US Department of Energy, Office of Science
Climate and Environment Division

Environmental Remediation Science
FY09 Second Quarter Performance Measure

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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 second of four quarterly reports, we describe how geophysical data can be used to estimate subsurface properties that influence flow and transport.

1. Introduction

As was described in the FY09 Q1 report, contaminant flow and transport, natural attenuation, and contaminant remediation efficacy are all influenced by subsurface hydrogeological and biogeochemical properties that vary over a wide range of spatial scales. Although geophysical data provide only indirect information about subsurface properties, recent research has illustrated the utility of these data for improving our understanding of heterogeneity and predictions of flow. In the Q1 report, we discussed the use of geophysical data for mapping subsurface architecture or features that influence flow. In this Q2 report, we extend that discussion to examine the use of geophysical data for estimating subsurface properties that influence flow and transport and illustrate hydrogeophysical advances that have been developed through DOE Environmental Remediation Science Program support.

2. Estimating Subsurface Properties that Control Flow and Transport

The ability to estimate hydrogeological or geochemical properties using a particular geophysical approach is a function of the relation between the property under consideration and geophysical attributes, the availability of direct measurements for calibration, the magnitude of the property variations and contrasts, and the spatial scale of the property variations relative to the measurement support scale of the geophysical technique (e.g., Hubbard and Rubin, 2005). In the simplest case, the property of interest can be *inferred* based on known geophysical responses to hydrological property variations. For example, electrical conductivity, which is typically greater in clay than in sandy sediments and is greater in saturated sediments than in the same dry sediments, has been used to infer the distribution of sedimentary units or saturation state. Such qualitative inference is the simplest approach for using geophysical data for subsurface characterization. This approach is widely used during reconnaissance characterization, where the geophysical interpretations are used to site wellbore drilling locations or regions that require more in-depth analysis.

Quantitative estimates of subsurface hydrogeochemical properties are also potentially obtainable using geophysical datasets. Such estimation requires two key components: a relationship or theory to link the geophysical measurements with the hydrogeological property of interest and a framework for interpreting the geophysical data in terms of the hydrogeochemical property of interest. The first component is referred to as a petrophysical relationship. Unfortunately, petrophysical relationships that link hydrogeochemical parameters (such as mean grain size, porosity, permeability and sediment geochemistry) within typical near-surface environments to geophysical attributes (such as seismic velocity, electrical resistivity, and dielectric constant) are not well understood. Although a significant amount of research has been performed to investigate petrophysical relationships used for petroleum reservoirs and mining applications, very little research has been performed to develop these relationships within the lower pressure and temperature environments common to contaminated sites. As such, there are only several general relationships that are commonly used within near surface geophysics, and even these are often used only to get a ‘ballpark’ estimate. Examples include the Topp’s empirical relationship (which relates dielectric constant values to moisture content; Topp et al., 1980) and Archie’s relationship (which relates bulk electrical conductivity to the electrical conductivity of water-saturated geologic materials; Archie, 1942). Mixing models have also been used within hydrogeophysics, whereby the effective geophysical measurement is expressed as a summation of the contributions from different components of a system (such as grains and pore fluid). Another common approach in hydrogeophysical applications is to develop site-specific empirical relationships between the geophysical measurements and the parameters of interest using co-located field data (such as data co-collected at a wellbore) or by developing relationships with laboratory measurements of site material. Difficulties in developing petrophysical relationships using co-located field data arise from the different sampling scales, measurement directions, and errors associated with wellbore hydrological measurements and geophysical ‘measurements’ acquired at or near a wellbore (e.g., Day-Lewis and Lane, 2004). Similarly, upscaling laboratory-derived relationships for use at the field scale also presents challenges (e.g., Moysey et al., 2004).

