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Comparing geophysical measurements to theoretical estimates for soil mixtures at low pressures

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Introduction

Interpretation of geophysical data collected at contaminated sites involves using relationships between measured geophysical properties such as seismic velocity and electrical conductivity, and desired hydrogeological parameters such as porosity and saturation. Empirical relationships developed in the oil industry (e.g., Wyllie et al., 1956, 1958) and theoretical relationships developed for consolidated rocks (e.g., Kuster and Toksöz, 1974) are inappropriate for most environmental applications since the depths involved are a few meters to a few hundred meters and the sediments are unconsolidated.

Developing appropriate relationships linking geophysical properties to fluid-flow properties is a key step in developing a technique for inverting geophysical field data for direct estimation of porosity, permeability, and saturation rather than inverting for seismic velocities or electrical conductivity. Solutions to the forward problem can be used to develop algorithms for the direct inversion.

Empirical relationships between geophysical and hydrogeological properties can be developed by making use of literature data for laboratory (e.g., Domenico, 1976; Chan and Knight, 1998) and field (e.g., Ramirez et al., 1993; Steeples et al., 1998) measurements of sediment properties. Literature data are sparse for elastic properties measurements, although recent measurements (Bonner et al., 1997, 1998; Trombino, 1998) contribute significantly to the available information on shear velocities in the top few meters of the subsurface where attenuation is high and measurements are difficult. Theoretical relationships have the advantage of not requiring extensive databases, since they rely on the physics of the problem rather than on the statistics of the material behavior.

In this paper, we focus on developing theoretical relationships for describing the elastic properties of the shallow subsurface. This work is part of a larger project for devoping a method for joint, direct inversion of elastic and electrical properties measurements to obtain hydrogeological parameters. Electrical properties are investigated elsewhere (Wildenschild et al., 1998).

Mixture Theories for Elastic Properties

The elastic properties of a rock or sediment depend on the elastic properties of the components, the relative volumes of the components making up the rock or soil, and the microstructure. If all the elastic properties and relative volumes of the component minerals and pore fluids and air are known, the properties of the whole rock or sediment can be estimated using a mixture theory. Some of the theoretical methods (e.g., Voigt, 1928; Reuss, 1929; Hashin, 1962; Hashin and Shtrikman, 1963) do not require an explicit description of the microstructure, and provide upper and lower bounds on elastic properties rather than providing a single estimated value for a given property. Other methods (e.g., Berryman, 1980; Walsh, 1980) require parameters describing some aspect of the microstructure. See Berryman (1995) for an overview of various mixture theories for modeling geophysical properties of multicomponent earth materials.

Theoretical relationships for estimating geophysical properties of sediments must contain microstructural assumptions that are compatible with the actual microstructures of the unconsolidated near-surface materials. For example, the self-consistent effective medium theory of Berryman (1980) treats all components as parts of a cluster of solid and fluid elements rather than as solid inclusions and pores embedded within a solid background material. The Reuss average (Reuss, 1929) contains the implicit assumption that the material being modeled is a fluid. Either of these theories may be useful for estimating elastic properties of unconsolidated materials that do not have a rigid framework.

Sand-Peat Velocity Data

For this investigation of theoretical methods for estimating sediment elastic properties, we used laboratory measurements of compressional and shear velocities of sand-peat mixtures at low pressures (Bonner et al., 1998; Trombino, 1998). Although other laboratory data sets are available in the exploration geophysics, marine geophysics, and soil mechanics literature (e.g., Rao, 1966; Domaschuk and Wade, 1969; Domenico, 1976; Hamilton and Bachman, 1982), few studies include both compressional and shear velocity measurements as a function of pressure at the extremely low pressures representing the shallow subsurface. The laboratory measurements described in Trombino (1998) were made at pressures between 0 and about 16 psi (about 0.1 MPa) in pressure increments of 1.5 psi, and represent the top few meters of the subsurface. Both compressional and shear velocities were measured for a set of samples containing various proportions of Ottawa sand and commercially available peat moss (Trombino, 1998). Such samples may be representative of shallow soils having a high organic content.

