos \theta}{r}
\]

where \( h_c \) is the capillary head, \( \rho_w \) is water density, \( g \) is gravitational acceleration, \( r \) is the radius of the capillary tube, \( \theta \) is the contact angle, and \( \gamma \) is the surface tension of water adhering to the tube wall. However, in our case the soil is layered and requires consideration of the influence of pore size variation in matric suction estimations (in Chapter 2).

### 1.2.5 Soil water characteristic curve (SWCC)

Soil water characteristic curve (SWCC) is an empirical curve that relates water saturation to capillary head (m) or capillary pressure (Pa). Different soil types usually have different SWCCs. At the same capillary pressure, clays have a larger water saturation value than sands (Fredlund and Xing, 1994). With a known water table and capillary head, SWCC can be converted to depth-versus-water saturation profiles. One
common empirical fitting of SWCC requires three fitting parameters (Van Genuchten, 1980):

\[
S_e = \left[ \frac{1}{1 + [ah]^n} \right]^m
\]  

(1.8)

where \( S_e \) is effective water saturation, \( h \) is capillary head, and \( a, n, m \) are empirical fitting parameters.

1.2.6 Fluid saturation and fluid-distribution pattern

Seismic velocity is influenced by pore fluid saturation. With the assumption of homogeneity, Biot-Gassmann theory (Biot, 1956; Gassmann, 1951) has been implemented to estimate velocities in porous material from matrix properties, fluid properties and fluid saturation (Mavko et al., 2009):

\[
K_{\text{eff}} = \frac{K_0 \left( \frac{K_m}{K_0 - K_m} + \frac{K_{fl}}{\phi(K_0 - K_{fl})} \right)}{1 + \frac{K_m}{K_0 - K_m} + \frac{K_{fl}}{\phi(K_0 - K_{fl})}}
\]

(1.9)

\[
G_{\text{eff}} = G_m
\]

(1.10)

where \( K_0 \) is the bulk modulus of the soil grains, \( K_m \) is the bulk modulus of the “dry” soil matrix, \( G_m \) is the shear modulus of the “dry” soil matrix, and \( K_{fl} \) is the bulk modulus of the pore fluids. Traditional Biot-Gassmann is accurate if stress does not change with water saturation as changes in stress will change the elasticity of the matrix.

Fluid-distribution pattern also affects seismic velocities. When media contain various pore throat sizes, it will likely induce "fingers" of heterogeneous fluid saturation. Additional, when fluid level drops because of evaporation or production, some fluid remains trapped in the pore spaces due to capillary pressure. In the case of heterogeneous (or patchy) saturation, velocity prediction depending on the relationship between the size of the patches to the frequency used (Knight et al., 1998).
1.3 References


CHAPTER 2: SEISMIC VELOCITY PREDICTION IN SHALLOW (< 30 M) PARTIALLY-SATURATED, UNCONSOLIDATED SEDIMENTS USING EFFECTIVE MEDIUM THEORY

2.1 Summary

Seismic velocity models of the near-surface (< 30 m) better explain seismic velocities when all elements of total effective stress are considered, especially in materials with large cohesive and soil suction stress such as clays. Traditional constitutive elastic models that predict velocities in granular materials simplify the effect of total effective stress by equating it to net overburden stress, while excluding interparticle stresses and soil suction stress. A new proposed methodology calculates elastic moduli of granular matrices in near-surface environments by incorporating an updated definition of total effective stress into Hertz-Mindlin theory and calculates the elastic moduli of granular materials by extending Biot-Gassmann theory to include pressure effects induced by water saturation changes and cohesion.

At shallow depths, when water saturation increases, theoretically calculated seismic velocities decrease in clay and increase in sand because interparticle stresses suppress the Biot-Gassmann effect. For standard sand and clay properties, net overburden stress becomes more influential than interparticle stresses at depths greater than 0.1 m in sand and 100 m in clay. Pore pressure in the new model also incorporates the effect of layer thickness and pore-size variation. Traditional calculation of pore pressure assumes a constant-pore-size medium, but may lead to an under- or overestimation of velocity by up to 20%. In clays, the variation of seismic velocity with water saturation is almost double the range predicted when only net overburden stress is considered to influence stress at...
the grain contacts. The proposed model predicts seismic velocities that compare well with measured field velocities from the literature.

2.2 Introduction

Currently, constitutive elastic models for granular materials are used to explain observed seismic velocities in sands (Bachrach et al., 1998; Velea et al., 2000) over shallow depths (< 30 m). However, velocity predictions may show improvement when additional sources of interparticle stress are considered such as those caused by capillarity (Tinjum et al., 1997) and cohesivity. These additional effects are especially significant in clay-rich soils. Through improved elastic models, observed seismic velocity can be inverted (Aster et al., 2013; Eberhart-Phillips et al., 1989) to better estimate parameters such as water saturation, porosity, matrix elastic moduli, or pressure.

The influences of pore content, matrix composition, and pressure on elasticity can be related through the elastic wave equation by implementing fluid substitution theory (Biot, 1956; Gassmann, 1951) and granular contact theory (Hertz, 1882; Mindlin, 1949). The Biot-Gassmann theory effectively explains the influence of pore constituent variations on elasticity and density of the porous media. When pore contents, such as water or air, have no shear resistance, the effective shear modulus is equal to the shear modulus of the granular matrix. In conventional Biot-Gassmann theory, elastic moduli of the granular matrix are considered constant. As water saturation increases in the pore space, a decrease in the seismic velocity is attributed to the Biot-Gassmann effect (Wulff and Burkhardt, 1997), because the bulk density increases more than the effective bulk modulus of the overall granular material.
Velocity predictions from Biot theory are frequency-dependent (Biot, 1956). When a seismic wave propagates through a fluid-filled porous medium at low frequencies (lower than critical frequency) (Mavko et al., 2009), Biot theory assumes fluids and matrix move in phase and so only a small amount of dissipation occurs. Critical frequency \( \omega_c \) defines the boundary between low and high frequencies in Biot theory: 

\[
\omega_c = \frac{\eta \phi}{\kappa \rho_f},
\]

where \( \eta \) is viscosity, \( \phi \) is porosity, \( \kappa \) is permeability and \( \rho_f \) is fluid density (Mavko et al., 2009). In this case, expressions derived from Biot theory are the same as those from Gassmann theory. When a wave propagates at high-frequencies (higher than critical frequency) (Mavko et al., 2009), Biot theory also predicts velocities of dissipative waves, which are caused by fluid and matrix moving out of phase. In some dispersion cases where Biot theory is not applicable, workers have developed other theories to predict wave propagation with velocity dispersion and attenuation, such as squirt-flow mechanism (Mavko and Jizba, 1991; Mavko and Nur, 1979) and an integration of Biot and squirt-flow model (Dvorkin and Nur, 1993).

Hertz-Mindlin contact theory (Hertz, 1882; Mindlin, 1949) is used to calculate the elastic moduli of elastic granular materials in terms of porosity, grain contact geometry, grain elasticity, and grain contact stress. Hertz-Mindlin theory predicts that seismic velocity \( V \) will increase as a power function of stress \( \sigma \) \( (V \propto \sqrt[\delta]{\sigma}) \) (Mindlin, 1949). In conventional Hertz-Mindlin theory, net overburden stress (Eaton, 1969) is typically used to represent stress at the grain contacts.

Total effective stress represents the average stress carried by the granular matrix and was first defined as total stress minus pore pressure (Terzaghi, 1943). Today, the
total effective stress is defined as the sum of net overburden stress and interparticle stresses (Bishop, 1960; Lu and Likos, 2006).

Interparticle stresses contribute to the total effective stress and include capillary stress arising from the interfacial tension between grains and the wetting phase (Tinjum et al., 1997), negative pore water pressure (Rinaldi and Casagli, 1999), and physicochemical stresses caused by van der Waals attractions, electrical double layer repulsion, and chemical cementation effects (Ikari and Kopf, 2011). Interparticle stresses can be classified into stresses in fully saturated media \( (\sigma_{co}) \), that confer cohesion to sediments, and stresses in unsaturated media that result as water saturation changes \( (\sigma'_s - \text{soil suction stress}) \) (Lu and Likos, 2006). Interparticle stresses are important in the near-surface \( (0-100 \text{ m}) \) because they increase the pressure at grain contacts and can be several orders of magnitude (MPa) larger than the net overburden stress.

Net overburden stress estimation can be difficult at depths near a changing water table, because the weight of sediment below the water table is effectively lowered by buoyancy (Turner, 1979). In this case, buoyancy is the displacement of water by sediments (Archimedes’ Principle) and results in a decrease in total effective stress on the granular matrix, and also the seismic velocity.

Several field studies demonstrate that both net overburden stress and interparticle stresses, particularly in shallow unconsolidated sediments, are important to consider when developing constitutive elastic models. However, interparticle stresses have yet to be included in constitutive elastic models for predicting seismic velocity of granular material (Dvorkin et al., 1999). In shallow unconsolidated sediments, seismic velocities can be underestimated if interparticle stresses are excluded when calculating pressure at
grain contacts. Lu and Sabatier (2009) document water saturation, temperature, stress, and compressional velocity in shallow soil over a two year period. The range in measured velocities (260-460 m/s) cannot be predicted by changes in net overburden stress (< 5 kPa) and must also include changes in interparticle stresses (> 350 kPa). In traditional elastic models, the exclusion of interparticle stresses for the case of deep (> 100 m), unconsolidated sediments remains valid where net overburden stresses are several orders of magnitude more than interparticle stresses (Dvorkin and Nur, 1996).

We propose a constitutive elastic model, suitable for use in unconsolidated clay as well as sand, and which estimates elastic moduli of elastic granular materials by extending conventional Hertz-Mindlin and Biot-Gassmann theory to incorporate interparticle stresses. An updated definition of total effective stress which includes interparticle stresses is incorporated into Hertz-Mindlin theory. Because total effective stress changes with water saturation, the bulk modulus and the shear modulus of the granular matrix ($K_{\text{matrix}}$ and $G_{\text{matrix}}$) vary throughout the full range of saturations. The elastic moduli of the granular matrix increase as the net overburden stress increases with depth and vary with interparticle stresses as water saturations change. Traditionally, Biot-Gassmann theory estimates elastic properties of granular materials by varying the elastic properties of the pore space as the pore constituents change in concentration but assumes that the elastic properties of the granular matrix are constant. However, Biot-Gassmann theory can also account for changes in the elastic properties of the granular matrix during changes in water saturation by updating the reference elastic moduli of the matrix through Hertz-Mindlin theory.
The influence of interparticle stresses is demonstrated by calculating theoretical seismic velocities from physical properties of sand and clay (Table 2.1) with varied total effective stresses and water saturations. Our modeled velocities are indistinguishable from those calculated from traditional Hertz-Mindlin and Biot-Gassmann methodologies at large confining pressures (> 5 MPa) and low interparticle stresses (< 2 kPa); however, calculated seismic velocities for materials with large interparticle stresses can be very different. Calculated seismic velocities are also compared successfully to measured field velocities (Lu and Sabatier, 2009) obtained at small confining pressures (< 5 kPa) and over a large total effective stress range (> 350 kPa) to validate the new model.

Table 2.1. Physical and theoretical properties and model parameters of sands and clays for seismic velocity calculations. Van Genuchten parameters (van Genuchten, 1980) are calibrated for capillary pressures in sands (psi) and clays (kPa).

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Sand</th>
<th>Reference</th>
<th>Clay</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain Shear Modulus (Pa)</td>
<td>4.5 x 10^10</td>
<td>Mavko et al. (2009)</td>
<td>9.9 x 10^9</td>
<td>Mavko et al. (2009)</td>
</tr>
<tr>
<td>Grain Bulk Modulus (Pa)</td>
<td>3.66 x 10^10</td>
<td></td>
<td>2.5 x 10^10</td>
<td></td>
</tr>
<tr>
<td>Grain Density (kg/m^3)</td>
<td>2650</td>
<td></td>
<td>2550</td>
<td></td>
</tr>
<tr>
<td>Grain Poisson’s Ratio</td>
<td>0.15</td>
<td>Mavko et al. (2009)</td>
<td>0.15</td>
<td>Mavko et al. (2009)</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.35</td>
<td></td>
<td>0.56</td>
<td></td>
</tr>
<tr>
<td>Water Density (kg/m^3)</td>
<td>1000</td>
<td></td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>Air Density (kg/m^3)</td>
<td>1.22</td>
<td></td>
<td>1.22</td>
<td></td>
</tr>
<tr>
<td>Gravitational Acceleration (m/s^2)</td>
<td>9.81</td>
<td></td>
<td>9.81</td>
<td></td>
</tr>
<tr>
<td>Coordination Number</td>
<td>1</td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Van Genuchten n Fitting Parameter</td>
<td>5.69</td>
<td></td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Van Genuchten α Fitting Parameter (1/m)</td>
<td>4.56</td>
<td>Engel et al. (2005)</td>
<td>0.01</td>
<td>Song et al. (2012)</td>
</tr>
<tr>
<td>Irreducible Water Content</td>
<td>0.024</td>
<td></td>
<td>0.10</td>
<td></td>
</tr>
<tr>
<td>Matrix Cohesion (Pa)</td>
<td>300</td>
<td>Krantz (1991)</td>
<td>16000</td>
<td>Bishop (1960)</td>
</tr>
</tbody>
</table>

2.3 Theory

Seismic velocities are related with effective moduli and density of media (e.g., Ikelle and Amundsen, 2005):
\[ V_p = \sqrt{\frac{K_{\text{eff}} + \frac{4}{3}G_{\text{eff}}}{\rho_{\text{bulk}}}} \]  \hspace{1cm} (2.1)

\[ V_S = \sqrt{\frac{G_{\text{eff}}}{\rho_{\text{bulk}}}} \]  \hspace{1cm} (2.2)

where \( V_p \) is the P-wave velocity, \( V_S \) is the S-wave velocity, \( K_{\text{eff}} \) is the effective bulk modulus, \( G_{\text{eff}} \) is the effective shear modulus, and \( \rho_{\text{bulk}} \) is the bulk density. The “\( \text{eff} \)” subscript is used to differentiate the elastic moduli of the bulk granular material from the elastic moduli of the granular matrix with the effect of pore fluids.

In equations 2.1 and 2.2, bulk density is the weighted mean of matrix and pore space densities. When the pore space is filled by a combination of water and air, the equation for bulk density becomes (Bourbie et al., 1992):

\[ \rho_{\text{bulk}} = \phi (S_w \rho_{\text{water}} + (1 - S_w) \rho_{\text{air}}) + (1 - \phi) \rho_{\text{grain}} \]  \hspace{1cm} (2.3)

where \( \phi \) is the porosity of the skeletal matrix, \( S_w \) is the water saturation, \( \rho_{\text{water}} \) is the density of water, \( \rho_{\text{air}} \) is the density of air, and \( \rho_{\text{grain}} \) is the grain density. Bulk density is needed for input into the elastic wave equation.

Biot-Gassmann theory (Biot, 1956; Gassmann, 1951) effectively explains the influence of pore constituent variations on elasticity and density of the porous media. The bulk modulus of the pore space is a weighted harmonic mean of the bulk moduli of the pore constituents. When pore contents such as water or air have no shear resistance, the effective shear modulus is equal to the shear modulus of the granular matrix. Biot-Gassmann theory is implemented to calculate effective bulk moduli and shear moduli (equations 2.1 and 2.2) for granular materials (mixture of grains, gas, and fluid) from elastic moduli of matrix (Mavko et al., 2009):
\[
\frac{K_{\text{eff}}}{K_0-K_{\text{eff}}} = \frac{K_{\text{matrix}}}{K_0-K_{\text{matrix}}} + \frac{K_{\text{pore}}}{\phi(K_0-K_{\text{pore}})}
\] (2.4)

\[
G_{\text{eff}} = G_{\text{matrix}}
\] (2.5)

where \(K_0\) is the bulk modulus of the grains and \(K_{\text{pore}}\) is the bulk modulus of the pore space.

When the two pore constituents are water and air, the bulk modulus of the pore space (\(K_{\text{pore}}\)) (equation 2.4) can be calculated (Mavko et al., 2009):

\[
\frac{1}{K_{\text{pore}}} = \frac{S_w}{K_{\text{water}}} + \frac{1-S_w}{K_{\text{air}}}
\] (2.6)

where \(S_w\) is water saturation, \(K_{\text{water}}\) is the bulk modulus of water, and \(K_{\text{air}}\) is the bulk modulus of air. In conventional Biot-Gassmann theory, elastic moduli of the granular matrix are considered to be constant. Note that variables with a “matrix” subscript are used instead of the “dry” subscript used in conventional Biot-Gassmann fluid substitution equations (Bachrach et al., 1998). The new notation is used to better show that we are using a reference matrix elasticity, whether wet or dry. In unconsolidated sediments \(G_{\text{eff}}\) is equal to \(G_{\text{matrix}}\) at a single depth and water saturation, but neither is constant throughout the full range of saturations. The depth and water saturation dependence of matrix elasticity is due to total effective stress contributions of net overburden stress and soil suction stress, respectively.

Matrix elastic moduli (equations 2.4 and 2.5) are calculated by Hertz-Mindlin theory (Hertz, 1882; Mindlin, 1949). Different from conventional Hertz-Mindlin theory, which only considers net overburden stress as effective stress, we incorporate both interparticle stresses (soil suction and cohesive stress) and overburden stress in the total effective stress \(P\) of our new model (Mavko et al., 2009):
\[
K_{matrix} = \frac{3 n^2 (1-\phi)^2 G^2}{18\pi^2 (1-\nu)^2} P \tag{2.7}
\]

\[
G_{matrix} = \frac{5-4\nu}{5(2-\nu)} \frac{3 n^2 (1-\phi)^2 G^2}{2\pi^2 (1-\nu)^2} P \tag{2.8}
\]

where \(n\) is grain coordination number, \(G\) is the grain shear modulus, \(\nu\) is the grain Poisson’s ratio, \(K_{matrix}\) is the bulk modulus of the skeletal matrix, \(G_{matrix}\) is the shear modulus of the skeletal matrix, and \(P\) is the total effective stress.

Total effective stress at the grain contacts is used to calculate matrix elasticity in Hertz-Mindlin theory (equations 2.7 and 2.8). In the absence of direct measurements, total effective stress can be estimated from the sum of net overburden stress \((\sigma_t - u_{\text{pore}})\) and interparticle stress \((\sigma'_s + \sigma_{co})\) acting on the granular matrix (Lu and Likos, 2006):

\[
P = (\sigma_t - u_{\text{pore}}) + \sigma'_s + \sigma_{co} \tag{2.9}
\]

where \(\sigma_t\) is the total external stress, \(u_{\text{pore}}\) is pore-pressure, \(\sigma'_s\) is soil suction stress (Lu and Likos, 2006), and \(\sigma_{co}\) is apparent tensile stress at the saturated state caused by cohesive or physicochemical forces (Bishop, 1960). Physicochemical forces are local forces arising from individual contributions from van der Waals attractions, electrical double layer repulsion, and chemical cementation effects (Lu and Likos, 2006). Soil suction is calculated from van Genuchten fitting parameters and water saturation (Song et al., 2012). Saturated cohesion is constant for different soil types and is taken from literature (Table 2.1).

The soil water characteristic curve (SWCC), relating suction stress and water content, is useful if water saturations need to be estimated above a given water table. SWCCs are expected to display hysteresis, a difference in suction stress between the wetting and draining stages because of the hydrophilic nature of soils. A SWCC can be
converted into a pressure head-water saturation profile by solving the above equation for capillary pressure \((u_a - u_w)\), and setting it equal to the weight of the water column supported above the water table (pore pressure equation). The pressure head can then be plotted against water saturation, creating a pressure head-water saturation profile. The work of van Genuchten (1980) is used to empirically fit capillary pressures and water saturations for different sediments:

\[
S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{1 + [\alpha (u_a - u_w)]^n}\right]^{\frac{n-1}{n}} \tag{2.10}
\]

where \(S_e\) is effective saturation, \(\theta\) is the volumetric water content, \(\theta_r\) is the residual water content, \(\theta_s\) is the saturated water content which is equivalent to porosity, \(\alpha\) and \(n\) are van Genuchten (1980) empirical fitting parameters, and \((u_a - u_w)\) is capillary pressure.

Soil suction stress (equation 2.9) is then derived from Van Genuchten’s fitting parameters for SWCC (Song et al., 2012).

\[
\sigma'_s = -\frac{S_e}{\alpha} \left(\frac{S_e^{\frac{n}{1-n}} - 1}{\frac{n}{1-n}}\right)^\frac{1}{n} \tag{2.11}
\]

2.3.1 Pore Pressure in Homogeneous Soils

For the derivation of pore pressure, we assume homogeneous soils can be represented by a medium with a constant pore size and no layering (Figure 2.1, a and c). The difference in the calculation of pore pressure (equation 2.9) can be up to 20% between that for a single pore-size medium (Figure 2.1, a and c) and a layered-soil medium (Figure 2.1, b and d).

In homogeneous soils, pore pressure \((u_{pore})\) is simply calculated from the weight of water column (Fredlund and Rahardjo, 1993):

\[
u_{pore} = \rho_{water} g h_b \tag{2.12}
\]
where $\rho_{water}$ is the density of water, $g$ is gravitational acceleration, and $h_b$ is the height of the sediment column supported by buoyancy.

![Simplified pore-size model](image)  
**Figure 2.1.** Simplified pore-size model used to calculate matric suction in three-layer soils. (a) A single, narrow pore size ($r_1$) occurs when the 3 layers ($h_1+h_2+h_3$) consist of homogeneous clay. (b) If the middle layer contains sand, the pore size is larger ($r_2$). (c) A single, thick pore size ($r_2$) occurs when the 3 layers ($h_1+h_2+h_3$) consist of homogeneous sand. (d) When the middle layer contains clay ($r_1$) sandwiched between sand ($r_2$), the narrowest pore size is in the center.

If normal stress from the weight of the sediment is much larger than horizontal stresses, the difference ($\sigma_t - u_{pore}$) becomes net overburden stress and is the weight of the sediment above the grain contact minus the local pore pressure (Terzaghi, 1943):

$Net\ overburden\ stress = \sigma_t - u_{pore} = \rho_{bulk}gh_a + (\rho_{bulk} - \rho_{water})gh_b \quad (2.13)$

where $\rho_{matrix}$ is the density of the solid matrix, and $h_a$ is the height of the sediment column not influenced by buoyancy.

### 2.3.2 Pore Pressure in a Clay-Sand-Clay Three-Layer Soil

In variable-pore-size layered soils that are not dominated by one type of soil, we examine the effects of a pore-size change with a simple, three-layered soil, using capillary tubes with various radii to conceptualize the calculations. Natural soils often have layers of alternating sand and clay composition. Usually, pore size in clay is smaller than in sand as the grain size of clay is smaller than sand (Taylor, 1948). We can simplify
more complicated field conditions by considering two idealized cases: one case where sand is sandwiched between clay layers (Figure 2.1, b) and another for clay sandwiched between sand layers (Figure 2.1, d). A three-layer pore-size model (Figure 2.1) that attempts to mimic a clay-sand-clay alternation has the thickest pore size in the middle layer. Pore pressure estimates are the same for the bottom layer (using equation 2.12) in both pore-size models, but different within top and middle layers (Figure 2.1, b and d).

In layered soil, pore pressure ($u_{pore}$) is equal to the total stress difference at the air-water interface and depends on layer thickness, pore-size variation and capillary head height. To simplify the derivation, we use a capillary tube to represent idealized pore size in soil (Figure 2.1). In equilibrium, pore pressure around a capillary tube is balanced by the weight of the water column pulled up by surface tension (Fredlund and Rahardjo, 1993). Three cases arise depending on the location of the capillary head within the three layers:

Case 1: when the capillary head ($h_{c1}$) is within the bottom clay layer ($h_{c1} < h_1$), pore pressure $u_{pore1}$ can be estimated by the weight of water column using equation 2.12.