Quantitative estimation of hydrogeochemical properties using geophysical methods also requires a method for integrating the sparse (yet direct) wellbore data with the more spatially extensive (yet indirect) geophysical datasets. Various approaches have been used to perform this estimation; the ‘best’ approach for a particular situation depends significantly on the availability and quality of the datasets; experience of the interpreter; conceptual model of the subsurface environment; and requirements for accuracy and uncertainty estimation. Examples of estimation categories include (e.g., Linde et al., 2006):

- Direct mapping, where the geophysical attributes are transferred to a hydrogeochemical property estimate using a petrophysical relationship. Although this is the simplest approach, it does not rigorously incorporate the wellbore data in the interpretation. If the developed petrophysical relationship is weak or non-stationary, the parameters estimated using the geophysical data can fail to match the measured data at wellbore locations.
- Geostatistical methods are widely used for incorporating hydrological and geophysical data. These techniques rely on spatial correlation information to interpolate between measurements in a least-squares sense. Because natural geologic materials often exhibit strong spatial organization, these methods have been widely used within the environmental sciences.
- Bayesian approaches have also proven to be useful for subsurface characterization, because they permit the incorporation of a-priori information (such as available from a

conceptual model or from wellbore datasets), quantify uncertainty, and provide a framework for incorporating additional datasets as they become available.

- Joint inversion and coupled modeling approaches, which jointly honor all datasets in the parameter estimation procedure.

The first three of these approaches involve a two-step hydrogeophysical procedure, whereby inversion of geophysical data is first performed to obtain estimates of geophysical attributes (e.g., radar velocity estimates are obtained through inversion of radar slowness measurements, and seismic attenuation estimates are obtained through inversion of seismic amplitude data). The geophysical attributes are considered hard data and are analyzed for correlation with direct borehole hydrogeological measurements, thereby providing the relationship between geophysical attributes and the hydrogeological parameters of interest. In the second step, the estimates of hydrological parameters are obtained using the geophysical data, petrophysical relationship, and direct borehole data through direct mapping, geostatistical, or Bayesian methods. Because application of the two-step technique for mapping hydrological parameters can be limited by errors associated with geophysical data acquisition and inversion procedures (as well as inferred relationships of geophysical attributes with petrophysical properties), joint inversion approaches have recently been developed to reduce errors in both geophysical and hydrological parameter estimation.

Summaries of several DOE-supported hydrogeophysical studies are given below. These case studies were chosen to illustrate the use of different types of petrophysical relationships, geophysical datasets, and approaches to estimate hydrogeochemcial properties that control flow and transport.

2.1 Estimation of Soil Water Content using a Direct Mapping Approach

In recent years, ground penetrating radar (GPR) has developed into a tool for mapping water content and movement within the vadose zone. Using a direct mapping approach, the velocity is first estimated by inverting the GPR travel time data. The velocity estimates are then converted to dielectric constant and then into estimates of water content using a petrophysical relationship. An example of the use of crosshole radar data for estimating volumetric water content is illustrated using data collected within the porous granular vadose zone of the DOE Hanford Site in Washington. Neutron probe data were collected at this site, calibrated using gravimetric techniques, and interpreted in terms of volumetric water content (Ward et al., 2000). Tomographic GPR data were collected and the inverted velocity values were used with a mixing model to convert the dielectric constant estimates to water content (Majer et al., 2001). Figure 1a shows the 2-D distribution of estimated volumetric water content between two wells, and Figure 1b shows a comparison of neutron probe values collected from an access tube located close to wellbore X3 with the estimates of water content obtained from the tomographic pixels along the column located approximately 0.25 m away from wellbore X3 (to avoid the geophysical distortion commonly encountered at the wellbore location). This figure illustrates that a simple mixing model was sufficient for estimating water content in multiple directions with a reasonable accuracy, and thus highlights the use of GPR for direct mapping of water content.

