US Department of Energy, Office of Science
Environmental Remediation Science Division (ERSD, now CESD)
FY09 First Quarter Performance Measure

The FY09 ERSD Overall PART charge to Lawrence Berkeley National Laboratory Environmental Geophysics Group is to 'test geophysical techniques that measure parameters controlling contaminant movement under field conditions in at least two distinct subsurface environments'. In this first of four quarterly reports, we describe how geophysical data can be used to quantify subsurface architecture that influences flow.

1. Introduction

Contaminant flow and transport, natural attenuation, and contaminant remediation efficacy are all influenced by subsurface hydrogeological and biogeochemical properties. Properties such as the spatial distribution of hydraulic conductivity, lithofacies, and fracture zonation, as well as the plume itself, impact further migration and remedial treatments. Developing a predictive understanding of subsurface flow is complicated by the disparity of scales across which controlling hydrological processes dominate (e.g., Gelhar, 1993). For example, the distribution of microfractures and geological layers both influence hydraulic conductivity and thus subsurface flow, albeit over dramatically different spatial scales. The level of subsurface characterization needed to guide environmental remediation efforts depends on many factors, including: regulatory and risk drivers, the level of heterogeneity relative to the spatial extent of the plume, and the spatial and temporal scales of interest. In some cases, reconnaissance efforts that delineate major characteristics of the study site may be sufficient (such as for estimating the mean plume behavior in low risk environments), while other investigations may require a much more intensive effort.

Conventional sampling techniques for characterizing or monitoring the hydrogeological properties that control flow typically involve collecting soil or fluid samples using borehole techniques. Established hydrological characterization methods (such as pumping, slug, and flowmeter tests) are commonly used to measure hydraulic conductivity in the vicinity of the wellbore (e.g., Butler, 2005). When the size of the study site is large relative to the scale of the heterogeneity or the scale associated with the remedial action, or when the heterogeneity is particularly complex, data obtained at point locations or within a wellbore may not capture sufficient information to describe the key controls on subsurface flow. The inability to collect the necessary measurements, using conventional characterization tools, at a high enough spatial resolution and over a large enough volume for understanding and predicting flow and transport processes, often hinders successful environmental remediation and stewardship.

Similar to how biomedical imaging procedures have reduced the need for exploratory surgery, integrating more spatially extensive geophysical measurements with direct borehole measurements holds promise for improved and minimally invasive characterization of subsurface environments. Because geophysical data can be collected from many different platforms (such as from satellites and aircraft, at the ground surface of the earth, and within and between wellbores), integration of geophysical data with direct hydrogeological or geochemical measurements can provide a minimally invasive approach for characterizing the subsurface at a variety of resolutions and over many spatial scales. In the last decade, many advances have been made that facilitate the use of geophysical data for hydrogeological characterization, as described by the books *Hydrogeophysics* (Rubin and Hubbard, 2005) and *Applied Hydrogeophysics* (Vereecken et al., 2006). Clearly, the main advantage of using geophysical data over conventional (wellbore based) measurements is that geophysical methods provide spatially extensive information about the subsurface in a minimally invasive manner. The greatest disadvantage is that the geophysical methods are indirect; they only provide proxy information about subsurface properties or processes relevant to contaminant remediation.

The use of geophysical data for aiding contaminant remediation investigation can be generally categorized into four broad categories (e.g., Hubbard and Rubin, 2005):

1. Mapping of subsurface architecture or features that influence flow (PART Report #1);
2. Estimating subsurface properties that influence flow and transport (PART Report # 2);
3. Monitoring subsurface processes associated with natural or engineered *in situ* perturbations relevant to environmental remediation (PART Report #3);
4. Use of geophysical data to improve the numerical representation of complex hydrobiogeochemical processes within predictive subsurface models (PART Report #4).

In this first PART Quarterly Report, we describe the use of geophysical data to quantify subsurface architecture or features that control flow. Subsequent PART Reports will address the other three topics. For each topic, we provide a short background and then highlight research advances that have been supported through the DOE Environmental Remediation Science Program of BER. Typically, we discuss the development of the characterization approach or framework, and then discuss the application of the approach to DOE relevant site(s). For each topic, we illustrate the use of developed geophysical characterization or monitoring approaches to a wide variety of hydrogeological environments (unsaturated/saturated, porous granular/fractured, arid/humid), subsurface contaminants (uranium, chromium, TCE, nitrate, strontium), scales (synchrotron investigations at the grain scale; laboratory column investigations, "local" field scales (study sites with dimensions of ~10 m or less), and/or plume field scales.

2. Geophysical Quantification of Subsurface Architecture or Features

Because geophysical attributes are often sensitive to contrasts in physical and geochemical properties, geophysical methods can be useful for mapping subsurface architecture and features that influence flow. Using geophysical methods for subsurface mapping is perhaps the most well-developed geophysical characterization approach, and it is most commonly performed using surface-based techniques. Examples of common mapping objectives for environmental remediation include: mapping the aquifer geometry (i.e., the stratigraphy), the depth to bedrock, the water table, and the location of major preferential flowpaths. The ability to distinguish hydrogeologically meaningful boundaries using geophysical data depends on the sensitivity of geophysical methods to subsurface physical properties or contrasts of these properties. From these measurements, the nature and distribution of subsurface materials can often be deduced. Common geophysical approaches for mapping hydrogeological targets include surface ground penetrating radar (GPR), electrical conductivity, electromagnetic, and seismic methods. For example, subsurface variations in elastic moduli and density associated with lithological heterogeneities can cause seismic waves to travel at different speeds. Information about these changes, and thus about the nature and distribution of the subsurface units, can be interpreted from analyzing the seismic arrival times. The contrasts in physical properties vary depending on which materials are juxtaposed, and the ability to detect these changes varies with the geophysical method employed. With methods such as surface seismic reflection or GPR, key interfaces are often manifested as laterally coherent wiggle traces and enable the production of a pseudo "cross section" of the subsurface. With methods such as surface electrical resistivity or seismic refraction, zonation of units that have distinct geophysical attributes (such as electrical conductivity or seismic P-wave velocity) is often used to infer lithological variations.