Case 2: when the capillary head ($h_{c2}$) rises into the middle sand layer ($h_1 < h_{c2} < h_1 + h_2$), pore pressure $u_{pore2}$ can be calculated as:

$$u_{pore2} = \left(\frac{r_1}{r_2}\right)^2 \rho_w g h_{c2} + \left(1 - \frac{r_1^2}{r_2^2}\right) \rho_w g (h_{c2} - h_1)$$  \hspace{1cm} (2.14)

where the $r_1$ and $r_2$ are narrow and thick pore sizes occurring in clay and sand, respectively. As the pore pressure is less in the middle layer than in the bottom layer, water will tend to stay in the bottom thin-throat layer longer before it eventually rises up into the second layer (Taylor, 1948).
Case 3: when the capillary head \((h_{c3})\) rises and enters the top clay layer \((h_2 < h_{c3} < h_1 + h_2 + h_3)\), pore pressure \(u_{pore3}\) becomes:

\[
u_{pore3} = \rho_w g h_{c3} + \left(\frac{r_2^2}{r_3^2} - 1\right) \rho_w g h_2 \tag{2.15}\]

Pore pressure can be misestimated if pore pressure calculation assumes only one homogeneous layer with a constant pore size for clay-sand-clay layered soils, such as in case 2, where pore pressure is overestimated, and in case 3, where pore pressure is underestimated.

2.3.3 Pore Pressure in a Sand-Clay-Sand Three-Layer Soil

Pore pressure may also be estimated for the case of a three-layer pore-size model (Figure 2.1, d) that attempts to mimic a sand-clay-sand alternation that has the narrowest pore size in the middle layer. We consider three cases:

Case 1: when the capillary head \((h'_{c1})\) is within the bottom sand layer \((h'_{c1} < h_1)\), pore pressure \(u'_{pore1}\) can be estimated by the weight of water column using equation 2.12.

Case 2: when the capillary head \((h'_{c2})\) rises into the middle clay layer \((h_1 < h'_{c2} < h_1 + h_2)\), pore pressure \(u'_{pore2}\) can be calculated as:

\[
u'_{pore2} = \left(\frac{r_2}{r_1}\right)^2 \rho_w g h_1 + \rho_w g (h'_{c2} - h_1) \tag{2.16}\]

Case 3: when the capillary head \((h'_{c3})\) rises and enters the top sand layer \((h_2 < h'_{c3} < h_1 + h_2 + h_3)\), pore pressure \(u'_{pore3}\) becomes:

\[
u'_{pore3} = \frac{r_2^2}{r_3^2} \rho_w g h_2 + \rho_w g (h'_{c3} - h_2) \tag{2.17}\]

Pore pressure can be misestimated if pore pressure calculation assumes only one homogeneous layer with a constant pore size for sand-clay-sand layered soils, such that in case 2, pore pressure is underestimated, and in case 3, pore pressure is overestimated. In
order to properly use our proposed model to match field data in layered soils, it is necessary to incorporate the effect of layer thickness and pore-size variation.

2.4 Theoretical Cases

In this section, we present several theoretical examples by assigning published values to parameters (Table 2.1) in the calculation of stresses and velocities, in order to present differences between traditional and our proposed models. As sand and clay are common unconsolidated sediments, the parameters we use to calculate theoretical results are for homogenous sand and clay soils. The variation of these properties vary less than 5% for sand, but may change by up to 20% for clay (Mavko et al., 2009). To simplify our examples, we choose one set of parameter values for sand and clay to represent typical trends of theoretical velocities or stresses. Different soil property values may lead to up to 10% changes in calculated velocities for clay and less than 3% changes for sand.

Unrealistically low coordination numbers (= 1, Table 2.1) have been previously used to match low seismic velocities in shallow sediments by taking into account the angular grain shape, which is contrary to the assumption of spherical contact in Hertz-Mindlin theory (Bachrach et al., 1998; Velea et al., 2000). However, the low coordination numbers can lower calculated velocity, but do not affect general velocity trends.

Our new model (equations 2.9 and 2.11) predicts that when water saturation changes, only soil suction stress contributes to the variation in total effective stress (Figure 2.2). Among the three stress terms in the calculation of total effective stress (equation 2.9), only soil suction stress is a function of effective water saturation (equation 2.11). Both overburden and cohesion are not affected by saturation changes.
Figure 2.2. Contribution of soil suction stress to total effective stress as a function of effective water saturation for (a) sand at 10 cm depth and (b) clay at 1 m depth. The difference between soil suction stress curve and total effective stress curve is attributed to net overburden stress and cohesion, which remain constant throughout saturation changes.
In order to highlight the influence of interparticle stresses on seismic velocity, we calculate velocities using either total effective stress (new model) or solely net overburden stress (traditional model) at constant depths in different soils (Figure 2.3). As the difference in velocity relies on the changes in stress and water saturation, they are the only variables that change within each example. We focus on using water saturation values greater than 10%, which are above residual water saturation, and less than 95% because compressional seismic velocities can increase by over $10^3$ m/s as water saturation approaches 100%. Normally, shallow soils are not fully saturated and observed velocities are on the order of $10^2$ m/s. We also focus on this range of water saturations because interparticle stresses increase above a base value within this range. At above 95% water saturation soil suction stress becomes negligible.

Field velocity profiles are sometimes depth-dependent, so we need to relate water saturation to depth for the prediction of field velocity. In our proposed model, we estimate the relationship between water saturation and depth from SWCCs (Figure 2.4). Pressure head-water saturation profiles converted from capillary pressure-water saturation curves (e.g. SWCC) are consistent with natural water saturation profiles (Desbarats, 1995). In the calculation of total effective stress (equations 2.9, 2.11 and 2.13), both net overburden stress and soil suction stress are depth-dependent. When depth changes, net overburden stress and soil suction stresses both contribute to the variation in sand and clay (Figure 2.5). Velocity-depth profiles (Figure 2.6) are calculated for sands and clays with stationary water tables to illustrate the decreasing effect of interparticle stresses as depth and net overburden stress increase.
Compressional ($V_P$) and shear-wave ($V_S$) velocities are calculated for (a) sand at 10 cm depth and (b) clay at 1 m depth. The different trends in $V_P$ and $V_S$ from incorporating total effective stress (dots, with soil suction and cohesion) and only net overburden stress (lines) are attributed to interparticle stresses.
Figure 2.4. Soil-water characteristic curves for (a) sand and (b) clay calculated from van Genuchten fitting parameters (Table 2.1). The capillary pressures are converted to pressure head for input into velocity-depth models for (c) sand and (d) clay. The water tables are at 0 m pressure head.
Figure 2.5. Contributions of soil suction stress, net overburden stress and cohesion to the calculation of total effective stress as a function of depth for (a) sand when water table is at the depth of 0.6 m and (b) clay when water table is at the depth of 100 m. Water table line (phreatic surface) shows where pressure head is equal to atmospheric pressure. Saturation at each depth is calculated from fitting parameters of soil water characteristic curve (Table 2.1).
Figure 2.6. Seismic compressional wave velocities ($V_p$) calculated by incorporating total effective stress (black) or only net overburden stress (grey) for (a) sand when water table is at the depth of 0.6 m and (b) clay when water table is at the depth of 100 m. Saturation at each depth is input into the model, calculated from soil parameters (Table 2.1).

2.5 A Verification with Field Measurements

To verify our proposed model, we compare our predictions to observed field velocities (Lu and Sabatier, 2009) (Figure 2.7). The uncertainty in soil property parameters (Table 2.1) and measured total effective stress (Lu and Sabatier, 2009) lead to
less than ±5% error in predicted velocity. Within error, the majority of field velocities fall
within predicted velocity range from our proposed model.

A traditional model fails to predict the variation in the observed field velocities
from ~250 to ~450 m/s (Figure 2.7). Without interparticle stresses (traditional model)
contributing to grain contact stress, we would expect pore constituent concentrations to
be the main variables affecting seismic velocity. However, changes in the bulk modulus
and density of the pore space only account for an ~14 m/s increase in seismic velocity.
The results (Figure 2.7) indicate large interparticle stresses (up to 20 kPa) are much more
influential on shallow seismic velocities (< 30 cm) than net overburden stress or pore
constituent concentrations.

![Figure 2.7](image.png)

Figure 2.7. A comparison of raw data (Lu and Sabatier, 2009) (dots) and predicted
velocities from our proposed model (solid line) as well as from a traditional model
(dashed line). Model input parameters are for clay (Table 2.1) with the exception of
coordination number, which is changed to 4.4 to provide the best fit to the data. The error
in calculated velocities is less than ±5%.
Field-velocity predictions require reasonable estimations of water saturation and total effective stress, both of which can be achieved from field measurements or estimated by our proposed model (using SWCC). For the velocity prediction in Figure 2.7, total effective stress and water saturation are from field measurements (Lu and Sabatier, 2009). Total effective stress is input for the range of observed stresses. Total effective stress and water saturation measurements are highly variable so we simplify water saturation input by correlating several water saturation and total effective stress values from the raw data. Water saturation is highest (53%) at the lowest effective stress and is assumed to decrease linearly until it reaches its lowest value (10%) at the largest effective stress. This relationship appears to hold true (±2% Sw) for the presented measurements. Total effective stress correlates with water saturation because of soil suction stress. The increase in velocity caused solely by changes in bulk modulus and density of the pore space is compared to measured velocities to further illustrate that interparticle stresses must be included in velocity calculations.

2.6 Discussion

In our proposed model, soil suction stress plays a more significant role in clay than in sand (Figure 2.2). In sands, soil suction stress contributes to less than 50% of total effective stress, while overburden stress is the dominant stress at most saturation values (Figure 2.2, a). In clays, soil suction stress contributes to ~80% of total effective stress except for effective water saturation reaches 100% (where soil suction stress is 0) (Figure 2.2, b). At shallow depths, clays (0-100 m) and sands (0-1 m) may have different seismic velocity trends with water saturation because of their respective interparticle stresses.
When interparticle stresses are included in our new model, there are significant differences in both values and trends of predicted seismic velocities from traditional models (Figure 2.3). When total effective stress is used to calculate pressure instead of only net overburden stress, theoretical seismic velocities can be up to 20% larger in sands and up to 60% larger in clays. In sand, over a range of 10-95% water saturation, the predicted seismic velocity increases with water saturation and the Biot-Gassmann effect is not apparent (Figure 2.3, a). In clays, velocity decreases as water saturation increases, but when interparticle stresses are considered (new model) the calculated velocities double the range predicted by traditional model (Figure 2.3, b). In comparison to sand, clay shows a larger variation in predicted velocities with changes in water saturation (Figure 2.3). This greater sensitivity of velocity to water saturation makes clays more suitable for water saturation modeling.

Some water table monitoring studies attribute a decrease in velocity to lowered water tables because of the Biot-Gassmann effect (Bachrach et al., 1998; Birkelo et al., 1987). However, calculations of seismic velocity that include interparticle stresses (new model) predict an increase in seismic velocity with increasing water saturation in sand (Figure 2.3, a) so that a lower seismic velocity may not be attributed solely to the Biot-Gassmann effect. Instead, a decrease in velocity may be caused by buoyancy. In normally-pressured sands, the net overburden stress gradient can decrease up to ~9800 Pa/m with the addition of water, due to buoyancy. Because of the decrease in the net overburden stress gradient, seismic velocities will decrease \((V \propto \sigma)\).

In our proposed model, the relative contributions of net overburden, soil suction and cohesive stresses to total effective stress depends on both depth and soil types (Figure
2.5). In sands, net overburden stress is the dominant stress except at the surface (< 5 cm depth). Also in sand, a local maximum arises in total effective stress just above water table (~50 cm depth) and it is attributed to the effect of soil suction stress. In clay, interparticle stresses (soil suction and cohesive stresses) dominate total effective stress until the water table is reached. Just above the water table, the sum of net overburden and soil suction stresses leads to a local maximum in total effective stress (~80 m depth) in clays. At the water table for both sand and clay, soil suction stress becomes 0 and the total effective stress becomes the sum of net overburden stress and cohesion. For example, in our case, net overburden stress equals the value of interparticle stresses at ~5 cm in sand and ~98 m in clay (Figure 2.5).

Velocity-depth profiles calculated using either total effective stress (as in our new model) or only net overburden stress (as in traditional model) are most different at the surface but converge near the water table (Figure 2.6). Calculated velocities have similar trends as depth increases and net overburden stress becomes the largest component of total effective stress. The minimum in velocity above water table in both sands and clays is a result from the maximum in total effective stress (Figures 2.5 and 2.6).

Interparticle stresses should be included in seismic velocity modeling of shallow unconsolidated sediments, even in sands which have very low capillary pressures and cohesion, but especially in clays which have very high interparticle forces. The large velocity variations measured by Lu and Sabatier (2009) at constant depths are better explained by interparticle stresses than density and elasticity changes during fluid substitution—these can only account for an ~8% velocity change (Figure 2.6). When predicting seismic velocities, interparticle stresses are particularly important at depths
less than 1 m in sands and 100 m in clays. At these depths, net overburden stress becomes a larger component of total effective stress than interparticle stresses. The proposed model remains applicable at large depths (> 1 km) where our calculated velocities at large net overburden stresses (> 5 MPa) are indistinguishable from previous models (Dvorkin and Nur, 1996).

Total effective stress is a required parameter in the proposed model. In the absence of direct measurements, total effective stress can be estimated from the SWCC but specific temperature-pressure and wetting/drying conditions must be considered. Hysteresis in the SWCC for clays during wetting and drying cycles accounts for as much as 30% differences in capillary pressures and is attributed to a change in contact angle between the wetting phase and the solid surface (Pham et al., 2005). Capillary pressure decreases by 3 kPa in sands as temperature increases from 20 to 80 °C (She and Sleep, 1998). Our proposed model indicates that the total effective stress can also be estimated by considering the effect of pore-size variation and layer thickness in clay and sand layered soils.

2.7 Conclusions

An improvement in our understanding of total effective stress (Lu and Likos, 2006) in constitutive elastic models allows improved predictions of seismic velocity in both shallow sands and clays. The added effect of interparticle stresses suppresses the Biot-Gassmann effect in shallow sediments. When interparticle stresses are included, as water saturation increases, the decrease in seismic velocity can be double that of the traditional models. A larger change in seismic velocity implies that water saturation can be modeled with more accuracy in shallow clays than in sands. At depths greater than 10
cm in sands and 100 m in clays, net overburden stress becomes a larger component of total effective stress than interparticle stresses in the modeled granular materials. The proposed model predicts seismic velocities that fit well with field measured seismic velocities under low confining pressures (< 5 kPa) and a large range of interparticle stresses (> 350 kPa).

2.8 References


Turner, J. S., 1979, Buoyancy effects in fluids: Cambridge University Press.


CHAPTER 3: SOIL DENSITY, ELASTICITY AND THE SOIL WATER CHARACTERISTIC CURVE INVERTED FROM FIELD-BASED SEISMIC P- AND S-WAVE VELOCITY IN SHALLOW (< 25 M DEPTH) NEAR-SATURATED (> 99%) LAYERED SOILS

3.1 Summary

Soil density, porosity, elastic moduli and the soil-water characteristic curve (SWCC) are important properties for soil characterization. However, geotechnical and laboratory tests for soil properties are costly and limited to point sampling sites. Seismic surveys can provide laterally continuous, seismic, soil property values that may complement geotechnical borehole tests with less cost. In this study, we propose a workflow to invert for soil properties and the SWCC from seismic P- and S-wave velocity-vs.-depth profiles interpreted from shallow (< 25 m depth) unconsolidated sediments under conditions of near-full saturation (> 99%). The inversion is performed by using the Covariance Matrix Adaptation Evolution Strategy to search automatically for optimal input soil property values by minimizing the misfit between field-based velocity profiles and predicted velocity profiles based on Hertz-Mindlin and Biot-Gassmann theories.

The results from seismic soil property inversion are validated by comparison to geotechnical as well as laboratory results conducted independently in the same area as the seismic survey. For each seismically recognizable layer, soil types are interpreted from the inverted soil density and elasticity, aided by the SWCC to help detect thin units that are below the original seismic resolution of the field data. There is flexibility to apply our suggested workflow in future studies. For a known geological setting, empirical relationships and other velocity prediction models could also be incorporated into the
suggested workflow to improve inversion results and extract additional information in soils.

3.2 Introduction

Soil properties such as density, elastic moduli, porosity, and the soil-water characteristic curve (SWCC) are important for assessing foundation stability (Bell, 1992), and monitoring of contaminant movement and soil aeration (Terzaghi, 1996). These soil properties depend on soil grain-size, mineral composition, overburden pressure and stress history (Fredlund and Xing, 1994). Soil properties can be measured directly in the laboratory (Van Genuchten, 1980), but these tests are costly and the necessary equipment may not be readily accessible. Laboratory soil property tests are performed on either core or bulk sediment samples, which may not be representative of in-situ sediments. The borehole locations are usually distant from each other (> 100’s m), so that lateral soil characteristics between boreholes are difficult to predict.

In this paper, we use an indirect inversion process to determine in-situ soil density, elastic moduli, porosity, and the SWCC by minimizing the misfit (cost function) between the predicted and field-derived velocity profiles (Figure 3.1, Appendix A). In order to perform the inversion, an optimization technique automatically searches for input soil-property-parameter values that can best explain the field velocity profiles. Compared to other seismic inversion techniques (such as widely-used full-waveform inversion), the major advantages of our inversion are that it uses a global optimization technique and requires only a velocity-vs.-depth profile which is interpreted from the seismic survey. A global optimization technique searches for a global minimal value of the misfit throughout the input parameter range. Unlike local optimization that is used by full-
waveform inversion, global optimization is not affected by starting parameters. Currently, full-waveform inversion often relies on reflections (Masoni et al., 2014), which can be hard to get in shallow near-saturated soils because of attenuation, especially for P-waves. For our inversion we incorporate both refraction and reflection first-arrivals through 1D P- and S- wave velocity-vs.-depth starting models (Lorenzo et al., 2014). Moreover, the inversion of one-dimensional velocity models is simpler and faster computationally than 2D or 3D waveform matching.

![Diagram](image)

Figure 3.1. The procedure of soil property inversion by minimizing misfit between predicted and field-based seismic velocities. Predicted velocities are calculated by Hertz-Mindlin and Biot-Gassmann model. CMA-ES is the optimization program to minimize misfit.

The SWCC shows the relationship between water saturation and capillary head (Van Genuchten, 1980), both of which are readily determined in our inversion. At the same capillary head, water saturation increases with soil plasticity (Fredlund and Xing, 1994). Therefore, water saturation is lower in sandy soils than in clayey soils. The SWCC is used to estimate other soil behavior parameters such as unsaturated shear strength,
permeability and pore size distribution (Fredlund, 1995; Fredlund and Rahardjo, 1993a; Fredlund et al., 1996).

Our velocity prediction model is based on Hertz-Mindlin contact theory (Hertz, 1882; Mindlin, 1949) and Biot-Gassmann fluid substitution theory (Biot, 1962; Gassmann, 1951) (Appendix B), as they are the currently acceptable constitutive models used to relate effective elasticity and soil properties in shallow unconsolidated sediments (Bachrach and Avseth, 2008; Bachrach et al., 1998; Bachrach et al., 2000; Bachrach and Nur, 1998; Dutta et al., 2010; Zimmer et al., 2006). The Hertz-Mindlin model uses grain elasticity, porosity and grain contact geometry under effective stress (Digby, 1981; Dvorkin and Nur, 1996; Walton, 1987) in order to calculate the isotropic elastic moduli of a homogeneous, granular matrix comprising identical spherical grains. The Hertz-Mindlin model also assumes dry, no-slip, spherical contacts between the grains and as a result the Poisson’s ratio for the grains is expected to be < 0.25. Biot-Gassmann fluid substitution theory accounts for pore fluid variation in a porous medium and estimates effective elastic moduli from dry matrix elasticity, grain elasticity and water saturation. Biot-Gassmann theory more accurately predicts velocities for data at low frequencies (10-200 Hz) than at higher frequencies (> 10 kHz) in unconsolidated soil (Wang, 2001). Seismic velocity is ultimately computed from the relationships between velocity, effective elasticity and bulk density (e.g., Ikelle and Amundsen, 2005).

The application of the Hertz-Mindlin model in clay-dominant sediments is debatable because the model is originally derived using spherical grains. For example, shear modulus is over-estimated by Hertz-Mindlin for angular grains (Bachrach et al., 2000) and clay grains have a platy shape. One heuristic approach is to lower the
coordination number for computing predicted velocities of angular grains (Bachrach et al., 1998; Velea et al., 2000). Particularly in shallow unconsolidated sediments, loosely packed, highly angular grains lead to a lower coordination number and higher porosity. As a result, high-porosity (~65%) clay has a relatively lower coordination number than medium-porosity (~40%) sand (Murphy, 1982). Hertz-Mindlin theory predicts elastic moduli successfully in clay-dominant rocks, such as shales (Avseth et al., 2005) and claystones (Takahashi and Tanaka, 2009).

Additional debate surrounds the application of a high Poisson’s ratio (> 0.25) with Hertz-Mindlin theory in wet sediments. In saturated unconsolidated sands (e.g., Dvorkin and Nur, 1996), as well as in near-fully-saturated clays (such as our case) the effective Poisson’s ratio can be larger than 0.25. Dvorkin and Nur (1996) use Hertz-Mindlin theory to predict velocities successfully in saturated-loose sands with a high effective Poisson’s ratio close to 0.5.

Another factor that needs to be considered for clay at shallow depth when using the Hertz-Mindlin model is the effective stress. In sand, the dominant stresses are overburden pressure and matric suction (cohesion is close to 0), whereas in clay, cohesion (up to 20 kPa) also plays a significant role. In this study, we modify the effective stress by also incorporating the effect of matric suction and cohesion. This modification helps to predict velocities in agreement with field velocities in clay-and-sand mixed soils (Crane, 2013).

Among the various optimization algorithms used to effectively search for those parameters that explain field velocity profiles, we use the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) (Hansen, 2011) (Appendix A). CMA-ES belongs to the
class of evolutionary algorithms, and is a stochastic, derivative-free algorithm used for non-linear local and global optimization (Mezura-Montes and Coello Coello, 2011). One of the advantages in CMA-ES over the genetic algorithm is its well-designed, internal, parameter-tuning mechanism which selects new candidates for input parameter values while approaching a best-fit between prediction and observation. The parameter-tuning mechanism is based on updating the covariance matrix between variables in the distribution (Hansen, 2011) as the candidate values converge toward the global optimum. In CMA-ES, population size is crucial to the success of global optimization – this number is designed to avoid a local optimum, increasing logarithmically with the number of unknown inputs (Hansen, 2006). CMA-ES is applied to model fluid flow (Bayer et al., 2009) and to facilitate groundwater remediation (Bayer and Finkel, 2007).

We attempt our inversion for seismic soil properties in near-fully-saturated soils of the lower Mississippi River swamps and marshes (Lorenzo et al., 2014), because the seismic velocity is most sensitive to water saturation at near-saturation conditions (water saturation > 99%). Near-saturated soils occur permanently or seasonally in wetlands, including coastal, floodplains, the margins of lakes, and other areas below groundwater level or where the precipitation is sufficiently high (Gilman, 1994). Both velocity prediction models (e.g., Bachrach and Nur, 1998) and field-based velocity profiles (e.g., Grellle and Guadagno, 2009) show that P-wave velocities change from ~200 to ~1500 m/s in the transition zone from near-saturated soils to saturated soils. As soil approaches full saturation, the pore water replaces almost all the air. The bulk modulus of water is more than 4 orders of magnitude larger than that of air (Table 3.1). As a result, higher water saturation yields a stiffer soil with an increased compressional velocity. As S-waves are
insensitive to pore fluids and travel more slowly than P-waves, S-waves are less attenuated by fluids and have more resolution (Harris, 2009). As a result, S-waves are sensitive to soil type changes (Hayashi et al., 2013) and S-wave reflections can be used to identify soil layers.