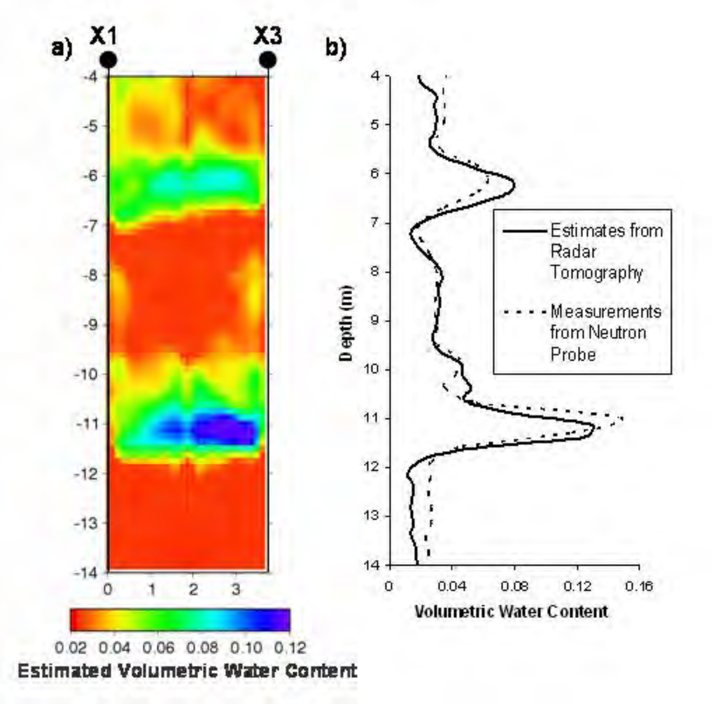

Figure 1 **(**a) Volumetric water content estimated using tomographic radar data, (b) comparison of tomographic estimates and neutron probe measurements of water content near borehole X3.

2.2. Estimation of Hydraulic Conductivity Zonation using a Discriminant Analysis approach.

Estimates of hydraulic conductivity zonation, or the location of units having higher and lower hydraulic conductivity, were obtained at the Cr(VI)-contaminated DOE Hanford 100H site using tomographic seismic and radar datasets with electromagnetic flowmeter data The reduced flowmeter measurements in the Hanford formation revealed that the hydraulic conductivity was bimodally distributed, suggesting that it would be most reasonable to estimate the distribution of higher and lower hydraulic conductivity zones in the Hanford formation, or hydrological zonation. To perform the estimation, we used an indicator approach and a linear discriminant analysis technique, which is a technique for categorizing a set of observations into several predefined classes. We divided the hydraulic conductivity into two classes: a class representing all values lower than a cutoff value of 10^{-3} cm/s, which was the median hydraulic conductivity value (i.e. indicator=0), and another class representing all values higher than the cutoff value (i.e. indicator=1). The mean log hydraulic conductivity values of the two categories were -3.47 and -2.33 cm/s, respectively, and the corresponding within-group standard deviations were lower than the overall standard deviation of the hydraulic conductivity dataset.

Using the linear discriminant approach, the defined cutoff value, and the tomographic data, we obtained the spatial distribution of the probability being in the higher hydraulic conductivity zone of the Hanford formation (Figure 2). Although the flowmeter data in the Hanford formation are quite sparse and the acquisition geometry and inversion approach impact the baseline geophysical images used for this interpretation, Figure 2 generally suggests that the probability of the hydraulic conductivity being higher than the median value is greater in the upper part of the sandy Hanford formation than in the lower part. These data were used during a Cr(VI) biostimulation experiment to guide the amendment injection as well as to help interpret the spatiotemporal distribution of amendments and biogeochemical transformations (Hubbard et al., 2008).

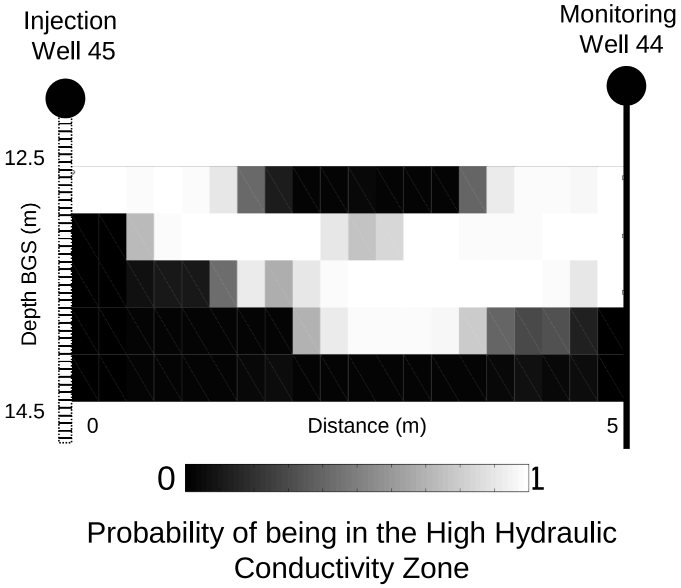

Figure 2. Estimate of hydraulic conductivity zonation obtained at the Hanford 100H Cr(VI) biostimulation site between the amendment injection and downgradient monitoring well using crosshole radar datatsets and a discriminant analysis approach (modified from Hubbard et al., 2008).

