Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring

P.A. Berge, J.G. Berryman, H. Bertete-Aguirre, B.P. Bonner, J.J. Roberts and D. Wildenschild

July 31, 2000
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Work performed under the auspices of the U. S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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JOINT INVERSION OF GEOPHYSICAL DATA FOR SITE CHARACTERIZATION AND
RESTORATION MONITORING

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Project Number: 55411
Grant Number: not applicable (DOE Lab; TTP #SF2-7-SP-22, Task A)
Grant Project Officers: not applicable (DOE Lab; Technical Program Officer K. V. Abbott,
DOE Oakland Field Office)
Project Duration: 10/01/96 to 9/30/99

LLNL report number UCRL-ID-128343
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**Relevance, Impact and Technology Transfer**

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Executive Summary

The purpose of this project was to conduct basic research leading to significant improvements in the state-of-the-art of geophysical imaging of the shallow subsurface. Geophysical techniques are commonly used for underground imaging for site characterization and restoration monitoring. In order to improve subsurface imaging, our objective was to develop improved methods for interpreting geophysical data collected in the field, by developing better methods for relating measured geophysical properties, such as seismic velocity and electrical conductivity, to hydrogeology parameters of interest such as porosity, saturation, and soil composition. We met our objectives using an approach that combined laboratory experiments, comparison to available field data, rock physics theories, and modeling, to find relationships between geophysical measurements, hydrogeological parameters and soil composition.

The primary accomplishments of this project in the last year (FY99) were that we completed our laboratory measurements of ultrasonic velocities in soils at low pressures and our measurements of complex electrical conductivity in those same soils; we used x-ray computed microtomography to image the microstructure of several soil samples; we used rock physics theories and modeling to relate the geophysical measurements to the microstructure and hydrological properties; we developed a theoretical technique for relating compressional and shear wave velocities to fluid distribution in porous media; we showed how electrical conductivity is related to clay content and microstructure; we developed an inversion algorithm for inferring soil composition given compressional and shear wave velocities and tested the algorithm on synthetic field seismic data; we completed two patent applications; we wrote three journal papers; and we made 15 presentations of our results at eight scientific meetings.
For the three-year project, we had accomplishments in the laboratory, in theoretical work, in modeling, and in developing an understanding of how to optimize field experiment design and what is actually measured in geophysical field experiments. During the three-year project, we made controlled laboratory measurements of ultrasonic velocities and complex impedances in man-made soils of known compositions under known saturation and pressure (analogous to depth) conditions. We then compared the results to theoretical models, other laboratory measurements from the literature, and to available field data. We investigated the role of microstructure, fluid and clay distribution, and chemical effects on measured geophysical properties. We developed some algorithms to relate certain measured geophysical properties to porosity and some aspects of soil composition and fluid distribution, and tested the algorithms on our laboratory data and synthetic field data. For certain simple cases, we can invert geophysical data to obtain information about porosity, saturation, and soil composition. We have presented the results from the three-year project in five journal papers, two patent applications, 17 presentations at ten scientific meetings, four technical reports, and on our project web site.

Before these results can be applied at DOE sites, further work is needed to investigate complicating factors such as effects of scaling from laboratory to field measurements, partial saturation, heterogeneity in soils at various scales, and technology transfer of research algorithms so that they eventually could be used by site engineers. Some of this work is being continued in a new EMSP project; in particular, the question of partial saturation for application to the vadose zone. We do have, however, some insights into geophysical field experiment design that may be useful for site engineers now.
We gained these insights from our laboratory and theoretical investigations and also from discussions with other geophysicists and site engineers at INEEL and PNNL workshops. Our recommendations for improving designs for geophysical field experiments to image the shallow subsurface are the following: Seismic field experiments should make every effort to collect both compressional and shear wave data because the two types of data can be used together to obtain information about fluid distribution in partially saturated sediments, and the two constitute independent data sets that increase the number of constraints for inversion codes. To minimize casing problems at sites such as Hanford where steel casing in boreholes may reduce the quality of electrical measurements, non-electrical geophysical methods such as seismic or microgravity measurements should be considered, and modeling can be used to optimize the design of any geophysical field experiment before the deployment. In areas where attenuation is expected to be high for a given type of geophysical measurement, measurements made in small sub-arrays can be combined using sophisticated inversion software to build an image beneath the entire field site. Multiple geophysical techniques should be used to characterize sites, since different types of geophysical measurement are sensitive to different characteristics of the subsurface. For complex regions, collecting different types of geophysical field measurements (e.g., electrical resistance tomography and electromagnetic induction tomography) will provide additional independent data sets to better constrain the estimates of subsurface structure and properties.

Details on relevance, impact, and technology transfer for this project may be found in the body of this report. Here we provide a brief summary, to aid DOE and potential research sponsors or future technology users.
The knowledge developed by our basic research in this EMSP project is relevant to critical DOE environmental management problems including needs for improving geophysical methods for subsurface characterization and monitoring in the vadose zone, for tank farms, and for subsurface contamination problems (e.g., statements of need in the DOE EM database: ID-6.1.02, ID-6.1.04, OH-F049, OK99-01, ORHY-03, RL-SS10, RL-SS31, and the PNNL Hanford Ground Water Vadose Zone Integration Project’s needs). The main results of this project are improved relationships between geophysical measurements, hydrological properties and soil composition. The improvements have the potential to reduce the cost and time required for geophysical field data interpretation and the subjectivity of the interpretation, by providing clear connections between what the geophysicist measures (e.g., seismic velocity, electrical conductivity) and what the site engineer needs (porosity, saturation, permeability estimates, soil composition and structure information). This could improve future cleanup costs and schedules by reducing costs and time required for site characterization, and risk would be reduced if the characterization involves less uncertainty due to improved reliability in the mapping between geophysical properties and hydrological properties.

