IMPROVED PARAMETERIZATION OF HYDROLOGICAL MODELS and REDUCTION OF GEOPHYSICAL MONITORING DATA AMBIGUITY THROUGH JOINT USE OF GEOPHYSICAL AND NUMERICAL MODELING METHODS

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ABSTRACT

In this presentation, we describe the benefits of using geophysical characterization data to parameterize numerical flow and transport models, as well as the use of numerical model predictions to reduce the ambiguity often associated with field-scale geophysical monitoring data. We will explore the twining between hydrogeophysical characterization, hydrological-biogeochemical modeling, and geophysical process monitoring through three different examples. The examples range from prediction of water balance within managed ecosystems to the prediction of system transformations during active remediation treatments. We illustrate that where approaches are sufficiently advanced (such as hydrogeophysical characterization), they can be helpful for constraining flow and transport prediction. However, where approaches are not yet well developed, such as field-scale geophysical monitoring of system transformations during remediation, numerical model predictions can be helpful for constraining interpretations of the geophysical responses.

1. INTRODUCTION

Numerical modeling of fluid flow and transport is often used to test hypotheses and to guide resource management. For example, numerical models are used to simulate contaminant plume transport and to design effective remediation plans, and to simulate aquifer depletion and to design sustainable resource allocation programs. Effective hydrological hypothesis testing using mathematical modeling requires parameterization of the hydrological and geochemical properties that exert significant control on flow and transport, such as hydraulic conductivity and the distribution of reactive solid phases. However, it is well recognized that the spatial variability of these properties can be large, and that it is extremely challenging to obtain information about these properties using conventional (borehole) data in a manner sufficient to parameterize most flow models. Through fusion approaches, geophysical data have the potential to provide quantitative estimates of important flow and transport parameters, as well as their associated estimation uncertainty, at a resolution and spatial scale that is useful for parameterizing flow and transport models.

Advanced numerical models have been developed to predict transformations in subsurface systems. These predictions can be useful for guiding the design of active remediation approaches, such as in-situ bioremediation or chemical oxidation, or for assessing the potential of natural attenuation as a remedial approach. In addition to requiring good initial characterization of hydrological and biogeochemical properties, such reactive transport models also require that the coupling of hydrological and biogeochemical processes is correctly represented within the model. As these models rely on many assumptions and often lack sufficiently resolved parameter inputs, methods to validate the numerical predictions at the field scale and over space and time are needed. As laboratory experiments have indicated the potential of geophysical data for monitoring transformations associated with remediation processes, such as the evolution of gas species, precipitates, and biofilms, these methods may eventually help in the validation of reactive transport models. Although geophysical field-scale monitoring datasets may eventually be helpful for validating predictions of transformations at the field-scale, development of such geophysical monitoring techniques is in an early stage, and unique interpretation of geophysical responses to system transformations (especially in the presence of natural heterogeneity and competing biogeochemical processes) is currently challenging.

In this presentation, we describe the benefits of using geophysical characterization data to populate numerical models as well as the use of numerical model predictions to reduce the ambiguity often associated with field-scale geophysical monitoring data. We will explore integration of hydrogeophysical characterization, hydrological-biogeochemical modeling, and geophysical monitoring information through three different examples, which illustrate both the benefits as well as the challenges currently associated with the joint use of geophysical and numerical modeling methods.

2. VINEYARD WATER BALANCE MODELING

Because water is a key control on the physiological status of grapevines, good water management can be used to optimize crop quality. It is generally accepted that moderate water stress on grapevines at early stages in the growing season controls canopy density and has a positive impact on the fruit characteristics (e.g., Dry et al., 2000; Williams, 2001). In areas where there is little rainfall during this time period, such as in the Napa Valley of California, water management typically entails irrigation. To optimize water stress, it is critical to understand how much irrigation water to apply and when to apply it.

