WATER RESOURCES RESEARCH GRANT PROPOSAL

Title: Spectral induced polarization (SIP) estimation of the hydraulic conductivity of unconsolidated sediments from Missouri

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Nature, Scope and Objectives of Research:

Methods, Procedures and Objectives of Research:

Overview: Measurements of the electrical properties of unconsolidated sediments are proposed as an approach to understanding sediment structural properties and for determining hydraulic conductivity. Hydraulic conductivity (*K*) quantifies the resistance to fluid flow exerted by an earth material and is hence a fundamental property of vast importance in ground water management and water quality. Reliable estimates of *K* are required if issues such as regulations on groundwater exploration and the prediction of the transport of contaminants are to be resolved properly. Use of the electrical technique known as 'Spectral Induced Polarization' (SIP) or 'Complex Resistivity' is proposed. Put simply, the technique measures the electrical properties of a material and the variation with frequency over a typical range of 0.01-1000 Hz. These electrical properties are related to important structural properties of the sediment and hence hydraulic conductivity.

Conventional field measurement of *K* suffers from well recognized limitations, in particular the cost and invasive nature of drilling operations and the difficulty in determining values at scales appropriate for use in models. Geophysical techniques provide a measurement of some physical Earth property (for example, electrical resistivity) and offer the following advantages: (1) densely sampled, spatially continuous information is obtained; (2) measurements are indirect and minimally invasive; (3) the scale of the measurement can be controlled through appropriate field survey design. A geophysical approach to the estimation of *K* could hence overcome the limitations of conventional hydrogeological approaches. The key is the determination of a geophysical procedure that provides a measurement of some parameter(s) that can be reliably related to hydraulic conductivity. This procedure should ideally involve the measurement of geophysical parameters that can be realistically obtained from a field survey.

Spectral Induced Polarization (SIP): Low frequency (0.01-1000 Hz) electrical properties are determined from measurements of the resistivity magnitude |*r*| and the phase shift *f* between a measured voltage sinusoid and an impressed current sinusoid. Stating in terms of complex conductivity *s** (1/ *r**),

$$\sigma^{*} = \sigma' + I\sigma'' \qquad (1)$$

the real and imaginary conductivities, s and s'' , are frequency dependent and defined from the measured parameters,

$$\sigma' = |\sigma| \cos \phi$$
$$\sigma'' = |\sigma| \sin \phi \qquad (2)$$

Two modes of electrical conduction in earth materials occur. The dominant mechanism is bulk (volumetric) conduction. In saturated sediments this conduction is primarily electrolytic, occuring through the interconnected pore volume. Bulk conduction can be modeled as,

$$\sigma^*(\omega) = \sigma_{static} + I\omega\varepsilon_o K_\infty \qquad (3)$$

where s_{static} is the low frequency bulk conductivity response of the sample and K_∞ is the high frequency bulk dielectric response of the sample. These parameters are considered independent of frequency and are primarily a function of the physical properties of the mineral grains and the saturating pore fluid. Archie's Law (1942) expresses s_{static} for saturated sediments as,

$$\sigma_{static} = \frac{\sigma_w}{F_*} \qquad (4)$$

where s_w is the electrolyte conductivity and F_* is the true Formation Factor measured at high fluid conductivity. F_* is related to the bulk structural properties (primarily porosity) of the matrix and for a clay-free material is given by,

$$F_* = a\phi^{-m} \qquad (5)$$

The bulk conduction model given in Eq. 3 does not account for the large enhancements in the low-frequency dielectric response observed in earth materials (Sen et al., 1981). A second mode of conduction is required to model this low frequency polarization. This mechanism is surface conduction, the result of electrochemical polarization that occurs at the grain-fluid interface. This polarization is frequency dependent and a function of the surface chemical and microgeometrical properties of the sample (Knight and Endres, 1990; Lesmes, 1993; Lesmes and Morgan, 1999). Assuming the complex conductivity response of the bulk rock and the surface electrochemical polarization mechanisms add in parallel (Lesmes and Frye, 1999) such that,

$$\sigma^* = \left(\sigma_{static} + I\omega\varepsilon_o K_\infty\right) + \left(\sigma'_{surf}(\omega) + I\sigma''_{surf}(\omega)\right) \qquad (6)$$

where s'_{surf} and s''_{surf} are the real and imaginary components of the complex surface conductivity s^*_{surf} .