2.3 Estimation of Hydraulic Conductivity using a Bayesian Approach

An example of hydrogeophysical property estimation performed within a Bayesian framework is the use of crosshole radar and seismic methods to provide multidimensional estimates of hydraulic conductivity at Oyster, VA bacterial transport site described by Hubbard et al. (2001). At this site, DOE supported a team of investigators to explore how physical and geochemical heterogeneity influenced the transport of bacteria that were injected into the subsurface in a manner used for bioaugmentation. Within the unconfined Atlantic Coastal Plain aquifer, tomographic data were used together with borehole flowmeter logs to develop a site-specific petrophysical relationship that linked radar and seismic velocity with hydraulic conductivity. To implement the Bayesian framework, a prior probability of hydraulic conductivity was first required, which was obtained through geostatistical kriging of the hydraulic conductivity values obtained at the wellbore location using the flowmeter logs. Within the Bayesian framework, these estimates were then ‘updated’ using the developed petrophysical relationship and estimates of radar and seismic velocity obtained using tomographic geophysical methods (Figure 3). The method yielded ‘posterior’ estimates of hydraulic conductivity (and their uncertainties) along the geophysical transects which exactly honored the wellbore measurements. The estimates were obtained at the high spatial resolution of the geophysical measurements (which had pixel dimensions of 0.25 m × 0.25 m).

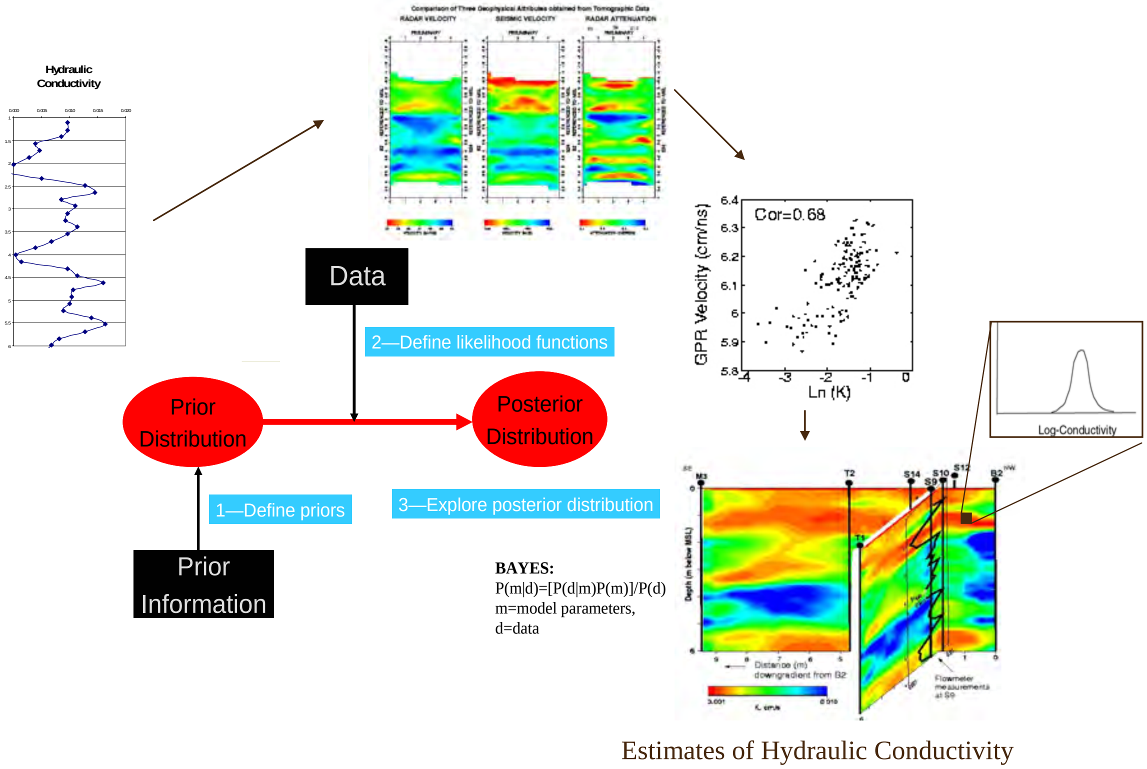

Figure 3. Example of Bayesian approach for integrating disparate datasets for the estimation of hydraulic conductivity distributions, where the mean value of the estimated hydraulic conductivity distributions within each 0.25 cm x 0.25cm pixel is shown on the bottom right (Modified from Hubbard et al., 2001).