Table 3.1. Key parameters with known values used in the Hertz-Mindlin and Biot-Gassmann models (Appendix A).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
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<tr>
<td>( g ) (m/s(^2))</td>
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</tr>
<tr>
<td>( \rho_w ) (kg/m(^3))</td>
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</tr>
<tr>
<td>( \rho_a ) (kg/m(^3))</td>
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</tr>
<tr>
<td>( K_w ) (Pa)</td>
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</tr>
<tr>
<td>( K_a ) (Pa)</td>
<td>1.01×10(^5)</td>
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3.3 Methods

3.3.1 Field-based Data

The field data we use for inversion include field-based P- and S-wave velocity-vs.-depth profiles interpreted from seismic surveys at two field sites (Figure 3.2). The seismic survey was conducted in the near-fully-saturated shallow soil (< 25 m) beneath a New Orleans flood-protection levee (Lorenzo et al., 2014). In these data, seismic frequency reaches 30 Hz. In velocity-vs.-depth profiles, there is ± 1 m error in layer depths (Lorenzo et al., 2014) and ± 2% error in P and S-wave velocities. The seismic survey line is ~100 m wide. As a result, velocity profiles represent the average of the survey width. Two sites (A and B) help validate the inversion results under a variety of water saturation conditions, and sand and clay percentages. At both sites, soil is composed of a majority of clay with several small sand units between the depths of 7.5 m to 15 m and these sand units are thicker at site A than at site B (Lorenzo et al., 2014).
Figure 3.2. Predicted and field-based P- and S-wave velocity-vs.-depth profiles and geotechnical CPT soil type profiles from the seismic survey area (Lorenzo et al., 2014) at (a) site A and (b) site B. Quality of inversion results can be quantified by the misfit between field and predicted velocity-vs.-depth profiles. Misfits are calculated by the sum of the normalized root-mean square error (NRMSE) between predicted and field velocity profiles. CPT soil type profile shown here is 100 m wide and covers the same area as seismic survey. At both sites, predicted velocities are calculated at discrete depths every 0.005 m. Depth error in field velocity is ±1 m. Errors in field velocities are < 2%. Soil types determined from the combination of density, elastic moduli and SWCC are labeled for each layer.
3.3.2 Velocity prediction model

The Hertz-Mindlin contact theory and Biot-Gassmann fluid substitution theory (Appendix B) predict seismic velocities from soil properties, water saturation and effective stress (Figure 3.1). Water saturation and effective stress are major factors that contribute to the increase in P-wave velocity from ~200 m/s to ~1200 m/s. In unconsolidated sediments, the Hertz-Mindlin model accounts for mechanical compaction from confining pressure, so that the predicted velocity is much more strongly dependent on effective stress than porosity (Avseth et al., 1998). In near-fully-saturated soil (> 99%), the velocity model predicts that a 1% change in water saturation leads to a 20% change in P-wave velocity, whereas a 1% change in soil properties (e.g., porosity, coordination number, density and elasticity) leads to less than a 1% change in P-wave velocity. In order to explain field velocity increases with depth (Figure 3.2) we also need to relate the changes in water saturation and effective stress with depth. We use SWCC to predict the relationship between depth and water saturation (Appendix B). Effective stress relates to the confining pressure as well as matric suction, and both of the parameters vary with depth. Matrix and effective density and elasticity are calculated using water saturation and effective stress, which are in turn themselves depth-dependent (Figure 3.1).

Accurate prediction of seismic velocity in shallow (< 25 m depth) unconsolidated sediments requires the incorporation of matric suction and cohesion into the estimation of effective stress in the Hertz-Mindlin and Biot-Gassmann models (Crane, 2013; Lu and Sabatier, 2009; Revil and Mahardika, 2013). In shallow, unconsolidated, clay-rich soil, matric suction and cohesion can be several orders of magnitude larger than overburden
pressure and dominate effective stress (Lu and Sabatier, 2009). Rock physics models (Bachrach and Nur, 1998) indicate seismic velocity is proportional to the $1/6$ th power of the effective stress. The incorporation of matric suction and cohesion in clay-rich soil almost doubles the predicted seismic velocity and brings results closer to real data (Crane, 2013). Cohesion is one kind of inter-particle stress and arises from physicochemical forces between mineral grains. Matric suction is equal to the total stress difference at the air-water interface ($u_a - u_w$). In equilibrium, matric suction ($u_a - u_w$) around a capillary tube is balanced by the weight of the water column pulled up by surface tension (Fredlund and Rahardjo, 1993b):

$$u_a - u_w = \rho_w gh_c$$

(3.1)

where $u_a$ is the atmospheric pressure, $u_w$ is the pore water pressure, $h_c$ is the capillary head, $\rho_w$ is water density and $g$ is gravitational acceleration (Table 3.1).

In shallow unconsolidated sediments, effective stress ($P_{eff}$) is the sum of the net overburden pressure ($\sigma - u_a$), matric suction ($u_a - u_w$), and cohesion ($\sigma_{co}$) (Lu and Likos, 2006):

$$P_{eff} = \sigma - u_a - S_w (u_a - u_w) + \sigma_{co}$$

(3.2)

where $\sigma$ is overburden pressure and equals $\rho_{eff} gh$ ($\rho_{eff}$ is effective density of soil with pore fluids, and h is the depth of soil); $u_a$ is assumed to be zero; $S_w (u_a - u_w)$ is the matric suction contribution weighted by the percentage of water saturation $S_w$ (Lu and Sabatier, 2009).

3.3.3 Parameter constraint before inversion

CMA-ES optimization is accelerated by constraining the uncertainty of input parameter values within reasonable ranges (Table 3.2) for local soil types. As our seismic survey was conducted on alluvial-deltaic soils (Lorenzo et al., 2014), the main soil types
to consider are organic clay, clay, and sand. Organic clay has lower cohesion (Waltham, 2001) and larger compressibility than clay (Robertson, 1990), because of the organic residue in clay. Input parameters in the velocity prediction model include pore fluid properties, soil properties and water-saturation related parameters. In order to give more flexibility to the search for optimal values by CMA-ES, we choose the largest published range of input parameter values for unconsolidated sediments (Table 3.2). For the correction of the over-estimated shear modulus in the Hertz-Mindlin model, we use a coordination number of 1 which is below a value with physical meaning. A coordination number of 1 is found to estimate velocity accurately in clay and sand mixtures (Crane, 2013). Pore fluids are assumed to be water and air, so their density and elastic properties are well known (Table 3.1). Because the maximum P-wave velocity throughout the profile is about 1400 m/s (Lorenzo et al., 2014) but below fully-saturated velocity values, around 1500 m/s (Grelle and Guadagno, 2009), for the purpose of SWCC calculation, the water table (value of 36 m) is assumed to be slightly below the depth of the profile.

Table 3.2. The 11 unknown parameters with published ranges used in the Hertz-Mindlin and Biot-Gassmann models (Appendix A). The ranges of each parameter span those in organic clay, clay and sand. These parameters are assumed to be constant within each seismically recognizable layer.

<table>
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<th>Parameters</th>
<th>Lower boundary</th>
<th>Upper boundary</th>
<th>References</th>
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<td>$C$</td>
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<td>8</td>
<td>Crane (2013), Allen (1985)</td>
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<tr>
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<td>Van Genuchten (1980)</td>
</tr>
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<td>$a$</td>
<td>0</td>
<td>1</td>
<td>Van Genuchten (1980)</td>
</tr>
<tr>
<td>$n$</td>
<td>0</td>
<td>49.9</td>
<td>Van Genuchten (1980), Leong and Rahardjo (1997)</td>
</tr>
</tbody>
</table>
3.3.4 Seismic soil property inversion

Soil property inversion is carried out separately within each seismically recognizable layer. Soil properties and the three fitting parameters in SWCC (Table 3.2) are the outputs from inversion when the misfit between the predicted and field velocity profiles reaches its minimum. From the fitting parameters, we then compute inverted SWCCs with an assumed water table (value of 36 m) (Figure 3.1). Three seismic layers can be determined from sharp changes in the field-derived S-wave seismic velocity profiles for both sites (Figure 3.2). We use CMA-ES optimization to minimize the misfit between the field-velocity profile and the predicted velocity profile by varying the input soil-property parameter values within reasonable ranges (Table 3.2). The soil property parameters used to explain the field velocity profile are the optimal values that represent the local soil characteristics. Based on the assumptions of the velocity prediction model and considering the resolution of the seismic data, we assume sediments are homogeneous and isotropic within each seismic layer. As a result, soil properties (Table 3.2) are constant within each seismic layer. Soil properties represent average values over the width of seismic survey area (~100 m) and over the depth of each layer. At each depth, water saturation is an average of patchy saturation over the seismic survey area (~100 m). Our seismic data have effectively low frequency (≤ 30 Hz), so that pore fluid heterogeneity is unresolvable with the dominant seismic wavelet (Johnson, 2001). In each seismic layer, the misfit between the field velocity profile and the predicted velocity profile is quantified by the normalized root-mean square error (NRMSE) at discrete depths every 0.005 m. NRMSE is calculated by normalizing the root-mean square of the
difference between the predicted and field-base velocities by the average of the field-based velocities.

The ± 2% velocity error and ± 1 m depth error from the original field velocity data propagate into errors in the inverted soil properties and water saturation. For example, the depth error in the inverted results is ± 1 m, which carries over from the depth errors (± 1 m) in the field-based velocity model. We estimate the final inversion errors via a Monte-Carlo simulation. First, we randomly generate 100 field-velocity-profile cases within their velocity error range of ± 2%. Then we invert for soil properties with the 100 different scenarios. The range of each resultant soil property value provides the estimated error.

3.3.5 Determination of soil types from inverted results

Inverted soil properties can be used to determine the soil types for each seismic layer by reference to published soil properties (Table 3.3). For different soil types, published density and elastic moduli vary over 70% (Table 3.3). Within single soil types, the variation in elastic moduli is about 20%-30% for clay, less than 5% for sand (Mavko et al., 2009), and about 50% for different organic clay (Mittal et al., 2004), because of different mineral content, overburden pressures and organic content. We assign soil types based on where the inverted soil properties fall within these ranges. If the inverted soil property value lies outside the range for one soil type alone but between the values for two soil types, we consider the soil type is a mixture of the two. Inverted soil property values that span the ranges of two or more soil types may indicate additional layering beyond the resolution of the seismic technique. SWCC can either be used to confirm a
heterogeneity or locate thin units in a heterogeneous layer that may not be sensed by inverted density and elastic moduli values.

Table 3.3. Common soil density and dynamic elastic moduli values for three different soil types (organic clay, clay and sand) used to calculate the average soil properties for each layer in geotechnical soil model.

<table>
<thead>
<tr>
<th>Soil type</th>
<th>Density (kg/m$^3$)</th>
<th>Bulk modulus (Pa)</th>
<th>Shear modulus (Pa)</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Organic clay</td>
<td>1.4</td>
<td>3.4×10$^6$</td>
<td>1.56×10$^5$</td>
<td>Walmsley (1977), Mittal et al. (2004)</td>
</tr>
<tr>
<td>Clay</td>
<td>2.6</td>
<td>2.1×10$^{10}$</td>
<td>7×10$^9$</td>
<td>Mavko et al. (2009)</td>
</tr>
<tr>
<td>Sand</td>
<td>2.65</td>
<td>3.66×10$^{10}$</td>
<td>4.5×10$^{10}$</td>
<td>Mavko et al. (2009)</td>
</tr>
</tbody>
</table>

3.4 Results

The predicted velocity-vs.-depth profile matches the field velocity-vs.-depth profile (Figure 3.2) in each of the three seismically recognizable layers with NRMSE less than 0.15 in all cases. The inverted density and elastic moduli correlate well in general with computed geotechnical results (Figure 3.3), except for the middle layer at site B (Figure 3.3, b).

The inverted soil density, elastic moduli profiles and the SWCC detect meaningful variations among three seismic recognizable layers and between sites A and B (Figures 3.3 and 3.4) as expected. The inverted soil property values are much larger at site A than site B, because the soil is sandier at the depth of the middle seismic layer (Figures 3.2 and 3.3).

The inverted water saturation, bulk density and porosity values at site B are also in agreement within an error of 15% to independent laboratory results from a well near site B (Figure 3.5). The largest mismatch arises in the bulk density and porosity profiles in the first layer.
Figure 3.3. Density, bulk modulus and shear modulus determined from seismic inversion and from geotechnical soil profile at (a) site A and (b) site B. Quality of inverted soil properties can be quantified by the misfit between the inverted soil properties and soil properties based on CPT soil profile. For most layers, the inverted soil property values fall within the error ranges of geotechnical results. The largest misfit of 70% arises in the middle layer at site B. Soil types determined from inverted density and elastic moduli are labeled for each layer.
Figure 3.4. SWCCs from seismic inversion at (a) site A and (b) site B. The error in inverted SWCC is 0.1%. SWCC can help identify the heterogeneity within a layer. The shift of SWCC to a lower value within the middle layer indicates the presence of sand within the middle clay-dominant layer at both sites. Soil types determined from the combination of density, elastic moduli and SWCC are labeled for each layer.
Figure 3.5. Water saturation, bulk density and porosity from seismic inversion at site B and laboratory tests from a well near site B. Quality of the inversion can be quantified by differences between inverted and laboratory results. Inverted water saturations are within 2% of laboratory results. In second and third layers, inverted bulk density and density are within 5% of laboratory results. In first layer, inverted bulk density and density have 15% comparing with laboratory results.

At both sites A and B, the inverted soil properties show some common trends that can be used to identify the soil types within the three different seismic layers. In both the top and bottom seismic layers, inverted soil density and elastic moduli values fall within the range for clay properties (Figure 3.3), but in addition, the relatively smaller values of the top seismic layer may indicate the presence of organic material. We note that for both sites, the water saturation (based on inverted SWCCs) shifts sharply to lower values across both the top and bottom boundary of the middle seismic layers (Figure 3.4). Laboratory data confirm a similar change to lower water saturation values at similar depths. For Site A, the inverted soil density and elastic moduli values are relatively larger
in the middle seismic layer than in the bottom layer. We interpret this to indicate that there may be additional sand within this clayey unit (Figure 3.3, a, middle layer).

Soil types indicated by the inverted cohesion values are in agreement with soil types determined from the inverted density and elasticity. Inverted cohesion values in the bottom seismic layers at both sites are close to 20 kPa and indicate that the soil type is possibly clay. Inverted cohesion values in the top seismic layers are about 50% lower than in the bottom layers and may indicate the presence of less cohesive organics. In the middle seismic layer at site A, the inverted cohesion value is close to 0 and indicates that the layer consists mainly of sand. In the middle seismic layer at site B, the inverted cohesion value is close to 20 kPa and indicates clayey soils.

3.5 Discussion

3.5.1 Validation of inversion results and interpretations

One measure of the usefulness of the inversion results for our three seismic layers is to compare them to other independent estimates of density and elastic moduli. If large differences appear between the two results, it may imply seismically unresolvable thin units. We assign known values of density and elasticity in soil (Table 3.3) to geotechnical soil behavior types determined by cone penetration testing (CPT) (Lorenzo et al., 2014) (Figure 3.2) in order to calculate an average geotechnical density and elasticity for three new equivalent layers. The vertical resolution of the CPT soil profile is ± 0.1m. Computed geotechnical soil properties will have range of values attributable to the variation of published soil properties (Table 3.3). A comparison of the inverted and computed geotechnical results of soil density and elastic moduli shows similar values and implications for soil types (Figure 3.3). The greatest difference between inverted and
geotechnical results occurs at depths equivalent to the middle layer at site B (Figure 3.3, b), where the inverted elastic moduli are almost 70% lower than those from the CPT. One explanation for this big difference is the presence of thin sand units (< 1 m) shown in the CPT soil profile (Figure 3.2, b, the middle layer). When seismic waves pass through these thin units (< 1 m at site B), the changes in soil density and elastic moduli may not be seismically resolvable. For example, a P-wave velocity of ~200-1200 m/s and a dominant frequency of 30 Hz, suggest a dominant wavelength of ~7-40 m. These thin sand units lead to a larger computed geotechnical soil property values than the inverted results derived from seismic profiles. At site A, the sand layers are sufficiently thick. Thus, the inverted soil property values are closer to the geotechnical results and inverted soil types are comparable (Figures 3.2 and 3.3). These lateral differences in sand layer thickness may also be responsible for the noticeable differences in density and elastic between the two sites (Figure 3.3).

Inverted SWCCs can help confirm heterogeneity or recognize thin units that cannot be sensed by soil density and elastic moduli alone. If the soil type changes, the water content at the same capillary head will also change (Fredlund and Xing, 1994). As the seismic velocity is most sensitive to the change in water saturation in near-saturation conditions (Bachrach and Nur, 1998), so may the SWCC inverted from seismic velocity resolve changes in average water saturation at the same capillary head and help determine soil type changes. In the middle seismic layers at both sites, the shift in the inverted SWCC to a lower value indicates the presence of sand units in the layer (Figure 3.4). If a clay layer contains sand units, the average water saturation will be lower than in a homogeneous clay layer at the same capillary head. A combination of the results of
inverted soil density, elastic moduli and SWCC suggests that middle layers at both sites may contain sand (Figure 3.4).

Inverted water saturation, bulk density and porosity appear consistent with results from laboratory tests from a well near Site B (Figure 3.5). Laboratory water content and bulk density are directly measured on soil cores from the well, and porosity is calculated from these measurements (Lorenzo et al., 2014). Trends in inverted results at site B match laboratory results throughout the well. Most of the inverted soil property values are within the error range of laboratory results. As velocity is more sensitive to the change in water saturation than other soil properties, inverted water saturation has the smallest error (± 0.1%) compared to errors in other inverted soil properties (which vary from ± 1% to ± 20%) (Figures 3.3, 3.4 and 3.5). In both inverted and laboratory results, water saturation shifts to lower values from the first layer to second layer, and shifts to higher values from the second to third layer. As previously mentioned, the shift in water saturation can help to detect seismically unresolvable thin layers. In the first organic clay layer, inverted and laboratory-based bulk density and porosity show the largest differences. One explanation of these differences is that the inverted soil properties represent average values over the seismic survey area (which covers ~100 m) and may not represent properties at the specific well location. In organic clay, soil properties may have a larger lateral variation because of the difference in organic content.

3.5.2 Comparison of inversion quality between different seismic layers

Within each seismic layer, corresponding soil behavior types (from CPT data) may vary and so not meet the homogeneity assumption of the velocity prediction model. The quality of inversion is best (with a small misfit of 2%) within the deepest layer
(Figure 3.2). The difference between inverted and geotechnical soil properties are also smallest within the deepest layers (Figure 3.3). For the top and middle seismic layers, the soil behavior types are a mixture of clay and organic content or sand. Only for the bottom seismic layer, is the soil type homogeneous clay. One of the assumptions of the Hertz-Mindlin and Biot-Gassmann is that the porous medium is homogenous (Wang, 2001). Thus, the inversion works best in the relatively homogeneous clay-rich layer in our three-layer seismic model.

Inversion results near the top of the first layer, corresponding to the very near surface soils (< 5m), unexpectedly predict a velocity that is higher than seen in the field velocity profile (Figure 3.2). An interesting possibility is that seismic velocity calculations overestimate the true saturation, which may be lowered by evaporation across the soil surface. In our velocity prediction model, water saturation is determined from the SWCC, which does not account for evaporation effects. As a result, the predicted water saturation from SWCC is greater than in the true field conditions, and the calculated P-wave velocity is larger than the actual field velocity.

There is flexibility with the application of our suggested workflow in future studies. Herein our attempt at soil property inversion begins with a general velocity prediction model but without any empirical relationship to either simplify the inversion process or reduce possible errors such as those arising from using the wrong empirical relationship for a certain field setting. Ideally, the incorporation of other empirical relationships, such as porosity vs. coordination number and porosity vs. depth, requires a good prior knowledge of the geological setting, which often is not the case. The influence of grain size distribution could also be taken into account because in the inversion results,
a poor sorting leads to a decrease in porosity and an increase in the coordination number. In this study, we use geological data from geotechnical and laboratory tests to validate our inversion results. Thus, for the inversion, we only use field velocity profiles without the support of extensive geological data. In other known geological settings, empirical relationships could be incorporated into the velocity prediction model to achieve a better inversion result. For example, the unexpected increase of porosity with depth observed using laboratory results (Figure 3.5) could be incorporated into the future work to improve inversion results. With the suggested workflow in this paper, other more complex velocity prediction models (such as those which include the effect of patchy saturation) could also be used to invert for additional soil-property and water-saturation information.

Although geotechnical borehole tests (± 0.1 cm in our case) may have higher vertical resolution than seismic-derived inverted results (> 1 m), seismic surveys advantageously provide continuous lateral seismic soil property values that may complement geotechnical borehole tests for less cost. Between geotechnical test sites, the inverted soil property results can highlight anomalies in the lateral changes of density, elasticity and water saturation (Figures 3.3 and 3.4). Based on the magnitude and the location of these anomalies, additional geotechnical tests can be proposed and sited efficiently. Another advantage is that soil property inversion employs seismic data, which sample in-situ lateral variations of pressure, saturation and organic content, if any are present. The inversion results can reflect these lateral variations in soil properties between geotechnical boreholes. Currently, seismic soil property inversion for water saturation is most sensitive if applied in near-fully-saturated conditions where the field P-
wave velocity can increase by over one order of magnitude with only a 1% change in the saturation, and is also most likely to detect lithological changes. Inverted soil stratigraphy of this type can improve with the improved resolution of seismic velocity field profiles.

3.6 Conclusions

In shallow (< 25 m) near-saturated soil (saturation > 99%), we invert for seismic soil properties by minimizing the misfit between field-based velocity profiles and predicted velocity profiles based on Hertz-Mindlin and Biot-Gassmann theories. CMA-ES optimizes the inversion results by searching for optimal input soil property values that can best explain field velocity profiles.

The inverted density and elastic moduli can be used to interpret major soil types and can detect variations in sand thickness between two field sites. By comparing inversion results to geotechnical results, the inverted soil properties appear valid in general except for one layer which probably contains seismically unresolvable sandy units.

The inverted SWCC can help recognize thin sand units that are below the original seismic resolution of the field data. Laboratory results validate the inversion results, as well as indicate that the results can be improved with a good prior empirical relationship between porosity and depth. The SWCC shifts to a lower value when the thin unresolvable layers are sandier than the clay-dominated soil. In combination, the inverted density, elastic moduli and SWCC correspond to soil types that are in agreement with soil types derived from geotechnical data (CPT).
For our three-layer seismic model at our two field sites, the inversion works best in the relatively homogeneous clay-rich bottom layer. Soil within this layer meets the assumption of homogeneity in Hertz-Mindlin and Biot-Gassmann theories.

Seismic surveys can provide continuous lateral seismic soil property values that may complement geotechnical borehole tests at lower cost. Inversion results can highlight anomalies in lateral changes of density, elasticity and water saturation in order to suggest additional geotechnical tests.

Although we use a general velocity model without any empirical relationship in the current workflow, there is flexibility to apply our suggested workflow in future studies. With a known geological setting, empirical relationships could be incorporated to improve the inversion results. Other velocity prediction models could also be used for the inversion of additional information on soils.

3.7 References


CHAPTER 4: SEISMIC VELOCITY INVERSION FOR PATCHY AND HOMOGENEOUS FLUID-DISTRIBUTION PATTERNS IN SHALLOW (< 1 M DEPTH), UNCONSOLIDATED SANDS

4.1 Summary

Knowledge of homogeneous and heterogeneous fluid-distribution patterns is important for the estimation of oil reserves, reservoir simulation, the interpretation of time-lapse seismic, and the selection of remediation techniques for groundwater contamination. However, problems exist in determining in-situ fluid-distribution patterns in unconsolidated sediments because laboratory tests on core samples may not be representative for in-situ conditions. In this study, we propose a seismic inversion method to determine in-situ fluid-distribution patterns that involves inverting experimental seismic P- and S-wave velocities using Hertz-Mindlin and Biot-Gassmann model with different averaging methods (Wood and Hill averages) and different saturation-related assumptions. This method can determine whether seismic velocity-versus-depth profiles are better explained assuming heterogeneous or homogeneous saturation patterns in shallow (< 1 m depth) unconsolidated sands.

During the imbibition and drainage of shallow unconsolidated sands, we observe a non-monotonic P-wave velocity-vs.-water saturation (or water level) relationship that is in consistent with other field and laboratory observations. This relationship can be explained by transitions between the lower Wood bound and the higher Hill bound, possibly caused by the alternation in the size of fluid patches between small and large during the wetting and drainage. Inverted results can be verified by a good correlation (difference <7%) between inverted and measured water saturation using moisture sensors.
4.2 Introduction

Partially-saturated unconsolidated sediments potentially contain a mixture of two or more fluids that can be distributed either homogenously or heterogeneously (in patches). However, the commonly applied laboratory ultra-sonic core tests for identifying fluid distributions are costly and may not represent in-situ conditions because of the disturbance of unconsolidated samples during core transportation, and the scaling issues with translating between ultra-high frequencies commonly used in laboratory studies and lower frequencies used in the field (Cadoret et al., 1995; Toms-Stewart et al., 2009). Moreover, there is a lack of understanding of the alternation of P-wave velocity ($V_P$) between decreasing and increasing trends when water level (WL) increases or decreases (namely non-monotonic $V_P$-WL relationship later in this paper) in either field tidal water-level change experiments (Bachrach and Nur, 1998) or laboratory water-level change experiments (Lorenzo et al., 2013; Velea et al., 2000). The fluid-distribution pattern influences seismic velocity, which affects the estimates of oil reserves, reservoir simulations (Dupuy and Stovas, 2014), and interpretation of time-lapse seismic during the monitoring of oil production (Calvert, 2005). Additionally, determining the saturation pattern can help select an adequate remediation technique for groundwater contamination based on whether the contaminants occur in patches or homogeneously (Dvorkin and Nur, 1998).