Combining real and imaginary components gives,

$$\sigma^* = \left(\sigma_{static} + \sigma'_{surf}(\omega)\right) + I\left(\omega\varepsilon_o K_\infty + \sigma''_{surf}(\omega)\right) \tag{7}$$

At low frequencies (<1000 Hz), we_oK_∞<< $s''_{surf}(w)$ such that the low frequency complex conductivity of the sample is given by (Lesmes and Frye, 1999),

$$\sigma^* = \frac{\sigma_w}{F_*} + \sigma'_{surf}(\omega) + I\sigma''_{surf}(\omega) \tag{8}$$

In this model the imaginary conductivity is only a function of the surface conductivity whereas the in-phase conductivity is a function of bulk and surface conductivity mechanisms. An equivalent circuit for this model is given in Fig. 1.

In terms of rock properties, s''_{surf} is closely related to the specific surface to porosity ratio S_{por} (Börner and Schon, 1991),

$$S_{por} = b\left(\sigma'_{surf}\right)^q \tag{9}$$

where *b* and *q* are empirical constants. As a consequence of the platy, needlelike structure of clay minerals, S_{por} and hence s''_{surf} increase with increasing clay content. For unconsolidated clay-sand mixtures s' is primarily a function of s_w< (but also affected by the clay content via s'_{surf}) whereas s'' is a function of clay content. A schematic taken from Slater and Lesmes (1999), summarizing the expected relationship between SIP electrical properties and saturated sediment properties is shown in Fig. 2.

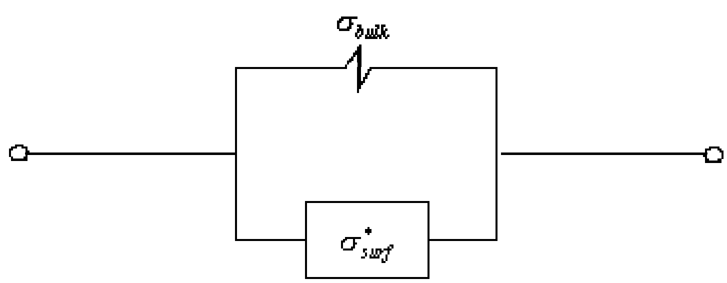

Figure 1: Simplified electrical model for sediments

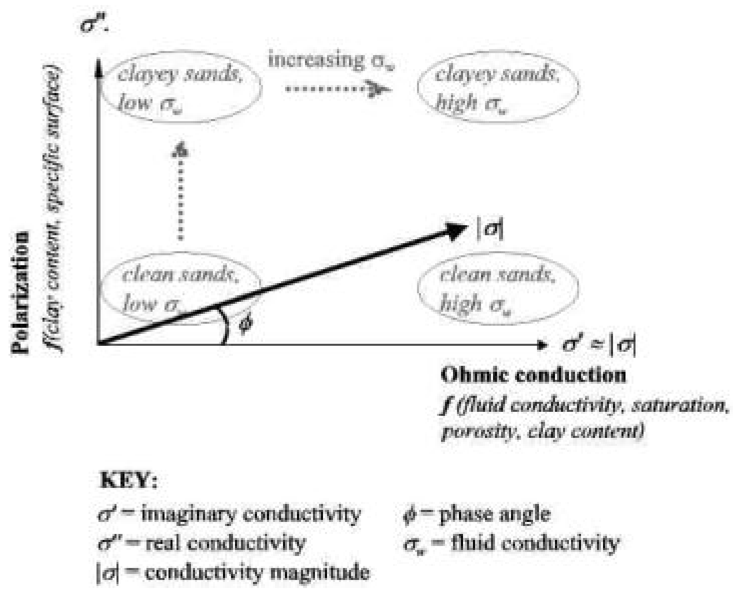

Figure 2: Expected relationship between SIP and saturated sediment properties

It is proposed to use these relationships to develop an SIP approach to the measurement of unconsolidated sediments from selected sites across Missouri.