Recommendations for field experiment design that we suggested were incorporated into plans for future geophysical experiments to be conducted at the Hanford site by the Office of River Protection. We are also coordinating work in a new EMSP project in order to collaborate with other EMSP P.I.’s to conduct field experiments at the LLNL Vadose Zone Observatory, at the small (a few meters) field scale.
Results of this project have advanced the understanding of the effects of microstructure, clays, and fluids (including some chemical effects) on measured geophysical properties. In addition to interest from DOE and other national laboratories, this project has generated interest from the California Dept. of Water Resources and various university researchers who want to compare their field measurements of soil elastic properties to our laboratory ultrasonic velocity data, because our lab measurements provide the first direct corroboration of very low velocities seen in field data for the top few meters of the subsurface. The results of this project include two patent applications. The equipment and expertise represented by those patent applications are being used in a new EMSP project (#70108) to further investigate and develop relationships between geophysical properties, hydrological properties and soil composition.
Research Objectives

The purpose of this project was to conduct basic research leading to significant improvements in the state-of-the-art of geophysical imaging for the near surface. The problem of improving subsurface imaging is important for several reasons: geophysical imaging can be used for characterization as well as for restoration monitoring; such imaging is cheaper and less invasive than drilling; and it provides information in areas between boreholes, at scales ranging from cm to km (e.g., Lines et al., 1993; Ramirez et al., 1993, 1995; Mathisen et al., 1995; Wilt et al., 1995a,b).

In order to improve subsurface imaging, our objectives were to develop improved methods for interpreting geophysical data collected in the field, by developing better methods for relating measured geophysical properties, such as seismic velocity and electrical conductivity, to hydrogeology parameters of interest such as porosity, saturation, and sediment composition. We met our objectives using an approach that combined laboratory experiments, rock physics theories, and modeling to find relationships between geophysical measurements, hydrogeological parameters and soil composition. We also compared our laboratory data to available field data.

This work was needed to address several shortcomings in current subsurface imaging practices. For example, current practice does not make use of recent advances in rock physics theories that relate geophysical properties to soil composition and hydrogeology parameters (e.g., Sen and Goode, 1992; Berge et al., 1993; Berryman, 1995). Current methods of combining various types of geophysical field data are not designed to provide objective interpretations of subsurface structure and properties, nor do they adequately exploit the complementary capabilities of seismic and electrical methods. Interpretation methods in common use for geophysical field data were developed for oil industry applications (e.g., Wyllie et al., 1956, 1958; Kuster and Toksöz, 1974) and are not optimized for the shallow depths and unconsolidated materials of environmental applications. Laboratory data collected for soils at low pressure conditions appropriate to the near-surface are sparse in the literature, increasing the difficulty of developing new interpretation techniques for geophysical field data from environmental sites.

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 wave velocity measurements as a function of pressure at the extremely low pressures representing the shallow subsurface, and few studies include both elastic and electrical properties measurements. Laboratory measurements made for this project contribute needed information about geophysical properties of shallow soils, particularly our innovative measurements of shear wave velocities that we obtained using a new sample-holder design (Trombino, 1998; Aracne-Ruddle et al., 1999a,b; Bonner et al., 1999a,b), and our ultrasonic and electrical properties investigations of how chemical effects due to clays influence geophysical measurements of soils (Bonner et al., 1997; Wildenschild et al., 2000).

Recent advances in field techniques for seismic measurements in shallow soils (e.g., Bachrach et al., 1998; Baker et al., 1998; Carr et al., 1998; Steeples et al., 1998) have produced data suggesting that shallow soils have much lower velocities than the conventional wisdom
expected. Geotechnical measurements also suggest that shallow soil velocities are low (e.g., Crouse et al., 1993; Boulanger et al., 1998). Our laboratory velocity measurements (Trombino, 1998; Aracne-Ruddles et al., 1999a,b; Bonner et al., 1999b) corroborate the low velocities found by those field measurements.

In addition to making the laboratory measurements, we used rock physics theories and modeling to relate measured geophysical properties to hydrogeological parameters and soil composition (Berge et al., 1999a; Berge and Bertete-Aguierre, 2000; Wildenschild et al., 2000). We also developed a new technique for relating ultrasonic compressional and shear wave velocities to hydrogeological parameters (Berryman, 1999; Berryman et al., 1999a, 2000).