The amount of irrigation water that a plant requires is a function of the microclimate and soil properties. Popular climate-based methods for guiding irrigation rely on weather data, empirical crop coefficients, and meteorological models to calculate the evapotranspiration (ETo) and irrigation requirements (e.g., White, 2003). Because moderate water stress in the early growing season is desirable, deficit irrigation strategies have been developed that strive to give the plant some fraction of its full evapotranspiration requirements. Although micrometeorological factors are often considered when developing an irrigation approach, the influence of small-scale soil variations and their control on water use and associated fruit quality is poorly understood. Part of this lack of understanding is the difficulty in characterizing the spatiotemporal variations in soil properties that are important to winegrapes, such as soil moisture, using conventional sampling or borehole measurement techniques. Success in modeling the dynamic interactions between soil, plan, and climate properties within vineyards has been thus far limited, due to the large variability of natural properties on the one hand, and the inherent inability to characterize them with sufficient accuracy and over large areas.

To improve such predictions, we have explored use of ground penetrating radar (GPR) for estimating soil water content over space and time within winegrape vineyards. We have used both 900 MHz GPR groundwave (Grote et al., 2003) and 100 MHz reflection techniques (Lunt et al., 2005; Hubbard et al., 2006) to provide spatially extensive estimates of soil water content distribution over time within two different California vineyards. For example, we tested the concept of using the GPR groundwave technique to estimate shallow (top 20cm) water content within a Robert Mondavi Vineyard, located in Napa Valley, California. The topography within the 3 acre study site is flat, and the vines are drip irrigated at a uniform rate across the block. GPR data were collected several times over a period of 18 months within the area using a 900 MHz PulseEKKO 1000 System. Using the GPR groundwave arrival travel time and the distance between the transmitting and receiving antenna, we estimated the electromagnetic velocity and subsequently the dielectric constant at each sampled location. As described by Grote et al. (2003), we used a site-specific relationship to transfer the GPR-obtained dielectric constant values into estimates of estimated water content. Independent comparison with conventional 'point' soil moisture measurements, obtained using time domain reflectometry (TDR) and gravimetric techniques revealed that the estimates of volumetric soil water content obtained using groundwave data were accurate to within 1% by volume.

An example of the soil water content estimated at one point in time using the 900 MHz GPR groundwave approach is shown in Figure 1a; such datasets were collected every few months over 1.5 years. Each dataset in the 3 acre site consisted of over 20,000 measurements, which is perhaps the highest density of shallow moisture measurements obtained to date in vineyards. We found that although the mean value of the water content estimates throughout the study block changed during the year, the spatial pattern remained fairly consistent and was controlled by soil texture. We also recognized a correlation between soil texture (shown in Figure 1b), soil moisture, and vegetation vigor (interpreted using remote sensing NDVI data). These results suggested that the surface GPR technique was valuable for providing accurate and dense information about soil properties in a non-invasive manner, and the study also illustrated the linkages between soil properties and vegetation responses.

We used a numerical model, parameterized with micrometeorological and spatially variable soils and plant data to predict spatially variable irrigation needs and date of critical water stress onset within the study site. For these simulations, we used the Vineyard Soil Irrigation Model (VSIM) (Pierce et al., 2003), which was modified from the Biome-BGC model (Running and Coughlan, 1988). VSIM is a simple water balance model that simulates the daily and seasonal water balance for a vineyard given information about the climate, soils, and leaf area index (LAI). In VSIM, water balance is described using a simple bucket model over the entire root zone of the plant, which considers the change in soil water storage over the root zone, precipitation, evapotranspiration from the soil-plant system, surface water runoff, and irrigation water input to the system. VSIM assumes the presence of two plant layers (cover crop and canopy) and one soil layer. The model is initialized with soil moisture information, which in our example was spatially variable and was obtained using the GPR data. Evapotranspiration within VSIM is based on reference evapotranspiration (ETo) and a crop coefficient (k_c), where crop ET (ETc) = ETo * k_c. VSIM relies on remotely-sensed imagery to quantify k_c and spatial variations in canopy density, and VSIM utilizes the California Irrigation Management Information System (CIMIS) meteorological station network to quantify daily and seasonal variations in climate. In VSIM, daily ETc and runoff are subtracted from soil moisture, while irrigation and rainfall during the growing season (if any) are added to soil moisture to keep a daily running calculation of water balance. The soil/leaf water potential is then obtained from the calculated soil moisture using relationships developed by Saxton et al. (1986). The Saxton models are based on soil texture, which in our example are defined to be spatially variable.