In this study, we propose a seismic inversion workflow to determine in-situ fluid-distribution patterns, by minimizing the difference between experimental and predicted velocity-versus-depth profiles. The predicted velocity-versus-depth profiles are calculated from rock physics models with assumptions of either heterogeneous or homogeneous
saturation patterns. For the inversion, we acquire the following experimental data: P- and S-wave velocity-versus-depth profiles from seismic survey and water saturation-versus-depth profiles from electrical measurements. The inversion results indicate that the non-monotonic $V_p$-WL relationship is attributable to the variation in fluid distribution patterns, and $V_p$ changes can be interpreted with transitions between the Hertz-Mindlin-Biot-Gassmann-Wood (HM-BG-Wood) bound and the Hertz-Mindlin-Biot-Gassmann-Hill (HM-BG-Hill) bound with the change in the size of patches.

The concept of homogeneous or heterogeneous (patchy) fluid-distribution pattern can be defined with the soil-water characteristic curve (SWCC) (Dvorkin and Nur, 1998), which shows the relationship between saturation and capillary head (or capillary pressure) (Van Genuchten, 1980):

$$S_e = \left[ \frac{1}{1 + [ah_c]^n} \right]^m$$

where $S_e$ is effective water saturation, $h_c$ is capillary head, and $a$, $n$, $m$ are empirical fitting parameters corresponding to various sediment properties. If the fluid-distribution pattern is homogeneous, the fluid is evenly distributed in the pore space and water saturation is constant within the sediment volume for a given capillary head. In contrast, if the fluid-distribution pattern is heterogeneous, the saturation within the patches (the relatively smaller zones) is higher or lower than the saturation within the surrounding area at a fixed capillary head (Dvorkin and Nur, 1998). The soil water characteristic curve within the patches is different than the curve within the adjacent area, depending on the heterogeneity in the sediment properties, such as porosity and permeability (Knight et al., 1998), interfacial tension, and wettability conditions (Riaz et al., 2007).
The most influential forces governing two-phase fluid flow during forced imbibition and gravity drainage are capillary, gravitational and viscous forces (Løvoll et al., 2005; Riaz et al., 2007). Viscous forces are negligible in an air-water system (Lopes et al., 2014), where the viscosities of the wetting (water) and non-wetting (air) fluids are very different. In an air-water system, the relative importance of gravitational and capillary forces determines the saturation characteristics. Gravitational forces pull water downward, while capillary forces drag and hold water in the pore spaces. Capillary forces decrease as water saturation increases, and vice versa. At low saturation, for example, at the beginning of imbibition, the capillary pressure is highest and creates capillary fingers that arise ahead of the water table. During imbibition, capillary pressure helps with the redistribution of water from large pores to surrounding small pores (Lopes et al., 2014). During gravitational drainage, initially, gravitational forces dominate until water drains to a low enough level that capillary pressure increases to reach equilibrium with gravitational forces, and drainage stops (DiCarlo, 2003).

Velocity prediction models that are applied in our inversion (Shen et al., 2015) are based on the commonly accepted Hertz-Mindlin (Hertz, 1882; Mindlin, 1949) and Biot-Gassmann (Biot, 1962; Gassmann, 1951) (HM-BG) theories, but with different averaging methods depending on patch size. When the patch size is small compared to the diffusion length, an average fluid bulk modulus can be given by the Wood (1941) average which uses a weighted harmonic mean of the bulk modulus of each pore fluid. The diffusion length mainly relates to rock permeability, fluid viscosity, and wave frequency \( \lambda = \sqrt{D/\omega} \), where \( \lambda \) is the diffusion length, \( \omega \) is the angular wave frequency, \( D = \kappa K_p/\eta \) is diffusivity, \( \kappa \) is permeability, \( \eta \) is fluid viscosity, and \( K_p \) is the poreelastic
modulus) (Norris, 1993). Applying the average fluid bulk modulus from the Wood average with the HM-BG theories, the HM-BG-Wood model is valid to determine the lower bound of seismic velocity (Müller et al., 2010). In contrast, if the patch size is much larger than the diffusion length, the average effective elasticity can be determined with the Hill (1963) average by using a weighted harmonic mean of the effective bulk and shear moduli of each patch (Müller et al., 2010). Applying the average effective elasticity from the Hill average with the HM-BG theories, the HM-BG-Hill model predicts the upper bound of seismic velocity. The HM-BG-Wood and -Hill bounds describe seismic velocity in the softest and the stiffest material, respectively (Mavko et al., 2009).

The observed seismic velocity and water saturation ($V_p-S_w$) relationships vary between different laboratory imbibition and drainage tests of limestone and sandstone core samples (Cadoret et al., 1995; Cadoret et al., 1998; Knight et al., 1998; Knight and Nolen-Hoeksema, 1990; Lebedev et al., 2009; Monsen and Johnstad, 2005; Murphy, 1982). The different observations are attributed to the differences in sediment heterogeneity and experiment setup (e.g., seismic frequency, injection rate, and the density and viscosity of pore fluids) (Homsy, 1987). Some observations show that the experimental $V_p-S_w$ relationship can be explained by the lower velocity bound from the HM-BG-Wood model during wetting, and the upper velocity bound from the HM-BG-Hill model during drainage (Cadoret et al., 1995; Knight and Nolen-Hoeksema, 1990; Monsen and Johnstad, 2005; Murphy, 1982). However, other experiments show a non-monotonic $V_p-S_w$ relationship that can be explained by the transitions between the HM-BG-Wood and the HM-BG-Hill bounds, depending on the change in patch size.
(Lebedev et al., 2009) and seismic frequency (Cadoret et al., 1995). During injection of water into a sandstone sample, Lebedev et al. (2009) observes that $V_p$ decreases slightly and follows the HM-BG-Wood bound at low water saturations. When water saturation exceeds 40%, $V_p$ sharply increases and can be interpreted by a transition from the HM-BG-Wood to HM-BG-Hill bound. Their results from X-ray computer tomography show that the interpreted transition from the HM-BG-Wood to HM-BG-Hill bound corresponds to the clustering of small fluid patches and the formation of larger patches.

4.2.1 The Hertz-Mindlin and Biot-Gassmann theories

In the HM-BG model, P-wave ($V_p$) and S-wave velocity ($V_s$) are calculated from the effective bulk modulus, shear modulus and density (Mavko et al., 2009):

\[ V_p = \sqrt{\frac{K_{eff} + \frac{4}{3}G_{eff}}{\rho_{eff}}} \]  \hspace{1cm} (4.2)

\[ V_s = \sqrt{\frac{G_{eff}}{\rho_{eff}}} \]  \hspace{1cm} (4.3)

where $K_{eff}$ and $G_{eff}$ are the effective bulk and shear moduli, respectively, and $\rho_{eff}$ is the effective density of the sand matrix with pore fluids.

Biot-Gassmann fluid substitution theory estimates effective bulk and shear moduli (equations 4.2 and 4.3) of the sand matrix and accounts for pore fluids (Mavko et al., 2009):

\[ K_{eff} = \frac{K_0 \left( \frac{K_m}{K_0 - K_m} + \frac{K_{fl}}{\phi (K_0 - K_{fl})} \right)}{1 + \frac{K_m}{K_0 - K_m} \cdot \frac{K_{fl}}{\phi (K_0 - K_{fl})}} \]  \hspace{1cm} (4.4)
\[ G_{eff} = G_m \]  

(4.5)

where \( K_0 \) is the bulk modulus of the sand grains, \( K_m \) is the bulk modulus of the “dry” sand matrix, \( G_m \) is the shear modulus of the “dry” sand matrix, and \( K_f \) is the bulk modulus of the pore fluids.

The matrix elastic moduli (equations 4.4 and 4.5) can be estimated using Hertz-Mindlin contact theory by assuming the sand grains are a pack of identical spheres (Mavko et al., 2009):

\[
K_m = \frac{3C^2(1 - \phi)^2G_0^2}{18\pi^2(1 - \nu)^2P_{eff}} 
\]

(4.6)

\[
G_m = \frac{5 - 4\nu}{5(2 - \nu)} \frac{3C^2(1 - \phi)^2G_0^2}{2\pi^2(1 - \nu)^2P_{eff}} 
\]

(4.7)

where \( C \) is grain coordination number, \( G_0 \) is the shear modulus of soil grains, \( \nu \) is the Poisson’s ratio of the soil grains, \( P_{eff} \) is the effective stress. To accurately predict velocity in shallow unconsolidated sediments, we incorporate the net overburden pressure \((\sigma - u_a)\), matric suction \((u_a - u_w)\), and cohesion \((\sigma_{co})\) in the estimation of effective stress \((P_{eff})\) (equation 4.11) (Lu and Likos, 2006):

\[
P_{eff} = \sigma - u_a - S_e(u_a - u_w) + \sigma_{co} 
\]

(4.8)

where \( \sigma \) is the overburden pressure and equals \( \rho_{eff}gh \) (\( \rho_{eff} \) is effective density of soil with pore fluids, \( g \) is the gravitational acceleration, and \( h \) is the depth of soil); \( u_a \) is atmospheric pressure; \( \sigma_{co} \) is the cohesion and can be up to 300 kPa in sand; \( S_e(u_a - u_w) \) is the matric suction contribution weighted by the effective water saturation \( S_e \) (Song et al., 2012). At equilibrium, matric suction \((u_a - u_w)\) equals the weight of the water column.
4.2.2 The Wood and Hill averages

The Wood (1941) average estimates the average bulk modulus of pore fluids ($K_{fl}$, in equation 4.4) using a weighted harmonic mean of the bulk modulus of each pore fluid (Mavko et al., 2009):

$$K_{fl} = \left( \sum_i \frac{f_i}{K_{fl_i}} \right)^{-1} \quad (4.9)$$

where $f_i$ is the volumetric fraction of the individual fluid and $K_{fl_i}$ is the individual fluid’s bulk modulus. To apply the Wood average for a scenario where the pore fluids are water and air, we assume two different water saturations exist, one in the patches ($S_{w1}$) and another in the surrounding area ($S_{w2}$). The average fluid bulk modulus with patchy saturation ($K_{fl}$, in equation 4.4) becomes:

$$\frac{1}{K_{fl}} = \frac{S_{w1}f_1}{K_w} + \frac{(1 - S_{w1})f_1}{K_a} + \frac{S_{w2}(1 - f_1)}{K_w} + \frac{(1 - S_{w2})(1 - f_1)}{K_a} \quad (4.10)$$

where $f_i$ is the volumetric fraction of the pore space in patches with water saturation $S_{w1}$, and $(1 - f_i)$ is the volumetric fraction of the pore space in adjacent areas with water saturation $S_{w2}$, $K_w$ and $K_a$ are the bulk modulus of water and air, respectively. In open shallow sediments, residual air and water may be trapped in small pore spaces and so the water saturation cannot reach either 0 or 100%.

In a special condition where there is one water saturation value for a given capillary pressure, the Wood average can be simplified to the commonly used averaging method in the Gassmann theory (Gassmann, 1951). In this case, the volumetric fraction (in equation 4.10) of patches is 0 or 100%. Then, the HM-BG model describes a
homogeneous saturation pattern. In the Gassmann model, the average fluid bulk modulus ($K_{fl}$, in equation 4.4) is simplified to (Mavko et al., 2009):

$$\frac{1}{K_{fl}} = \frac{S_w}{K_w} + \frac{(1 - S_w)}{K_a}$$

(4.11)

where $S_w$ is the water saturation at a fixed capillary pressure. In this case, the HM-BG-Wood model is simplified to the commonly used HM-BG model (Mavko et al., 2009).

The Hill (1963) average determines the average effective bulk and shear moduli ($K_{eff}$ and $G_{eff}$, in equations 4.2 and 4.3) by using a weighted harmonic mean of the effective bulk and shear moduli of each patch:

$$\frac{1}{K_{eff} + \frac{4}{3} G_{eff}} = \sum_i f_i \frac{1}{K_{eff_i} + \frac{4}{3} G_{eff_i}}$$

(4.12)

where $f_i$ is the volumetric fraction of each patch, and $K_{eff}$ and $G_{eff}$ are the bulk and shear moduli of the sand matrix with pore fluids in each patch, respectively. In each patch, water is homogeneously distributed. If we assume there are two different water saturations ($S_{w_1}$ and $S_{w_2}$) in patches and surrounding area, then equation 4.12 becomes:

$$\frac{1}{K_{eff} + \frac{4}{3} G_{eff}} = \frac{f_1}{K_{eff_1} + \frac{4}{3} G_{eff_1}} + \frac{(1 - f_1)}{K_{eff_2} + \frac{4}{3} G_{eff_2}}$$

(4.13)

where $f_i$ is the volumetric fraction of patches with water saturation $S_{w_1}$, $(1 - f_i)$ is the volumetric fraction of the adjacent area with water saturation $S_{w_2}$, $K_{eff_1}$ and $K_{eff_2}$ are the effective bulk moduli of the sand matrix with pore fluids in patches and in adjacent areas, respectively, and $G_{eff_1}$ and $G_{eff_2}$ are the effective bulk moduli of the sand matrix with pore fluid in patches and in adjacent areas, respectively.
4.3 Seismic Acquisition and Inversion

To test our seismic inversion method for fluid distribution patterns, we conduct a seismic survey during imbibition and drainage experiments in a \( \sim 6 \times 9 \times 0.6 \) m sand-filled tank (Figure 4.1, Appendix C). We collect P- and S-wave pseudo-walkaway seismic data during wetting at 6 different water levels (WL1-6, from 0 to 0.46 m), during draining at 5 different water levels (WL7-11, from 0.46 to 0.02 m), and for a reference test (WL0) in air-dry sand with residual water saturation. Each time we change the water level, we wait between 2 and 4 hours for the water to reach equilibrium in 5 monitoring wells (Figure 4.1, a, measured by water level sensors).

![Figure 4.1. Experiment equipment layout of accelerometers (triangles), shot locations (stars), moisture sensors (rhombus or half rhombus). All units are in cm. (a) Sand tank contains 5 monitoring wells (circles). The body of sand in the tank is 55 cm thick. The dashed rectangle (inset) is shown in Figure 1, b. (b) In the seismic acquisition system, there are 48 accelerometers (triangles), buried in two rows at 3 cm below the top of the sand. Half of the accelerometers are buried vertically in one row and their corresponding vibration source (stars) sits vertically. The other half of the accelerometers are buried horizontally in another row and their corresponding vibration source (stars) is buried horizontally. The accelerometers are placed 1.5 cm apart (center to center) for a total array length of 34.5±0.2 cm. There are a total of 6 shots for each pseudo-walkaway survey. The first shot offset is 3 cm (center to center) and each subsequent shot location is moved 36 cm. The total survey length is 217.5±2 cm. The location errors are estimated at 1%-5% of numbers shown.]
A previous wetting experiment was conducted in the same sand tank with a similar acquisition system, but the sand had at least two layers (Lorenzo et al., 2013). Since the previous experiment, we attempted to homogenize the grains using shovels with a blade size of ~0.15×0.2 m. Now, sand sieve analysis indicates that there is ~5% difference in grain size distribution parameters, such as mean, sorting, skewness, and kurtosis among 10 samples we collect from various locations and depths (Table 4.1, Appendix F). These grain size variations indicate the heterogeneity in sands (Appendices E and G) and possibly lead to the heterogeneity in saturation pattern during the wetting and draining.

Table 4.1. Statistical parameters of grain size (Folk and Ward, 1957) by sand sieve analysis for 10 samples from various locations and depths in sand tank after “homogenization”. The grain size parameters show variations in mean, sorting, skewness and kurtosis.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Mean (mm)</th>
<th>Mean (phi)</th>
<th>Sorting</th>
<th>Skewness</th>
<th>Kurtosis</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.3393039</td>
<td>1.55935</td>
<td>0.50271</td>
<td>-0.05406</td>
<td>1.00922</td>
</tr>
<tr>
<td>2</td>
<td>0.3338287</td>
<td>1.58282</td>
<td>0.49264</td>
<td>-0.04258</td>
<td>1.04724</td>
</tr>
<tr>
<td>3</td>
<td>0.3422802</td>
<td>1.54675</td>
<td>0.52116</td>
<td>-0.063</td>
<td>1.02432</td>
</tr>
<tr>
<td>4</td>
<td>0.3473495</td>
<td>1.52554</td>
<td>0.497</td>
<td>-0.02641</td>
<td>0.97075</td>
</tr>
<tr>
<td>5</td>
<td>0.3571915</td>
<td>1.48523</td>
<td>0.54523</td>
<td>-0.14979</td>
<td>1.01593</td>
</tr>
<tr>
<td>6</td>
<td>0.3456107</td>
<td>1.53278</td>
<td>0.50482</td>
<td>-0.04576</td>
<td>0.99724</td>
</tr>
<tr>
<td>7</td>
<td>0.3372943</td>
<td>1.56792</td>
<td>0.49256</td>
<td>-0.04177</td>
<td>1.02035</td>
</tr>
<tr>
<td>8</td>
<td>0.3412048</td>
<td>1.55129</td>
<td>0.49328</td>
<td>-0.03972</td>
<td>1.00075</td>
</tr>
<tr>
<td>9</td>
<td>0.3403544</td>
<td>1.55489</td>
<td>0.4877</td>
<td>-0.04146</td>
<td>0.98799</td>
</tr>
<tr>
<td>10</td>
<td>0.3447350</td>
<td>1.53644</td>
<td>0.48772</td>
<td>-0.03827</td>
<td>0.98525</td>
</tr>
</tbody>
</table>

The seismic acquisition system uses an ultra-high frequency (up to 20 kHz) magnetostrictive vibrator and 48 single-component accelerometers (Table 4.2). The seismic wavelength is ~4 cm (with a velocity of order 10^2 m/s and a dominate frequency of ~2.5 kHz). At each water level, we collect six shot gathers with a total survey width of 2.17 m (Figure 4.1). The vibration source is oriented both vertically and horizontally.
Twenty-four accelerometers are buried (3 cm depth) in one row and oriented with the most sensitive axis parallel to source vibration direction. Another 24 accelerometers are buried (also at 3 cm) in another row and oriented with the most sensitive axis orthogonally to the source so they can capture SH-waves (Figure 4.1, b).

Table 4.2. Descriptions for the seismic, moisture and water level acquisition equipment used in our experiments. More details for the seismic acquisition system are described in Lorenzo et al. (2013).

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accelerometer</td>
<td>48 piezo-electric accelerometers (ACH01 from Measurement Specialties Inc.); linear response in 2 to 20 kHz range with a sensitivity of ~9 ±1 mV/g.</td>
</tr>
<tr>
<td>Vibration source</td>
<td>Magnetostrictive ultrasonic transducer (Model CU-18 from Etrema Products Inc.); the source wavelet is a Ricker wavelet with a vibration frequency up to 20 kHz and a central frequency at 10 kHz.</td>
</tr>
<tr>
<td>Moisture sensor</td>
<td>Five capacitance/frequency domain sensors (EC-5 from Decagon Devices Inc.); the maximum measurement volume is 240 ml for a cylindrical volume with a radius of ~3 cm and a height of ~10 cm; the accuracy is ±2%; the resolution is 0.001 m³/m³; the measurement range is from 0 to saturation; the operating temperature is -40 to 60 °C.</td>
</tr>
<tr>
<td>Water level sensor</td>
<td>Five submersible pressure transducers (WL400 from Global Water Instrumentation Inc.); the accuracy is ±0.1%; the operating temperature is -40 to 85 °C.</td>
</tr>
</tbody>
</table>

To determine one dimensional $V_P$ and $V_S$-versus-depth profiles, we forward ray trace (Cerveny, 2001) the travel times of refracted and reflected first arrivals of P- and S-waves (Figure 4.2). The error in velocity is less than ±2% (from ±$10^{-4}$ s error in travel time). We extract $V_P$ and $V_S$ at the depths of 0.1 and 0.37 m (Figure 4.3) from $V_P$- and $V_S$-versus-depth profiles (Figure 4.2) to show velocity changes with various water levels (velocity-WL relationship) at a given depth. These depths are chosen to represent the central portion of two zones with distinct velocity gradients (Figure 4.2).
Figure 4.2. Representative seismic data sets and interpreted $V_p$-versus-depth profiles at different water levels: (a) WL2, (b) WL4, and (c) WL6, out of 12 total. On left, variable-area plots display seismic amplitudes interpolated among shades of gray with positive seismic amplitudes in black and negative amplitudes in white. Amplitudes are rebalanced through division by the root-mean-square average at each recorded accelerometer with a window width of 0.002 s. Band-pass frequency filtering between 200 and 5000 Hz is applied to suppress noise. Synthetic seismic events, forward-modeled using the first arrivals of refracted and reflected rays (dashed lines) are drawn over seismic panels. $V_p$-versus-depth profiles used to calculate distance-traveltime locations for seismic rays are shown highlighted with solid black lines to the right of each data set. Key seismic arrivals in data are labeled near calculated synthetic events. Reflected synthetic events are convex-downward and refracted synthetic events have a straight or slightly convex-upward shape. Faint, early linear arrival is interpreted as air-blast. Rayleigh waves have a larger slope than refracted and reflected waves. The mismatch in traveltime ($\sim 10^{-4}$ s) leads to a +/-2% error in velocity.
Figure 4.3. $V_P$ and $V_S$-water level (WL) relationships during wetting and draining. (a) $V_P$ values in the sand tank (this paper) come from two different depths of 0.1 m (indicated by differently shaded triangles) and 0.37 m (shown by differently shaded circles). Also shown for comparison are $V_P$ values (as rhombi) from a sandy beach study (Bachrach and Nur, 1998) and $V_P$ values from a laboratory test in Ottawa Sand (as crosses) (Velea et al., 2000). (b) $V_S$ values in the sand tank (this paper) come from two different depths of 0.1 m (as solid black triangles) and 0.37 m (as solid black circles). The top horizontal water level axis shows water depths measured from the top of the sand (Bachrach and Nur, 1998), whereas the bottom axis shows water level height measured from the bottom of the sand in the sand tank (this paper). In the sand tank experiment (this paper), during wetting, the water level increases up to 0.46 m in 6 stages (WL1 to WL6, labeled as “1-6”). During draining, the water level decreases to 0.02 m in 5 stages (WL7 to WL11, labeled as “7-11”). The water level height for the dry reference test is labeled as “0”. Based on the magnitude of $V_P$, velocities can be grouped in to four cases: WL1-WL3 (solid grey circles and triangles), WL4, WL5 (grey circles and triangles with black outline), WL6 (hollow circles and triangles) and WL7-WL11, WL0 (solid black circles and triangles). Within each case, $V_P$ values differ less than ±3% from each other.
To determine fluid-distribution patterns, we assume the saturation distribution pattern is either homogeneous or heterogeneous, and then use rock physics models with different fluid distribution assumptions to best match experimental $V_p$ and $V_S$-versus-depth profiles (Appendix A). The inversion results include the SWCC within the patches and within the surrounding area, as well as the volumetric fraction of the patchiness. We minimize the misfit between experimental and predicted $V_p$ and $V_S$-versus-depth profiles for each water level, aided by the Covariance Matrix Adaptation Evolution Strategy optimization (Shen et al., 2015). The best fit for the experimental data relies on the lowest RMS misfit to arrive at the preferable inversion result. Velocity prediction models are based on the HM-BG model, but have three different averaging methods depending on their respective fluid distribution assumptions: (1) HM-BG for homogeneous saturation (average using equation 4.11), (2) HM-BG-Wood for small-sized patchy saturation (average using equation 4.10), and (3) HM-BG-Hill for large-sized patchy saturation (average using equation 4.13).

To compare with the inverted saturation results from seismic velocity and verify the quality of the inversion, we also measure volumetric water content during experiments with five moisture sensors buried horizontally in the sand at different depths (0.1 m, 0.19 m, 0.28 m, 0.37 m, and 0.46 m). These capacitance/frequency domain sensors detect the volumetric water content by measuring the dielectric constant of the sand (Table 4.2). The readings from moisture sensors are collected for 90 seconds (at the rate of 1 sample/sec) each time after the water level reaches equilibrium and before seismic acquisition. We self-calibrate the sensors by determining a linear relationship between the sensor’s voltage readings and volumetric water content measured from
gravimetric sampling methods using oven-drying (Czarnomski et al., 2005; Dane and Topp, 2002) for both air-dry and wet sands in the sand tank (Appendix D). The volumetric water content for each water level is calculated with the self-calibrated linear relationship from the average voltage of the 90-second voltage readings.