Although this project was fully funded by EMSP and did not include collaborators from outside LLNL, the project benefitted from the generosity of many scientists and engineers from other organizations. Many of our colleagues provided advice and even some field data that we compared to our laboratory measurements. We acknowledge the support of the following individuals and organizations:

In October, 1996, Robin Newmark of LLNL provided cores from 2 LLNL boreholes for our laboratory measurements, and also provided field data from logs of clay-bearing soils from the LLNL Site Initiative. The Gas Research Institute (GRI) invited the lead P.I. to attend the GRI Permeability Logging Forum in February, 1997, in Houston, TX, to discuss state-of-the-art geophysical methods for borehole logging and obtaining permeability estimates using geophysical methods. Herb Wang of the University of Wisconsin met with the P.I.’s and discussed techniques for ultrasonic velocity measurements in soils while he was visiting LLNL in June and July of 1997. Brian Vianni of LLNL provided advice on microstructure and geochemistry of clays in discussions with the P.I.’s in August and September, 1997. Ross Boulanger of U.C. Davis and Andrew Taber of Taber Consultants invited the lead P.I. to attend a workshop on geotechnical field measurements in soils in February, 1999. In March, 1999, Ross Boulanger and his collaborator Mike Driller of the California Dept. of Water Resources provided field data from borehole logs of organic-rich soils for comparison to our lab measurements made in similar soils.

Methods and Results

For this project, we made laboratory measurements of elastic wave velocities, electrical properties, porosity, and permeability for artificial soil samples made from sand/clay and sand/peat mixtures and a few natural soils. We used x-ray computed tomography (XCT) to image the microstructure of some samples. We also used rock physics theories, modeling, and comparison to available field data to develop relationships between geophysical measurements, microstructure, soil composition, and fluid-flow properties of the soil samples. Our results are summarized below. Details on our methods and results are given in the publications from this project, which are listed in a later section of this report.

We used the pulse transmission technique (Sears and Bonner, 1981) to measure ultrasonic compressional and shear wave velocities for dry and fully saturated soil samples made from mixtures of Ottawa sand and a second phase, using either peat moss or Wyoming bentonite, a
swelling smectite, for the second phase (Trombino, 1998; Aracne-Ruddle et al., 1999a,b). This allowed us to investigate geophysical properties for silty sands and sandy soils with organic components, for simple systems under controlled conditions. Measurements were made at room temperature, at pressures between about 0.01 and about 0.11 MPa to simulate the top few meters of the subsurface. We developed a new type of sample holder to make it possible to detect shear waves in unconsolidated samples at low pressures. This new sample holder is the subject of a patent disclosure (Bonner et al., 1999a). Details of the experimental procedures are given by Trombino (1998) and Aracne-Ruddle et al. (1999b). Figures 1 and 2 show the measured compressional (Vp) and shear wave (Vs) velocities for dry sand-peat and sand-clay samples. Velocity results and related uncertainties are described in detail elsewhere (Bonner et al., 1997, 1999b; Aracne-Ruddle et al., 1998, 1999a,b; Trombino, 1998; Berge et al., 1998, 1999a). Our main findings are that the microstructure controls the velocities; the velocities are low, a few hundred m/s in dry samples, with compressional velocity values being about twice the shear velocity values; velocities and amplitudes depend on the amount and distribution of fluid in saturated and drained samples; and the velocity gradients at the lowest pressures are strongly influenced by grain packing. Comparison of our laboratory velocity measurement results to available field data (e.g., Crouse et al., 1993; Taylor and Wilson, 1997; Bachrach et al., 1998; Boulanger et al., 1998; Steeples et al., 1998) showed agreement between velocities measured in the lab and field for soils of similar types, a lab pressures equivalent to the appropriate depth for the field measurements.

We measured complex impedance in the frequency range of 0.01 to 100 kHz for fully-saturated soil samples made from mixtures of Ottawa sand and Wyoming bentonite, as for the velocity samples. We also made a few measurements on clay-rich soil samples from the LLNL site, but controlled measurements of the artificial soil samples were our primary source of investigating how the amount and arrangement of clay affect geophysical properties. Different configurations of sand and clay, including dispersed mixtures, discrete clay clusters, and layers, were used to investigate effects of clay on electrical conduction. Pore fluid conductivity was varied from about 5 x 10^{-3} S/m to about 6 S/m, using various solutions of filtered deionized water and NaCl or CaCl₂. We designed a technique for making samples by packing sand and clay in heat-shrink tubing with sintered Hasteloy frits at both ends and AgCl-coated silver wires inside. This sample design allowed us to make electrical measurements using the 4-electrode method described by Olhoeft (1985), and to measure hydraulic permeability by a constant flow technique without removing the sample from the measurement apparatus. The sample design also allowed us to make XCT images of these same samples at the LLNL x-ray imaging facility. Electrical measurements were made at room temperature and at pressures up to about 0.3 MPa, equivalent to about the top 10 to 20 m of the subsurface. Figure 3 shows single-frequency results at 1 kHz, for sand-clay mixtures having various microstructures and pore fluid compositions. Details of experimental methods, results, and uncertainties for electrical properties measurements, porosities, and permeabilities of these samples are described in Wildenschild et al. (1999a,b; 2000). Our main findings are that electrical properties depend greatly on the arrangement of the clay; surface conduction may be significant; permeability is independent of fluid composition as expected, but does depend on porosity and clay content, dropping by about 2 orders of magnitude for samples containing about 10 percent dispersed clay as compared to clean sand samples.
Our ultrasonic and electrical properties measurements showed that geophysical properties are greatly dependent on microstructural details such as the amount and distribution of clay or peat and fluids. For example, Figure 4 illustrates how microstructure controls velocities for the sand-peat samples. To assist our investigations of the effects of microstructure on geophysical properties, we used the LLNL x-ray facility to make XCT images of some of our samples, using the technique described by Bonner et al. (1994) and Roberts and Lin (1996). Figure 5 shows an example of one of our relatively large-scale images. Other images at various scales were included in various presentations and publications for this project (e.g., Aracne-Ruddle et al., 1999a,b; Berge et al., 1998, 1999a; Wildenschild et al., 1998, 1999a,b). The images provide direct observations of the sample microstructure, and thus aid our interpretation of geophysical data with respect to microstructural influences.