Comparison of the geophysically obtained hydraulic conductivity estimates and tracer breakthrough data suggested that the tomographic estimates were extremely useful in helping to reduce the ambiguity associated with interpreting bacterial and chemical transport data collected during tracer tests at the DOE Oyster bacterial transport site (Johnson et al., 2001). Even though this site was fairly homogeneous (the range of hydraulic conductivity was approximately one order of magnitude) and had extensive borehole control (i.e., wellbores every few meters), it was difficult to capture the variability of hydraulic conductivity using borehole data alone with sufficient accuracy to ensure reliable transport predictions. By comparing numerical model predictions with tracer test measurements at the Oyster Site, Scheibe and Chien (2003) found that "conditioning to geophysical interpretations with larger spatial support significantly improves the accuracy and precision of model predictions" relative to wellbore based datasets. This study suggested that the geophysically based methods provided information at a reasonable scale and resolution for understanding field-scale processes. This is an important point, because it is often difficult to take information gained at the laboratory scale or even from discrete wellbore samples and apply it at the remediation field scale.

2.4 Estimation of Sediment Geochemistry using a sampling-based Bayesian approach.

Estimation of sediment geochemistry is also extremely important for prediction of contaminant evolution and transport, because sediment geochemistry controls sorption, bioavailability and bacterial attachment, and other critical processes. As such, sediment geochemistry greatly impacts the mobility of contaminants and their susceptibility to remedial treatments. Traditional methods for characterizing geochemical heterogeneity typically involve collecting a subsurface sample and subsequently performing laboratory analysis (such as Fe(II) and Fe(III) extraction using the Ferrozine method; Roden and Lovely, 1993). Because these methods require core samples for analysis and are labor-intensive, there are typically far fewer measurements of sediment geochemistry available for environmental remediation studies relative to hydrogeological measurements.

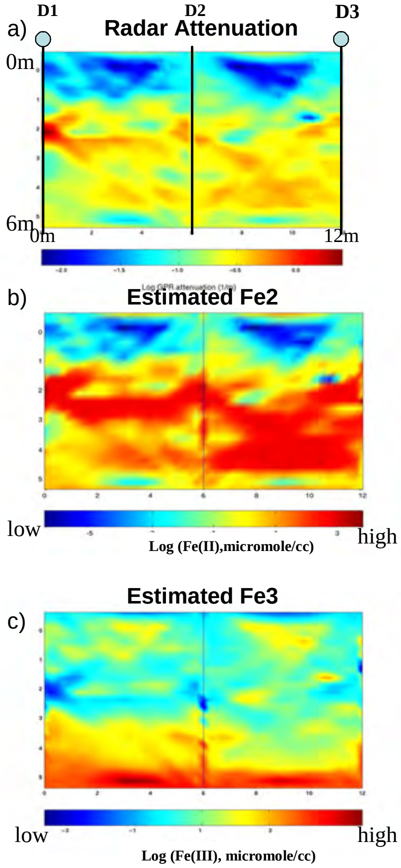

Figure 4. (a) Radar attenuation values obtained through inversion of crosshole radar tomographic amplitude data. (b) Estimates of Fe2 and (c) Fe3 obtained using the geophysical measurements and site-specific chemical-physical relationship (modified from Chen et al, 2004).

Because geophysical measurements often respond to physical property variations, it is also possible to quantitatively exploit physio-chemical relationships (if they exist) to quantitatively estimate sediment geochemistry distribution using geophysical methods. Recent DOE-supported research has illustrated the use of high resolution tomographic ground penetrating radar measurements and site-specific physio-chemical relationships to estimate lithofacies and Fe(II) and Fe(III) within a Bayesian framework (Chen et al., 2004). In this case, the geophysical data were not directly sensitive to the geochemical parameters. Instead, the radar amplitudes were sensitive to lithology (i.e., radar amplitudes were more attenuated in units with a larger clay fraction), and the lithology was in turn related to the distribution of Fe(II) and Fe(III) at the site. The developed estimation approach exploited this mutual dependence to estimate lithology and sediment geochemical parameters along 2-D cross-sections using tomographic radar amplitude data. Because of the complexity of the estimation (several parameters were simultaneously estimated), the posterior distribution was obtained through sampling based Markov Chain Monte Carlo approaches. Figure 4a illustrates the 2-D geophysical estimates of radar attenuation obtained from inversion of GPR amplitude data. Figures 4b and 4c illustrate the mean values of the estimated Fe (II) and Fe (III) distributions, respectively; variances associated with these estimates are available but are not shown in the figure. Cross-validation exercises revealed that the estimates obtained using the geophysical data were highly accurate and greatly improved the 2-D identification of the geological and geochemical properties. This study provided perhaps the highest-resolution field-scale characterization of geochemical properties performed to date. Scheibe et al. (2006) in turn used the spatially variable, geophysically obtained lithofacies and sediment geochemistry as parameterization for reactive transport simulations. The simulations illustrated the importance of understanding linked hydrological and sediment geochemical property distributions for predicting the distribution of contaminants, remediation amendments, and subsequent biogeochemical reactions associated with remediation.