4.4 Results

$V_p$-WL relationships are non-monotonic in both the shallow (represented by the depth at 0.1 m) and deep (represented by the depth at 0.37 m) sand (Figure 4.3, a). No general trend can be observed throughout the imbibition or drainage and no trend is available for more than 4 water levels. During imbibition, $V_p$ values oscillate from peak to trough twice. The peaks of the $V_p$ value occur in air-dry sand (WL0) and WL4. $V_p$ reaches the lowest value at the highest water level (WL6). During drainage, the $V_p$-WL relationship has a transition between increasing and decreasing trends, and the peak of $V_p$ value occur at WL9 (Figure 4.3, a).

In contrast to the non-monotonic $V_p$-WL relationship, the $V_s$-WL relationship is monotonic during the wetting and drainage of the sand (Figure 4.3, b). $V_s$ values decrease throughout the wetting (WL1-6) and increase throughout the drainage (WL7-11).

Based on the similarity of inversion results and the $V_p$-versus-depth profiles among 12 water levels (WL0 to WL11), we distinguish 4 representative cases for 4 different groups to summarize the results. $V_p$-versus-depth profiles and inversion results differ by less than 7% in different cases.

Case 1: during the earliest stage of wetting (WL1-3, represented by WL2), velocity-versus-depth profiles are best fit by the HM-BG-Wood model (Figures 4.4, a and 4.3, a). Case 2: during the middle stage of wetting (WL4 and WL5, represented by WL4),
velocity-versus-depth profiles are best fit by the HM-BG-Hill model (Figures 4.4, b and 4.3, a). Case 3: when water level is the highest (WL6), velocity-versus-depth profiles are best fit by both the HM-BG-Wood and the HM-BG models (Figures 4.4, c and 4.3, a). Case 4: during draining (WL7-11, WL0, represented by WL10), velocity-versus-depth profiles are best fit by the HM-BG-Hill model (Figures 4.4, d and 4.3, a).

Figure 4.4. A comparison between representative experimental $V_p$-versus-depth profiles (in solid black lines) and inverted $V_p$-versus-depth profiles using the HM-BG (in solid grey lines), the HM-BG-Hill (grey dashed lines) and the HM-BG-Wood (grey dotted lines) models for (a) WL2, which is representative of inversion results for WL1-3 and is best fit by the HM-BG-Wood model, (b) WL4, which is representative of inversion results for WL0, 4 and 5, and is best fit by the HM-BG-Hill model, (c) WL6, which is best fit by both the HM-BG and HM-BG-Wood models, and (d) WL10, which is representative of inversion results for WL7-11 and is best fit by the HM-BG-Hill model.
The measurement of quality for the inversion results can be shown by the good correlation between inverted water saturation with measured in-situ water saturation. The inverted water saturation agrees with the measured water saturation with a difference less than 7% for all water levels (Figure 4.5). The error is ±2% in measured water saturation (from instrument error). The inverted water saturation has an error of ±10%, which is determined using a Monte-Carlo method after 100 inversion attempts (Shen et al., 2015). The difference between inverted and measured water saturation is within the error of inverted water saturation.

Figure 4.5. A comparison of representative water saturation-depth profiles from inversion (hollow circles) and measurements by moisture sensors (black solid circles) at different water levels: (a) WL2, (b) WL4, (c) WL6, and (d) WL10. The error in the inverted water saturation is ±10% and in the measured water saturation is ±2%.
4.5 Discussion

Although our experiment is conducted once, similar observed non-monotonic $V_P$-WL relationships have been described in other laboratories (Lorenzo et al., 2013; Velea et al., 2000) and field tidal experiments (Bachrach and Nur, 1998). Consistent with the observations made by Bachrach and Nur (1998) and Velea et al. (2000) (Figure 4.3, a), there are two oscillations in $V_P$ values during imbibition and the $V_P$ value is the lowest at the highest water level. During drainage, the transition from an increasing to a decreasing trend in our $V_P$-WL relationship is in agreement with the observation made by Velea et al. (2000) (Figure 4.3, a). However, Bachrach and Nur (1998) only observe an increasing trend during the drainage (Figure 4.3, a). One possible explanation for this difference is that the time durations of the two drainage processes are different: the drainage in our experiment lasts for ~15 hours, while in Bachrach and Nur (1998)’s it lasts ~2 hours. As a result, their experiment may not have captured the decreasing trend in $V_P$-WL relationship during the drainage.

The assumptions behind each rock-physics model can be used to interpret the fluid-distribution pattern at water levels. When the HM-BG-Wood model best describes the velocity-versus-depth profiles (WL1-3, Figures 4.4 and 4.6), it suggests that the patch sizes are small in comparison to the diffusion length (~1 cm in our unconsolidated sands) at the beginning of the wetting. However, when the HM-BG-Hill model provides a better fit to the velocity-versus-depth profile, we can interpret that the size of the patches is larger than the diffusion length (> 1 cm) (WL0, 4, 5, 7-11, Figures 4.4 and 4.6). In the air-dry sand (WL0), the matric suction contribution weighted by water saturation (equation 4.8) is minimum and so the effective pressure in highest. The high effective
pressure may also lead to the relatively high $V_p$ value. At WL6 (highest), the best fit by both HM-BG and HM-BG-Wood models indicates that the saturation pattern is homogeneous (Figures 4.4 and 4.6). For WL6, the inversion results from HM-BG-Wood show that no patches exist.

Figure 4.6. $V_p$-$S_w$ relationships during wetting. (a) $V_p$ values (as hollow circles) come from the sand tank at the depth of 0.1 m (this paper). Also shown for comparison are $V_p$ values (as crosses) come from observations in sandstone core samples (Lebedev et al., 2009). The vertical axis for $V_p$ in the sand tank (this paper) is on the left, whereas for the sandstone core (Lebedev et al., 2009) is on the right. Theoretical HM-BG-Hill and HM-BG-Wood bounds for unconsolidated sands in this paper are shown by gray and black solid lines, respectively. Theoretical HM-BG-Hill and HM-BG-Wood bounds for sandstone (Lebedev et al., 2009) are shown by gray and black dashed lines, respectively. (b) $V_p$ values (as hollow circles) come from the sand tank at the depth of 0.37 m (this paper). Average water saturation for each $V_p$ value in the sand tank is calculated using arithmetic average of the water saturation at each depth. The numbers from 0 to 6 indicate different water levels from WL0 to WL6 in the sand tank experiments.
We can interpret that the transition in $V_p$-$S_w$ relationships between the HM-BG-Wood and the HM-BG-Hill bounds are attributed to the variation in the patch size relative to the diffusion length (Figures 4.4 and 4.6). At low water saturation (WL1-3), the $V_p$-$S_w$ relationship follows the HM-BG-Wood bound (Figures 4.4 and 4.6). We interpret that the patches are small sized (< 1 cm) at the beginning of wetting. When the inverted average water saturation (arithmetic mean) is more than ~45% (WL4, Figure 4.5, b), $V_p$ values have a transition from the HM-BG-Wood to HM-BG-Hill bound (Figures 4.4b and 4.6a) or between the two bounds (Figures 4.4 and 4.6). We interpret that the large-sized patches (> 1 cm) start to form during the middle stage of wetting. The transition from HM-BG-Wood behavior to HM-BG-Hill behavior (WL1 to WL5) is consistent with a previous laboratory study, which shows that the transition happens when small patches cluster as water saturation exceeds 40% (Figure 4.6) (Lebedev et al., 2009). When water level is the highest (WL6), $V_p$ values have a transition from the HM-BG-Hill back to the HM-BG-Wood bound (Figures 4.4 and 4.6). We interpret that the water distribution is relatively homogeneous with small-sized residue-air patches at the highest water level. During drainage, the $V_p$-$S_w$ relationship follows the HM-BG-Hill behavior (Figure 4.4, d) and this result is in agreement with previous laboratory observations (Cadoret et al., 1995; Knight and Nolen-Hoeksema, 1990; Monsen and Johnstad, 2005; Murphy, 1982). We interpret that the patches are large-sized (> 1 cm) during drainage.

Based on the interpretation of patch size during the wetting and draining, we can also infer a model for the development of fluid-distribution patterns at different water levels/saturations (Figure 4.7). At the beginning of wetting, small-sized patches are
formed because of large capillary forces at low saturation (Lopes et al., 2014). Water rises initially along more permeable pore throats and forms capillary fingers (Figure 4.7, a). When the water saturation is more than 45%, capillary fingers start to cluster and form large-sized patches as water migrates from large pores to small pores. After water redistribution, water saturations are higher in the sand patches with higher permeability and porosity (Figure 4.7, b). The size of large patches is likely comparable to the size of the shovel-sized patches in the sand tank (~0.15×0.2 m). When the water level almost reaches the top of the sand, large patches are connected and so water is distributed homogeneously, but residual air may be trapped in small pore space when pore pressure dropped below irreducible air pressure (Figure 4.7, c) (Faybishenko, 1995). During the drainage, large-sized patches remain, because no capillary finger can be formed during drainage owing to the hydrophilic nature of the sand. Water tends to drain from sand patches with higher permeability and porosity first, and residual water may be trapped in patches with less permeability and porosity. At the end of drainage (in air-dry sand), large patches with less permeability and porosity ends up with higher residual water saturation compared to the patches with higher permeability and porosity.

Figure 4.7. Illustrations of the inferred development in the size of patches as water level (or water saturation) increases for (a) at low saturation, small-sized patches are formed due to capillary fingering effect, (b) when water saturation >45%, large-sized patches are formed from the clustering of small fingers, (c) when water level almost reaches the top of the sand, small residual-air patches are trapped in small pore spaces as large water patches connect.
4.6 Conclusions

In-situ fluid-distribution patterns can be derived by the inversion of $V_p$ and $V_S$-versus-depth profiles using the HM-BG model with different averaging methods depending on the assumption related with a particular fluid-distribution pattern. The inverted water saturation matches the measured water saturation with an error less than 7%.

The observed non-monotonic $V_p$-WL relationship from water-level change experiments is best explained by alternating between the HM-BG-Wood and HM-BG-Hill bounds, and we interpret the alternations are possibly caused by the variation in patch size during the wetting and draining of the sand. At low water saturation, $V_p$ values follow the HM-BG-Wood bound which indicates small-sized patches are possibly formed because of capillary fingering effect. When water saturation is more than 45%, $V_p$-$S_w$ relationship shows a transition from the HM-BG-Wood to the HM-BG-Hill bound and we interpret the transition as caused by a change in patch size from small to large. When water level almost reaches the top of the sand, the $V_p$-$S_w$ relationship shows a transition from the HM-BG-Hill back to HM-BG-Wood bound and we interpret this transition as caused by a change from large water-saturated patches to small-sized residual-air patches. During drainage, $V_p$ values follow the HM-BG-Hill bound which indicates the patches are large-sized because no capillary finger can be formed due to the hydrophilic nature of the sand.

4.7 References


CHAPTER 5: CONCLUSIONS

Seismic velocity prediction models better explain seismic velocities when total effective stress incorporates both overburden and interparticle stresses, especially for shallow (< 30 m) unconsolidated sediments with large cohesive and capillary pressures such as clays. The proposed model predicts seismic velocities that compare well with observed field velocities from previous shallow soil measurements. Interparticle stresses interfere constructively or destructively with the Biot-Gassmann effect, depending on physical properties of the type of soil. When interparticle stresses are included, theoretical seismic velocities show an overall decrease in clay and increase in sand as water saturation increases. The effect of interparticle stresses is more influential at very shallow depth. Net overburden stress becomes more influential than interparticle stresses at depths greater than 1 m in sand and 100 m in clay. In clay, the theoretical seismic velocities double the range predicted by traditional model, which incorporates only net overburden stress. Velocity is more sensitive to water saturation in clays than sands, which implies that water saturation can be modeled with higher accuracy in clays.

In shallow (< 25 m) near-saturated soil (saturation > 99%), seismic soil properties are successfully inverted by minimizing the misfit between field-based velocity profiles and predicted velocity profiles based on Hertz-Mindlin and Biot-Gassmann theories, aided by Covariance Matrix Adaptation Evolution Strategy optimization. The inverted soil density, elastic moduli, soil-water characteristic curve (SWCC) and soil types determined from these soil properties match geotechnical results from a soil profile interpreted from cone penetration tests. The inverted water saturation, density and porosity also validated by laboratory data from a well. The inverted density and elastic
moduli can be used to interpret major soil types and can detect variations in sand thickness between two field sites. The inverted SWCC can help recognize thin sand units that are below the original seismic resolution of the field data. The SWCC shifts to a lower value when the thin unresolvable layers are sandier than the clay-dominated soil. In combination, the inverted density, elastic moduli and SWCC correspond to soil types that are in agreement with soil types derived from geotechnical data. This work can be applied to determine lateral change in soil properties and stratigraphy between geotechnical borehole tests and guide the location of necessary geotechnical boreholes in near-saturated soil. The suggested workflow in our study has flexibility to incorporate other empirical relationships for known geological settings in order to improve inversion results, or use different velocity models for the extraction of additional information in soils.

In shallow (< 1 m) unconsolidated sediments, in-situ fluid-distribution patterns can be determined by the inversion of P- and S-wave velocity-versus-depth profiles using Covariance Matrix Adaptation Evolution Strategy optimization. The assumption of the best-fitting models, include Hertz-Mindlin-Biot-Gassmann-Hill (HM-BG-Hill) and Hertz-Mindlin-Biot-Gassmann-Wood (HM-BG-Wood) models, can be used to imply the fluid-distribution pattern. Inverted results are verified by a match between the inverted and observed water saturation from electrical measurements. Seismic data from a lab-scale sand tank during imbibition and drainage shows a non-monotonic P-wave velocity ($V_P$)-water saturation ($S_w$) relationship, which is consistence with previous observations. The inversion results show transitions in which model can best fit the experimental velocity data between the HM-BG-Wood model and the HM-BG-Hill model, possibly as
the size of fluid patches alternate between small and large during the imbibition and drainage. At low water saturation, small-sized patches are possibly formed because of capillary fingering effect and $V_p$ values follow the HM-BG-Wood bound. When water saturation is more than 45%, small fluid patches start to cluster and form large-sized patches preferably in sand patches with higher permeability and porosity. $V_p$-$S_w$ relationship shows a transition from the HM-BG-Wood to HM-BG-Hill bound. When water level almost reaches the top of the sand, large patches are connected but small-sized patches with residue air are trapped in small pore space. $V_p$-$S_w$ relationship shows a transition from the HM-BG-Hill back to HM-BG-Wood bound. During drainage, the patches are large sized because no capillary finger can be formed due to the hydrophilic nature of the sand, and $V_p$ values follow the HM-BG-Hill bound.
APPENDIX A: MATLAB OPTIMIZATION SCRIPTS

The following Matlab optimization scripts are designed to minimize the misfit between the predicted and experimental velocity-versus-depth profiles in Chapter 3 and 4. The optimization scripts include one main script “purecmaes.m” and several subscripts such as “hmbg_sand2WL2.m”, “hmbg_siteA_layer1.m”, etc.. The main script is used with each subscript separately for different optimization scenarios.

The following is matlab code using the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) to minimize the misfit between predicted and observed data. The open-source script is wrote by Nikolaus Hansen (Hansen, 2011).

This main code requires a subscript to calculate the misfit. The input misfit function (the parameter called “strfitnessfct”) and the number of variables (the parameter called “N”) for the use of minimizing the misfit predicted and experimental velocity-versus-depth profiles were edited. In this example, the misfit function (“strfitnessfct”) is called “hmbg_sand2WL2”, which is a subscript that calculates the misfit between predicted and experimental velocities. The number of variables (“N”) is set to 10, because that is the number of unknown variable in the subscript “hmbg_sand2WL2.m”. To optimize other misfit, these two parameters (commented as “need to be edited”) can be edited according to the name of the subscript that calculates the misfit and the number of unknown variables that used in the subscript.

The following is the script for purecmaes.m:

```matlab
function xmin=purecmaes

% (mu/mu_w, lambda)-CMA-ES
```
% CMA-ES: Evolution Strategy with Covariance Matrix Adaptation
% for nonlinear function minimization.
%
% This code is "an excerpt" from cmaes.m and implements the key
% parts of the algorithm. It is intended to be used for READING
% and UNDERSTANDING the basic flow and all details of the CMA-ES
% *algorithm*. To run "serious" simulations better use the cmaes.m
% code: it is longer, but offers restarts, far better termination
% options, and, in particular, supposedly quite useful output.
%
% Author: Nikolaus Hansen, 2003-09.
% Edited by Jie Shen
% e-mail: hansen[at]lri.fr
%
% License: This code is released into the public domain (that is,
% you may use and modify it however you like).
%
% URL: http://www.lri.fr/~hansen/purecmaes.m
%
% References: See end of file. Last change: April, 29, 2014

% --------------------- Initialization ---------------------
% User defined input parameters (need to be edited)
strfitnessfct = 'hmbg_sand2WL2';
% name of objective/fitness function (need to be edited),

% the example here uses the subscript called “hmbg_siteA_layer1”

N = 10;

% number of objective variables/problem dimension (need to be edited),

% in the subscript “hmbg_siteA_layer1”, there are 10 unknown parameters.

xmean = rand(N,1);   % objective variables initial point

sigma = 0.5;          % coordinate wise standard deviation (step size)

stopfitness = 1e-10;  % stop if fitness < stopfitness (minimization)

stopeval = 1e3*N^2;   % stop after stopeval number of function evaluations

% Strategy parameter setting: Selection

lambda = 4+floor(3*log(N));  % population size, offspring number

mu = lambda/2;              % number of parents/points for recombination

weights = log(mu+1/2)-log(1:mu);  % muXone array for weighted recombination

mu = floor(mu);

weights = weights/sum(weights);  % normalize recombination weights array

mueff=sum(weights)^2/sum(weights.^2); % variance-effectiveness of sum w_i x_i

% Strategy parameter setting: Adaptation

cc = (4 + mueff/N) / (N+4 + 2*mueff/N);  % time constant for cumulation for C

cs = (mueff+2) / (N+mueff+5);  % t-const for cumulation for sigma control

cl = 2 / (((N+1.3)^2+mueff);  % learning rate for rank-one update of C

cmu = min(1-cl, 2 * (mueff-2+1/mueff) / (((N+2)^2+mueff));  % and for rank-mu update
\[ \text{damps} = 1 + 2 \cdot \max(0, \sqrt{(\text{mueff} - 1)/(N + 1)}) - 1 + \text{cs}; \] % damping for sigma

% usually close to 1

% Initialize dynamic (internal) strategy parameters and constants
\[
\text{pc} = \text{zeros}(N,1); \quad \text{ps} = \text{zeros}(N,1); \quad \% \text{ evolution paths for } \text{C} \text{ and } \sigma
\]

\[
\text{B} = \text{eye}(N, N); \quad \% \text{ B defines the coordinate system}
\]

\[
\text{D} = \text{ones}(N, 1); \quad \% \text{ diagonal D defines the scaling}
\]

\[
\text{C} = \text{B} \cdot \text{diag}(\text{D}^2) \cdot \text{B}'; \quad \% \text{ covariance matrix } \text{C}
\]

\[
\text{invsqrtC} = \text{B} \cdot \text{diag}(\text{D}^{-1}) \cdot \text{B}'; \quad \% \text{ C}^{-1/2}
\]

\[
\text{eigeneval} = 0; \quad \% \text{ track update of } \text{B} \text{ and } \text{D}
\]

\[
\chi_N = N^{0.5} \cdot (1 - 1/(4 \cdot N) + 1/(21 \cdot N^2)); \quad \% \text{ expectation of}
\]

\[
\quad \% \quad \|N(0,1)\| = \text{norm} \left( \text{randn}(N, 1) \right)
\]

\[
\text{out.dat} = []; \quad \text{out.datx} = []; \quad \% \text{ for plotting output}
\]

% ------------------- Generation Loop -------------------------------

\[
\text{counteval} = 0; \quad \% \text{ the next 40 lines contain the 20 lines of interesting code}
\]

while \text{counteval} < \text{stopeval}

\[
\% \text{ Generate and evaluate lambda offspring}
\]

\[
\text{for } k = 1: \text{lambda},
\]

\[
\text{arx(:,k)} = \text{xmean} + \text{sigma} \cdot \text{B} \cdot (\text{D} \cdot \text{randn}(N, 1)); \quad \% \text{ m + sig } \cdot \text{Normal}(0, \text{C})
\]

\[
\text{arfitness}(k) = \text{feval}(\text{strfitnessfct}, \text{arx(:,k)}); \quad \% \text{ objective function call}
\]

\[
\text{counteval} = \text{counteval} + 1;
\]

end
% Sort by fitness and compute weighted mean into xmean

[arfitness, arindex] = sort(arfitness); % minimization
xold = xmean;
xmean = arx(:,arindex(1:mu)) * weights; % recombination, new mean value

% Cumulation: Update evolution paths
ps = (1-cs) * ps ...
   + sqrt(cs*(2-cs)*mueff) * invsqrtC * (xmean-xold) / sigma;
hsig = sum(ps.^2)/(1-(1-cs)^(2*counteval/lambda))/N < 2 + 4/(N+1);
pc = (1-cc) * pc ...
   + hsig * sqrt(cc*(2-cc)*mueff) * (xmean-xold) / sigma;

% Adapt covariance matrix C
artmp = (1/sigma) * (arx(:,arindex(1:mu)) - repmat(xold,1,mu)); % mu difference vectors
C = (1-c1-cmu) * C ... % regard old matrix
   + c1 * (pc * pc' ... % plus rank one update
   + (1-hsig) * cc*(2-cc) * C) ... % minor correction if hsig==0
   + cmu * artmp * diag(weights) * artmp'; % plus rank mu update

% Adapt step size sigma
sigma = sigma * exp((cs/damps)*(norm(ps)/chiN - 1));
% Update B and D from C
if counteval - eigeneval > lambda/(c1+cmu)/N/10  % to achieve O(N^2)
eigeneval = counteval;
C = triu(C) + triu(C,1);  % enforce symmetry
[B,D] = eig(C);           % eigen decomposition, B==normalized eigenvectors
D = sqrt(diag(D));        % D contains standard deviations now
invsqrtC = B * diag(D.^-1) * B';
end

% Break, if fitness is good enough or condition exceeds 1e14, better termination methods are advisable
if arfitness(1) <= stopfitness || max(D) > 1e7 * min(D)
    break;
end

% Output
more off;  % turn pagination off in Octave
disp([num2str(counteval) ': ' num2str(arfitness(1)) ' ' ...
    num2str(sigma*sqrt(max(diag(C)))) ' ' ...
    num2str(max(D) / min(D))]);
% with long runs, the next line becomes time consuming
out.dat = [out.dat; arfitness(1) sigma 1e5*D'];
out.datx = [out.datx; xmean'];
dlmwrite('out_xmean.txt', xmean);
dlmwrite('out_C.txt', C);
end % while, end generation loop

% ----------------- Final Message and Plotting Figures ---------------------
disp([num2str(counteval) ': ' num2str(arfitness(1))]);

xmin = arx(:, arindex(1)); % Return best point of last iteration.
    % Notice that xmean is expected to be even
    % better.
figure(1); hold off; semilogy(abs(out.dat)); hold on; % abs for negative fitness
semilogy(out.dat(:,1) - min(out.dat(:,1)), 'k-'); % difference to best ever fitness, zero is
not displayed

    title('fitness, sigma, sqrt(eigenvalues)'); grid on; xlabel('iteration');
figure(2); hold off; plot(out.datx);

    title('Distribution Mean'); grid on; xlabel('iteration')
This program is a subscript for the input misfit function in the main code “puremaes.m”. This subscript calculates the misfit between predicted and field P- and S-wave velocity-versus-depth profiles using the Hertz-Mindlin and Biot-Gassmann (HM-BG) model in Chapter 3. In this example, the experimental velocity data is from layer 1 at site A at Marrero levee (“Vpmod_A.txt” and “Vsmod_A.txt”, Chapter 3). For other field data, the name of the input field data .txt file needs to be edited (commented as “can be edited”).