We compared our laboratory measurement results to various rock physics theories to investigate the relationships between geophysical measurements, microstructure, soil composition, and fluid-flow properties for our samples. The paragraphs below describe results from our comparison of measured electrical properties and ultrasonic velocities to predictions from rock physics theories, followed by paragraphs describing results from our work on developing relationships between measured geophysical properties, hydrological properties and soil composition.

Electrical properties data are often interpreted using the empirical Archie’s law (Archie, 1942), which can be modified to include a surface conduction term (Waxman and Smits, 1968). Johnson et al. (1986) derived a linear relationship between bulk, fluid, and surface conductivities that provides a theoretical basis for this empirical expression and gives physical meaning to the constants in the expression. This theory has been shown to apply to clay-bearing rocks (e.g., Sen et al., 1988), but it has not been used previously for unconsolidated materials. We quantified the influence of microstructural properties on electrical properties for our sand-clay samples by calculating formation factors, Lambda-parameters, and surface conductances from our data, and then we compared our surface conductances to estimates from the theory of Johnson et al. (1986). We obtained good agreement, and we found that high and low bounds on the expected surface and bulk conductance in a sand-clay system can be determined from measurements made on samples having a few different microgeometries, including dispersed clay, clay layers, and clay clusters. These results could be applied to natural systems. Details of our theoretical results are presented in Wildenschild et al. (2000).

Empirical relationships developed in the oil industry to obtain porosity and saturation estimates from seismic velocity data (e.g., Wyllie et al., 1956, 1958) are not suitable for near-surface applications and soils. Similarly, statistical approaches based on laboratory measurements made on reservoir rocks with pore fluids and confining pressures optimized for oil industry applications (e.g., Han et al., 1986) are not optimal for estimating porosity, clay content, and saturation in shallow soils. We have chosen to use approaches that make use of the physics of the problem, rather than relying on empirical or statistical methods, to relate velocities to porosity, saturation, and soil composition.

Porosity, saturation, and composition in soils and rocks can be estimated using rock physics theories that relate the mechanical properties (e.g., seismic velocity, bulk modulus, shear
modulus, density) of component minerals and fluids, and the relative amounts of the minerals and fluids, to the measured properties of a rock or soil. Such effective medium theories make simple assumptions about the microstructure and its effects on measured properties (see Berryman, 1995 for a review). We applied several effective medium theories to model our ultrasonic velocity measurements for the sand-clay and sand-peat mixtures, and obtained useful velocity estimates when appropriate microstructure assumptions were made. We found that the self-consistent effective medium theory of Berryman (1980), illustrated in Figure 6, provided estimated velocities that are in good agreement with measured velocities for some of our soil samples (Figure 7). Details of our theoretical results for velocities are presented in Berge and Berryman (1999) and Berge et al. (1999a, b). In addition to the effective medium theory modeling, we also did some theoretical work to develop effective medium theories and to improve our understanding of the role of microstructure in controlling mechanical properties. These results are presented in several theoretical papers (Berryman and Pride, 1998; Pride and Berryman, 1998; Berryman and Berge, 1999; Berryman et al., 1999b).