Procedures: SIP measurements using instrumentation based around a NI 4551 two-channel dynamic signal analyzer are proposed (Fig. 3a). The resistance magnitude and phase shift (relative to a standard high-quality resistor) are measured. An AD624 pre-amplifier is used across the sample channel to boost the input impedance of the instrumentation to ~10^9 Ohm, minimizing spurious phase effects that may arise due to instrument electronics. Non-polarizing Ag-AgCl electrodes are used to minimize effects of electrode polarization that can occur at the fluid/electrode interface. Sample hydraulic conductivity determination will result from standard constant head or falling head methods, with K calculated from Darcy's Law.

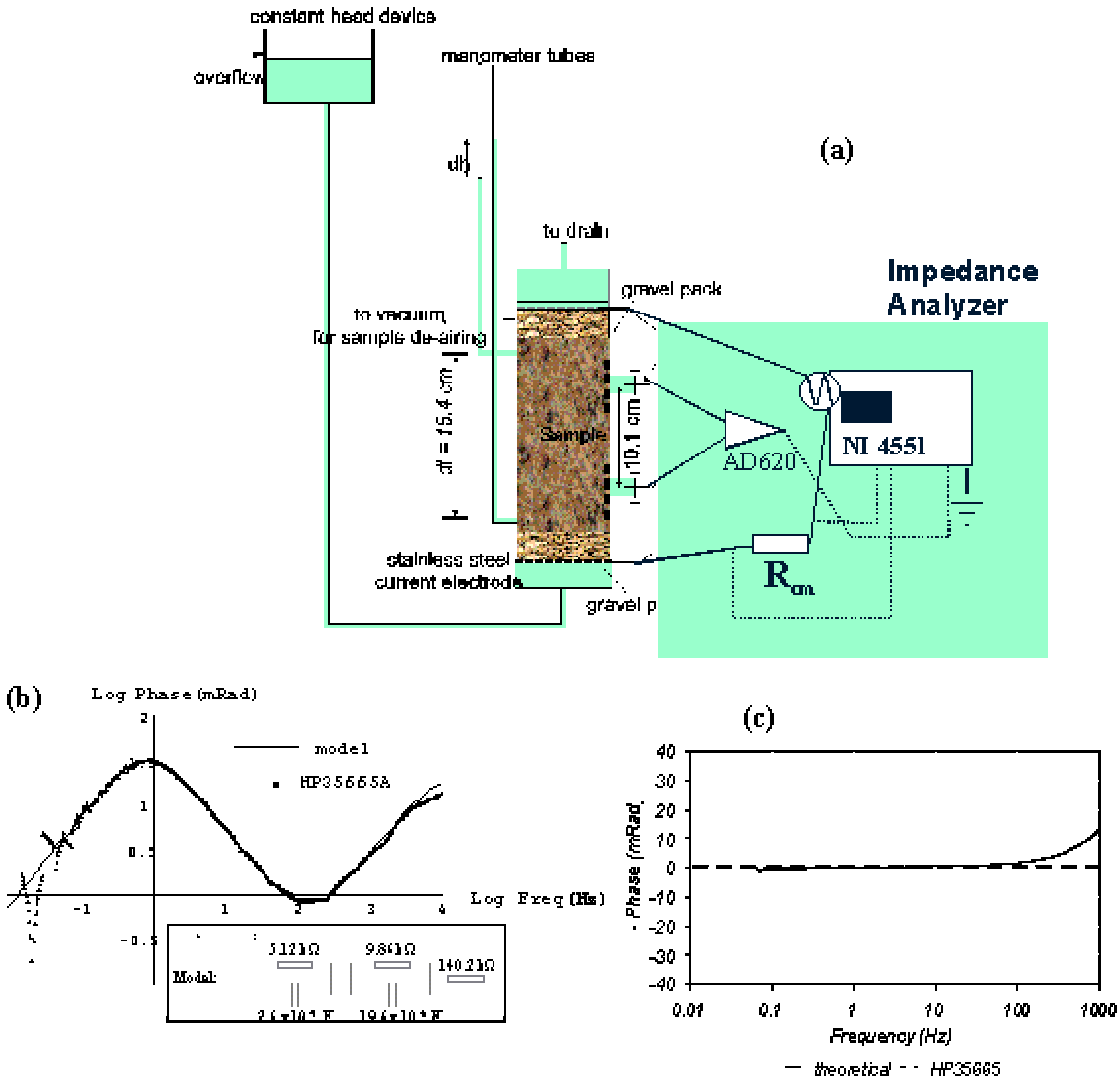

Figure 3: (a) Instrumentation for the measurement of SIP properties and hydraulic conductivity (b) HP35665A calibration on a capacitor-resistor network (c) 'HP35665 measured' and 'theoretical' phase angle for water (e_r = 80 and s = 10 S/m)

Errors in the phase are the primary concern as the low frequency dielectric contribution to the electrical properties of a material is small, such that phase angles are typically less than 40 mRad. Capacitive and electromagnetic coupling between wires in the external circuit [making connections to the sample] must be minimized to prevent spurious phase measurements. One option is shielding of the external wiring. However, previous calibration measurements made by the author, using an equivalent impedance analyzer (the Hewlett Packard HP35665A), indicate that shielding is not necessary in the frequency range 0.1-1000 Hz, provided the length of external wiring is kept as small as possible. Figure 3b shows calibration measurements made on a capacitor-resistor network, directly replacing the sample. The phase measurements closely match the predicted measurements up to 3000 Hz (excluding below 0.1 Hz where the instrument is not reliable). Deviations due to the circuitry only occur above 3000 Hz (outside the range of investigation). The major contributing factor to errors in the phase measurement on sediment samples is the polarization that occurs at the measuring electrode-fluid interface. A