Sample construction and laboratory measurement techniques are described in detail in Trombino (1998) and will not be repeated here. Briefly, the samples were made by combining known masses of sand and peat moss in a specially-designed jacket and then velocities were measured by the standard ultrasonic pulse transmission technique (e.g., Sears and Bonner, 1981). The mass fraction of peat in each sample is well-known, but the volume fraction is less certain since the density of peat moss varies with porosity and humidity. Literature values for peat moss density range from about 0.1 to 0.4 g/cm^3 (Carmichael, 1984; Ahrens and Johnson, 1995). The uncertainty in the relative volume of the peat moss in each sample is not expected to affect our modeling results significantly. Samples having peat mass fractions of 0, 1, 3, 10, 20, and 30 percent were constructed (Trombino, 1998) and velocities were measured at room temperature and ambient humidity for nominally dry samples. Measured velocities had typical uncertainties of about 5 to 10 percent. Attenuation was so high in the sample having the most peat (sample 30) that no reliable velocity measurements are available for that sample. Shear velocity measurements are not reliable for the sample having 10 percent peat by mass fraction (sample 10). (Future digital filtering and examination of the data in the frequency domain are expected to yield additional velocity information for signals having high attenuation.) Table 1 presents some of the velocity data after corrections were made to the raw data in Trombino (1998) and Bonner et al. (1998). (Not all available pressures are shown in this table.)

Theoretical Estimates of Sand-Peat Velocities

The microstructure of the pure sand sample (sample 0) and the sample having the lowest volume concentration of peat (sample 1) can be thought of as a collection of lightly-packed sand grains, with occasional peat particles filling in some pore space or replacing some sand grains in sample 1. The samples having the highest concentrations of peat (sample 20 and sample 30) have microstructures that can be thought of as closely-packed blobs of porous peat separated by some air-filled pores and containing isolated sand grains. The sand grains cannot form a continuous network after the sand concentration drops below about 60 percent by volume, since that is the concentration at which a packing of uniform spheres would become disconnected (e.g., Bernal and Mason, 1960). The samples having intermediate amounts of peat (sample 3 and sample 10) have microstructures such that the peat gradually fills pore space in the sandpack, reducing the sand porosity without significantly reducing the total amount of air space in a sample and without causing the sand grains to become isolated from each other. We used the density of quartz, 2.65 g/cm^3 (e.g., Wilkens et al., 1984), and of the solid component of peat moss, 1.57 g/cm^3 (Carmichael, 1984), to find the relative amounts of quartz, air, and the solid component of peat in the sand-peat samples, and also give estimates of the densities and porosities of the sand and peat components of the samples in Table 2.

In addition to knowing relative volumes of component materials, for our theoretical estimates of the sand-peat sample velocities we need to know the elastic properties of the components. The bulk and shear moduli and densities of quartz (38 GPa, 44 GPa, 2.65 g/cm^3) and of air (0.000152 GPa, 0, 0.00129 g/cm^3) are well-known (e.g., Wilkens et al., 1984; Weast and Astle, 1982). We do not have estimates of the bulk and shear moduli for peat moss. Since most minerals have bulk and shear moduli that lie in the range of about 5 to 100 GPa, we can try various values such as 5, 10, and 20 GPa for the bulk and shear moduli of the solid component of peat to find out how much the results will depend on the exact values of these moduli. Alternatively, we can assume that the moduli can be approximated by using moduli values calculated from the measured velocities of sample 20, which has a high concentration of peat.