Comparison between direct measurements and geophysical attributes is necessary to interpret the geophysical data in a hydrogeologically meaningful manner. The most common approach is one that capitalizes on expert skills and intuition in the comparison of wellbore information (such as depths to key lithological interfaces) and the geophysical signatures. This methodology allows for incorporation of information that is often very difficult to quantify. For example, because the spatial distribution of hydrological properties is largely a function of ancient depositional and geological processes, interpretation of subsurface geometries between wellbores is often performed within the context of a geological model. This approach might be as simple as recognizing the lateral continuity of geological layers or the expected geometry of a particular depositional facies, or it might be as extensive as development of a hydrofacies model (e.g., Kolterman and Gorelick, 1996). If a linkage between the direct wellbore and the indirect geophysical dataset can be developed, then the geophysical dataset can then be used to extrapolate the information away from the wellbore. However, with this approach, it is often difficult to quantify the uncertainty associated with the components of the problem, such as the conceptual model, the hydrogeological parameter estimate, and the geophysical data inversion procedure.

Stochastic methods provide a systematic framework for assessing or handling some of the complexities that arise when integrating geophysical and hydrogeological data and also provide estimates of parameter uncertainty. For example, Bayesian methods permit incorporation of a-priori information into the estimation approach, and provide a framework for incorporating additional data as they become available. The relatively new field of hydrogeophysics focuses on the development and application of frameworks that permit integration of hydro- and geophysical data for quantitative subsurface characterization. Although the majority of the significant DOE-supported hydrogeophysical advances are mainly associated with the use of geophysical data for quantitative estimation of surface parameters and processes that control flow and transport (which will be the focus of the 2009 PART Reports #2 and #3 respectively), as is described below, DOE has also supported some research that entails both traditional and stochastic approaches for delineating architecture and subsurface features relevant to flow and transport using geophysical datasets.

Below, we describe the use of geophysical data for mapping subsurface architecture or features relevant to flow through focusing on three key examples, including the delineation of: (1) stratigraphy; (2) fracture zonation; (3) plume boundaries.

2.1 Stratigraphic Interpretation

In this section, we illustrate two traditional uses of geophysical data for delineation of stratigraphy and its control on subsurface flow. The first example is associated with a DOE-supported field-scale bacterial transport study that was conducted within an uncontaminated sandy Pleistocene aquifer near Oyster, Virginia, where the overall project goal was to evaluate the importance of heterogeneities in controlling the field-scale transport of bacteria that are injected into the ground for contaminant remediation (bioaugmentation). The second example is associated with a DOE-supported study at the TCE-contaminated P-Area of the Savannah River Site, which also is located within Atlantic Coastal Plain sediments. To develop a predictive understanding of the long tailing often observed with tracer tests and contaminant transport in sand-clay systems such as these, investigators at the Savannah River Site are making an ongoing effort to explore the benefit of utilizing dual porosity representations in transport models. Both examples illustrate the utility of geophysical methods for improving the understanding of subsurface architecture.

At the DOE Oyster bacterial transport site, surface ground penetrating radar (GPR) data were used in conjunction with retrieved sediment cores, cone penetrometer (CPT) data and electromagnetic flowmeter data to interpret the subregional and local stratigraphy. The surface, common-offset GPR datasets at the South Oyster Site were collected using a PulseEKKO 100 system with 100 and 200 MHz central frequency borehole antennas. Radar data were collected at two spatial scales within what are called the "reconnaissance" and "detailed" data grids and were processed using conventional flows (e.g., Yilmaz, 1988). The total traverse distance of these data, collected at a minimum line spacing of 25 m, was 4,350 m. The CPT data were interpreted in terms of lithology indicator logs (following Robertson et al., 1986), the flowmeter data were used with wellbore slug tests to interpret interval hydraulic conductivity at the local field scale, and grain-size analysis using core samples were performed and used to interpret core-scale hydraulic conductivity.

On the basis of the GPR data reflection strength, continuity, and character (Vail et al., 1987), and through comparison with lithological-hydrological information provided by the wellbore data, investigators identified reflectors as bounding surfaces that separate wedge-shaped, seaward dipping and tapering, thin sequences. An example of the interpreted subregional stratigraphy from a reconnaissance GPR line is shown in Figure 1a**,** where the two-way travel times of the radar reflections have been converted to approximate depths using an average velocity function obtained from nearby radar velocity tomograms. This radar profile reveals the water table, as well as the series of reflectors bounding the successive sequences of the Wachapreague Formation. The deepest of these (the red reflector) marks the unconformable base of the Wachapreague Formation. The dip of this surface steepens as it approaches the surface towards the western (landward) margin of the study area, and emerges as a regionally recognized subaerial surface (the Mappsburg Scarp). A comparison of the surface radar and CPT responses reveals lithological variations in the dip direction within the sedimentary sequences bounded by the annotated unconformities.

The locations of two "local-scale" bacterial transport study sites were chosen based on the subregional stratigraphic information obtained from surface reconnaissance GPR and CPT dissolved-oxygen-content data. The goal was to choose sites located in the same stratigraphic interval, but with different groundwater chemistries. Indeed, the location of the original study sites were altered based on the subregional GPR data, because one of the flowcells was originally located up-dip of the Mappsburg Scarp (i.e., landward), whereas the other was located in the down-dip (shallow marine) environment. Figure 1b shows an example of a detailed GPR data cube associated with one of the local flow cells; the reflection character of the surface GPR data was used to assess the geologic complexity of the subsurface at the local scale. More details of this GPR study are given in Hubbard et al. (2001).

To assess the value of various conditioning data for improving flow predictions, Scheibe and Chien (2002) performed simulations using synthetic aquifers constructed with different types of available characterization data. They compared the simulations with bromide breakthrough measurements collected during tracer tests at the local scale sites. The mapped GPR horizons were input as layers, and two different approaches were used to assign hydraulic conductivity values between the interfaces. Their simulations suggested that the layered surface GPR model only slightly improved flow predictions over those obtained using homogeneous hydraulic conductivity values, based on subregional calibrations. As will be described in PART Report #2, use of tomographically obtained hydraulic conductivity estimates greatly improved the flow predictions. In this particular study, the surface GPR datasets were most useful for guiding location and installation of the flow cells: the reconnaissance GPR dataset was most useful for citing the location of the detailed flow cells, and the detailed 3D GPR datasets were most useful for guiding the wellbore layout within the flow cell itself.