After analyzing our laboratory data, we developed an algorithm for inverting Vp and Vs measurements to obtain information about the composition and distribution of soils in the subsurface. We used our laboratory ultrasonic measurements and field data from the literature (e.g., Taylor and Wilson, 1997; Boulanger et al., 1998) to create synthetic field data examples with realistic noise (Bertete-Aguirre and Berge, 1999; Berge and Bertete-Aguirre, 2000). These examples simulate seismic compressional and shear wave velocity data collected to image the shallow subsurface in realistic situations (e.g., Boulanger et al., 1998; McGuire et al., 1998). To recover the soil distribution in the shallow subsurface from the simulated field data, we developed an inversion code. We built a grid to represent the shallow subsurface, in which each cell in the grid is assumed to have constant soil composition, constant density, and constant velocity. (Gradients and more complicated structure can be accommodated by using finer gridding.) For a given point at a given depth, the code calculates the misfit between the observed (synthetic, in our example) seismic velocity and linear fits to laboratory ultrasonic velocity measurements at the appropriate pressure (e.g., data from Figures 1, 2). The misfit in each cell in the grid is given by the L2 norm (square of the difference of the velocities). The code repeats this procedure for all the possible soil types for which laboratory data are available, for Vp and Vs, over all cells of the grid. The code assigns a soil type to each cell by choosing the soil that gives the minimum misfit for the velocities. Figure 8 shows results for one simulated field example for three cases: (1) subsurface soil distribution constrained by using only Vp velocity distributions, (2) constrained only by Vs velocity distributions, and (3) constrained by using both Vp and Vs. These results show that by using Vp, Vs sets of data we are able to get a better mapping of the subsurface than the one obtained using Vp only. The ambiguity of the subsurface reconstruction is reduced by adding Vs data that further constrain the solution space, obtaining better imaging of the soil distribution. This implies that field seismic experiments will be more successful for underground imaging if both compressional and shear wave velocity data are collected. Using electrical properties data to provide additional independent constraints would further improve the results. This suggests that multiple geophysical methods should be used for characterizing field sites, whenever possible. Details of this work are presented in Bertete-Aguirre and Berge (1999) and Berge and Bertete-Aguirre (2000).
Although this project focused on dry and fully-saturated soils, our laboratory measurements on some drained samples and dry samples in the presence of humid air indicated that partial saturation effects on mechanical properties are significant for soils at low pressures (Bonner et al., 1997). Future work on a new EMSP project will investigate this subject more fully, but we were able to obtain some theoretical results in this area. These results are the subject of a patent disclosure (Berryman, 1999). We developed a new method for obtaining information about fluid saturation and fluid distribution in soils and rocks from compressional and shear wave velocity data. For wave propagation at low frequencies in a porous medium, the Gassmann-Domenico relations are well-established for homogeneous partial saturation of a liquid (Gassmann, 1951; Domenico, 1974). Although these relations provide the correct expressions for velocities in terms of the mechanical properties (bulk modulus, shear modulus), densities, and relative amounts of component minerals and fluids in a rock or soil, it has not been possible to invert these relations easily to determine porosity and saturation when the velocities are known. Also, the distribution of saturation, whether it is homogeneous or patchy (e.g., Berryman et al., 1988; Endres and Knight, 1989), is another important parameter that we would like to know. We determined that by expressing velocities in terms of ratios of densities and the Lamé elastic parameters (see Sheriff, 1994 for definition), the part of the elastic behavior that is influenced by the presence of fluid can be separated from the part that theoretically should be independent of fluid effects. Resulting cross-plots of these ratios produce diagrams that yield information about the porosity, saturation, and whether saturation is homogeneous or patchy, for a given rock or soil. We tested the method using velocity data from the literature (e.g., Murphy, 1984; Knight and Nolen-Hoeksema, 1990). Detailed results are presented in Berryman et al. (1999a, 2000). These results provide a promising basis for future development of inversion algorithms to relate velocities to porosity and saturation in partially-saturated soils and rocks.

In addition to the results described above, another result of our work on this project is insight into improving the designs for field experiments at contaminated sites. We gained this insight from our laboratory and theoretical investigations. Our understanding evolved further during discussions with geophysicists and site engineers while attending the INEEL Science Integration Workshop at INEEL in October, 1998, and two workshops held at PNNL in November, 1999 and January, 2000 after the end of this EMSP project. Our best recommendations for improving designs for geophysical field experiments are the following:

Seismic experiments should make every effort to collect both compressional and shear wave data because the two types of data can be used together to obtain information about fluid distribution in partially saturated sediments (Berryman et al., 2000), and the two constitute independent data sets that increase the number of constraints for inversion codes. This means using vibrational and impact sources for seismic reflection or refraction experiments; using P-S probes or tools for borehole logging; or using cone penetrometers with instrumented tips for P and S waves. This is all readily-available off-the-shelf technology, and the additional time and expense involved in deploying extra field equipment is well worth the effort because the additional data can greatly increase the value of the experiment.

To minimize casing problems at sites such as Hanford where steel casing in boreholes may reduce the quality of electrical measurements, non-electrical geophysical methods such as seismic or microgravity measurements should be considered. Modeling can be used to optimize
the design of any geophysical field experiment before the deployment. Data from surface measurements such as ground-penetrating radar may be used to supplement electrical resistance tomography data.

In areas where attenuation is expected to be high for a given type of geophysical measurement, measurements made in small sub-arrays can be combined using sophisticated inversion software to build an image beneath the entire field site. Modeling before the field deployment can provide information about how to design the subarrays (e.g., instrument spacing, number of receivers). For complex regions, collecting different types of geophysical field measurements (e.g., electrical resistance tomography and electromagnetic induction tomography) will provide additional independent data sets to better constrain the estimates of subsurface structure and properties.

Figures

The following figures illustrate the results presented in the Methods and Results section.
Figure 1. Results from laboratory ultrasonic measurements of compressional and shear wave velocities for sand-clay samples (Aracne-Ruddle et al., 1999b; Bonner et al., 1999b).

