VADOSE ZONE CHARACTERIZATION TECHNIQUES DEVELOPED BY EMSP RESEARCH

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ABSTRACT

This paper discusses research contributions made by Environmental Management Science Program (EMSP) research in the area of geophysical characterization of the subsurface. The goal of these EMSP research projects is to develop combined high-resolution measurement and interpretation packages that provide accurate, timely information needed to characterize the vadose zone. Various types of geophysical imaging techniques can be used to characterize the shallow subsurface. Since individual geophysical characterization tools all have specific limitations, many different techniques are being explored to provide more widespread applicability over a range of hydrogeologic settings. A combination of laboratory, field, theoretical, and computational studies are necessary to develop our understanding of how contaminants move through the vadose zone. This entails field tests with field-hardened systems, packaging and calibration of instrumentation, data processing and analysis algorithms, forward and inverse modeling, and so forth. DOE sites are seeking to team with EMSP researchers to leverage the basic science research investment and apply these advances to address subsurface contamination issues that plague many U.S. Department of Energy (DOE) sites.

INTRODUCTION

This paper discusses EMSP research projects that have developed geophysical imaging techniques for vadose zone characterization under the auspices of Environmental Management Science Program (EMSP). The U.S. Department of Energy (DOE) seeks to harvest the results of the EMSP research and, integrating them with the site operations, apply them to characterization of waste burial grounds and disposal sites throughout the DOE complex. These geophysical imaging techniques enable non-destructive characterization of subsurface conditions and processes from a limited number of boreholes and/or surface measurements. Accurate site characterization is important for contaminant and containment structure monitoring to decide whether waste can be safely left in place or if remediation is required. These basic science projects have the potential to improve our knowledge of subsurface properties and structures, which in turn leads to better decision-making regarding remediation and long-term stewardship strategies.

NEED FOR GEOPHYSICAL CHARACTERIZATION

Our understanding of the subsurface structure and properties of a site is derived from field observations. Non-invasive, high-resolution imaging of the shallow subsurface is needed to detect buried waste and to verify integrity of containment structures. A variety of geophysical methods used to provide subsurface characterization data are discussed herein, including electromagnetic (EM), radar, electrical, seismic, and nuclear magnetic resonance. These techniques enable information from limited test wells to be extrapolated to a larger area, without having to drill holes every few meters.

Geophysical imaging can be used to non-invasively map subsurface structures and contamination and investigate whether contaminants are leaking into the lower geological horizons via transport pathways. Accurate characterization of the subsurface beneath DOE waste sites is essential to assess the inventory, distribution, and movement of contaminants; develop improved predictive methods for liquid flow and

contaminant transport; assess risk; provide a foundation for the selection of remediation alternatives; and enable effective performance monitoring of corrective actions. Figure 1 shows how EMSP basic research provides tools and techniques that are used to protect groundwater supplies for future generations.