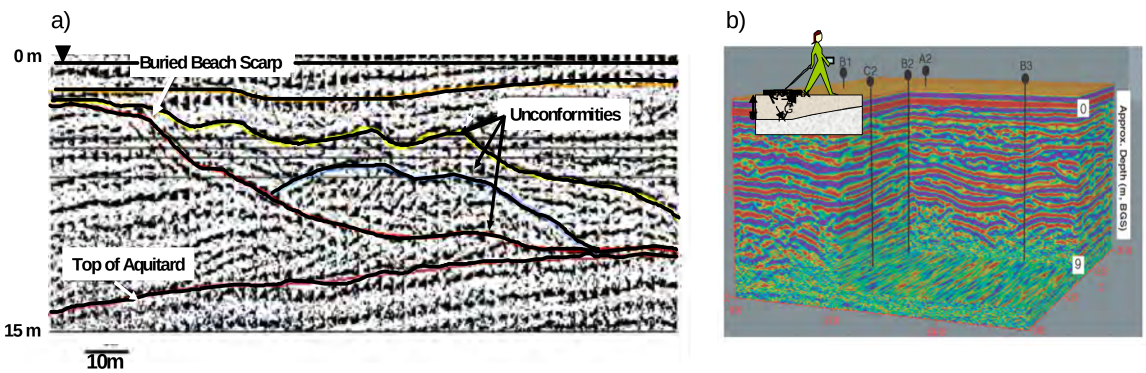

Figure 1. Example of the use of subregional (left) and local scale (right) surface GPR datasets to delineate subsurface stratigraphy at the DOE Oyster Bacterial Transport Site in Oyster, Virginia (modified from Hubbard et al., 2001)

The second example illustrates the use of surface seismic reflection methods for delineating subsurface stratigraphy at the TCE-contaminated P-Area of the Savannah River Site. To characterize the subsurface, several datasets were collected, including: a pseudo 3D surface seismic survey; vertical seismic profiles (VSP); tomographic radar, electrical, and seismic datasets; CPT, gamma, and resistivity logs; concentration data; flowmeter data, and core data. At this site, the study was confined to the upper 45 m of Atlantic Coastal Plain sediments, with the water table about 15 m below ground surface. The initial conceptual model of the subsurface at the site (obtained using CPT and log data) was of alternating layers of sand and clays, with the location of the TCE plume located in the saturated section between two clay layers: an “upper” and a “middle” clay. Although the general geologic dip and the groundwater flow direction are to the southeast, the plume had an east-west flow direction. The intent of the (ongoing) characterization effort is to use the surface seismic to constrain the architecture of the subsurface (described here) and to develop an integration approach that permits estimation of clay versus sand fraction over the entire plume area (discussed in PART Report # 2). Since sand versus clay fraction drives mass transfer in dual porosity systems, such lithofacies information is needed to parameterize the transport model.

The seismic datasets were collected in an iterative manner: multi-offset and azimuthal VSP surveys were first conducted and used to guide the seismic survey design. The surface survey was collected using a 120-channel Geometrics system with 40 Hz geophones, receiver, and shot spacings of 1 m, a sample rate of 0.5 m, a target fold of 30, and a record length of 500 ms. An accelerated weight drop was used as the source, and 4–6 stacks were used per shot for a total of 2,906 shots. Data processing was performed using conventional steps (i.e., Yilmaz, 1987) and with an emphasis on suppressing surface waves and highlighting coherent reflectors in the vadose and saturated systems. Processing was performed as a 3D volume, rather than as a series of 2D lines, to facilitate interpretation. The final (migrated and depth converted) dataset consisted of 86 crossline and 17 in-line profiles that encompassed a 170 m (length) by 150 m (width) by 34 m (depth) volume (Figure 2a).

To link the seismic reflectors to geological interfaces, the pseudo 3D seismic dataset was compared with information available from wellbore gamma, resistivity, core, and CPT datasets (Figure 2b). This integration revealed the presence of buried channel complexes not included in the initial conceptual model. The primary buried channel, located in the plume region, was incised through the defined upper and middle clays (i.e., through the zone previously identified from wellbore data alone as the contaminated zone). Comparison of the spatial relationship between the TCE plume and the mapped primary channel (Figure 2c) suggests that the primary channel may act as a conduit for the TCE plume, causing a narrowing of the plume and migration in a direction offset from the geologic dip and hydrological gradient. This example, which is described in more detail by Addison et al. (2009), provides an excellent illustration of the traditional use of surface geophysical methods to delineate subsurface architecture and improve site conceptual models. Hydrogeological property estimation using multiscale datasets and associated dual-domain transport modeling are currently under way to quantify the impact of this architecture on plume migration at this site.