The theoretical methods that we used for this paper were the Hashin-Shtrikman bounds (Hashin and Shtrikman, 1963), the Voigt and Reuss averages (Voigt, 1928; Reuss, 1929), which are also strict upper and lower bounds, and Berryman's (1980) self-consistant effective medium theory. See Berge et al. (1995) for a discussion of microstructural considerations for these various methods. See Berryman (1995) for mathematical expressions for velocities and moduli for these methods. Table 3 presents the compressional and shear moduli estimates found for the peat moss samples using these methods. (Note that no particular pressure is specified for these estimates since they use only moduli and volume concentrations of component solids and air, which do not vary significantly at low pressures.) The values used for the bulk and shear moduli of the solid component of peat moss for the results presented in the table were 10 GPa for both moduli. We also tried using values of 5 GPa and 20 GPa in various combinations for both moduli. We found that the resulting estimates were not very sensitive to the exact values used for the peat moduli, and the results shown in the table are typical.

Discussion

The Hashin-Shtrikman bounds (HS+ and HS- in Table 3) provide strict upper and lower limits on the velocities. Comparison of these values with the measured velocities in Table 1 shows that the bounds do lie above and below the measured velocities as expected, but are so far apart that they do not provide useful estimates of the measured velocities. The bounds lie far apart for any material containing solids and gases (e.g., Berge et al., 1995). Note, however, that the lower bounds on compressional and shear velocities are non-zero for these unconsolidated samples.

The Voigt and Reuss averages (V and R in Table 3) also give strict upper and lower bounds on the velocities. The Reuss average is an exact result for a fluid. These do not provide useful estimates of the measured sand-peat velocities, as they lie even further apart than the Hashin-Shtrikman bound estimates. The measured velocities fall between the Voigt and Reuss averages, as expected. The Reiss average lower bound on shear velocity vanishes because this is the exact result for a fluid.

The self-consistent estimate (SC in Table 3) is too high for the pure sand sample, which has a well-understood microgeometry and well-known component properties. This is a more appropriate model for a loosely-consolidated sandstone than for an unconsolidated sand sample. The SC estimated velocities drop with increasing peat concentration, but are much too low for the highest concentrations of peat, approaching zero (and violating the HS- and V lower bounds) for samples 10 and 20. This implies that the changes being modeled are too extreme, perhaps because the components considered in the microstructure include quartz and air, which have extremely different elastic properties.

After examining the above results, we decided to try applying the self-consistent method again, but using porous peat moss and sand as the basic components of the microstructure instead of using quartz, air, and the solid component of peat. In order to do this, we used the measured velocities and density of sample 0 to obtain bulk and shear moduli and the density for the sand component of the sand-peat samples, and we used the measured velocities and density of sample 20 to obtain the bulk and shear moduli and density for the porous peat component of the sand-peat samples.Here we assumed that sample 20 was entirely composed of peat moss, for the purposes of this SC modeling. We used the relative volume concentrations of sand and peat given in Table 2 for samples 1, 3, and 10 for calculating our new SC estimates of the velocities for these three samples at various pressures. Since the measured velocities were available at several pressures for sample 0 and sample 20, we were able to estimate velocities for samples 1, 3, and 10 at several pressures. The results of this SC modeling are presented together with the observed velocities for comparison, in Table 4.

Conclusions

We obtained good estimates of measured velocities of sand-peat samples at low pressures by using a theoretical method, the self-consistent theory of Berryman (1980), using sand and porous peat to represent the microstructure of the mixture. We were unable to obtain useful estimates with several other theoretical approaches, because the properties of the quartz, air and peat components of the samples vary over several orders of magnitude. Methods that are useful for consolidated rock cannot be applied directly to unconsolidated materials. Instead, careful consideration of microstructure is necessary to adapt the methods successfully. Future work will include comparison of the measured velocity values to additional theoretical estimates, investigation of Vp/Vs ratios and wave amplitudes, as well as modeling of dry and saturated sand-clay mixtures (e.g., Bonner et al., 1997, 1998).

Our results suggest that field data can be interpretted by comparing laboratory measurements of soil velocities to theoretical estimates of velocities in order to establish a systematic method for predicting velocities for a full range of sand-organic material mixtures at various pressures. Once the theoretical relationship is obtained, it can be used to estimate the soil composition at various depths from field measurements of seismic velocities. Additional refining of the method for relating velocities to soil characteristics is useful for developing inversion algorithms.