2.5 Estimation of Permeability and Water Content though Joint Hydrogeophysical Inversion

In this example, we illustrate the joint inversion of geophysical and hydrological data, which effectively circumvents some of the obstacles commonly encountered during the previously discussed two-step hydrogeophysical approach and takes advantage of the complementary nature of geophysical and hydrological data. As was illustrated by the example shown in Section 2.1, the use of GPR methods for mapping water distributions in the subsurface is now well established; this mapping is made possible by correlation between the soil water content and measured dielectric constant. However, in general, GPR measurements cannot be directly related to the soil hydraulic parameters needed to make hydrological predictions in the vadose zone (such as the absolute permeability and the parameters describing the relative permeability and capillary pressure function). On the other hand, time-lapse GPR data can contain information that can be indirectly related to the soil hydraulic properties, since soil hydraulic properties influence the time- and space-varying changes in water distribution, which in turn affect GPR data.

Kowalsky et al. (2004) developed an approach for incorporating time-lapse GPR travel time and measurements of hydrological properties into a hydrological-geophysical joint inversion framework for estimating soil hydraulic parameter distributions. Coupling between the hydrological and GPR simulators is accomplished within the framework of iTOUGH2 (Finsterle, 1999). Inversion is performed using a maximum *a posteriori* (MAP) method that utilizes concepts from the pilot point method. One of the benefits of this approach is that it directly uses GPR travel times without requiring creation of velocity tomograms, thus alleviating difficulties inherent to tomographic inversion and allowing for sparser GPR data sets, relative to those required for conventional tomography. This joint inversion method was later extended to account for uncertainty in the petrophysical function (water content relationship to the dielectric properties) and to increase the flexibility of GPR data characteristics (to include multiple offset data acquisition in three dimensions), allowing increased resolution and accuracy of soil hydraulic parameter estimates (Kowalsky et al., 2005; Finsterle and Kowalsky, 2008).

This approach was applied to time-lapse neutron probe and tomographic radar travel time data collected at the 200 East Area of the U.S. Department of Energy (DOE) Hanford site in

Washington during an infiltration test. Unknown parameters estimated using the joint inversion approach included log-permeability values at pilot point locations (which are used to create three-dimensional permeability distributions), porosity, a parameter of the petrophysical function (the dielectric constant of the solid component of the soil), and the water injection rates, which were not measured precisely. Joint inversion resulted in estimates of hydrological parameter distributions, such as permeability (Figure 5), which can be used to parameterize flow models for predicting fluid distributions at future times.