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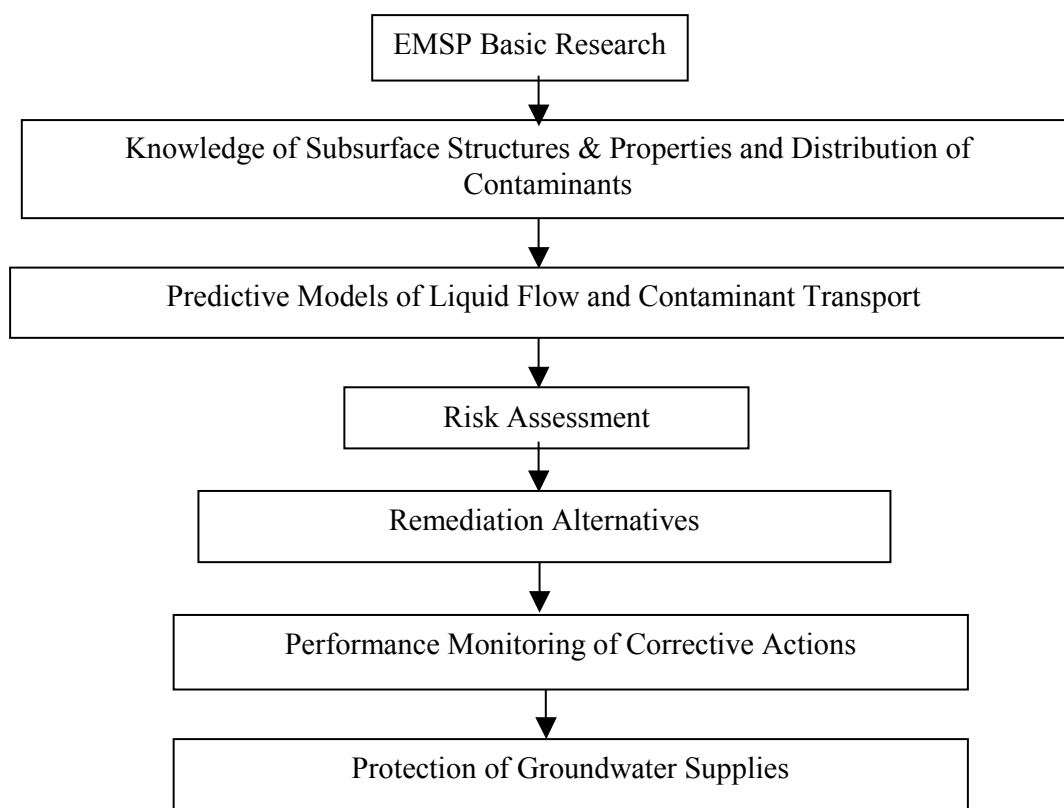
Figure 1. EMSP Basic Research as the Foundation for Protection of Groundwater Supplies

Stewardship plans for protecting groundwater supplies rely on an accurate predictive capability for contaminant transport in the subsurface. Current abilities to predict and optimally manage fluid flow and contaminant transport processes in the subsurface are limited by inadequate descriptions of subsurface heterogeneities (i.e., those occurring naturally and those created by waste interaction with the porous medium) that may influence the distribution of contaminants. Consequently, predictive models have often failed to provide accurate results and have underestimated transport rates.

The technical foundation for making decisions concerning the vadose zone requires knowledge of subsurface processes and properties, developing and integrating numerical and experimental capability, and performing simulations to assess the effectiveness of remediation strategies. Engineers and scientists must be able to represent and visualize the subsurface structure and properties as part of a whole-earth system in order to integrate computational predictions of relevant processes with subsurface data. A combination of multidisciplinary laboratory, computational, and field-scale studies are necessary to test specific hypotheses and provide a comprehensive understanding of vadose zone behavior. Characterization of the subsurface environment is a necessary precursor to developing isolation, stabilization, and treatment strategies, since the subsurface properties coupled with physicochemical and biological processes affect contaminant fate and transport. The purpose of such analysis is to predict the potential for infiltration to cause movement of contaminants in the vadose zone before they migrate into the groundwater, where they are difficult and costly to remediate. Knowledge of contaminant levels and

distribution throughout the subsurface is necessary to develop remediation and long-term stewardship monitoring strategies.

INTERPRETATION OF GEOPHYSICAL IMAGES

Geologic mapping provides critical information on subsurface features and the distribution of hydrologic properties. In the unsaturated zone, soil properties change dramatically with moisture content. Subsurface hydrology is a particularly important aspect of site characterization, because subsurface water and vapor transport are the primary natural pathways for the movement of contaminants to the accessible environment (1). To convert between geophysical and hydrological properties requires the application of petrophysical models. Improved relationships between geophysical measurements, hydrological properties, and soil composition are needed. A more reliable mapping between geophysical properties and hydrological properties would provide information that could ultimately be used to reduce cleanup costs, accelerate schedules, and reduce risk.

Improved methods for interpreting geophysical data collected in the field are needed. Two- and three-dimensional, EM forward modeling and inversion algorithms play an important role in environmental site characterization. Inversion algorithms are frequently used to "invert" or transform certain field measurements (such as radar, EM, and remote sensing data) into high-resolution images that provide more readily usable information.