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Table 1. Measured Velocities in Sand-Peat Samples

Sample	Pressure (psi)*	Vp (m/s)	Vs (m/s)
Sample 0	0	238±5%	126±1%
	1.56	228±5%	127±2%
	3.12	255±3%	138±2%
	6.24	296±3%	178±3%
	7.80	317±5%	184±2%
	15.6	378±5%	218±3%
Sample 1	0	137±8%	---
	1.56	142±7%	---
	3.12	218±%	---
	6.24	194±5%	113±5%
	15.6	240±8%	160±5%
Sample 3	1.56	228±8%	150±4%
	3.12	218±5%	133±3%
	6.24	260±6%	139±5%
	15.6	350±8%	169±4%
Sample 10	0	396±12%	---
	1.56	387±12%	---
	3.12	380±10%	---
	6.24	373±10%	---
	15.6	353±13%	---
Sample 20	6.24	91.3±6%	74.9±5%
	7.80	119±8%	85.2±5%
	15.6	424±15%	110±5%

*1 MPa = 145 psi

Table 2. Relative Volume Concentrations of Sand-Peat Sample Components

Sample	Sample 0	Sample 1	Sample 3	Sample 10	Sample 20	Sample 30
Sample Dens. (g/cm^3)	1.69	1.56	1.45	1.08	0.974	0.840
Sand Rel. Vol.	100%	88±4%	80±4%	40±3%	30±2%	22±2%
Sand Dens. (g/cm^3)	1.69	1.69-1.83	1.69-1.86	2.62-2.65	2.65	2.65
Sand Porosity	36%	31-36%	30-36%	0-1%	0%*	0%*
Peat Rel. Vol.	0%	12±4%	20±4%	60±3%	70±2%	78±2%
Peat Dens. (g/cm^3)	---	0.10-0.18	0.18-0.26	0.18-0.25	0.28-0.36	0.32-0.38
Peat Porosity	---	89-94%	83-89%	84-89%	77-82%	76-80%
Quart Rel. Vol.	0.64	0.583	0.531	0.366	0.294	0.223
Air Rel. Vol.	0.36	0.407	0.441	0.565	0.582	0.618
Peat Solid Rel. Vol.	0	0.00998	0.0277	0.0688	0.124	0.159

*indicates isolated quartz grains

Table 3. Theoretical Estimates of Velocities for Sand-Peat Mixtures

Sample	HS-	HS+	R	V	SC
Sample 0, Vp (m/s)	15.8	5260	15.8	6050	4110
Vs (m/s)	0.00179	3460	0	4090	2640
Sample 1, Vp (m/s)	15.5	5150	15.5	6030	3350
Vs (m/s)	0.00172	3390	0	4080	2110
Sample 3, Vp (m/s)	15.4	5070	15.4	5990	2170
Vs (m/s)	0.00169	3320	0	4050	1340
Sample 10, Vp (m/s)	15.8	4780	15.8	5860	0.0123
Vs (m/s)	0.00165	3110	0	3960	0.00281
Sample 20, Vp (m/s)	16.4	4620	16.4	5680	0.00593
Vs (m/s)	0.00169	3000	0	3830	0.00181

Table 4. SC Estimates of Velocities for Mixtures of Sample 0 Sand and Sample 20 Peat

Sample	Pressure (psi)*	Measured Vp (m/s)	Measured Vs (m/s)	SC Est. Vp (m/s)	SC Est. Vs (m/s)
Sample 1	0	137	---	215	115
	6.24	194	113	268	161
	15.6	240	160	372	234
Sample 3	1.56	228	150	197	106
	6.24	260	139	247	147
	15.6	350	169	373	245
Sample 10	0	396	---	108	51.0
	6.24	373	---	114	55.0
	15.6	353	---	405	310

*1 MPa = 145 psi