truly non-polarizing electrode is difficult to manufacture, and the magnitude of the electrode polarization will depend upon the electrode quality, as well as the electrolyte chemistry. Figure 3c shows the phase measurements when the sample is replaced with water. In this case, the theoretical phase is effectively zero between 0.1-1000 Hz. Measurements attributed to electrode polarization occur above 100 Hz, with a maximum deviation of 13 mRad at 1000 Hz. Such a calibration curve is used to correct measurements on sediment samples for electrode polarization.

Sample selection: Measurements on unconsolidated sediments obtained from selected sites across northwestern Missouri are planned. Quaternary sediments comprising of unconsolidated clay, silt, sand, gravel and till mantle a large part of this area. The primary sediments in the area are glacial till, alluvium and loess. The glacial drift is the most variable deposit, with ablation till intercepted by lenses of outwash deposits and buried valley deposits. The varying composition of the Quaternary sediments results in considerable hydraulic conductivity variability. Skelton et al. (1982) report transmissivities (the hydraulic conductivity integrated over an aquifer height) varying between 270-11,000 m/day. To maximize variability in hydraulic conductivity, sample selection will include the glacial drift, outwash deposits, Missouri River alluvium, alluvium from tributaries and loess deposits. Consultation with UMKC faculty and regional environmental consultancy firms will assist in suitable site selection. Parameters to control during electrical measurements include electrolyte conductivity and sample temperature. Repeat measurements for at least three values of electrolyte conductivity will reveal the effect of electrolyte variability. A Coulter laser particle size analyzer is available for rapid and accurate determination of grain size distribution over the range of particle size 0.4–2000 mm. Hydrometer measurements will resolve grain size distribution for clay-rich sediments. A sub-contract with Micromeritics Inc., to supply specific surface measurements obtained using the multi-point nitrogen BET method, is proposed.