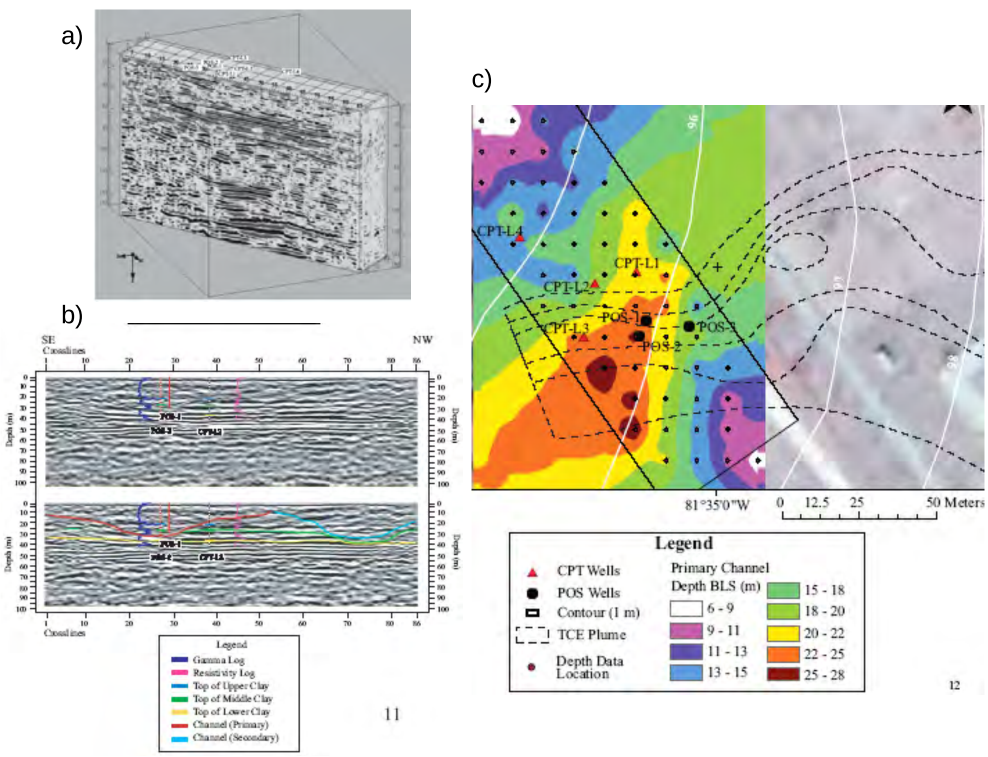

Figure 2. Surface seismic reflection datasets collected at the TCE contaminated Savannah River Site. (a) Pseudo 3D processed seismic data cube. (b) Example of the comparison between geophysical log and seismic reflectors. (c) Comparison of the TCE plume boundary (obtained using wellbore data) with the location of the mapped buried primary channel (obtained using seismic reflection data); the contaminant source is located to the right of the displayed image (modified from Addison et al., 2009).

2.2 Fracture Delineation at the Local and Plume Scales

Because fracture zones often serve as fast (preferential) flow paths, fracture mapping is often a key objective in contaminated, fractured subsurface environments. Delineation of subsurface fractures using traditional wellbore methods is typically challenging because wellbores often do not intersect the fracture plane. Because of the contrast between the physical and fluid properties associated with the matrix and the fractured region, geophysical methods hold potential for aiding in the delineation of fracture zones. For example, because seismic velocity is sensitive to the stiffness of a material, and because a fractured rock is less stiff than the surrounding matrix, fracture zones should be associated with lower P-wave velocity relative to surrounding areas (e.g., Hayles et al., 1996). Similarly, since fracture zones commonly serve as fluid fast paths, and because electrical conduction in subsurface materials is predominantly electrolytic in nature (i.e., conducted through fluids), electrical methods hold potential for providing information about fracture zonation. For example, Lane et al. (1995) used azimuthal resistivity methods, which involves the acquisition of data along surface-based transects that extend radially from a common center point, to indicate the principal fracture strike orientation in crystalline bedrock.

Recent DOE-supported work has focused on quantifying fracture zonation at both the local and the plume scale at the contaminated Oak Ridge National Laboratory Field Research Center (ORNL IFRC) in Tennessee, through integrating seismic and hydrogeological datasets. The saturated section of interest at this site is contaminated with uranium, nitrate, and other contaminants associated with the S-3 seepage basin. Underlying this research center is the Nolichucky Shale bedrock, and overlying the shale is unconsolidated materials that consist of weathered bedrock (referred to as saprolite) and a thin top layer of man-placed fill. The saprolite overlying the Nonlichucky Shale is approximately 13 m thick at the study site. To a depth of ~10 m, the saprolite is clay-rich and has low permeability. Between the clay rich saprolite and the bedrock is a transition zone of fractured bedrock weathered to varying degrees. The transition zone tends to be a zone of higher permeability than the surrounding saprolite and bedrock, because of a combination of higher fracture density and low clay content (Watson et al., 2005). Understanding the distribution of fracture zonation at the site is expected to be critical for defining fastpaths of the subsurface contaminants throughout the site.

Recent DOE-supported efforts have focused on the development of joint inversion approaches using seismic and hydrological datasets to infer the distribution of fracture zonation at the local and plume scales. Traditional uses of geophysical datasets to infer fracture zonation include collecting and inverting the datasets for geophysical attributes (such as velocity and attenuation), and then comparing those attributes with fracture-based measurements (such as from borehole logs or cores) to obtain information about the spatial distribution of fractures. Such two-step approaches are generally effective when good site-specific petrophysical relationships between the inverted geophysical attributes and the fracture properties are easily obtainable, when the developed petrophysical relationships are approximately uniform over the region of interest, or when only approximate information about the fracture zonation is required. However, they are ineffective or even fail in some situations, such as when geophysical inversion errors are large or when the petrophysical models are difficult to obtain, (e.g., at the ORNL IFRC, where anisotropy confounds development of an azimuthally consistent petrophysical model). Because it is well recognized that inversion of both seismic tomographic and surface refraction datasets are subject to uncertainty and artifacts, are often overly smooth and require expert knowledge to determine inversion choices, and have spatially varied resolution, recent research has focused on the development of inversion techniques that jointly honor all available datasets (i.e., seismic P-wave travel times—not inverted seismic slowness or velocity values—and wellbore hydrogeological measurements) in the inversion process.

In the first (local-scale) fracture zonation example, a Bayesian joint inversion approach was developed to integrate tomographic seismic-travel-time and borehole-flowmeter data for fracture zonation estimation, in a region of the ORNL IFRC where a combined *in situ* and *ex situ* bioremediation-based approach was being tested. The key treatment zone for the bioremediation was the fracture zone at the base of the weathered saprolite. Within the Bayesian framework, the seismic travel time (rather than the inverted seismic slowness or its inverse velocity) and the borehole flowmeter data were considered as data, and the seismic slowness and hydrological zonation indicators at each pixel as unknown random variables. Using a probabilistic petrophysical model developed from site data to link the seismic response to fracture zonation, investigators used a sampling based Markov Chain Monte Carlo method to obtain posterior estimates of the unknown variables. Figure 3a illustrates the geophysically obtained estimates along transects within the treatment region that run both parallel and perpendicular to geologic dip. These figures indicate the "probability of being within a high hydraulic conductivity fracture zone" at the site. These estimates revealed that the target biostimulation zone had a varying thickness and dip, and was sometimes laterally discontinuous. Indeed, comparison of conservative tracer and uranium biostimulation experimental results (Wu et al., 2005) at the study site with the fracture estimation suggested that the stochastic seismic estimation method was useful for delineating zones that were hydraulically isolated from the amendment injection area (Figure 3b). The details of this study are provided in Chen et al. (2006).