Figure 2. Results from laboratory ultrasonic measurements of velocities for sand-peat samples (Trombino, 1998; Berge et al., 1999a; Bonner et al., 1999b), with linear fits to velocity gradients and comparison to field data from the literature (e.g., Crouse et al., 1993).
Figure 3. Bulk sample conductivity vs. fluid conductivity for sand-clay samples, for single-frequency measurements at 1 kHz (Wildenschild et al., 1999a,b). See Wildenschild et al. (2000) for additional measurements.
Figure 4. Inferred approximate arrangement of sand grains and peat in sand-peat samples (Berge et al., 1999a,b). Grey circles indicate sand grains, light grey areas indicate pores in the sand pack, and black-and-white areas indicate peat (which is porous). At low concentrations, peat slowly replaces a few sand grains and fills a few pores in the sand pack as the peat concentration is increased. Peat can act as a cement between grains in the sand pack, at moderate concentrations. Eventually, at high concentrations, the sand grains are isolated in a peat matrix. Velocities change systematically with these changes in microstructure.
Figure 5. XCT image of 5-cm-diameter sand-clay sample (Berge et al., 1998; Wildenschild et al., 1998). Clusters of clay (about .5 to 1 cm diameter) show up inside the cylindrical sample; sand is black. Bright rings are the wire electrodes used for the electrical properties measurements.
Figure 6. Cartoon (Berge and Berryman, 1999) illustrating how Berryman’s (1980) physically-realizable self-consistent effective medium theory works. The porous material is treated as an effective medium made up of a sphere of aggregated pores and grains embedded in the effective medium such that scattered energy from individual pores and grains is equivalent to scattered energy from the embedded sphere, and that scattering must vanish for the aggregate sphere embedded in the effective medium. Scattering coefficients are adjusted to accomplish this.
Figure 7. Comparison of measured velocities and estimates from Berryman’s (1980) self-consistent (SC) effective medium theory and other theories, for sand-peat samples (Berge et al., 1999a). The SC theoretical estimates assume the samples are made of sand grains and porous peat for samples having high concentrations of peat, and samples having low concentrations of peat are assumed to be sand packs mixed with porous peat.
Figure 8. Subsurface soil distribution recovered using constraints from (a) Vp only, (b) Vs only, (c) Vp and Vs, for a synthetic field data example where synthetic seismic velocities were available for a 10x10 grid with grid cells that were each 1.5 m in the vertical direction and 5 m in the horizontal direction (Bertete-Aguirre and Berge, 2000). The true soil distribution (top) is recovered with much better resolution if both kinds of velocity data are available.
Relevance, Impact and Technology Transfer

This section addresses specific questions on relevance, impact, and technology transfer, in order to help DOE communicate project information to potential technology users, commercial partners, or sponsors of continuing research.

a. How does this new scientific knowledge focus on critical DOE environmental management problems?

For this project, we conducted basic research to advance the state-of-the-art of geophysical imaging of the shallow subsurface. Our results improve the understanding of relationships between geophysical measurements, hydrological properties and soil composition. These results can be used to improve interpretation of geophysical data collected at environmental sites. This knowledge is relevant to critical DOE environmental management problems including needs for improving geophysical methods for subsurface characterization and monitoring in the vadose zone, for tank farms, and for subsurface contamination problems. In the DOE EM database, many statements of need for various sites refer to needs for improvements in geophysical imaging of the subsurface (e.g., ID-6.1.02, ID-6.1.04, OH-F049, OK99-01, ORHY-03, RL-SS10, RL-SS31, and the PNNL Hanford Ground Water Vadose Zone Integration Project’s needs). Although this is basic research and the results are not ready for technology transfer or site demonstrations, we will continue this work in future EMSP projects (e.g., EMSP project #70108) and work towards technology transfer. We also have made recommendations for improvements in the design of geophysical field experiments for characterization and monitoring at DOE contaminated sites.

b. How will the new scientific knowledge that is generated by this project improve technologies and cleanup approaches to significantly reduce future costs, schedules, and risks and meet DOE compliance requirements?

The main results of this project are improved relationships between geophysical measurements, hydrological properties and soil composition. The improvements have the potential to reduce the cost and time required for geophysical field data interpretation and the subjectivity of the interpretation, by providing clear connections between what the geophysicist measures (e.g., seismic velocity, electrical conductivity) and what the site engineer needs (porosity, saturation, permeability estimates, soil composition and structure information). This could improve future cleanup costs and schedules by reducing costs and time required for site characterization, and risk would be reduced if the characterization involves less uncertainty due to improved reliability in the mapping between geophysical properties and hydrological properties.

c. To what extent does the new scientific knowledge bridge the gap between broad fundamental research that has wide-ranging applications and the timeliness to meet needs-driven applied technology development?

This was a basic research project. It did provide, however, some information that is immediately applicable to improving the design of geophysical field experiments for site characterization. Our
laboratory measurements and modeling gave us some insight into ways to improve the collection of geophysical data in the field.

Our results show that whenever possible, it is beneficial to collect multiple geophysical data sets (e.g., seismic, electrical resistivity) at a site, and that seismic field experiments should be designed to collect both compressional and shear wave velocity data whenever possible.

Compressional and shear velocity data together provide information on saturation and fluid distribution, and having several independent data sets improves reconstruction of subsurface structure from inversion codes. We recommend that seismic experiments use both impact and vibrational sources for surface reflection and refraction lines, that suspension logging should use P-S tools, and that cone penetrometers be used with instrumented tips for Vp and Vs data collection.

Additional recommendations for field experiments are that seismic and microgravity techniques be used in areas where metal casing causes problems for electrical methods; that modeling prior to conducting experiments will provide information for optimizing experiment design (e.g., source frequencies and strengths, number and separation distances for surface sensors and boreholes) and thus will improve field results; and that areas of high attenuation can be imaged by using many small sub-arrays with close spacing and then by combining the results using sophisticated inversion software to build an image beneath the entire field site.

d. What is the project’s impact on individuals, laboratories, departments, and institutions? Will results be used? If so, how will they be used, by whom, and when?