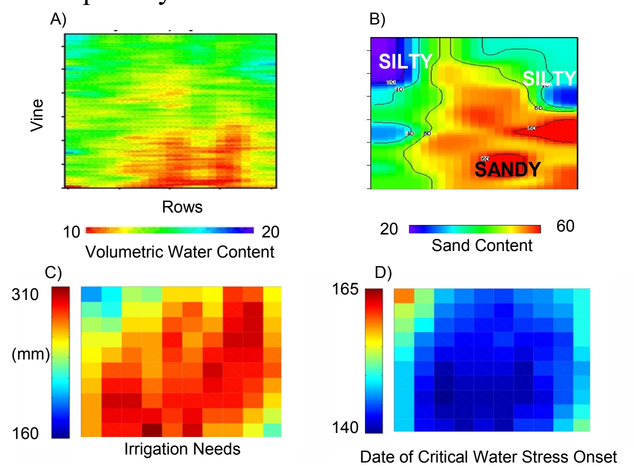

FIGURE 1. (A) estimation of water content obtained throughout the study block using 900 MHz GPR data; (B) Soil textures measured using conventional techniques; (C) Estimates of irrigation needs throughout the growing season based on micrometeorological as well as spatially variable plant and soils data; (D) Estimates of the date of critical water stress onset, an important parameter in controlling winegrape quality, based on micrometeorological and spatially variable plant and soils data.

Simulations from VSIM provided spatially variable estimates of soil moisture, water stress onset, and irrigation needs over the study site. Comparison of the soil moisture simulations with the GPR-obtained soil moisture estimates over time suggested that the model performed adequately. Figure 1c shows the temporal distribution of the onset of critical water stress within the vineyard block predicted using VSIM, while Figure 1d shows the required cumulative irrigation over the vineyard block during the growing season. These plots show that the sandier and typically drier portion of the study site demands more irrigation water than does the more silt-rich and consistently wetter soils, and that the sandy area requires water earlier in the growing season than the more silt-rich areas. As too much water or too early application of water reduces grape quality, these results suggest that the current practice of applying uniform irrigation water from the same starting date across the block to sate the 'thirstiest' (sandy) portions of the block likely results in decreased fruit quality and water efficiency in the more silty regions. The results also suggested that variability in soil properties most influenced the date of first water stress onset, but variability in plant properties (LAI) most influenced the total seasonal simulated irrigation needs. With predictions such as those shown in 1c and 1d, vineyard management zones can be defined, which can be farmed preferentially to increase both fruit quality and water savings. This example illustrates the benefit of GPR-obtained information for both initializing and validating predictions of water balance in a manner helpful for guiding precision agriculture.

3. ENVIRONMENTAL FLOW AND TRANSPORT MODELING

Field and laboratory scale transport experiments have suggested that both physical heterogeneity of an aquifer system, such as hydraulic conductivity, and geochemical heterogeneity, such as iron oxide distribution, control microbial transport behavior at the field-scale. Physical heterogeneity can be important because the pore throat sizes associated with particular lithofacies may restrict transport of bacteria (or their nutrients), and geochemical heterogeneity can be important due to electrostatic interactions, which often results in preferential attachment of bacteria to solid grain surfaces. As bacteria are being increasingly used to remediate subsurface contaminants, understanding transport in the presence of natural physical and chemical heterogeneity is a prerequisite for numerical transport predictions that are being used to develop contaminant remediation design. The scarcity of hydrological and geochemical data obtained using conventional (wellbore) sampling techniques, however, limits the ability to adequately populate numerical models and ultimately accurately predict chemical and bacterial transport.