The following are the script for hmbg_siteA_layer1.m:

```matlab
function diff = hmbg_siteA_layer1(x)
% This is a subscript for CMA-ES.
% Output: the misfit between predicted and field P- and S-wave velocities (Vp and Vs),
% using the Hertz-Mindlin and Biot-Gassmann (HM-BG) model
% which incorporates matric suction.
% This is an example with field data collected within layer 1 at Site A at Marraro Levee.
% Author: Jie Shen
% Date: 9_2013

% [1] Reject values outside optimization range
rangemin = -3;
rangemax = 3;
if min(x(:))<rangemin || max(x(:))>rangemax % Outside parameter range
diff=1e6*max([max(x) abs(min(x))]);
```

hmbg_siteA_layer1.m
% f=inf;
return
e

% Define the ranges of 10 unknown parameters in HM-BG model,
% assuming soil are composed of sand, clay and organic clay (can be edited).
% x is a matrix with the size of (10, 1),
% which are 10 unknown in the HM–BG model,
% e.g., x = [RHO0, K0, G0, PHI, C, Co, VWCr, m, a, n].
% Parameter range input in CMA-ES is -3 to 3, so we need to
% convert our parameter ranges into the limit of -3 to 3.

OptRange=[-3;3];
RHO0 = interp1(OptRange, [1400;2650],x(1));
% x (1) is RHO0-the density of mineral (kg/m^3).
K0 = interp1(OptRange, [3.4E6;3.66E10],x(2));
% x (2) is K0-the bulk modules of the mineral (Pa).
G0 = interp1(OptRange, [1.56E5;4.5E10],x(3));
% x (3) is G0-the shear modules of the mineral (Pa).
PHI = interp1(OptRange, [0.35;0.8],x(4));
% x (4) is PHI-porosity.
C = interp1(OptRange, [1;8],x(5));
% x (5) is C-the contact number.
Co = interp1(OptRange, [0;20000],x(6));
% x (6) is Co-the cohesive stress (pa).

\[ VWCr = \text{interp1(OptRange, [0;0.436],x(7))}; \]

% x (7) is VWCr-the volumetric water content of the residue water.

\[ m = \text{interp1(OptRange, [0;1],x(8))}; \]

% x (8) is m-fitting parameters for soil water characteristic curves (SWCC)

\[ %m=(n-1)/n \]

\[ a = \text{interp1(OptRange, [0;1],x(9))}; \]

% x (9) is a-fitting parameters for SWCC.

\[ n = \text{interp1(OptRange, [0;49.9],x(10))}; \]

% x (10) is n-fitting parameters for SWCC.

% xnew is a string for output.

\[ xnew = [\text{RHO0, K0, G0, PHI, C, Co, VWCr, m, a, n}]; \]

% Define 6 known parameters (can be edited).

\[ \text{WT} = 36; \]

% WT-estimated water table (m).

\[ g = 9.80665; \]

% g-gravitational acceleration constant (m/s^2).

\[ \text{RHOa} = 1.18; \]

% RHOa-the density of air (kg/m^3).

\[ \text{RHOw} = 1000; \]

% RHOw-the density of water (kg/m^3).

\[ \text{Ka} = 1.01\times10^5; \]
% Ka-bulk modulus of air (Pa).
Kw = 2.2*10^9;
% Kw-bulk modulus of water (Pa).

% Read the experimental Vp profile (model) (can be edited),
% read .txt which saves field P-wave velocity data,
% the example here read a file called “Vpmod_A.txt”.
Pmod=load('Vpmod_A.txt');
Zpmod= Pmod(:,1);
%Zpmod is a column, Zpmod-the P-wave depth points;
Vpmod= Pmod(:,2);
%Vpmod is a column, Vpmod-the P-wave velocity points;

% Read the experimental Vs profile (model) (can be edited),
% read .txt which saves field S-wave velocity data,
% the example here read a file called “Vsmod_A.txt”.
Smod=load('Vsmod_A.txt');
Zsmod= Smod(:,1);
%Zsmod is a column, Zsmod-the S-wave depth points;
Vsmod= Smod(:,2);
%Vsmod is a column, Vsmod-the S-wave velocity points;

% Define the depth range and depth interval (can be edited).
% This is an example with a depth range of 2.5m to 7.5m, with an interval of 0.005m.

\[ z = 2.5:0.005:7.5; \]

% \( z \) is a vector, \( z \)-depth (m) varying from 2.5m to 7.5m with 0.005 interval.

\[ z = z'; \]

% Convert \( z \) to a column \( z' \), \( z' \)-depth (m).

% Interpolate the \( V_p \) and \( V_s \) models linearly into \( V_p \) and \( V_s \) field data and output in .txt.

\[ Vpdat = \text{interp1}(Zpmod, Vpmod, z); \]

% \( Vpdat \) is a column, \( Vpdat \)-the field P-wave velocity.

\[ Vsdat = \text{interp1}(Zsmod, Vsmod, z); \]

% \( Vsdat \) is a column, \( Vsdat \)-the field S-wave velocity.

\[ \text{dlmwrite('Vpdat.txt', Vpdat);} \]

\[ \text{dlmwrite('Vsdat.txt', Vsdat);} \]

% Predict \( V_p \), \( V_s \) using the HM-BG model.

\[ h = WT-z; \]

% \( h \) (vector)-pressure head (m).

\[ Pc = \text{RHOw.*g.*h./6894.75729;} \]

% \( Pc \) (vector)-matric suction/capillary pressure (psi).

\[ Se = (1/(1+(a.*Pc).^n)).^m; \]

% \( Se \) (vector)-effective water saturation.

\[ Sw = (\text{VWCr} + Se.*(	ext{PHI-VWCr}))./\text{PHI;} \]

% \( Sw \) (vector)-water saturation.
RHOeff=PHI.*(Sw.*RHOw+(1-Sw).*RHOa)+(1-PHI).*RHO0;

% RHOeff (scalar)-effective bulk density with pore fluids (kg/m3).

Peff=(RHO0-Se.*RHOw).*g.*z;

% Peff (vector)-overburden pressure (Pa).

NU=(3.*K0-2.*G0)./(2.*(3.*K0+G0));

% NU-the poisson's ratio.

Km=(((C.^2.*(1-PHI).^2.*G0.^2)./(18.*pi.^2.*(1-NU).^2)).*Peff).^((1/3);

% Km (vector)-matrix bulk modulus from HM (Pa).

Gm=((5-4.*NU)./(5.*(2-NU))).*(((3.*C.^2.*(1-PHI).^2.*G0.^2)/(2.*pi.^2.*(1-NU).^2)).*Peff).^((1/3);

% Gm (vector)-matrix shear modulus from HM (Pa).

Kfl=1./(Sw./Kw+(1-Sw)./Ka);

% Kfl (vector)-bulk modulus of pore fluids (Pa).

Keff=(K0.*(Km./(K0-Km)+Kfl./(PHI.*(K0-Kfl))))./(1+(Km./(K0-Km)+Kfl./(PHI.*(K0-Kfl)));

% Keff (vector)-effective bulk modulus from BG (Pa).

Vp=((Keff+(4/3).*Gm)./RHOeff).^((1/2);

% Vp (vector)-predicted P-wave velocity using HM-BG (m/s).

Vs=(Gm./RHOeff).^((1/2);

% Vs (vector)-S-wave velocity using HM-BG (m/s).

diffp=rms(Vp-Vpdat);

% diffp (scalar)-the rms=(Vp^2-Vpdat^2)/sample number in Vp

% between predicted and field data (m/s).
diffs=rms(Vs-Vsdat);

% diffs(scalar)-the rms=(Vp^2-Vpdat^2)/sample number in Vs
  % between predicted and experimental data (m/s).
diff=diffp+diffs;

% diff(scalar)-total misfit/difference between calculated and field velocity (m/s).

% output optimal properties into a .txt file when the misfit is minimal,
  % between predicted and experimental velocities.
dlmwrite('hmbg_siteA_layer1.txt',xnew);
end
hmbghill_sand2WL2.m

This program is a subscript for the input misfit function in the main code “puremaes.m”. This subscript calculates the misfit between predicted and experimental P- and S-wave velocity-versus-depth profiles using the Hertz-Mindlin- Biot-Gassmann-Hill (HM-BG-Hill) model in Chapter 4. In this example, the experimental velocity data is from sand tank at water level 2 during wetting (“WL2_P” and “WL2_S”, Chapter 4). For other experimental data, the name of the input experimental data .txt file needs to be edited (commented as “can be edited”).

The following are the script for hmbghill_sand2WL2.m:

function diff = hmbghill_sand2WL2(x)

% This is a subscript for CMA-ES.

% Output: the misfit between predicted and experimental

%P- and S-wave velocities (Vp and Vs),

% using the Hertz-Mindlin-Biot-Gassmann-Hill (HM-BG-Hill) model

%which incorporates matric suction.

% This is an example with experimental data collected

%from sand tank at water level 2 during wetting.

% Author: Jie Shen

% Date: 3_2015

%[1] Reject values outside optimization range

rangemin =-3;

rangemax = 3;
if min(x(:))<rangemin || max(x(:))>rangemax % Outside parameter range
    diff=1e6*max([max(x) abs(min(x))]);
    % f=inf;
    return
end

% Define the ranges of 12 unknown parameters in HM-BG-Hill model,
% assuming the sand is quartz (can be edited).
% In patchy saturation, the sand body refers to the adjacent area
% that surrounding sand patches.
% x is a matrix with the size of (12, 1),
% which are 12 unknown in the HM-BG-Hill model,
% e.g., x = [C, Co, Fp, m1, a1, n1, VWCr1, m2, a2, n2, VWCr2, WT].
% Parameter range input in CMA-ES is -3 to 3, so we need to
% convert our parameter ranges into the limit of -3 to 3.
OptRange=[-3;3];
C = interp1(OptRange, [1;8],x(1));
% x (2) is C-the contact number.
Co = interp1(OptRange, [0;300],x(2));
% x (2) is Co-the cohesive stress (pa).
Fp = interp1(OptRange, [0;0.5],x(3));
% x (3) is the volumetric fraction of the patches.
m1 = interp1(OptRange, [0;1],x(4));
% x (4) is m-fitting parameters of sand body for SWCC; m=(n-1)/n.

a1 = interp1(OptRange, [0;1],x(5));

% x (5) is a-fitting parameters of sand body for SWCC.

n1 = interp1(OptRange, [0;60],x(6));

% x (6) is n-fitting parameters of sand body for SWCC.

VWCr1 = interp1(OptRange, [0;0.436],x(7));

% x (7) is VWCr-the volumetric water content of the residue water of sand body.

m2 = interp1(OptRange, [0;1],x(8));

% x (8) is m-fitting parameters of sand patches for SWCC; m=(n-1)/n.

a2 = interp1(OptRange, [0;1],x(9));

% x (9) is a-fitting parameters of sand patches for SWCC.

n2 = interp1(OptRange, [0;60],x(10));

% x (10) is n-fitting parameters of sand patches for SWCC.

VWCr2 = interp1(OptRange, [0;0.436],x(11));

% x (11) is VWCr-the volumetric water content of the residue water of sand patches.

WT = interp1(OptRange, [0.55;5],x(12));

% x (12) is WT-water table (m).

% xnew is a string for output.

xnew = [C, Co, Fp, m1, a1, n1, VWCr1, m2, a2, n2, VWCr2, WT];

% Define 9 known parameters, assuming the sand is quartz (can be edited).

RHO0 = 2650;

% RHO0-the density of mineral (kg/m³).
K0 = 4.4E10;
% K0-the bulk modules of the mineral (Pa).
G0 = 3.66E10;
% G0-the shear modules of the mineral (Pa).
PHI = 0.42;
% PHI-porosity.
g = 9.80665;
% g-gravitational acceleration constant (m/s²).
RHOa = 1.18;
% RHOa-the density of air (kg/m³).
RHOw = 1000;
% RHOw-the density of water (kg/m³).
Ka = 1.01*10^5;
% Ka-bulk modulus of air (Pa).
Kw = 2.2*10^9;
% Kw-bulk modulus of water (Pa).

% Read the experimental Vp profile (model) (can be edited),
% read .txt which saves experimental P-wave velocity data,
% the example here read a file called “WL2_P.txt”.
Pmod=load('WL2_P.txt');
Zpmod= Pmod(:,1);
% Zpmod is a column, Zpmod-the P-wave depth points;
Vpmod= Pmod(:,2);

%Vpmod is a column, Vpmod-the P-wave velocity points;

% Read the experiemntal Vs profile (model) (can be edited),
%read .txt which saves experimental S-wave velocity data,
%the example here read a file called “WL2_S.txt”.
Smod=load('WL2_S.txt');
Zsmod= Smod(:,1);
%Zsmod is a column, Zsmod-the S-wave depth points;
Vsmod= Smod(:,2);
%Vsmod is a column, Vsmod-the S-wave velocity points;

% Define the depth range and depth interval (can be edited).
% This is an example with the sand tank depth
%from 0.03m to 0.55m, with an interval of 0.005m.
z=0.03:0.005:0.55;
% z is a vector, z-depth (m) varying from 0.03m to 0.55m with 0.005 interval.
z=z';
% Convert z to a column z', z'-depth (m).

% Interpolate the Vp and Vs models linearly into
%Vp and Vs experimental data and output in .txt.
Vpdat=interp1(Zsmod,Vsmod,z);
Vpdat is a column, Vpdat-the experimental P-wave velocity.

Vsdat=interp1(Zsm, Vsmod, z);

Vsdat is a column, Vsdat-the experimental S-wave velocity.

dlmwrite('Vpdat.txt', Vpdat);
dlmwrite('Vsdat.txt', Vsdat);

% Predict Vp, Vs using the HM-BG-Hill model.

h = WT-z;

% h (vector)-pressure head (m).

Pc=RHOw.*g.*h./6894.75729;

% Pc(vector)-matric suction/capillary pressure (psi).

Se_body=(1./(1+(a1.*Pc).^n1)).^m1;

%Se(vector)-effective water saturation of sand body.

Se_patch=(1./(1+(a2.*Pc).^n2)).^m2;

%Se(vector)-effective water saturation of sand patches.

Sw_body=(VWCr1+Se_body.*(PHI-VWCr1))./PHI;

% Sw(vector)-water saturation of sand body outside patches.

Sw_patch=(VWCr2+Se_patch.*(PHI-VWCr2))./PHI;

% Sw(vector)-water saturation of sand patches.

Sw=Fp.*Sw_patch+(1-Fp).*Sw_body;

% Sw(vector)-effective water saturation of sand within patches.

RHOeff=PHI.*(Sw.*RHOw+(1-Sw).*RHOa)+(1-PHI).*RHO0;

%RHOeff (scalar)-effective bulk density with pore fluids (kg/m^3).
Peff\_body=(\text{RHOeff-Se\_body}.*\text{RHOw})*g.*z+Co;

\% Peff\_body (vector)-effective pressure of sand body outside patches (Pa).

Peff\_patch=(\text{RHOeff-Se\_patch}.*\text{RHOw})*g.*z+Co;

\% Peff\_patch (vector)-effective pressure of sand patches (Pa).

NU=(3.*K0-2.*G0)/(2.*(3.*K0+G0));

\%NU-the poisson's ratio.

Km\_body=(((C.^2.*(1-PHI).^2.*G0.^2)./(18.*pi.^2.*(1-NU).^2)).*Peff\_body).^(1/3);

\%Km\_body (vector)-matrix bulk modulus of sand body from HM (Pa).

Km\_patch=(((C.^2.*(1-PHI).^2.*G0.^2)./(18.*pi.^2.*(1-NU).^2)).*Peff\_patch).^(1/3);

\%Km\_patch (vector)-matrix bulk modulus of sand patches from HM (Pa).

Gm\_body=((5-4.*NU)/(5.*(2-NU))).*((3.*C.^2.*(1-PHI).^2.*G0.^2)/(2.*pi.^2.*(1-NU).^2)).*Peff\_body).^(1/3);

\%Gm\_body (vector)-matrix shear modulus of sand body from HM (Pa).

Gm\_patch=((5-4.*NU)/(5.*(2-NU))).*((3.*C.^2.*(1-PHI).^2.*G0.^2)/(2.*pi.^2.*(1-NU).^2)).*Peff\_patch).^(1/3);

\%Gm\_patch (vector)-matrix shear modulus of sand patches from HM (Pa).

Kfl\_body=1./(Sw\_body./Kw+(1-Sw\_body)./Ka);

\%Kfl\_body(vector)- bulk modulus of pore fluids of sand body outside patches (Pa).

Kfl\_patch=1./(Sw\_patch./Kw+(1-Sw\_patch)./Ka);

\%Kfl\_patch(vector)- bulk modulus of pore fluids in sand patches (Pa).

Keff\_body=(K0.*(Km\_body./(K0-Km\_body)+Kfl\_body./(PHI.*(K0-Kfl\_body))))./(1+(Km\_body./(K0-Km\_body)+Kfl\_body./(PHI.*(K0-Kfl\_body))));

\%Keff\_patch (vector)-effective bulk modulus from BG of sand body (Pa).
Keff\_patch=(K0.*(Km\_patch./(K0-Km\_patch)+Kfl\_patch./(PHI.*(K0-Kfl\_patch))))/(1+(Km\_patch./(K0-Km\_patch)+Kfl\_patch./(PHI.*(K0-Kfl\_patch))));

%Keff\_patch(vector)-effective bulk modulus from BG(Pa) of sand patches.

Meff\_body=Keff\_body+4/3.*Gm\_body;

%Effective elastic modulus of sand body.

Meff\_patch=Keff\_patch+4/3.*Gm\_patch;

%Effective elastic modulus of sand patches.

Meff=1./((Fp.*PHI)./Meff\_patch+((1-Fp).*PHI)./Meff\_body);

%Effective elastic modulus of sand body and patches.

Geff=1./((Fp.*PHI)./Gm\_patch+((1-Fp).*PHI)./Gm\_body);

%Effective elastic modulus of sand body and patches.

Vp=(Meff./RHOeff).^(1/2);

%Vp (vector)-P-wave velocity (m/s).

Vs=(Geff./RHOeff).^(1/2);

%Vs (vector)-S-wave velocity (m/s).

diffp=rms(Vp-Vpdat);

% diffp1(scalar)-the rms=(Vp^2-Vpdat^2)/sample number in Vp,

%between calculated and experimental data (m/s).

diffs=rms(Vs-Vsdat);

% diffs1(scalar)-the rms=(Vp^2-Vpdat^2)/sample number in Vs,

%between calculated and experimental data (m/s).

diff=diffp+diffs;

%diff (scalar)-the total misfit/difference
% between predicted and experimental velocity (m/s).

% output optimal properties into a .txt file when the misfit is minimal,

% between predicted and experimental velocities.


dlmwrite('hmmbghill_sand2WL2.txt', xnew);

end
hmbgwood_sand2WL2.m

This program is a subscript for the input misfit function in the main code “puremaes.m”. This subscript calculates the misfit between predicted and experimental P- and S-wave velocity-versus-depth profiles using the Hertz-Mindlin- Biot-Gassmann-Wood (HM-BG-Wood) model in Chapter 4. In this example, the experimental velocity data is from sand tank at water level 2 during wetting (“WL2_P” and “WL2_S”, Chapter 4). For other experimental data, the name of the input experimental data .txt file needs to be edited (commented as “can be edited”).

The following are the script for hmbgwood_sand2WL2.m:

function diff = hmbgwood_sand2WL2(x)
% This is a subscript for CMA-ES.
% Output: the misfit between predicted and experimental
% P- and S-wave velocities (Vp and Vs),
% using the Hertz-Mindlin-Biot-Gassmann-Wood (HM-BG-Wood) model
% which incorporates matric suction.
% This is an example with experimental data collected
% from sand tank at water level 2 during wetting.
% Author: Jie Shen
% Date: 3_2015

% [1] Reject values outside optimization range
rangemin = -3;
rangemax = 3;
if min(x(:))<rangemin || max(x(:))>rangemax  % Outside parameter range
diff=1e6*max([max(x) abs(min(x))]);

  % f=inf;
  return

  end

  % Define the ranges of 12 unknown parameters in HM-BG-Wood model,
  % assuming the sand is quartz (can be edited).
  % In patchy saturation, the sand body refers to the adjacent area
  %that surrounding sand patches.
  % x is a matrix with the size of (12, 1),
  %which are 12 unknown in the HM-BG-Wood model,
  %e.g., x = [C, Co, Fp, m1, a1, n1, VWCr1, m2, a2, n2, VWCr2, WT].
  % Parameter range input in CMA-ES is -3 to 3, so we need to
  %convert our parameter ranges into the limit of -3 to 3.
  OptRange=[-3;3];
  C = interp1(OptRange, [1;8],x(1));
  % x (2) is C-the contact number.

  Co = interp1(OptRange, [0;300],x(2));
  % x (2) is Co-the cohisive stress (pa).

  Fp = interp1(OptRange, [0;0.5],x(3));
  % x (3) is the volumetric fraction of the patches.
  m1 = interp1(OptRange, [0;1],x(4));
% x (4) is m-fitting parameters of sand body for SWCC; m=(n-1)/n.

a1 = interp1(OptRange, [0;1],x(5));

% x (5) is a-fitting parameters of sand body for SWCC.

n1 = interp1(OptRange, [0;60],x(6));

% x (6) is n-fitting parameters of sand body for SWCC.

VWCr1 = interp1(OptRange, [0;0.436],x(7));

% x (7) is VWCr-the volumetric water content of the residue water of sand body.

m2 = interp1(OptRange, [0;1],x(8));

% x (8) is m-fitting parameters of sand patches for SWCC; m=(n-1)/n.

a2 = interp1(OptRange, [0;1],x(9));

% x (9) is a-fitting parameters of sand patches for SWCC.

n2 = interp1(OptRange, [0;60],x(10));

% x (10) is n-fitting parameters of sand patches for SWCC.

VWCr2 = interp1(OptRange, [0;0.436],x(11));

% x (11) is VWCr-the volumetric water content of the residue water of sand patches.

WT = interp1(OptRange, [0.55;5],x(12));

% x (12) is WT-water table (m).

% xnew is a string for output.

xnew = [C, Co, Fp, m1, a1, n1, VWCr1, m2, a2, n2, VWCr2, WT];

% Define 9 known parameters, assuming the sand is quartz (can be edited).

RHO0 = 2650;

% RHO0-the density of mineral (kg/m³).
K0 = 4.4E10;
% K0-the bulk modules of the mineral (Pa).
G0 = 3.66E10;
% G0-the shear modules of the mineral (Pa).
PHI = 0.42;
% PHI-porosity.
g = 9.80665;
% g-gravitational acceleration constant (m/s^2).
RHOa = 1.18;
% RHOa-the density of air (kg/m^3).
RHOw = 1000;
% RHOw-the density of water (kg/m^3).
Ka = 1.01*10^5;
% Ka-bulk modulus of air (Pa).
Kw = 2.2*10^9;
% Kw-bulk modulus of water (Pa).

% Read the experimental Vp profile (model) (can be edited),
% read .txt which saves experimental P-wave velocity data,
% the example here read a file called “WL2_P.txt”.
Pmod=load('WL2_P.txt');
Zpmod= Pmod(:,1);
% Zpmod is a column, Zpmod-the P-wave depth points;
Vpmod= Pmod(:,2);

%Vpmod is a column, Vpmod-the P-wave velocity points;

% Read the experimental Vs profile (model) (can be edited),
% read .txt which saves experimental S-wave velocity data,
% the example here read a file called “WL2_S.txt”.
Smod=load('WL2_S.txt');
Zsmod= Smod(:,1);
%Zsmod is a column, Zsmod-the S-wave depth points;
Vsmod= Smod(:,2);
%Vsmod is a column, Vsmod-the S-wave velocity points;

% Define the depth range and depth interval (can be edited).
% This is an example with the sand tank depth
% from 0.03m to 0.55m, with an interval of 0.005m.
z=0.03:0.005:0.55;
% z is a vector, z-depth (m) varying from 0.03m to 0.55m with 0.005 interval.
z=z';
% Convert z to a column z', z'-depth (m).

% Interpolate the Vp and Vs models linearly into
% Vp and Vs experimental data and output in .txt.
Vpdat=interp1(Zpmod,Vpmod,z);
%Vpdat is a column, Vpdat-the experimental P-wave velocity.

Vsdat=interp1(Zsmod,Vsmod,z);

%Vsdat is a column, Vsdat-the experimental S-wave velocity.

dlmwrite('Vpdat.txt',Vpdat);
dlmwrite('Vsdat.txt',Vsdat);

% Predict Vp, Vs using the HM-BG-Wood model.

h= WT-z;

% h (vector)-pressure head (m).