Results of this work have been presented at several EMSP workshops and also at the Advanced Vadose Zone Characterization Workshop that was held in Richland, WA, Jan. 19-20, 2000, sponsored by the PNNL Hanford Groundwater/Vadose Zone Integration Project. Recommendations for field experiment design that we suggested were incorporated into plans for future geophysical experiments to be conducted at the Hanford site by the Office of River Protection. The P.I. for this project is also a participant in the Non-invasive Characterization Work Group for the DOE Complex-Wide Vadose Zone Science and Technology Roadmap for Characterization, Modeling and Simulation of Subsurface Contaminant Fate and Transport. Insights gained in this project and resulting advancements in the area of petrophysics (relating geophysical measurements to hydrological properties and soil composition) have been included in current drafts of the roadmapping report in sections describing the current state-of-the-art of petrophysical relationships. The research in this EMSP project is being continued in a new EMSP project (#70108), and future results will be communicated to DOE EM site managers and engineers when ready for technology transfer. All of the research was conducted at LLNL and the co-investigators are all affiliated with LLNL. We hired three undergraduate students and one graduate student to work on the project during the summers, and thus this project contributed to the education of those individuals. The students learned to do laboratory experiments in the LLNL experimental geophysics laboratory. The students wrote reports and were co-authors of presentations at scientific meetings (e.g., Bonner et al., 1997, 1999b; Rowe, 1997; Trombino, 1998; Aracne-Ruddell et al., 1999a). The graduate student is a co-author on a patent application (Bonner et al., 1999a). This work did not involve any student dissertations or theses.
e. Are larger scale trials warranted? What difference has the project made? Now that the project is complete, what new capacity, equipment or expertise has been developed?

As a result of this work, we are coordinating work in the new EMSP project in order to collaborate with other EMSP P.I.’s to conduct field experiments at the LLNL Vadose Zone Observatory, at the small (a few meters) field scale, and we have made recommendations for field experiments to be conducted at the Hanford site, as mentioned above.

The results of this project include two patent applications (described below, in the Patents section). The equipment and expertise represented by those patent applications, i.e. the laboratory apparatus and methods developed in this project, are being used in a new EMSP project (#70108) to further investigate and develop relationships between geophysical properties, hydrological properties and soil composition.

f. How have the scientific capabilities of collaborating scientists been improved?

This project involved several researchers from LLNL. We did not have outside collaborators from other laboratories, but we did have several students who worked on the project during the summers (see above, section on impact on individuals, and below, section on personnel supported). They learned how scientific research is conducted and improved their laboratory and computer skills as well as their scientific writing ability.

g. How has this research advanced our understanding in the area?

As described above in the Methods and Results section, we have advanced the understanding of the effects of microstructure, clays, and fluids (including some chemical effects) on measured geophysical properties. We have developed new relationships between geophysical properties, hydrological properties and soil composition.

We have also developed new tools (see Patents section) for making measurements of shear wave velocities in the laboratory for soils at low pressures, and for relating velocities to porosity and saturation in soils and rocks. These new tools may be of use to geotechnical companies who need to measure soil properties in the laboratory, and to geophysical interpreters who need alternatives to traditional methods such as AVO (amplitude-variation-with-offset) used to interpret seismic field data.

As discussed above, we have gained insight into improving the design of geophysical field experiments as a result of our research.

h. What additional scientific or other hurdles must be overcome before the results of this project can be successfully applied to DOE Environmental Management problems?

We need to continue this work in the new EMSP project (#70108) to further develop the relationships between geophysical measurements, hydrological properties and soil composition. The case of partial saturation has not been investigated completely, nor have we adequately
addressed the scaling of results between laboratory and field. The heterogeneities at a field site require that we understand uncertainties related to partial saturation, scaling, and other effects.

In addition to continued research, application of our results would require working on technology transfer, since our algorithms are not in the form of computer codes that site engineers could apply.

i. Have any other government agencies or private enterprises expressed interest in the project?

As noted above, this work was presented to the PNNL Hanford Ground Water Vadose Zone Integration Project when the lead P.I. was invited to speak at the Advanced Vadose Zone Characterization Workshop that was held in Richland, WA, Jan. 19-20, 2000. The California Dept. of Water Resources has expressed interest in the laboratory measurements of ultrasonic velocities in soils, for comparison to their field measurements of shallow soil properties in regions where they are performing seismic hazards assessments. The ultrasonic velocity results also have generated a lot of interest from university researchers, particularly from individuals working on seismic field experiments for measuring velocities in the shallow subsurface. Our lab measurements provide the first direct corroboration of very low velocities seen in field data for the top few meters of the subsurface.

Project Productivity

The project was on schedule and the work plan was not revised. We accomplished our goals of making the necessary laboratory measurements by developing laboratory techniques for simultaneous measurement of compressional and shear wave velocities in unconsolidated sediments at low pressures, and for measurement of complex electrical properties and permeability in the same sample followed by microstructural imaging using the same sample holder so that the microstructure is not disturbed. We collected a large data set of geophysical properties measured in the laboratory as a function of pressure, for samples of various compositions, as well as microstructural images of several samples. We met our goal of improving our understanding of the role of microstructure and effects of clay on measured geophysical properties by making the laboratory measurements and performing microstructural imaging. We used rock physics theories, modeling, and comparing lab data to available field data, in order to meet our goal of developing relationships between geophysical properties and porosity, fluid content, and soil composition. We also developed a new technique for relating P and S velocities to saturation. This contributed to meeting our goal of developing methods for combining geophysical information from different data sets to infer composition and hydrological properties. We showed that multiple geophysical data sets can improve subsurface imaging. We did not conduct a field experiment because it was beyond the budget and time limit of the project once we understood the complexity involved, but we did compare our laboratory results to available field data and we developed recommendations for improving field experiment design, as well as insight into combining different types of geophysical data collected in the field.
Personnel Supported