RESULTS OF EMSP GEOPHYSICAL RESEARCH

Various types of geophysical imaging techniques are being investigated by EMSP researchers to characterize the contents of waste pits and trenches – electromagnetic (EM) induction, ground-penetrating radar (GPR), electrical resistivity, seismic, and nuclear magnetic resonance (NMR). Since individual geophysical characterization tools all have specific limitations, many different techniques are being explored to provide more widespread applicability over a range of hydrogeologic settings. The goal of these research projects are to develop combined high resolution measurement and interpretation packages that provide accurate, timely information needed to characterize the vadose zone. These geophysical projects couple field characterization techniques with data acquisition, data processing algorithms, and/or software development to interpret the data. Modeling is a very necessary counterpart to experimental investigation. A combination of laboratory, field, theoretical and computational studies are necessary to develop our understanding of the vadose zone. Each EMSP project discussed in this paper addresses an aspect of the field characterization problem. The following subsections describe both completed research or research in progress and the research contribution.

Electromagnetic Induction Techniques

Electromagnetic (EM) induction techniques provide a measure of the electrical conductivity of the subsurface. The source is a magnetic field generated by currents in wire coils, whereby sources and receivers are either located in boreholes or on the surface. A high-frequency impedance methodology that uses a window in the EM spectrum (1.0 to 100 MHz) between GPR and low-frequency induction techniques is used to yield high-resolution mapping of electrical conductivity, as well as the permittivity of near surface formations. Measurements made in this frequency range can resolve small buried targets and determine both the electrical conductivity and dielectric permittivity, which are related to shallow subsurface geochemistry and geohydrology. EM methods are sensitive to the amount and composition of fluid present in porous media. Monitoring soil moisture and electrical conductivity can provide indications of contaminant transport. EM methods have been shown to be effective in environmental site

characterization, but there is a need for increased resolution for waste form characterization, verification, and monitoring activities.

- *Detection of Buried Metal Objects (EMSP Projects #60162 and 86992).* Software and hardware enhancements to the existing Very Early Time Electromagnetic (VETEM) prototype instrument have enabled physical modeling experiments, numerical forward and inverse modeling, and field demonstrations. The VETEM system was deployed at Pits 4, 9, and 10 in the Subsurface Disposal Area at the Radioactive Waste Management Complex at the Idaho National Engineering and Environmental Laboratory. VETEM is designed to produce high-resolution electromagnetic images of the shallow (0 to 5 m) subsurface when the electrical conductivity of the earth is too high for GPR to be effective, such as in the clay capping material covering the waste pits. Data from Pits 4 and 10 were obtained using a VETEM system towed by an all-terrain vehicle equipped with a global positioning system that provides decimeter lateral positional accuracy. Inversion of the VETEM data provides depth estimates. VETEM was used to obtain geophysical images of the location and estimated depths of Pit 9 waste, and this information is used to support remediation operations (2).

- *Forward and Inverse Modeling (EMSP Project # 70220).* A full, three-dimensional, nonlinear inversion algorithm, which uses a scattered-field solution approach, is being developed for impedance data. Inversion algorithms are typically very complex and compute intensive. Rigorous 2D and 3D inversion codes are needed to bound the range of applicability of the approximate methods. The research team is currently: (a) implementing full non-linear 2D/3D inverse solutions that incorporate source coordinates and polarization characteristics, (b) using these solutions to study improvements in image resolution that can be obtained by making measurements in the near- and mid-field regimes using multiple source fields, (c) collecting data at the Hanford site with recently developed earth impedance measurement systems, and (d) interpreting the field data with the newly developed inversion capability, as well as with additional, independent information, such as well logs from boreholes (3).

- *Surface and Borehole Electromagnetic Imaging (EMSP Project # 55011).* Another EMSP research project has produced a forward modeling capability based upon a three-dimensional, finite-difference, Fourier-domain code to produce forward predictions of electrical and magnetic fields for a given source configuration, and to compute the adjoint operator to be used in the inversion method. An adjoint method of data inversion was developed to allow higher resolution and contrast images than previously possible. Data from crosswell and surface-to-borehole tests have been analyzed using the new inversion methods (4).