Related research

Weller and Börner (1995) and Börner et al. (1996) have investigated the value of SIP for the determination of hydraulic conductivity of loosely consolidated sandstones. These workers applied a constant phase angle (CPA) model (Jonscher, 1981) to interpret SIP data. The CPA model expresses the complex resistivity, r^*, in terms of only two parameters,

$$\rho^* = \rho_n (i\omega)^{1-P} \qquad (10)$$

where r_n is the 1 Hz resistivity and (1-P) is an exponent describing the frequency dependence. The formation factor and the specific surface are determined from the real and imaginary components of s^* $(1/r^*)$ as per equations 4 and 9. Borner et al. (1996) then apply a modified version of an empirical Kozeny-Carmen like equation, proposed by Pape et al. (1982) for the determination of K,

$$K = 475 \frac{1}{FS_{por}^{3.1}} \quad (11)$$

Weller and Börner (1995) utilized equation 11 to calculate the *K* variation along a 5 m deep borehole drilled through weathered schist from SIP data. Comparison of the SIP estimates with *K* estimates obtained from sieve analysis showed some correlation, with the methods showing similar trends with depth (Fig. 4). However, the differences in *K* derived from the two techniques frequently reached two orders of magnitude.

The discrepancy between the data in Figure 4 may have numerous sources, including (1) poor hydraulic conductivity estimation from the grain size distribution, and (2) incorrect Formation Factor evaluation in the presence of significant clay content (matrix conduction).

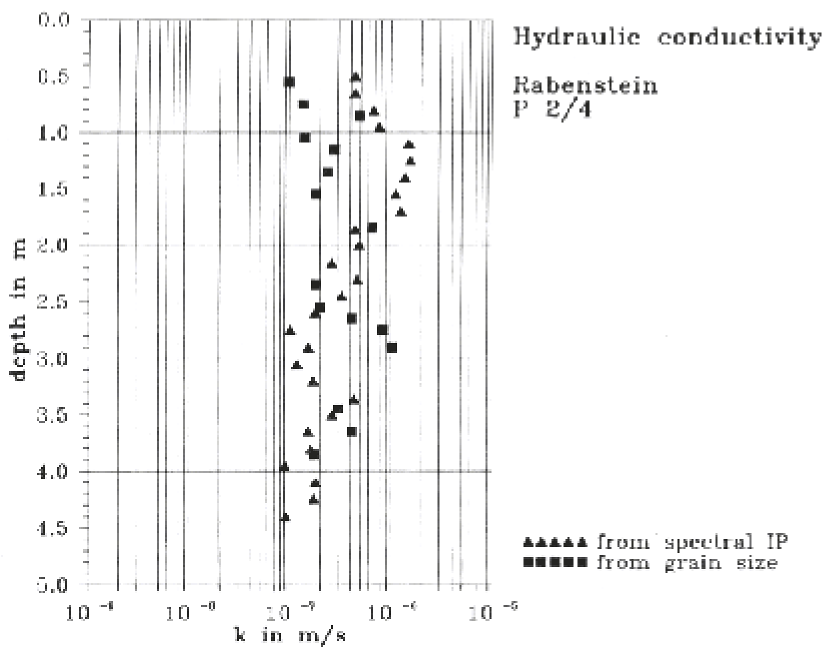

Figure 4: Observed relationship between electrically determined hydraulic conductivity and that obtained from grain size analysis for a 5 m deep borehole (after Weller and Börner, 1995).

Preliminary results obtained by the author, while conducting postdoctoral research at the University of Southern Maine, indicate that for unconsolidated sediments the SIP parameters are closely related to *K* (Figure 5). In this work *K* was directly measured from flow tests. Although no measurements of specific surface were made, the imaginary conductivity (low-frequency dielectric constant) shows a strong correlation with *K*. The range in hydraulic conductivity exceeds three orders of magnitude (see Figure 5). A similar range is expected for the Quaternary sediments of northwestern Missouri, given the highly heterogeneous nature of the material.