This project provided partial support (approximately .2 to .3 FTE level of effort for each) for several geophysicists at LLNL:
Patricia A. Berge, James G. Berryman, Hugo Bertete-Aguirre, Brian P. Bonner, Jeffery J. Roberts

LLNL technical support personnel were also partially supported (approximately .1 to .2 FTE level):
Chantel M. Aracne-Ruddle, Carl O. Boro, Eric D. Carlberg

Partial support (approximately .5 FTE level of effort) was provided for one post-doctoral researcher at LLNL:
Dorthe Wildenschild

Several students were hired to work at LLNL during the summers:
Edgar D. Hardy, David J. Hart, Christen D. Rowe, Cosette N. Trombino

Publications

The results in these publications are described in the Methods and Results section above. Copies of many of these documents may be viewed online or downloaded at the URL http://www.llnl.gov/tid/lof/ by performing a search using the UCRL number of the document or the author name. They are also available on our project web site (Berge and Rowe, 1998) at the URL http://www.llnl.gov/ees/esd/expgeoph/Berge/EMSP/

a. Publications in peer-reviewed journals and books


b. Technical reports and conference proceedings


c. Accepted/submitted publications

Interactions

a. Participation/presentations at meetings, workshops, conferences, seminars

The Gas Research Institute invited the lead P.I. to attend the GRI Permeability Logging Forum in February, 1997, in Houston, TX, to discuss state-of-the-art geophysical methods for borehole logging and obtaining permeability estimates using geophysical methods.

Ross Boulanger of U.C. Davis and Andrew Taber of Taber Consultants invited the lead P.I. to attend a workshop on geotechnical field measurements in soils in February, 1999. In March, 1999, Ross Boulanger and his collaborator Mike Driller of the California Dept. of Water Resources provided field data from borehole logs of organic-rich soils for comparison to our lab measurements made in similar soils.

The P.I.’s had discussions with various geophysicists and site engineers while attending the INEEL Science Integration Workshop at INEEL in October, 1998, and two workshops held at PNNL in November, 1999 and January, 2000 after the end of this EMSP project. Discussions with P.I.’s on other EMSP projects, in particular projects that involve geophysical field measurements or techniques (e.g., J. G. Berryman of LLNL, E. L. Majer of LBL, D. Steeples of U. Kansas, C. Carrigan of LLNL, B. Faybishenko of LBL, R. Knight of U. British Columbia) are on-going and may lead to future collaborations. Many university researchers who are conducting seismic experiments to measure velocities in the shallow subsurface have expressed interest in the laboratory velocity measurements because these lab measurements corroborate very low velocities observed in the field.

b. Consultative and advisory functions to other laboratories and agencies

The lead P.I. was invited to present results of this work at the Advanced Vadose Zone Characterization Workshop that was held in Richland, WA, Jan. 19-20, 2000, sponsored by the PNNL Hanford Groundwater/Vadose Zone Integration Project. Our recommendations for field experiment design were incorporated into plans for future geophysical experiments to be conducted at the Hanford site by the Office of River Protection. The lead P.I. for this project is also a participant in the Non-invasive Characterization Work Group for the DOE Complex-Wide Vadose Zone Science and Technology Roadmap for Characterization, Modeling and Simulation of Subsurface Contaminant Fate and Transport, and participated in the May, 2000 roadmapping workshop in Salt Lake City as well as the July, 2000 workshop in San Diego. Insights gained in this project and resulting advancements in the area of petrophysics (relating geophysical measurements to hydrological properties and soil composition) have been included in current drafts of the roadmapping report in sections describing the current state-of-the-art of petrophysical relationships.

c. Collaborations

We are coordinating work in the new EMSP project (#70108) in order to collaborate with other EMSP P.I.’s to conduct field experiments at the LLNL Vadose Zone Observatory, at the small (a
few meters) field scale, and may possibly participate in an experiment at Hanford. The new EMSP project includes making laboratory measurements on soil samples from the Hanford site.

Transitions

As noted above, our recommendations for field experiment design were incorporated into plans for future geophysical experiments to be conducted at the Hanford site by the Office of River Protection. Results from our patent applications (see below) may be used by the DOE, other federal agencies or by industry in the future.

Patents


Future Work

The research in this EMSP project is being continued in a new EMSP project (#70108. We are coordinating work in the new EMSP project in order to collaborate with other EMSP P.I.’s to conduct field experiments at the LLNL Vadose Zone Observatory, at the small (a few meters) field scale, and we have made recommendations for field experiments to be conducted at the Hanford site, as mentioned above.

In the new EMSP project, we are investigating partial saturation by making laboratory measurements of ultrasonic velocities in partially saturated soils. We are also using x-ray imaging to examine the microstructure of the samples. We will continue to develop relationships between geophysical measurements and hydrological properties and soil composition. We have not adequately addressed the scaling of results between laboratory and field. The heterogeneities at a field site require that we understand uncertainties related to partial saturation, scaling, and other effects.

In addition to continued research, application of our results would require working on technology transfer, since our algorithms are not in the form of computer codes that site engineers could apply.

Literature Cited


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Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract number W-7405-ENG-48 and supported specifically by the Environmental Management Science Program of the DOE Office of Environmental Management and the Office of Science.