- *High Frequency Electromagnetic Impedance Measurements (EMSP Projects # 60328 and 73776).* Another research team is seeking to interpret the EM impedance data by simultaneously inverting electrical conductivity and permittivity using a single data set. Proof of concept of the methodology has been successfully demonstrated using commercial EM instruments. Currently, electronics of these instruments are carefully redesigned and repackaged for improved performance and field deployment (5,6)

Ground Penetrating Radar

Ground penetrating radar (GPR) uses microwaves to detect buried objects and provide information about the variation in dielectric properties of the subsurface.

- *Spatial Variability Of Subsurface Moisture Content (EMSP Project #70115).* Three-dimensional maps of subsurface moisture content are being constructed from GPR data. One approach involves obtaining estimates of water content for a radar-sampled volume of the subsurface. A critical part of this research is quantifying the uncertainty in water content estimates due to heterogeneity below the scale of the sampled volume. A second approach involves working directly with the radar image to quantify the spatial variability in water content. Researchers are using a modified version of GSLib for geostatistical analysis of GPR images. Field test at the Sisson and Lu site at Hanford have yielded encouraging results when the analysis of the radar data is compared with the information about water content obtained from neutron probe data (7).

- *DNAPL Detection (EMSP Project #70052).* A suite of methodologies for the direct detection of dense non-aqueous phase liquid (DNAPL), specifically chlorinated solvents, is being developed via material property estimation from surface GPR data. Most organic liquids have lower dielectric permittivity and conductivity than water, so a contrast in properties is induced when DNAPL displaces water. To identify zones of DNAPL contamination, a research team led by John Bradford is examining three aspects of reflected wave behavior—propagation velocity, frequency dependent attenuation, and amplitude variation with offset (AVO). Velocity analysis provides a direct estimate of electric permittivity, attenuation analysis provides a measure of conductivity, and AVO behavior provides an estimate of the permittivity ratio at a reflecting boundary. Preliminary work shows significant potential for quantitative direct detection methodologies in identifying shallow DNAPL source zones (8).

- *Improvements for Challenging Field Conditions (EMSP Project #86992).* A recently funded EMSP project seeks to extend the limits of performance of GPR in challenging environments via improvements in hardware and in the numerical computations. Key features include:

  (a) greater dynamic range through real time sampling and receiver gain improvements
  (b) modified, fully characterized antennas with current sensors to allow dynamic measurement of the changing radiated waveform
  (c) modified deconvolution and depth migration algorithms exploiting the new antenna output information
  (d) development of automatic, full waveform inversion made possible by the known radiated pulse shape
  (e) a modified visualization package for efficient subsurface interpretation (9).

Electrical Resistivity

Electrical resistivity tomography (ERT) is a direct current (DC) resistivity technique that measures electric potentials generated by a current source either on the earth's surface or in the subsurface. These potentials are sensitive to the bulk electrical properties, indicative of porosity, the amount and connectivity of pore fluid, and the pore fluid chemistry. ERT data require an inversion algorithm for producing a subsurface image. ERT can be used to observe changes in the water's movement. Mathematical inversion of the resistivity measurements can be used to derive a three-dimensional image of the electrical resistivity of the subsurface by taking advantage of water's ability to conduct electricity much more readily than rock.

- *Spectral Induced Polarization (EMSP Projects #55300 and 73836).* EMSP research is aiming to resolve the EM coupling problem with spectral induced polarization (SIP), by directly including EM induction in the three-dimensional IP modeling inversion codes. EM coupling noise presents a critical limitation for field implementation of SIP and conventional correction methods are

inadequate. This project treats EM coupling as a data signal rather than a useless noise signal, to extend the usable frequency range of the data to greater than 1 KHz (10). In 2001, the team performed electrical surveys using electrical-impedance tomography (EIT) to detect DNAPL contamination at the Savannah River Site. EIT was chosen since it is the only geophysical method that has been demonstrated in the laboratory to have high sensitivity to organic compounds (11).