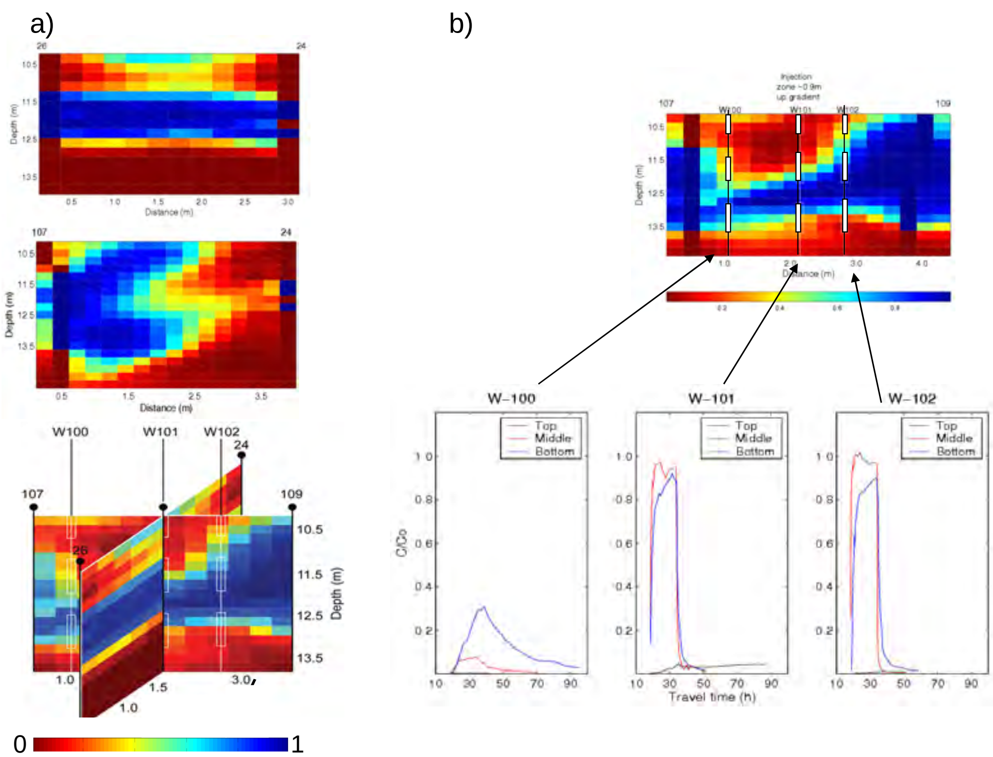

Figure 3. Estimates of natural fracture zonation obtained using seismic tomographic slowness measurements data within a stochastic estimation framework (modified from Chen et al., 2006): (a) estimates along the strike (top) and dip (middle) direction, as well as composite fence diagram (bottom); (b) comparison of the estimated fracture zonation with bromide breakthrough datasets (from Wu et al., 2006) associated with multilevel samplers.

The second example focuses on the development and testing of a Bayesian approach for estimating fast paths/fracture zonation along the length of the plume at the ORNL IFRC. This research is motivated by the recognition that the use of seismic datasets within a Bayesian framework permitted the estimation of fracture zonation at the local scale (see above); that surface-based seismic refraction datasets collected along the length of the ORNL IFRC plume reveal the presence of a buried low-velocity feature (which may indicate the location of a fast flow path); and that wellbore data (such as CPT push probes and electromagnetic flowmeter data) contain information about rock competency or flow (respectively) near the wellbore region. Conventional inversion of surface-based seismic refraction datasets yields a 2D cross section of P-wave velocity estimates, where the spatial distribution of the estimates often depends on the assumptions and parameters (such as smoothing) used in the inversion algorithm. As discussed above, calibration of the geophysical data using such a two-step approach can be confounded by the choice of inversion parameters and discrepancies between the wellbore and surface seismic measurement support scales.

To circumvent this limitation, an aspect of ongoing research at the ORNL IFRC focuses on developing and testing a watershed approach that simultaneously inverts the surface geophysical and wellbore datasets in a single step, thereby jointly honoring all available (multiscale) datasets and minimizing errors associated with the two-step process in the quantification of subsurface architecture. Particularly important at the ORNL IFC is the delineation of the low-velocity zone (that may influence preferential flow) and key interface geometry, needed as input to the site-wide flow model. Within a developed Bayesian framework, the seismic first-arrival times (not the inverted seismic-velocity values) and wellbore information about key interfaces are considered as input. A staggered-grid finite-difference method (with second-order precision in time and fourth-order precision in space) was used to forward model the full seismic waveform in 2D with subsequent automated travel-time picking. Seismic slowness and indicator variables of key interfaces are considered as unknown variables in the framework. By conditioning to the seismic travel times and wellbore information (i.e., picks of interface depths, depth of resistance of push probes), we are able to estimate the probability of encountering key interfaces (i.e., between fill, weathered saprolite, low-velocity zone, and consolidated materials) as a function of location and depth within the watershed. Application of the approach to synthetic and real field data indicate that the developed method is effective and that the incorporation of local-scale depth constraints provided by wellbore datasets in the inversion procedure significantly reduces uncertainty in the zonation estimation obtained using surface seismic refraction datasets. An example of the Bayesian-obtained inversion compared to conventional inversion of surface seismic refraction datasets collected at the ORNL IFRC is shown in Figure 4. The developed approach differs from the conventional approach (of inverting surface datasets into 2D estimates of seismic velocities and using that to interpolate wellbore data or infer boundaries), in that it explicitly incorporates wellbore data into the inversion of the geophysical data in terms of aquifer architecture and provides estimates of uncertainties. To our knowledge, this is the first plume/watershed joint inversion procedure that has been developed to quantify shallow subsurface architecture and associated uncertainties using seismic refraction datasets.