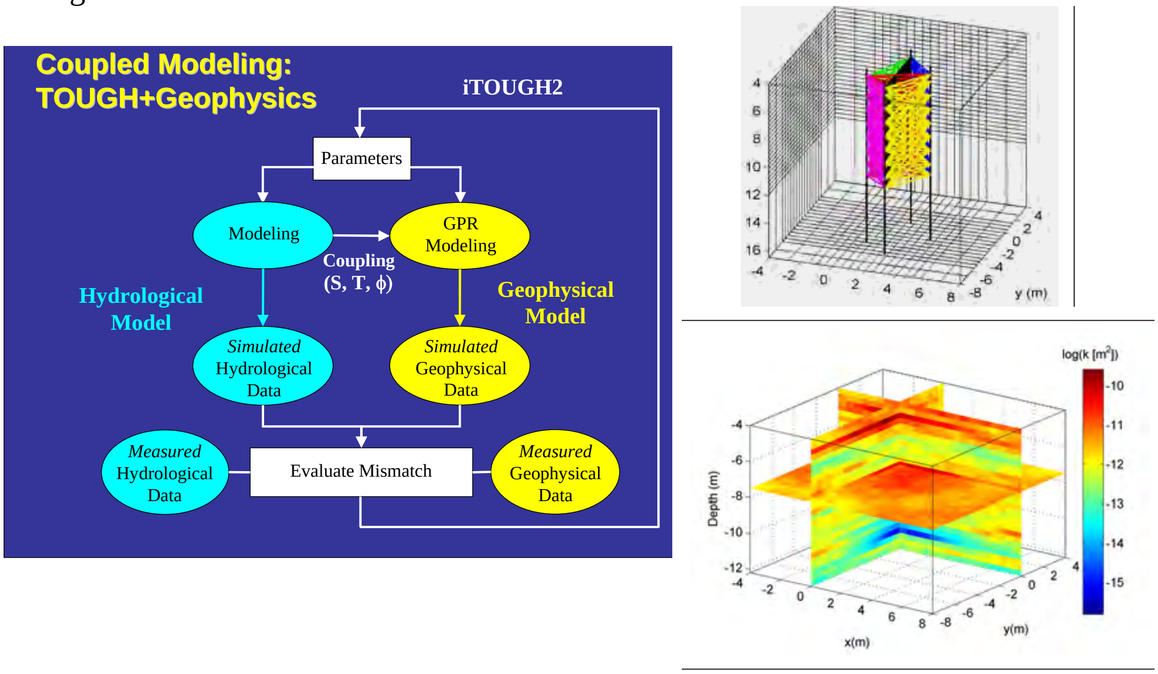

Figure 5. Estimation of hydraulic conductivity along selected slices in 3D volume obtained through joint consideration of hydrological and geophysical phenomena within coupled modeling framework (from Kowalsky et al, 2005).

3. Summary and Outlook

The examples presented above illustrated the use of different geophysical attributes (radar velocity, seismic velocity, and radar attenuation) to estimate different hydrogeophysical properties (soil moisture, hydraulic conductivity, hydraulic zonation, and sediment geochemistry) using direct mapping, Bayesian, and joint inversion approaches. The case studies illustrated the utility of the hydrogeophysical estimation methods in a variety of subsurface environments, including: unsaturated, saturated, clean, and Cr(V) contaminated aquifers. Understanding the full capacity of geophysical methods for environmental remediation characterization and monitoring is expected to improve through: increased laboratory and field experimentation; development of petrophysical relationships and theory; improved understanding of geochemical to geophysical measurement scaling issues; 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. In particular, the following topics describe challenges that are currently being explored through DOE research and that, once tackled, should greatly extend the utility of geophysical methods for guiding environmental remediation.

- Most of the case studies described in previous sections were tested at the ‘local’ scale (i.e., tens of meters length scales or less), where the scale disparity between the wellbore and geophysical measurements is not great. The importance of characterizing critical subsurface properties with sufficient confidence over plume-relevant scales is recognized. However, there have been few hydrogeophysical examples of property estimation using datasets that sample a variety of hydrobiogeochemical properties over a range of scales (from core samples to wellbores to surface datasets).

- Because hydrological and mineralogical (sediment geochemical) properties often co-vary as a function of geological processes, a significant opportunity exists to develop organizing principles, strategies, and frameworks that exploit these dependencies and provide information about properties that influence both flow and transport. Although this concept was illustrated in the example given in Section 2.4, the concepts could similarly be useful for mapping more regional variations in linked hydrogeochemcial properties.

- Although improvements in hydrogeophysical approaches (e.g., Rubin and Hubbard, 2004) and reactive transport modeling (e.g., Steefel et al., 2005) have been realized in recent years, there have been few attempts to test and document the synergies that come from integration of characterization, modeling, and monitoring datasets for improving environmental remediation. The examples provided in Section 2.3 (geophysically obtained hydraulic conductivity estimates used to parameterize a flow model) and Section 2.5 (coupled hydro-geophysical modeling) are two of the few in the hydrogeophysical literature that have been used to predict flow for improving environmental remediation. Further studies are needed to quantify the improvement inflow and transport prediction associated with including geophysical-based parameterizations.

With the continuing hydrogeophysical and biogeophysical research that is currently underway within DOE and the broader hydrogeophysical community, we expect that the use of geophysical methods for exploring complex and coupled hydrobiogeochemical subsurface processes associated with contaminant remediation to increase in frequency and to become more routine in practice.

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