- *Hybrid Hydrological/Geophysical Inverse Technique (EMSP Projects #55332, 70267, and 86890).* Hydrologic data is being combined with cross-borehole GPR (XBGPR) and ERT in a hybrid hydrological/geophysical inverse technique to better understand contaminant movement in the vadose zone. During the first three-year EMSP award, the researcher and his team obtained hydrologic and geophysical data at the Sandia-Tech Vadose Zone Facility infiltration test site in New Mexico. This dataset was used in both forward and inverse hydrologic algorithms to describe the relationship between in situ moisture content and matric potential, as well as the saturated hydraulic conductivity. The second three-year EMSP research focuses on the use of geophysical imaging to estimate transport processes in unsaturated conditions. The researchers have developed a new anisotropic ERT inversion code for commercial applications and a new aquifer test method, called hydraulic tomography, for characterizing aquifer heterogeneity (12). Research funded by a sequential EMSP award seeks to thoroughly evaluate how well ERT and XBGPR can resolve subsurface hydrological features and processes within the vadose zone, provide synthetic data sets for other researchers to use for testing and assessment, and assess an interactive method for determining subsurface flow and transport properties within the vadose zone.

- *Four-Electrode Resistivity (EMSP Project #70012).* Complex electrical resistivity measurements are being refined for monitoring DNAPL contamination in the subsurface. The work is based on a four-electrode electrical resistivity measurement, where two electrodes are used to impose a sinusoidal current and the remaining two electrodes sense the response voltage of the sample. Strong electrical signatures are characteristic of certain organic solvents, notably toluene, perchloroethylene (PCE), and trichloroethylene (TCE), in clay-bearing soils (13). This technique is potentially useful to detect the presence of DNAPLs along interfaces between basalt and the clay-bearing interbeds.

Seismic Techniques

Seismic methods measure the travel times of acoustic waves and have the potential to fully depict the contours and connectivity of subsurface aquitards and other essential structures for design of groundwater remediation programs. Use of seismic imaging methods can potentially reduce the uncertainty about contaminant pathways due to the scarcity of test wells and the untestable assumptions of geostatistical interpolation methods (14). Images of shallow structures can be obtained from the periphery of the waste site and do not require access to the surface above the structure.

- *Integrated Suite of Imaging and Inverse Techniques (EMSP Projects #60115 and 73962).* An integrated suite of imaging and inverse techniques for two-dimensional and three-dimensional seismic data in the near vertical to wide-angle propagation regime is being developed. The researcher and his team are presently extending Kirchhoff inversion, depth focusing, and full waveform inversion methods to three-dimensional imaging of the shallow subsurface. The researchers conducted an extensive three-dimensional seismic experiment at a groundwater contamination site in Utah, using a 0.22-caliber rifle as the seismic source. This team has produced a three-dimensional map of a shallow paleo-channel along which DNAPLs are confined at the base of a shallow aquifer (14).

- *Surface-Wave Group-Velocity Tomography (EMSP Project #86870).* An analysis technique for surface-wave group-velocity tomography is being developed to map the primary fluid pathways in shallow soils. Measurements of perturbations in the shear wave velocity of the soil are made by measuring changes in seismic response induced by fluid flow. The observed changes in surface-wave velocity are then used to map areas where fluids have modified the fluid pressure and, hence, the shear-wave velocity. Areas experiencing the greatest pressure and material properties changes would indicate primary flow paths and zones that are most likely amenable to remediation by extraction or flushing. The technique could be used prior to remediation to detect flow paths and, hence, help design an optimal remediation process, or during remediation to detect and determine which zones are reached by the remediation. The sensitivity of shear waves to fluid content could eventually allow surface-wave tomography to track fluid (i.e., water or organic contaminants in soils) movement with time. Information such as the time variations in the depth of the water table would be provided without having to drill wells to obtain single-point values (15).

- *Automated Geophone Planting (EMSP Projects #60199 and 73731).* Complementary site characterization capabilities of three-component shallow (compressional) P-wave seismic reflection techniques and GPR methods at ultra-shallow depths are being explored. Traditional shallow seismic-reflection methods have been capable of imaging the subsurface from about 2 to 30 m, but are ineffective in the very near surface regime. By modifying the field layout of the geophones and using an alternative seismic source (a single shot from a 0.22-caliber rifle), it has been possible to image subsurface depths of 0.6 to 2.1m. An automated geophone-planting device to quickly and automatically plant large numbers of geophones is under development (16).