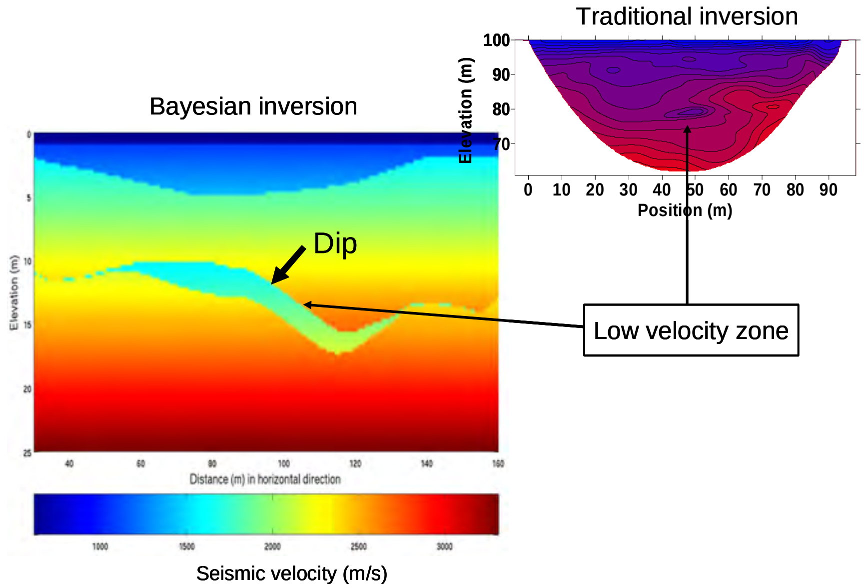

Figure 4. Estimated 2D velocity profile obtained using synthetic seismic refraction data within the developed Bayesian framework with constraints from several boreholes, showing the ability of the estimation framework to more discretely identify the base of the fill, top of the saprolite, and low seismic velocity transition zone at the ORNL IFRC relative to traditional inversion procedures (modified from Chen et al., 2008).

2.3 Plume Delineation

In addition to delineating subsurface geometry and fracture zonation, delineation of the contaminant plume boundary is often a subsurface characterization objective. Plume "mapping" has primarily been performed using surface electrical methods, which capitalize on the commonly observed direct relationship between electrical conductivity and total dissolved solids (TDS). Such plume mapping is also a difficult target, because electrical signatures respond to pore-fluid ionic strength as well as material properties, temperature, and other factors (e.g., Lesmes and Friedman, 2005), and it is often difficult to deconvolve the different contributions to the geophysical signal. However, if the contrast between the concentration of the uncontaminated groundwater and the plume is great enough so that the contribution of lithological (and other) variations on the electrical signature can be considered to be negligible, electrical methods can be used to delineate approximate plume boundaries.

An example of the use of surface electrical data to approximately delineate plume boundaries at the ORNL IFRC is illustrated in Figure 5 (modified from Watson et al., 2005). At this site, ion chromatography of wellbore groundwater samples indicate that nitrate concentrations range from the tens of thousands of parts per million (ppm) near the (S-3 ponds) source area to thousands of ppm (and less) in the downgradient regions, whereas the uranium is currently located in the source-zone region. Understanding the distribution of the nitrate is important for considering the potential future uranium transport flowpaths. Because the nitrate concentrations are so high at this site, it was believed that associated variations in TDS would predominantly impact the surface electrical responses. Consequently, an electrical resistivity survey was conducted using an AGI/Sting 56 electrode system. Both dipole-dipole and Schulmberger array geometries were used with 1 m and 2 m electrode spacings. Widely available software that relies on least-squares approaches (Loke and Barker, 1996) was used to invert the data for 2D distributions of electrical resistivity estimates.

Figure 5 illustrates an inverted surface electrical resistivity profile located adjacent to the source area in the downgradient direction. The profile reveals a shallow, unsaturated section of high electrical resistivity, as well as a deeper region in the saturated section that has very low electrical resistivity values. Comparison of surface and wellbore data indicated that zones of low electrical resistivity (or high electrical conductivity) were correlated with zones that have higher concentration of nitrate pore waters. Figure 5b provides a comparison of the fluid and effective resistivity values obtained from the wellbore and surface datasets, respectively. Where the matrix and fluid properties are constant, Archie’s law (Archie, 1942) should yield a linear relationship between fluid and effective resistivity (the latter obtained from inversions of the surface datasets). In this case, there is significant scatter in the cross plot, which suggests that the material properties vary spatially and that without taking this into account, the surface electrical datasets cannot be used to quantify the spatial distribution of nitrate concentration. Instead, the datasets were used to define a boundary of high nitrate concentration, using an indicator approach. With this approach, resistivity values less than 12.2 Ohm-m were used to estimate regions of the plume having a concentration greater than 3,000 ppm, based on a site-specific relationship. Figure 5c illustrates the approximate boundary of the high-nitrate portion of the plume obtained using this indicator method and the surface electrical-resistivity transects.