Pc=RHOw.*g.*h./6894.75729;

% Pc(vector)-matric suction/capillary pressure (psi).

Se_body=(1./(1+(a1.*Pc).^n1)).^m1;

%Se(vector)-effective water saturation of sand body.

Se_patch=(1./(1+(a2.*Pc).^n2)).^m2;

%Se(vector)-effective water saturation of sand patches.

Sw_body=(VWCr1+Se_body.*(PHI-VWCr1))./PHI;

% Sw(vector)-water saturation of sand body.

Sw_patch=(VWCr2+Se_patch.*(PHI-VWCr2))./PHI;

% Sw(vector)-water saturation of sand patches.

Sw=Fp.*Sw_patch+(1-Fp).*Sw_body;

% Sw(vector)-effective water saturation of sand body and patches.

Se=Fp.*Se_patch+(1-Fp).*Se_body;

% Se(vector)-effective water saturation of sand and patches.
\[ \text{RHO}_{\text{eff}} = \Phi_{\text{i}} \cdot (\text{Sw} \cdot \text{RHO}_{\text{w}} + (1-\text{Sw}) \cdot \text{RHO}_{\text{a}}) + (1-\Phi_{\text{i}}) \cdot \text{RHO}_{0}; \]

% \text{RHO}_{\text{m}} (\text{scalar}) - effective bulk density with pore fluids (kg/m³).

\[ \text{Peff} = (\text{RHO}_{\text{eff}} - \text{Se} \cdot \text{RHO}_{\text{w}}) \cdot \text{g} \cdot \text{z} + \text{Co}; \]

% Peff (vector) - effective pressure (Pa).

\[ \text{NU} = (3 \cdot \text{K}_{0} - 2 \cdot \text{G}_{0}) / (2 \cdot (3 \cdot \text{K}_{0} + \text{G}_{0}); \]

% NU - the poisson's ratio.

\[ \text{Km} = \left( \left( \text{C}^{2} \cdot (1 - \Phi_{\text{i}})^{2} \cdot \text{G}_{0}^{2} \right) / \left( 18 \cdot \pi^{2} \cdot (1 - \text{NU})^{2} \right) \right) \cdot \text{Peff} \cdot (1/3); \]

% Km (vector) - matrix bulk modulus from HM (Pa).

\[ \text{Gm} = \left( (5 - 4 \cdot \text{NU}) / (5 \cdot (2 - \text{NU})) \right) \cdot \left( \left( \text{C}^{2} \cdot (1 - \Phi_{\text{i}})^{2} \cdot \text{G}_{0}^{2} \right) / \left( 2 \cdot \pi^{2} \cdot (1 - \text{NU})^{2} \right) \right) \cdot \text{Peff} \cdot (1/3); \]

% Gm (vector) - matrix shear modulus from HM (Pa).

\[ \text{Kfleff} = 1 / \left( \left( \text{Sw}_{\text{patch}} \cdot \text{Fp} \cdot \Phi_{\text{i}} \right) / \text{Kw} + \left( (1 - \text{Sw}_{\text{patch}}) \cdot \text{Fp} \cdot \Phi_{\text{i}} \right) / \text{Ka} + \left( \text{Sw}_{\text{body}} \cdot (1 - \text{Fp}) \cdot \Phi_{\text{i}} \right) / \text{Kw} + \left( (1 - \text{Sw}_{\text{body}}) \cdot (1 - \text{Fp}) \cdot \Phi_{\text{i}} \right) / \text{Ka} \right); \]

% Bulk modulus of pore fluids (Pa) of sand body and patches.

\[ \text{Keff} = (\text{K}_{0} \cdot (\text{Km} / (\text{K}_{0} - \text{Km}) + \text{Kfleff} / (\Phi_{\text{i}} \cdot (\text{K}_{0} - \text{Kfleff})))) / (1 + (\text{Km} / (\text{K}_{0} - \text{Km}) + \text{Kfleff} / (\Phi_{\text{i}} \cdot (\text{K}_{0} - \text{Kfleff}))) ; \]

% Keff _patch(vector) - effective bulk modulus from BG (Pa) of sand body and patches.

\[ \text{Meff} = \text{Keff} + 4/3 \cdot \text{Gm}; \]

% Effective elastic modulus of sand body and patches.

\[ \text{Vp} = (\text{Meff} / \text{RHO}_{\text{eff}}) \cdot (1/2); \]

% Vp (vector) - P-wave velocity (m/s).

\[ \text{Vs} = (\text{Gm} / \text{RHO}_{\text{eff}}) \cdot (1/2); \]

% Vs (vector) - S-wave velocity (m/s).
diffp=rms(Vp-Vpdat);

% diffp (scalar)-the rms=(Vp^2-Vpdat^2)/sample number in Vp,

% between predicted and experimental data (m/s).

diffs=rms(Vs-Vsdat);

% diffs (scalar)-the rms=(Vs^2-Vsdat^2)/sample number in Vs,

% between predicted and experimental data (m/s).

diff=diffp+diffs;

% diff (scalar)-the total misfit (difference),

% between predicted and experimental velocity (m/s).

% output optimal properties into a .txt file when the misfit is minimal,

% between predicted and experimental velocities.

dlmwrite('hmbgwood_sand2WL2.txt',xnew);

end
hmbg_sand2WL2.m

This program is a subscript for the input misfit function in the main code “puremaes.m”. This subscript calculates the misfit between predicted and experimental P- and S-wave velocity-versus-depth profiles using the Hertz-Mindlin and Biot-Gassmann (HM-BG) model in Chapter 4. In this example, the experimental velocity data is from sand tank at water level 2 during wetting (“WL2_P” and “WL2_S”, Chapter 4). For other experimental data, the name of the input experimental data .txt file needs to be edited (commented as “can be edited”).

The following are the script for hmbg_sand2WL2.m:

function diff = hmbg_sand2WL2(x)

% This is a subscript for CMA-ES.
% Output: the misfit between predicted and experimental
% P- and S-wave velocities (Vp and Vs),
% using the Hertz-Mindlin and Biot-Gassmann (HM-BG) model
% which incorporates matric suction.
% This is an example with experimental data collected
% from sand tank at water level 2 during wetting.
% Author: Jie Shen
% Date: 3_2015

% [1] Reject values outside optimization range
rangemin = -3;
rangemax = 3;
if min(x(:))<rangemin || max(x(:))>rangemax % Outside parameter range

diff = 1e6*max([max(x) abs(min(x))]);

% f=inf;
return
end

% Define the ranges of 7 unknown parameters in HM-BG model,

% assuming the sand is quartz (can be edited).

% x is a matrix with the size of (7, 1),
% which are 7 unknown in the HM-BG model,
% e.g., x = [C, Co, VWCr, m, a, n, WT].

% Parameter range input in CMA-ES is -3 to 3, so we need to
% convert our parameter ranges into the limit of -3 to 3.

OptRange=[-3;3];
C = interp1(OptRange, [1;8],x(1));
% x (1) is C-the contact number.
Co = interp1(OptRange, [0;300],x(2));
% x (2) is Co-the cohesive stress (pa).
VWCr = interp1(OptRange, [0;0.436],x(3));
% x (3) is VWCr-the volumetric water content of the residue water.
m = interp1(OptRange, [0;1],x(4));
% x (4) is m-fitting parameters for soil water characteristic curves (SWCC)
 %m=(n-1)/n
a = interp1(OptRange, [0;1],x(5));
% x (5) is a-fitting parameters for SWCC.
n = interp1(OptRange, [0;49.9],x(6));
% x (6) is n-fitting parameters for SWCC.
WT = interp1(OptRange, [0.55;5],x(7));
% x (7) is WT-water table (m).
% xnew is a string for output.
xnew = [C, Co, VWCr, m, a, n, WT];

% Define 9 known parameters, assuming the sand is quartz (can be edited).
RHO0 = 2650;
% RHO0-the density of mineral (kg/m³).
K0 = 4.4E10;
% K0-the bulk modules of the mineral (Pa).
G0 = 3.66E10;
% G0-the shear modules of the mineral (Pa).
PHI = 0.42;
% PHI-porosity.
g = 9.80665;
% g-gravitational acceleration constant (m/s²).
RHOa = 1.18;
% RHOa-the density of air (kg/m³).
RHOw = 1000;
% RHOw-the density of water (kg/m³).

Ka = 1.01*10^5;

% Ka-bulk modulus of air (Pa).

Kw = 2.2*10^9;

% Kw-bulk modulus of water (Pa).

% Read the experimental Vp profile (model) (can be edited),
% read .txt which saves experimental P-wave velocity data,
% the example here read a file called “WL2_P.txt”.

Pmod=load('WL2_P.txt');

Zpmod= Pmod(:,1);

%Zpmod is a column, Zpmod-the P-wave depth points;

Vpmod= Pmod(:,2);

%Vpmod is a column, Vpmod-the P-wave velocity points;

% Read the experimental Vs profile (model) (can be edited),
% read .txt which saves experimental S-wave velocity data,
% the example here read a file called “WL2_S.txt”.

Smod=load('WL2_S.txt');

Zsmod= Smod(:,1);

%Zsmod is a column, Zsmod-the S-wave depth points;

Vsmod= Smod(:,2);

%Vsmod is a column, Vsmod-the S-wave velocity points;
% Define the depth range and depth interval (can be edited).
% This is an example with the sand tank depth
% from 0.03m to 0.55m, with an interval of 0.005m.

z=0.03:0.005:0.55;

% z is a vector, z-depth (m) varying from 0.03m to 0.55m with 0.005 interval.

z=z';

% Convert z to a column z', z'-depth (m).

% Interpolate the Vp and Vs models linearly into Vp and Vs experimental data and output in .txt.
Vpdat=interp1(Zpmod,Vpmod,z);

%Vpdat is a column, Vpdat-the experimental P-wave velocity.

Vsdat=interp1(Zsmod,Vsmod,z);

%Vsdat is a column, Vsdat-the experimental S-wave velocity.
dlmwrite('Vpdat.txt',Vpdat);
dlmwrite('Vsdat.txt',Vsdat);

% Predict Vp, Vs using the HM-BG model.

h= WT-z;

% h (vector)-pressure head (m).
Pc=RHOw.*g.*h./6894.75729;

% Pc(vector)-matric suction/capillary pressure (psi).
Se=(1./(1+(a.*Pc).^n)).^m;

%Se(vector)-effective water saturation.

Sw=(VWCr+Se.*(PHI-VWCr))./PHI;

% Sw(vector)-water saturation.

RHOeff=PHI.*(Sw.*RHOw+(1-Sw).*RHOa)+(1-PHI).*RHO0;

%RHOeff (scalar)-effective bulk density with pore fluids(kg/m3).

Peff=(RHO0-Se.*RHOw).*g.*z;

% Peff (vector)-overburden pressure (Pa).

NU=(3.*K0-2.*G0)./(2.*(3.*K0+G0));

%NU-the poisson's ratio.

Km=((C.^2.*(1-PHI).^2.*G0.^2)./(18.*pi.^2.*(1-NU).^2)).*Peff).^(1/3);

%Km (vector)-matrix bulk modulus from HM (Pa).

Gm=((5-4.*NU)./(5.*(2-NU))).*(((3.*C.^2.*(1-PHI).^2.*G0.^2)/(2.*pi.^2.*(1-NU).^2)).*Peff).^(1/3);

%Gm (vector)-matrix shear modulus from HM (Pa).

Kfl=1./(Sw./Kw+(1-Sw)./Ka);

%Kfl(vector)- bulk modulus of pore fluids (Pa).

Keff=(K0.*(Km./(K0-Km)+Kfl./(PHI.*(K0-Kfl))))./(1+(Km./(K0-Km)+Kfl./(PHI.*(K0-Kfl))));

%Keff (vector)-effective bulk modulus from BG(Pa).

Vp=((Keff+(4/3).*Gm)./RHOeff).^(1/2);

%Vp (vector)-predicted P-wave velocity using HM-BG (m/s).

Vs=(Gm./RHOeff).^(1/2);
%Vs (vector)-S-wave velocity using HM-BG (m/s).

diffp=rms(Vp-Vpdat);

% diffp(scalar)-the rms=(Vp^2-Vpdat^2)/sample number in Vp,
% between predicted and experimental data (m/s).

diffs=rms(Vs-Vsdat);

% diffs(scalar)-the rms=(Vs^2-Vsdat^2)/sample number in Vs,
% between predicted and experimental data (m/s).

diff=diffp+diffs;

% diff(scalar)-total misfit/difference between calculated and experimental velocity (m/s).

% output optimal properties into a .txt file,
% when the misfit between predicted and experimental velocities is minimal.

dlmwrite('hmbg_sand2WL2.txt',xnew);

end

References

Hansen, N., 2011, The CMA evolution strategy: A tutorial,
APPENDIX B: VELOCITY PREDICTION MODEL

The following velocity prediction model is used in Chapter 3. Seismic P-wave velocity \((V_P)\) and S-wave velocity \((V_S)\) are calculated from effective elastic moduli and bulk density (Dvorkin and Nur, 1996):

\[
V_P = \sqrt{\frac{\frac{K_{eff} + \frac{4}{3}G_{eff}}{\rho_{eff}}}{}} \quad (B-1)
\]

\[
V_S = \sqrt{\frac{G_{eff}}{\rho_{eff}}} \quad (B-2)
\]

where \(K_{eff}\) is the effective bulk modulus, \(G_{eff}\) is the effective shear modulus, and \(\rho_{eff}\) is the effective density of the soil matrix with pore fluids and expressed as (Dvorkin and Nur, 1996):

\[
\rho_{eff} = \phi(S_w\rho_w + (1 - S_w)\rho_a) + (1 - \phi)\rho_0 \quad (B-3)
\]

where \(\phi\) is the porosity, \(S_w\) is the water saturation, \(\rho_w\) is the density of water, \(\rho_a\) is the density of air, and \(\rho_0\) is the density of soil grains.

Effective elastic moduli are calculated by Gassmann fluid substitution theory (Dvorkin and Nur, 1996):

\[
K_{eff} = \frac{K_0 \left( \frac{K_m}{K_0 - K_m} \phi \left( \frac{K_{fl}}{K_0 - K_{fl}} \right) \right)}{1 + \frac{K_m}{K_0 - K_m} \phi \left( \frac{K_{fl}}{K_0 - K_{fl}} \right)} \quad (B-4)
\]

\[
G_{eff} = G_m \quad (B-5)
\]

where \(K_0\) is the bulk modulus of the soil grains, \(K_m\) is the bulk modulus of the “dry” soil matrix, \(G_m\) is the shear modulus of the “dry” soil matrix, and \(K_{fl}\) is the bulk modulus of the pore fluids.
We assume pore fluid to be water and air, so that bulk modulus of the pore fluids is (Dvorkin and Nur, 1996):

\[ K_{fl} = \left( \frac{S_w}{K_w} + \frac{1-S_w}{K_a} \right)^{-1} \]  

(B-6)

where \( K_w \) is the bulk modulus of water, and \( K_a \) is the bulk modulus of air.

Matrix elastic moduli are estimated using Hertz-Mindlin contact theory (Dvorkin and Nur, 1996):

\[ K_m = \frac{3 C^2 (1-\phi)^2 G_0^2}{18 \pi^2 (1-\nu)^2} P_{eff} \]  

(B-7)

\[ G_m = \frac{5-4 \nu}{5 (2-\nu)} \frac{3 C^2 (1-\phi)^2 G_0^2}{2 \pi^2 (1-\nu)^2} P_{eff} \]  

(B-8)

where \( C \) is the coordination number, \( G_0 \) is the shear modulus of soil grains, \( \nu \) is the Poisson’s ratio of the soil grains, \( P_{eff} \) is the effective stress.

SWCC fitting function determines the relationship between effective water saturation \( S_e \) and capillary head \( h \) (Van Genuchten, 1980):

\[ S_e = \left[ \frac{1}{1+|a h|^n} \right]^m \]  

(B-9)

where \( a, n, m \) are fitting parameters.

Water saturation is related with effective water saturation as (Van Genuchten, 1980):

\[ S_w = \frac{S_e (\phi - \theta_r) + \theta_r}{\phi} \]  

(B-10)

where \( \theta_r \) is the residual volumetric water content.

References

APPENDIX C: SAND TANK WATER LEVEL EXPERIMENTS

The following are details and procedures for the sand tank water level experiments in Chapter 4. In order to optimize our data collection capabilities, we make improvements to the previous acquisition system (Lorenzo et al., 2013). We incorporate 5 soil moisture meters (capacitance/frequency domain sensors) that utilize conductivity to measure water content from the sand tank. In order to reduce noise, we place the acquisition cards into grounded metal boxes and expand the previous 8-channel amplifier to include 16 more channels and two additional amplifier boxes. We enlarge the acquisition system from 8 to 48 accelerometers by applying a custom switch box which can select 24 adjacent channels at a time. After these improvements, the new setup of the seismic acquisition system is as shown in Figure C.1.

Figure C.1. Schematics of improved acquisition system.

1. Moisture meter placement

24-channel NI-PCI-6251 Digital Acquisition Cards (DAC)
24-channel A/D input for accelerometers
QSC RMX 2450 audio
Etrema CU-18 mechanical vibrator source
24-channel in-house amplifiers
48-channel custom switch box
48 ACH-01 accelerometers

Computer 1
Computer 2

NI-PCI-6251 DAC
6 WL400 Water Level Sensors

5 EC-5 Soil Moisture Sensors
1.1 Five moisture meters are inserted near the middle monitoring well at five different depths at $9 \pm 1$ cm intervals starting from $9 \pm 1$ cm above the bottom of the sand tank (Figure C.2). The moisture meters are placed horizontally with the center of each meter $96 \pm 2$ cm away from the North wall of the sand tank (Figure C.3).

Figure C.2. Five moisture meters buried at various depths.

Figure C.3. Overhead picture of the sand tank with 5 wells (in white) looking North. The yellow cables in each well are connected to five pressure and temperature sensors.
1.2 Five moisture meters are connected to a terminal box (Figure C.4). The terminal card for the moisture meters is connected to one PCI-based acquisition card (Figure C.1) that is installed in a computer.

2. Pressure-Temperature (P-T) sensor placement

2.1 Five P-T sensors are placed in each of the five monitoring wells (Figure C.2) and one P-T sensor in the water away from the sand body.

2.2 Six P-T sensors are connected to a terminal box (the same box as for the moisture meters). The terminals for P-T sensors are connected to a second PCI-6251 acquisition card in a computer.

3. Seismic acquisition system connection

3.1 Forty-eight accelerometers (Figure C.4a) are connected to 48 input channels on the switch box (Figure C.4b). The 24 output channels on the switch box are connected to a total of 24 input channels on the three amplifiers (Figure C.4c). Each amplifier has eight input channels. Eight output channels on each amplifier are connected to eight input channels on each terminal box of the acquisition card (Figure C.4c). There are a total of three terminal boxes connected to three acquisition cards that installed in a computer (Figure C.4c).

3.2 Two 12V batteries are connected for each of the three amplifiers for the accelerometers.

3.3 An output channel on one of the terminal boxes is connected to the amplifier for the mechanical vibrator. The mechanical vibrator is connected to its audio amplifier (Figure C.4c).

4. Geometric layout of accelerometers and shots (Figure 4.1 in Chapter 4)
4.1 For the P-wave seismic survey, there are 24 sensors (P-wave/vertical sensors) connected to even channels of the switch box. The switch box is a self-designed box to select half of the 48 channels at once (Figure C.4b). The P-wave vibration source is placed vertically, while P-wave sensors lay out in a row with their sensitive sides facing down (Figure C.5a). The row of P-wave sensors is parallel to the North wall of the sand tank and 95 ± 1 cm away from the North wall. The distance between each sensor is 1.5 ± 0.1 cm (from center to center) and the total length of sensors is 34.5 ± 0.5 cm (from center to center). The center of the first sensor (on the west end) is 205 cm away from East Wall of the sand tank (Figure C.5). Sensors are buried 3 ± 0.1 cm from the top of the sand (measured from the center of sensor).

Figure C.4. The seismic acquisition system with (a) 48 accelerometers connected to (b) the switch box and then connected to (c) the amplifiers (white) and terminal boxes (grey cubes) for acquisition cards (in the silver computer). The amplifier (black) is for output signal to the vibration source.
4.2 For the S-wave seismic survey, the other 24 sensors (S-wave/horizontal sensors) are connected to odd-numbered channels of the switch box. The S-wave vibration source is placed vertically, while S-wave sensors lay out in a row with their detector sides placed horizontally (Figure C.5b). The row of S-wave sensors is parallel to the North wall of the sand tank and 98 ± 1 cm away from the North wall. The distance between each sensor is 1.5 ± 0.1 cm (from center to center) and the total length of sensors is 34.5 ± 0.5 cm (from center to center). The center of the first sensor (on the west end) is 205 cm away from East Wall of the sand tank (Figure C.6). Sensors are buried 3 ± 0.1 cm from the top of the sand (measured between the centers of each sensor). The sand body is 55 cm thick.

![Figure C.5. The layout for shot 1 of (a) the P-wave and (b) the S-wave seismic survey.](image)

4.3 There are six shots for each pseudo-walk-away seismic survey. The tip of the vibration source (measured from its center) is buried at 3 ± 0.1 cm from the top of the sand for both P- (Figure C.5a) and S- wave survey (Figure C.5b). Shot points are spaced 36 cm apart. The offset between the 1st shot and the 1st sensor is three cm (Figure C.5).

6. A reference seismic survey in the air-dry sand tank (three month)

6.1 During the P-wave seismic survey, even-numbered channels are selected on the switch box. The vibration source is placed vertically in the same row as the P-wave sensors. A pseudo-walk-away P-wave seismic survey is conducted for a total of six shots
(Figures C.5a and C.6a). P-wave seismic signals are vertically (time-wise) stacked 10 and 100 stacks.

6.2 During the S-wave seismic survey, odd-numbered channels are selected on the switch box. The vibration source is placed horizontally in the same row as S-wave sensors. A pseudo-walk-away S-wave seismic survey is conducted for a total of six shots (Figures C.5b and C.6b). S-wave seismic signals are vertically (time-wise) stacked 10 and 100 stacks.

![Figure C.6](image1.png)  
Figure C.6. The layout for shot 6 of (a) the P-wave and (b) the S-wave seismic survey.

7. Seismic surveys during the imbibition and drainage

7.1 During the imbibition, we increase water levels six times. A ruler is used to measure estimated depths of water in each well over time until water in the wells reaches equilibrium (2-4 h) before the experiment for that water level begins. Water levels are then recorded with 5 pressure-temperature (P-T) sensors in 5 monitoring wells. Accurate water levels are the average of recorded readings by P-T sensors. Water levels are 7 cm at water level 1 (WL1), 20 cm for WL2, 29 cm for WL3, 36 cm for WL4, 40 cm for WL5, and 46 cm for WL6 (Figure C.7).

7.2 During the drainage, we decrease water levels five times from WL6 in wetting tests. After water is drained from the sand tank, a ruler is used to measure estimated
depths of water in each well over time until water in the wells reaches equilibrium (2-24 h). Accurate water levels are the average of recorded readings from pressure-temperature sensors in 5 monitoring wells. Water levels are 5 cm for WL7, 27 cm for WL8, 19 cm for WL9, 13 cm for WL10, and 2 cm for WL11 (Figure C.8).

7.3 At each water level, we repeat Step 6.1 to conduct P-wave pseudo-walk-away seismic surveys when water reaches equilibrium in all five wells.

7.4 At each water level, we repeat Step 6.2 to conduct S-wave pseudo-walk-away seismic surveys when water reaches equilibrium in all five wells.

Figure C.7. Wetting tests for (a) WL 1 at 7cm; (b) WL 2 at 20cm; (c) WL 3 at 29cm; (d) WL 4 at 36cm; (e) WL 5 at 40cm; (f) WL 6 at 46cm.
Figure C.8. Drainage tests for (a) WL 7 at 35cm; (b) WL 8 at 27cm; (c) WL 9 at 19cm; (d) WL 10 at 13cm; (e) WL 11 at 2cm.

References

APPENDIX D: THE CALIBRATION OF EC-5 MOISTURE Meters

The following explains the calibration of EC-5 moisture meters using in-situ sands. Procedure is revised from Dane and Topp (2002) and Czarnomski et al. (2005).