In this study, we explored the utility of tomographic data for providing multi-dimensional estimates of hydraulic conductivity (Chen et al., 2001; Hubbard et al., 2001) and sediment geochemistry (Chen et al., 2005) in association with a chemical and bacterial injection experiment performed near the town of Oyster, Virginia. We used crosshole radar velocity information conditioned to borehole flowmeter hydraulic conductivity measurements within a Bayesian framework to provide hydraulic conductivity probability distribution functions at each 0.25cm by 0.25 cm pixel along the geophysical transects. Crosshole GPR amplitude data were used to estimate lithofacies and sediment Fe(II) and Fe(III) at a related Oyster site using Markov Chain Monte Carlo approaches. As the GPR amplitudes are sensitive to lithofacies, and lithofacies is often correlated with iron oxide distribution, the approach exploited this mutual dependence on lithology to provide estimates of lithological and sediment geochemical parameter spatial distributions. With both estimation procedures, cross-validation exercises revealed that the hydraulic conductivity and sediment geochemistry estimates obtained using the geophysical data were accurate and greatly improved the 2-D identification of the properties over estimates obtained using conventional measurements only.

The estimates obtained using geophysical data were used within two different studies to evaluate the benefit of high resolution conditioning data for improving flow and transport simulations. By comparing numerical model predictions conditioned to conventional and geophysically-obtained measurements at the Oyster Site, Scheibe and Chien (2003) found that conditioning the models to the geophysical estimates of hydraulic conductivity significantly improved the accuracy and precision of the model predictions relative to those obtained using borehole data alone. In a related study, Scheibe et al. (2006) integrated field-scale geophysical, hydrological, and geochemical data from the Oyster site to build a two-dimensional stochastic numerical model of a synthetic, uranium contaminated aquifer. As was observed at the Oyster site, the physical and geochemical parameterization datasets were correlated. Figures 2a and 2b illustrate example estimates of hydraulic conductivity and Fe(III) obtained using GPR amplitudes at the Oyster site, and are representative of the information used to parameterize the synthetic aquifer. Bioremediation of the synthetic contaminated aquifer was then simulated through modeling the injection of an electron donor amendment. The code incorporated coupling between ferrous iron sorption onto ferric iron surfaces and microbial growth and transport dynamics. Figure 2c illustrates amendment distribution and Figure 2d illustrates biofilm distribution, both at 200 days after injection. The study revealed how small scale heterogeneity, such as that identified using the tomographic data, were important in controlling amendment distribution, microbial attachment, and the timing of uranium reduction in response to biostimulation. Of key importance in both modeling studies is that the geophysical-based methods provided hydrological and geochemical information at a *reasonable scale and resolution for improving the prediction of field-scale processes*.

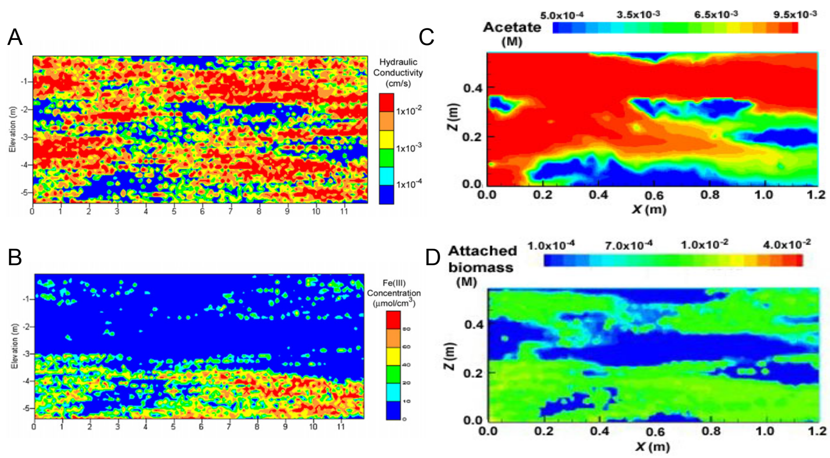

FIGURE 2. (A) Realization of the simulated hydraulic conductivity distribution; (B), Realization of the simulated Fe(III) distribution; (C) Simulated distribution of sodium acetate at the end of 200 days of simulated biostimulation. The initial distribution of acetate was uniform with zero concentration; (D) Simulated distribution of biomass at the end of 200 days of simulated biostimulation. The initial distribution of biomass was uniform with cell density of 2.0×10^{-5} M.