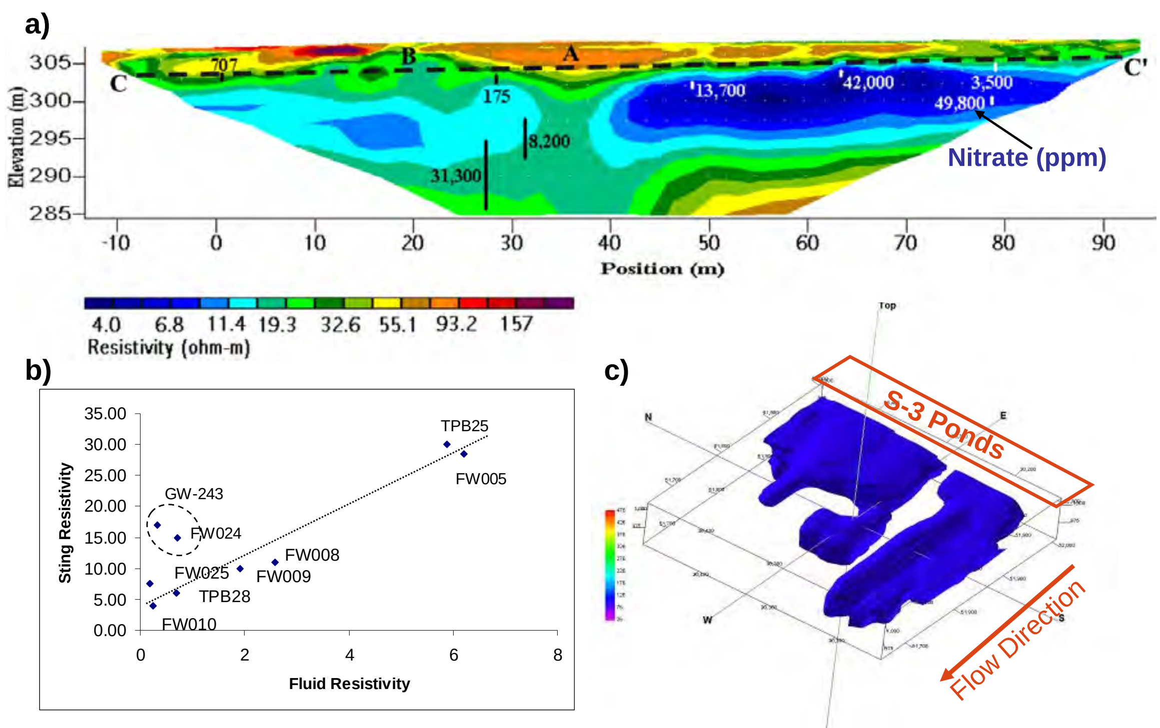

Figure 5. Use of surface electrical datasets at the ORNL IFRC to delineate the approximate plume boundary: (a) example surface electrical profile showing distribution of inverted electrical resistivity as well as nitrate concentrations obtained from wellbore sampling; (b) comparison of electrical resistivity obtained using the surface electrical data collected using a Sting system and the wellbore (fluid) resistivity values; (c) estimation of the distribution of the portion of the nitrate plume having a concentration greater than 3,000 ppm obtained using the surface electrical datasets and a site-specific indicator relationship between electrical resistivity and nitrate concentration (modified from Watson et al., 2005).

In a similar study, Rucker and Fink (2007) used surface electrical profiles to delineate a nitrate plume at the BC Cribs area of the Hanford Reservations in Washington (Figure 6). At this site, because nitrate is a key contaminant of concern (technetium) and because the nitrate concentrations are also very high, electrical methods were considered to be a reasonable approach for delineating the approximate boundary of the plume. Drilling is planned to verify the geophysically obtained plume distribution.

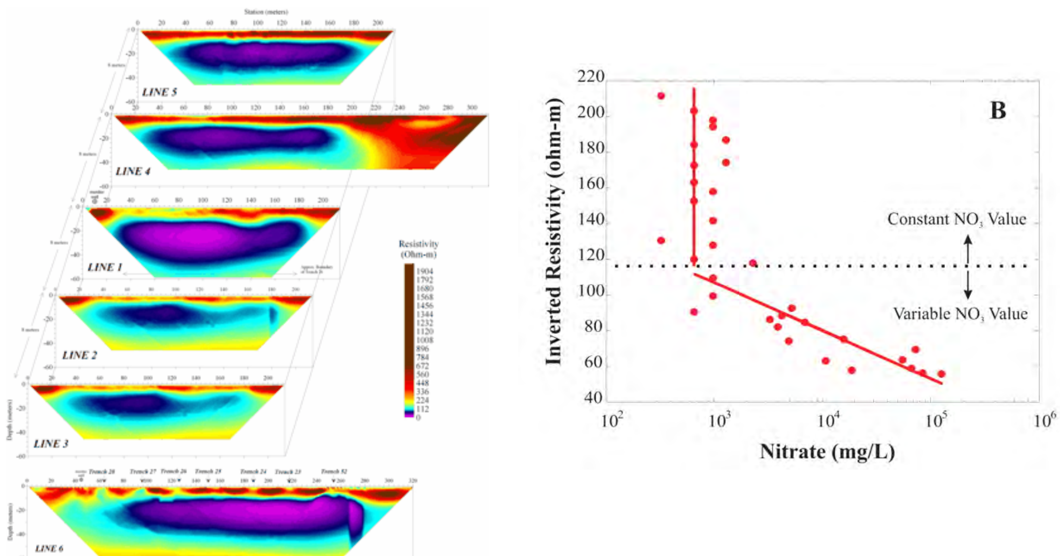

Figure 6. (a) Inverted electrical resistivity profiles at the BC crib area of the contaminated Hanford, Washington Reservation, where the low electrical resistivity (high electrical conductivity) regions were interpreted as the plume boundaries; (b) observed relationship between electrical conductivity and nitrate concentration at a single wellbore location within and above the interpreted plume (modified from Rucker and Fink, 2007).

3. Summary and Existing Challenges

This report illustrates the potential that geophysical methods have for the most common characterization objective: mapping the subsurface architecture or features that may impact flow and transport.

- Two case studies illustrated the traditional use of surface GPR and surface seismic-reflection methods for inferring subsurface stratigraphy, whereby surface geophysical datasets were compared with (or “tied to”) log data to permit qualitative interpolation of stratigraphic information between wells. In the GPR case study, the data were most useful for choosing the locations of the detailed bacterial transport study sites. In the seismic case study, the data were useful for identifying a buried channel that appears to have impacted plume direction and geometry; the revised conceptual model is being assessed through numerical modeling. These studies were conducted in saturated and unsaturated sections of granular porous Atlantic Coastal Plain sediments. The subsurface of the GPR study was “clean”, whereas the subsurface associated with the seismic study (Savannah River Site P-Area) was contaminated with TCE.
- Two case studies illustrated the use of seismic methods and stochastic approaches for quantifying architecture/fracture zonation at the uranium-contaminated ORNL IFRC site in Tennessee. One example illustrated the use of a Bayesian approach to jointly invert seismic

travel time and wellbore data to estimate the "probability of being in a high hydraulic conductivity fracture zone." The other approach extended the Bayesian method to the watershed scale and used surface refraction travel-time and wellbore data to delineate key interfaces and low-velocity zones (suspected to represent preferential flowpaths).

- Two case studies illustrated the use of surface electrical datasets for delineating approximate boundaries nitrate plumes at the Tc-contaminated BC Cribs of the Hanford Site and at the U-contaminated ORNL IFRC. Both case studies revealed that (1) variations in saturation, lithology, and/or plume location prohibited a one-to-one mapping of electrical conductivity in terms of nitrate concentrations, and that (2) in regions of high nitrate concentration, the electrical response is primarily influenced by TDS and indicator approaches can be useful for delineating approximate plume boundaries.