- *Improvements to Seismic Data Interpretation (EMSP Projects #55411 and 70108).* EMSP research is being undertaken to relate measured geophysical properties, such as seismic velocity and electrical conductivity, to hydrogeology parameters of interest, such as porosity, saturation, and soil composition. The approach combines laboratory experiments, comparison to available field data, rock physics theories, and modeling to find relationships between geophysical measurements, hydrogeological parameters, and soil composition. Controlled laboratory measurements were conducted to determine ultrasonic velocities and complex impedances in man-made soils of known compositions under known saturation and pressure conditions to simulate prescribed depths. Researchers compared their measurements to theoretical models, other laboratory measurements from literature, and available field data and investigated the role of microstructure, fluid and clay distribution, and chemical effects on measured geophysical properties. The researchers have developed and tested algorithms to relate measured geophysical properties to porosity, soil composition, and fluid distribution (17).

Nuclear Magnetic Resonance

Magnetic resonance imaging (MRI) can be used to observe and quantify the location and size of individual pores containing DNAPL, water, and vapor flow through sediments. MRI provides three-dimensional images of the phases within the pores as a function of time.

- *Magnetic Resonance Imaging of Soil Columns (EMSP Project #70045).* MRI has been used to observe and quantify the location and size of individual pores containing DNAPL, water, and vapor flow in soil columns. In conjunction with MRI, constitutive relations are being developed for use in modeling techniques to describe the transient distribution of phases inside a column

experiment. Column experiments in the laboratory with decane have shown that MRI signal intensity is linearly correlated to the amount of decant trapped in the columns (18).

- *Measurements of Adsorbed Organic Contaminants (EMSP Project #54699).* Experiments were performed to measure the nuclear magnetic resonance (NMR) response of a water-saturated sand in its "clean" state and with various amounts of adsorbed oil. It was shown that NMR measurements can be a useful way of detecting trace amount of adsorbed organic contaminants in geological porous media. This research also provided results about the paramagnetic effects of Fe(III) on NMR data that must be taken into account to accurately interpret NMR measurements in the near-surface environment (19).

- *NMR Downhole Logging Tool (EMSP Project #86804).* A newly awarded EMSP project is investigating the capability and limitations of low-field NMR relaxation decay-rate measurements for determining environmental properties affecting DNAPL flow in the subsurface. The oil and gas industry uses NMR measurements to determine porosity and hydrocarbon content and to estimate formation permeability in deep subsurface formations. These determinations rely on NMR's ability to distinguish between water and hydrocarbons in the pore space and to obtain the distribution of pores sizes from relaxation decay-rate distributions. The potential of NMR decay-rate distributions for characterizing DNAPL fluids in the subsurface and understanding their flow mechanisms has not been exploited. Near-surface, unsaturated, vadose zone environments provide unique challenges for using NMR. These challenges are being addressed through systematic laboratory experiments and a program of research to extend and adapt current-field NMR measurements to near-surface environmental problems. The product of this research will be a downhole logging tool that is sensitive to microbiological influences on TCE fate and distribution (20).

SUMMARY

EMSP-sponsored projects with geophysical research relevant to vadose zone characterization throughout the DOE complex have been presented. A variety of geophysical techniques with complementary capabilities (e.g., EM induction, GPR, electrical resistivity, seismic, and NMR) are being pursued to provide a more complete picture of vadose zone properties and processes. Since individual geophysical characterization tools all have specific limitations, a suite of integrated measurements is sought to provide a better understanding of contaminant fate and transport in the vadose zone. A combination of laboratory, field, theoretical, and computational studies are necessary to develop our understanding of the vadose zone. Research transfer of scientific findings, methodology improvements, and the latest interpretation algorithms to practicing environmental geophysicists and site engineers is essential to support clean-up operations at contaminated sites.

ACKNOWLEDGMENTS

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