1. Equipment needed

1.1 A shovel and a ruler (length is 1m): For removal of soil above the depth that is measured.

1.2 A homemade volumetric soil sampler (volume is $V_{\text{sample}}$) with a flat cap: The volumetric soil sampler is used to sample a known volume ($V_{\text{sample}}$) soil from the in-situ soil near the EC-5. The homemade soil sampler is made from a centrifuge tube by cutting the sharp end off and sharpen the edge of the cut off end.

![A homemade volumetric soil sampler](image)

Figure D.1. A homemade volumetric soil sampler.

1.3 Fifty plastic centrifuge tubes. The total sample number is 100, because: (1) there are 5 sensors; (2) Each sensor with be calibrated for 5 different depths; (3) For each depth, 2 samples will be collected; (4) The calibration will run once in relatively dry sand and once in relatively wet sand. The deformation temperature for the centrifuge tube is ~90°C, while the melting point is ~122°C.

1.4 A scale (Figure D.2).
Figure D.2. A scale with a precision of $10^{-4}$g.

1.5 A drying oven that can maintain a relatively stable temperature at 85°C.

1.6 An icing knife to wipe off excess sand from the edge of the volumetric meter.

A funnel and a glass stir rod to transfer sand from volumetric meter to centrifuge tube (Figure D.3).

![Figure D.3. (a) An icing knife, and (b) a funnel and a glass stir rod.](image)

2. In the relatively dry sand tank, collect readings from moisture meters and soil samples (This procedure is to calibrate the sensor when the upper 0-10cm sand is air-dry with residual water)

2.1. Drain the sand tank and leave the sand tank dry in room temperature until the upper 0-10cm sand is air-dry. Pre-weigh the 50 centrifuge tubes ($M_{\text{tube1}}$, Figure D.4).
Figure D.4. Pre-weigh the centrifuge tubes to measure $M_{\text{tube1}}$.

2.2. In the drained sand tank, choose five sample locations on the uppermost part where the experiments will be conducted. The area for each location is a 1*1m square to avoid interference when dig down to the sand at depth. The 5 sample locations are located between monitoring wells. Insert the five EC-5 moisture meters in the middle of the 1*1m squares vertically into the 0-10cm sands (Figure D.5). Wait for one minute before take any measurements. Measure the voltage output of each sensor three times by reading the voltage after every one minute for three minutes. Take an average of the three readings and write down as “Avg. reading 0-10cm (mV)”.

Figure D.5. EC-5 measurement in sand at the depth of 0-10 cm: (a) during the insertion of one sensor, and (b) after all sensors are inserted.
2.3. Without removing the moisture meter, use the homemade volumetric soil sampler to collect 2 samples. To collect sample, first vertically insert the volumetric soil sampler into the sand 3 cm away from the moisture meter. 3 cm is chosen because the effect range of the moisture meter is up to 5 cm away from it. The soil 3 cm away is also less disturbed by inserting the moisture meters than that closer to the moisture meters. Use hand to push the sampler down until the sand overflows the top end of the sampler. Use the icing knife to remove the excess soil above the sampler. Carefully remove the soil surrounding the top of the sampler and use a flat cap to cap the sampler. To retrieve the sampler and intact sand core, remove the sand surrounding the sampler and cap one end of the sampler. Place a hand underneath the sampler and use palm to hold up the sampler (make sure sand in palm flows over the edge). Get the sample out and flip the sampler upside down attempting to not disturb the packing. Use the icing knife to remove the excess sand above the sampler (Figure D.6).

2.4 To transfer sand from the sampler to a tube, pour the sand through the funnel into pre-weighed centrifuge tube (tap the funnel and tube to make sure no material is left in the funnel). Cap the tube after transferring the sand and label the tube.

2.5. Pull out the moisture meter. Use the shovel to remove the 0-10 cm sand and use a ruler to help measure the depth range of the sand.

2.6. Repeat Step 2.2-2.5 for the depth range of 10-20 cm, 20-30 cm, 30-40 cm, 40-50 cm in the sand (Figure D.7).

2.7 Weigh the wet samples in the centrifuge tubes ($M_{\text{wet}}$).
Figure D.6. Detail process of in-situ sand sample collection from top to bottom and left to right.

Figure D.7. EC-5 measurement in sand at the depths of (a) 10-20 cm, (b) 20-30 cm, and (c) 30-40 cm. The dark color sand shown at the depths of 20-30 cm and 30-40 cm has more moisture than the light color sand.
2.8 Dry the 50 samples in the centrifuge tube in the oven at 85°C for 24h (Figure D.8). Cap the tubes as soon as removed from the oven and wait for the samples to cool down to room temperature before weighing.

Figure D.8. The drying process for (1) placing 50 samples on a rack, (2) removing caps, and (3) drying samples in the oven.

2.9 Weigh dry samples in pre-weighed centrifuge tubes ($M_{\text{dry}}$).

2.10 Pour the 50 samples in the centrifuge tube out.

3. In the relatively wet sand tank, collect readings from moisture meters and soil samples. This procedure allows a larger water content range for the calibration of moisture sensors.

3.1. Fill the sand tank with water to about 50 cm and wait for 26h (Figure D.9). The water in the monitoring well is 38cm. Pre-weigh the 50 centrifuge tubes ($M_{\text{tube2}}$).

Figure D.9. The sand tank filled with ~50 cm water.

3.2 Repeat Steps 2.2-2.10 (Figure D.10).
Figure D.10. Sample collection in wet sand from (a) to (c).

4. Calculations

Volumetric water content for the 50 samples first put into a centrifuge tube:

\[ V_{\text{MC}} = \frac{V_{\text{water}}}{V_{\text{sampler}}} \] \hspace{1cm} (D-1)

\[ V_{\text{water}} = \frac{(M_{\text{wet}} - M_{\text{dry}})}{\rho_{\text{water}}} \] \hspace{1cm} (D-2)

where \( V_{\text{sampler}} \) is the volume of the homemade volumetric sampler, \( M_{\text{wet}} \) is the weight of the wet soil and in the plastic bag, \( M_{\text{dry}} \) is the weight of the dry soil and tube with lid on.

5. Results

The results of the moisture sensor calibration are shown in Figure D.11 and Table D.1. The first five equations are self-calibrated using the sand in the sand tank, while the manufacturer’s calibration is given by the Decagon Manual. The calibration of each sensor is similar to the manufacturer’s calibration, but not exactly the same (Figure D.11f). The experimental error during the VWC measurement is less than 6%. The experimental error source is expected to be related to sample loss during sampling and transferring. The sampling error is less than 5%. In damp sand, there is a less than 1mm gap between the volumetric sampler tube and the sand sample because of the cohesion of the sand grain is relatively larger in damp sand. The overestimation in volume may lead to the underestimation in the measurement in dry bulk density and porosity in damp sand. There will be also less than 1% error because some water may be left in the sampler and funnel during transportation from sampler to the tube, especially for the wetter samples.
The error introduced into the procedure by manual handling of sample is much larger than the error produced by the electronic weighing of sample.

Figure D.11. The samples and trend line for moisture sensor calibration: (a) to (e) are the calibration for sensor 1-5, and (f) is the comparison of the calibration between difference sensors and factory calibration.
Table D.1. The calibration of the EC-5 sensors.

<table>
<thead>
<tr>
<th>EC-5 sensors</th>
<th>Calibration equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensor 1</td>
<td>\text{VWC} = 0.9921 \times \text{Voltage (V)} - 0.3704</td>
</tr>
<tr>
<td>Sensor 2</td>
<td>\text{VWC} = 1.3595 \times \text{Voltage (V)} - 0.513</td>
</tr>
<tr>
<td>Sensor 3</td>
<td>\text{VWC} = 1.1381 \times \text{Voltage (V)} - 0.4164</td>
</tr>
<tr>
<td>Sensor 4</td>
<td>\text{VWC} = 1.2775 \times \text{Voltage (V)} - 0.4673</td>
</tr>
<tr>
<td>Sensor 5</td>
<td>\text{VWC} = 1.0625 \times \text{Voltage (V)} - 0.3745</td>
</tr>
<tr>
<td>Factory calibration</td>
<td>\text{VWC} = 1.16 \times \text{Voltage (V)} - 0.481</td>
</tr>
</tbody>
</table>

References


APPENDIX E: BULK DENSITY MEASUREMENTS FOR IN-SITU SAND

The following bulk density measurements are conducted for in-situ sand in our sand tank (Chapter 4). The procedure is revised from Dane and Topp (2002).

1. Equipment preparation

   The same as Step 1 in the Calibration for EC-5 Moisture Meters (Appendix D).

2. Collect soil samples -- In the relatively dry sand tank

   The same as Step 2 in the Calibration for EC-5 Moisture Meters (Appendix D).

3. Oven dry soil samples and measure the weight of dry samples

   The same as the Step 2.7-2.9 in the Calibration of EC-5 Moisture Meters (Appendix D).

4. Calculations

   Bulk density of dry sand:

   \[ \rho_{\text{dry}} = \frac{(M_{\text{dry}} - M_{\text{tube1}})}{V_{\text{Sampler}}} \]  \hspace{1cm} (E-1)

   where \( V_{\text{Sampler}} \) is the volume of the homemade volumetric sampler, \( M_{\text{dry}} \) is the weight of the dry soil and tube with lid on, \( M_{\text{tube1}} \) is the weight of the centrifuge tube with lid on.

   Porosity of dry sand:

   \[ \rho_{\text{dry}} = (1 - \Phi) \times \rho_{\text{quartz}} \]  \hspace{1cm} (E-2)

   where \( \Phi \) is the porosity, \( \rho_{\text{quartz}} \) is the density of quartz.

   From equation E-2, we can get porosity of dry sand:

   \[ \Phi = 1 - \frac{\rho_{\text{dry}}}{\rho_{\text{quartz}}} \]  \hspace{1cm} (E-3)

5. Results

   The results of the bulk density are shown in Table E.1. The average bulk density is 1.53 g/cm\(^3\) and the error is less than 6%. The bulk density varies with depth and the
variation is less than 5%, which is within the experimental error. The average porosity of the dry sand is 42%. The experiment error source is the same as explained in Appendix D.

Table E.1. The bulk density of sand in the sand tank.

<table>
<thead>
<tr>
<th>Depth</th>
<th>Density (Sensor 1) (g/cm³)</th>
<th>Density (Sensor 2) (g/cm³)</th>
<th>Density (Sensor 3) (g/cm³)</th>
<th>Density (Sensor 4) (g/cm³)</th>
<th>Density (Sensor 5) (g/cm³)</th>
<th>Average dry bulk density (g/cm³)</th>
<th>Average Porosity (air-dry)</th>
<th>Porosity (wet)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-10 cm</td>
<td>1.530</td>
<td>1.595</td>
<td>1.561</td>
<td>1.547</td>
<td>1.578</td>
<td>1.562</td>
<td>0.410</td>
<td>0.371</td>
</tr>
<tr>
<td>10-20 cm</td>
<td>1.494</td>
<td>1.540</td>
<td>1.518</td>
<td>1.585</td>
<td>1.586</td>
<td>1.545</td>
<td>0.417</td>
<td>0.434</td>
</tr>
<tr>
<td>20-30 cm</td>
<td>1.499</td>
<td>1.483</td>
<td>1.498</td>
<td>1.482</td>
<td>1.458</td>
<td>1.484</td>
<td>0.440</td>
<td>0.469</td>
</tr>
<tr>
<td>30-40 cm</td>
<td>1.561</td>
<td>1.601</td>
<td>1.538</td>
<td>1.532</td>
<td>1.504</td>
<td>1.547</td>
<td>0.416</td>
<td>0.459</td>
</tr>
<tr>
<td>Average</td>
<td>1.521</td>
<td>1.555</td>
<td>1.529</td>
<td>1.537</td>
<td>1.531</td>
<td>1.535</td>
<td>0.421</td>
<td>0.433</td>
</tr>
</tbody>
</table>

References

APPENDIX F: GRAIN SIZE ANALYSIS

The following is grain size analysis results of the sand tank in Chapter 4.

Before homogenization, there were three to four layers in the sand tank (Figure F.1). Four samples have been taken for each layer for grain size analysis (Table F.1).

![Figure F.1. Cross-section of the pre-homogenized sand tank. Four layers can be recognized and are labeled from top to bottom as dark brown sand, light brown sand, reddish brown sand and white sand (in a patch). Solid lines represent boundaries that we interpreted with more confidence, while dashed lines are estimated boundaries and dashed lines with question marks are unsure boundaries we interpreted with less confidence.](image)

During homogenization of the sand tank, the sand is “homogenized” using shovels with a blade size of ~0.15×0.2 m. After the homogenization, we collect 10 samples from various depths and locations in the sand tank for grain size analysis (Table F.1).

The grain size was analyzed by Dr. Cristina Gama, a visiting Fulbright scholar in the Coastal Studies Institute at LSU. Before doing the grain size analysis, the sand sample
is oven-dried at 30°C. The equipment for grain size is Gilson-Autosiever. The result is shown in Table F.1.

Table F.1. Statistical parameters of grain size (Folk and Ward, 1957) by sand sieve analysis. Sample 1 to 4 are dark brown sand, light brown sand, reddish brown sand and white sand, respectively. Sample 5 to 14 are homogeneous sand.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Mean (mm)</th>
<th>Mean (phi)</th>
<th>Sorting</th>
<th>Skewness</th>
<th>Kurtosis</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.339303919</td>
<td>1.55935</td>
<td>0.50271</td>
<td>-0.05406</td>
<td>1.00922</td>
</tr>
<tr>
<td>6</td>
<td>0.333828724</td>
<td>1.58282</td>
<td>0.49264</td>
<td>-0.04258</td>
<td>1.04724</td>
</tr>
<tr>
<td>7</td>
<td>0.342280261</td>
<td>1.54675</td>
<td>0.52116</td>
<td>-0.063</td>
<td>1.02432</td>
</tr>
<tr>
<td>8</td>
<td>0.347349518</td>
<td>1.52554</td>
<td>0.497</td>
<td>-0.02641</td>
<td>0.97075</td>
</tr>
<tr>
<td>9</td>
<td>0.357191586</td>
<td>1.48523</td>
<td>0.54523</td>
<td>-0.14979</td>
<td>1.01593</td>
</tr>
<tr>
<td>10</td>
<td>0.345610751</td>
<td>1.53278</td>
<td>0.50482</td>
<td>-0.04576</td>
<td>0.99724</td>
</tr>
<tr>
<td>11</td>
<td>0.337294337</td>
<td>1.56792</td>
<td>0.49256</td>
<td>-0.04177</td>
<td>1.02035</td>
</tr>
<tr>
<td>12</td>
<td>0.341204836</td>
<td>1.55129</td>
<td>0.49328</td>
<td>-0.03972</td>
<td>1.00075</td>
</tr>
<tr>
<td>13</td>
<td>0.340354479</td>
<td>1.55489</td>
<td>0.4877</td>
<td>-0.04146</td>
<td>0.98799</td>
</tr>
<tr>
<td>14</td>
<td>0.344735075</td>
<td>1.53644</td>
<td>0.48772</td>
<td>-0.03827</td>
<td>0.98525</td>
</tr>
</tbody>
</table>

1. Mean

Mean grain sizes and sorting are expressed in phi (φ) units. Krumbein (1934) redefined grain size using what was termed phi (φ) grain size:

$$\phi = - \log_2 d$$

(F-1)
or

\[ d = 2^{-\phi} \]  \hspace{1cm} (F-2)

where \( \phi \) is the Krumbein phi scale (Krumbein, 1934), \( d \) is the diameter of the particle in millimeter.

An estimate of the mean particle size (Folk and Ward, 1957) is:

\[ M = \frac{\phi_{16} + \phi_{50} + \phi_{84}}{3} \]  \hspace{1cm} (F-3)

where \( \phi_{16}, \phi_{50} \) and \( \phi_{84} \) are the phi size corresponding to the 16%, 50% and 84% marks on the cumulative frequency distribution curve, respectively. They represent the percentage of the sample that is coarser than the particular phi size.

Based on Folk and Ward (1957) grain size parameters, the mean grain size indicates the sands are medium sand. The mean varies from 0.33 to 0.38mm in the sand tank before homogenization, while the means are between 0.33 to 0.35mm in homogenized sand.

2. Sorting/Standard Deviation

Sorting is the measure of degree of scatter. The standard deviation is then a measure of sorting. The inclusive graphic standard deviation is found by the formula (Folk and Ward, 1957):

\[ \sigma_\phi = \frac{\phi_{84} - \phi_{16}}{4} + \frac{\phi_{95} - \phi_{5}}{6.6} \]  \hspace{1cm} (F-4)

where \( \phi_{5}, \phi_{16}, \phi_{84}, \) and \( \phi_{95} \) are the phi size corresponding to the 5%, 16%, 84% and 95% marks on the cumulative frequency distribution curve, respectively. They represent the percentage of the sample that is coarser than the particular phi size.
Before homogenization, the sorting for the sand is moderate well (Sample 1 and 2) to well (Sample 3 and 4) sorted. The homogenized sands tend to have better sorted cases (Sample 6, 8, 11-14), but still have some moderate sorted cases (Sample 5, 7, 10).

3. Skewness

The skewness is the measure of the degree of lopsidedness. A normal distribution, which is perfectly symmetrical curve, the skewness is 0. The inclusive graphic skewness is estimated by (Folk and Ward, 1957):

\[ SK_\phi = \frac{\phi_{16} + \phi_{84} - 2\phi_{50}}{2(\phi_{84} - \phi_{16})} + \frac{\phi_{5} + \phi_{95} - 2\phi_{50}}{2(\phi_{95} - \phi_{5})} \] (F-5)

where \( \phi_{5}, \phi_{16}, \phi_{50}, \phi_{84}, \) and \( \phi_{95} \) are the phi size corresponding to the 5%, 16%, 50%, 84% and 95% marks on the cumulative frequency distribution curve, respectively. They represent the percentage of the sample that is coarser than the particular phi size.

For a normal distribution, which has a perfectly symmetrical curve, the skewness is 0. A positive skewness indicates that the samples are weighted towards the coarse sizes. A negative skewness indicates that the samples weighted towards the finer sizes.

In the sand tank, skewness shows that before homogenization, sands are coarser in part of the sand tank (Sample 1 and 2) and are finer in other part of the sand tank (Sample 3). The distribution of the homogenized sand is symmetric (except Sample 9).

4. Kurtosis

Kurtosis is the degree of peakedness. Many curves have the normal skewness value, but turn out to be non-normal when the kurtosis is computed. Kurtosis measures the ratio of the sorting in the extremes of the distribution compared with the sorting in the central part. The graphic kurtosis is given by the formula (Folk and Ward, 1957):

\[ K_\phi = \frac{\phi_{95} - \phi_{5}}{2.44(\phi_{75} - \phi_{25})} \] (F-6)
where $\phi_5$, $\phi_{25}$, $\phi_{75}$, and $\phi_{95}$ are the phi size corresponding to the 5%, 25%, 75%, and 95% marks on the cumulative frequency distribution curve, respectively. They represent the percentage of the sample that is coarser than the particular phi size.

For a normal distribution, the graphic kurtosis is 1. Kurtosis is sensitive and valuable test of the normality of a distribution. Even when many curves have a normal skewness value, they turn out to be non-normal when the kurtosis is computed. If the kurtosis is greater than 1, the curve is relatively better sorted in the central area than in the tails. Curves that are more peaked than the normal distribution curve are termed "leptokurtic" (Folk and Ward, 1957). If the kurtosis is less than 1, the distribution curve is called "platykurtic" (Folk and Ward, 1957).

The sand tank grain size distribution tends to be “platykurtic” before homogenization, while the homogenized sand grain size distribution tends to be more “leptokurtic”.

As the result of the sand grain size distribution shows, the homogenization of the sand effectively to narrow the range of the mean, keep the well sorted sand, make the distribution symmetric, and make the distribution more concentrated to the peak.

References


Krumbein, W. C., 1934, Size frequency distributions of sediments: Journal of sedimentary Research, 4, no. 2.
APPENDIX G: XRD ANALYSIS

The following are the X-ray diffraction (XRD) analysis results of the sand composition in sand tank in Chapter 4.

In average, the sand is composed of ~98% of quartz, ~1% of K-feldspar and ~1% of plagioclase (Table G.1). Some coal, plastic and glitter can be also found (estimated <0.1%), but the amorphous materials are not detected by XRD analysis.

Table G.1. Sand composition determined from XRD analysis for Sample 5-14 (in Appendix F) from “homogenized” sand tank.

<table>
<thead>
<tr>
<th>After Homogeneous</th>
<th>Quartz (%)</th>
<th>K-feldspar (%)</th>
<th>Plagioclase (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample 5</td>
<td>98.6766</td>
<td>0.7349</td>
<td>0.5885</td>
</tr>
<tr>
<td>Sample 6</td>
<td>98.2924</td>
<td>1.0214</td>
<td>0.6863</td>
</tr>
<tr>
<td>Sample 7</td>
<td>98.848</td>
<td>0.6224</td>
<td>0.5296</td>
</tr>
<tr>
<td>Sample 8</td>
<td>97.1667</td>
<td>1.6509</td>
<td>1.1824</td>
</tr>
<tr>
<td>Sample 9</td>
<td>97.2693</td>
<td>1.2604</td>
<td>1.4703</td>
</tr>
<tr>
<td>Sample 10</td>
<td>98.051</td>
<td>1.137</td>
<td>0.812</td>
</tr>
<tr>
<td>Sample 11</td>
<td>97.7481</td>
<td>1.0006</td>
<td>1.2513</td>
</tr>
<tr>
<td>Sample 12</td>
<td>98.1944</td>
<td>1.0474</td>
<td>0.7581</td>
</tr>
<tr>
<td>Sample 13</td>
<td>97.9672</td>
<td>0.9769</td>
<td>1.0559</td>
</tr>
<tr>
<td>Sample 14</td>
<td>97.4112</td>
<td>1.0532</td>
<td>1.5356</td>
</tr>
<tr>
<td>Average</td>
<td>97.96249</td>
<td>1.05051</td>
<td>0.987</td>
</tr>
</tbody>
</table>

The XRD analysis and preparation were conducted by Wanda LeBlanc, a researcher in the LSU X-ray diffraction & geochemistry lab. The process of sample preparation and XRD is the following:

1. Sample preparation:
   (1) 2 grams of sample was weighed.
   (2) The weighed samples were pass through a 30 mesh sieve.
   (3) The weighed sample that did not pass through the sieve was hand ground in a corundum mortar and pestle until it passed through the 30 mesh sieve.
   (4) The 2 grams of sample were then placed in the McCrone microcronizer
grinding jar for grinding.

(5) 10 ml of ethanol was added to the McCrone grinding jar.

(6) The samples was ground for three minutes.

(7) The samples was poured out of the jar into a centrifuge tube.

(8) Additional ethanol was used to retrieve all the samples.

(9) The centrifuge tube was then placed in a low speed centrifuge.

(10) The sample was centrifuged for 20 minutes at 2500 rpm.

(11) The excess ethanol was poured out of the centrifuge tube.

(12) The centrifuge tube was placed in a 60 degree oven overnight to dry.

(13) The sample was then allowed to come to room temperature.

(14) The sample was mixed to be homogeneous.

(15) The sample was then poured into side mount aluminum holders.

2. XRD test:

(1) The samples were placed in the Bruker/Siemens D5000 diffractometer.

(2) Samples were run from 3 degrees to 75 degrees at a 0.04 degree/ 2.00 second scan

(3) The diffractometer ran at 30 kV and 40 mA.

3. Result analysis:

(1) The completed samples were processed using Jade 6 software.

(2) The quantitative concentrations were calculated utilizing XRDPHil a program developed for Dr. Ray Ferrell, Jr. (Cook et al., 1975). In XRDPHil, any concentration below 10% has a 20% uncertainty, and any concentration above 10% has a 10% uncertainty.
References

**VITA**

Jie Shen, a resident of China, completed a Bachelor's of Science in Resource Exploration at China University of Geosciences in Beijing, completing a thesis on Analysis of Inversion Structures in Bongor Basin, Chad. After college, Jie was inspired by her grandfather, who is a noted geologist in China, to continue the pursuit of a Ph.D. in geology and geophysics. During graduate school, Jie maintained a 3.9 GPA, but was still able to pursue educational extracurricular activities as well. Jie has presented her research at several conferences, has participated in the Imperial Barrel Award competition, and took an internship during the third summer at Shell Exploration & Production Company in New Orleans, Louisiana, where she has accepted a full time offer upon completion of her doctoral work.