Understanding the full capacity of geophysical methods for subsurface architecture delineation is expected to improve through increased experimentation; development of petrophysical relationships and theory; and improved understanding of scaling issues; through the development of estimation approaches for integrating multi-scale hydrobiogeochemical-geophysical datasets; and through comparison and integration of field data and reactive transport model predictions (Hubbard and Rubin, 2005). With the hydrogeophysical research currently under way within the community, we expect that the use of geophysical methods for exploring complex subsurface structure associated with contaminant remediation to increase in frequency and to become more quantitative in nature. As will be illustrated by the ensemble of the four 2009 PART Reports, the DOE Environmental Remediation Science Division has supported a large fraction of the hydrogeophysical and biogeophysical methodology development and testing, which should contribute significantly to their Long Term Measure of "incorporation of physical, chemical and biological processes into decision making for environmental remediation and long-term stewardship."

Authors

This report was developed by Susan Hubbard (LBNL) with contributions from Adrian Addision and Mike Waddell (USC), Greg Baker (UT), Jinsong Chen (LBNL) and David Watson (ORNL).

References Supported Through DOE ERSP Funding

Addision, A., M.G. Waddell, C.C. Knapp, D.T. Brantley and J.M. Shafer, Developing a robust geologic conceptual model using pseudo 3D P-wave seismic reflection data, Environmental Geosciences, volume 16(1), 1-16, 2009.

Chen, J., S. Hubbard, J. Peterson, K. Williams, M. Fienen, P.Jardine, and D. Watson, Development of a joint hydrogeophysical inversion approach and application to a contaminated fractured aquifer, Water Resour. Res., 42, W06425, doi:10.1029/2005WR004694, 2006.

Chen, J., S. Hubbard, V. Korneev, D. Gaines, G. Baker and D. Watson, Stochastic inversion of seismic refraction data with borehole depth constraints for watershed-scale characterization of aquifer geometry, *Eos Trans. AGU, 89*(53), Fall Meet. Suppl., Abstract H44C-06, 2008.

Hubbard, S. and Y. Rubin, Hydrogeophysics, Chapter 1 in Hydrogeophysics, Y. Rubin and Susan Hubbard, eds., Springer, The Netherlands, Water and Science Technology Library, V. 50, p. 3-7, 2005.

Hubbard, S., Chen, J., Peterson, J., Majer, E., Williams, K., Swift, D., B. Mailliox and Y. Rubin, Hydrogeological Characterization of the D.O.E. Bacterial Transport Site in Oyster Virginia using Geophysical Data, *Water Resources Research* , 37(10), 2431-2456, 2001.

Rubin, Y. and S. Hubbard, Hydrogeophysics, Springer, Netherlands, Water and Science Technology Library, V. 50, 523 p., 2005.

Scheibe T.D., and Y.J. Chien, An Evaluation of Conditioning Data for Solute Transport Prediction, Ground Water 41(2):128-141, 2003.

Watson, D. B., W. E. Doll, T. J. Gamey, J. R. Sheehan, and P. M. Jardine, Plume and lithologic profiling with surface resistivity and seismic tomography. *Ground Water* 43(2):169–177, 2005.

Wu, W.M. et al., Field scale bioremediation of uranium in a highly contaminated aquifer I: Conditioning of a treatment zone, Environmental Science and Technology, V(40), 3978-3985, 2006.

Additional References (Other)

Archie, G.E., The electrical resistivity log as an aid in determining some reservoir characteristics, Trans. Amer, Inst. Mining Metallurgical and Petroleum Engineers, 146, 54-64, 1942.

Butler, J., Hydrogeological Methods, Chapter 2 in Hydrogeophysics, Eds. Y. Rubin and S. Hubbard, Springer, Netherlands, 23–25, 2005.

Gelhar, L., Stochastic Subsurface Hydrology, Prentice Hall, New Jersey, 1993.

Hayles, J.G. Serzu, M.H., Lodha, G.S., Everitt, R.A., and Tomsons, D.K. Cross-hole seismic and single-hole geophysical surveys to characterize an area of moderately fractured granite, *Canadian Journal of Exploration Geophysics*, Vol. 32, No. 1, p. 6-23, 1996.

Kolterman, C.E. and Gorelick, S.M.. Heterogeneity in sedimentary deposits: a review of structure-imitating, process-imitating, and descriptive approaches. *Water Resour. Res.* 32, pp. 2617–2658, 1996.

Lane, J.W. Jr., F.P. Heini, W.M. Watson, Use of a square-array direct current resistivity methods to detect fractures in crystalline bedrock in New Hampshire. Ground Water, 33(3), 476-485, 1995.

Lesmes, D. and S. Friedman, The relationship between the electrical and hydrogeological properties of rocks and soils, Chapter 4 in Hydrogeophysics, Eds. Y. Rubin and S. Hubbard, Water Science and Technology Library, V. 50, Springer, Netherlands, 2005.

Loke, M.H. and R.D. Barker, Rapid least-squares inversion of apparent resistivity pseudosections using a quasi-Newton method, Geophysical Prospecting, 44, 131-152, 1996.

Robertson, P.K., R.G. Campanela, D. Gillespie, and J. Greig, Use of piezometer cone data, in Proceedings of the ASCE Specialty Conference In Situ ’86: Use of In Situ Tests in Geotechnical Engineering, 1263-1280, Am. Soc. of Civ. Eng., Reston, VA 1986.

Rucker, D.F. and J.B. Fink, Inorganic plume delineation using surface high resolution electrical resistivity at the BC Cribs and Trenches Site, Hanford. Vadose Zone Journal, 6:946-958, 2007.

Vail, P.R., Seismic stratigraphy interpretation utilizing sequence stratigraphy, in Bally, A.W., ed., Atlas of Seismic Stratigraphy: American Association of Petroleum Geologists, Studies in Geology, v. 27, p. 1-10, 1987.

Vereecken, H., A. Binley, G. Cassiani, A. Revil, and K. Titov, Applied Hydrogeophysics, Nato Science Series, Vol 71, 383 p., 2006.

Yilmaz, O., *Seismic Data Processing*, Society of Exploration Geophysicists, Tulsa, OK, 1988.