4. BIOGEOCHEMICAL PROCESS MONITORING USING GEOPHYSICAL APPROACHES

In addition to the natural variability in biogeochemical and hydrological properties, many remediation approaches being implemented induce dynamic transformations in natural systems, as was illustrated by the example given above. Potential alterations resulting from remediation treatments include, for example, dissolution and precipitation of minerals, surface complexation, gas evolution, sorption, oxidation and reduction (inorganic and microbially mediated), biofilm generation, and changes in permeability and porosity. Most of these parameters/processes are coupled, with many resulting from redox transformations accompanying the specific remediation approach. For example, mineralization, gas evolution, and biofilm generation may block the pore space and reduce hydraulic conductivity, rendering it more difficult to introduce treatment into the subsurface via injection or to withdraw groundwater via pumping. To advance solutions for remediation of contaminated sites, both monitoring and modeling approaches are needed that can elucidate and predict reactions associated with coupled biological, chemical and hydrologic processes. As was described in

Section 3, the development of advanced codes to simulate coupled processes is currently underway.

Over the last few years, we have investigated the capability of geophysical methods for remotely detecting changes in biogeochemical properties using geophysical methods during laboratory and field scale remediation treatments. At the laboratory scale, we have explored the use of (1) radar velocity and seismic amplitude measurements for detecting the onset and evolution of gas during denitrification (Williams et al., 2002; Hubbard and Williams, 2004), (2) Self Potential (SP) measurements for characterization of redox conditions (Williams et al., 2005), (3) Induced Polarization (IP) methods to track changes in iron mineralogy during sulfate reduction (Williams et al., 2005; Ntarligiannis et al., 2005), and (4) combined seismic and IP methods to monitor biomass accumulation. Our laboratory studies to date indicate that minimally invasive, high-resolution geophysical methods hold potential for monitoring and elucidating individual processes that occur during remediation. However, under natural conditions, these processes do not occur in isolation; they occur as a function of spatially variable initial conditions. Our field scale work indicates that at this time, it is often difficult to distinguish the response of competing biotic and abiotic reactions on geophysical signatures. For example, a reduction in electrical conductivity may represent a decrease in solute concentration or an increase in the pore space gas concentration that ultimately leads to pore throat blocking and isolation of the pores.

Several advancements are needed to reduce the ambiguity of geophysical responses to system transformations that will allow these methods to be useful at the field scale for validating reactive transport models and for assessing the efficacy of remediation. We are currently evaluating four different approaches for reducing such uncertainty: (1) conducting laboratory experiments in the presence of multiple reactions while collecting geophysical and biogeochemical-hydrological data; (2) development of better petrophysical models to link the geophysical signatures with biogeochemical properties; (3) development of estimation frameworks that can incorporate the direct and indirect data and petrophysical models to find the most likely interpretation; and (4) iteration of the geophysical monitoring results with reactive transport modeling to ultimately improve both methods.

In this final example, we illustrate how coupling of geophysical monitoring data and reactive transport models help to reduce the ambiguity associated with the geophysical responses. This investigation is part of a larger scale study to assess the potential of a slow release polylactate compound to remediate chromium (VI) in the groundwater at the 100H area of the Hanford Site in Washington. The geophysical data were used to monitor amendment distribution, detect system transformations, and investigate the control of heterogeneity on the distribution and reactions. In the initial modeling phase, hydrological zonation estimates obtained using geophysical data provided constraints to the initial simulation of repeated injection and pumping tests using the Toughreact code (Xu et al., 2006). Using tomographic methods in a monitoring mode, we found that both radar and seismic methods were useful for tracking the amendment distribution, and that heterogeneity played a significant role on the distribution (Hubbard et al., 2005). Radar amplitude data indicated the formation of an electrically resistive ‘reaction halo’ that formed around the polylactate and persisted over time. Unique interpretation of this response remains challenging, as several transformations are possible at this site during organic carbon amendment. These include the disappearance of solutes, the increase in both dissolved and exsolved gas phases, and an increase in amorphous precipitates, such as FeS. Reactive transport modeling and detailed laboratory experiments were used to test different hypothesis and ultimately to reduce the ambiguity associated with the geophysical monitoring data interpretation. We expect that as we gain experience with the use of geophysical methods to monitor transformations associated with active remediation, that such methods may in turn be useful for validating and improving the numerical model predictions.

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