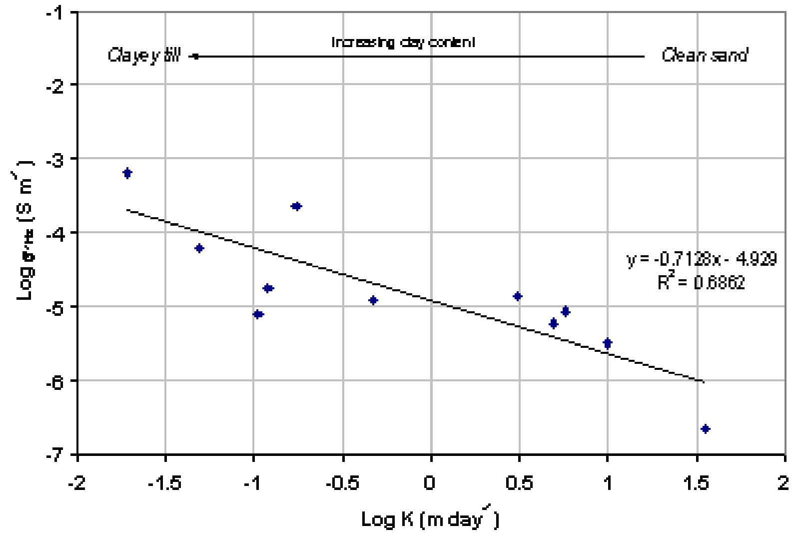

Figure 5: Relationship between imaginary conductivity at 1 Hz and hydraulic conductivity as obtained for unconsolidated sediments collected from sites in Maine

Sturrock et al. (1999) present data suggesting that hydraulic conductivity estimation from SIP can be improved by incorporating some measure of the grain size distribution, as well as the specific surface, into the model. This work again focused on loosely consolidated sandstone samples. They utilized a model for permeability in terms of packing, sorting and grain size effects as proposed by Berg (1970),

$$k(Darcy) = 5.1\times10^{-6}\phi^{5.1}MD^{2}e^{(-1385PD_{\phi})} \qquad (10)$$

where f is porosity in percent, MD is median grain size diameter in millimeters and PD_f is a phi percentile deviation of the grain size distribution given as $PD_{90\%}$-$PD_{10\%}$ in phi units. The SIP estimate of the grain size distribution was obtained from fitting the SIP data to a Cole-Cole type dispersion model, stated here in terms of complex permittivity,

$$\varepsilon^{*} = \varepsilon_{\infty} + \frac{\varepsilon_{o} - \varepsilon_{\infty}}{1+\left(I\omega\tau_{o}\right)^{1-\alpha}} \qquad (11)$$

where e * is the complex permittivity, e_{∞} is the high frequency permittivity limit, e_o is the low frequency permittivity limit, t_o is the peak relaxation time of the distribution and a is a value between 0 and 1 which relates to the spread of the distribution. The median grain size and the grain size distribution are determined from t_o and a respectively and applied in equation 10. Sturrock et al. (1999) compared the model of Weller and Börner (1995) based on surface area with this proposed model based on grain size distribution. They found a large improvement in permeability estimation when using the grain size distribution model. However, their published dataset only consisted of 10 samples.

Two current models for the determination of hydraulic conductivity from SIP measurements hence exist. Both models have only been applied to a limited number of samples. This work will determine the applicability of both models to unconsolidated sediments of Missouri. A reliable model for the estimation of the hydraulic conductivity of unconsolidated sediments of Missouri from SIP measurements will result.

Training potential

Employment of a graduate level Geosciences Masters student for the proposed nine month duration of the project is anticipated. Training in aspects of the following areas, (1) hydrogeology, (2) geophysics, (3) instrumentation, (4) electrochemistry, (5) geotechnics and (6) computer modeling, will follow. In addition, the graduate student will present the results at an international conference following completion of the project. It is the author's responsibility to develop graduate level teaching and research in the fields of Hydrogeology and Applied Geophysics. A funded research project in these fields would enhance the training potential of students interested in Hydrogeology and Applied Geophysics at UMKC.

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RELEVANCE OF PROJECT

Relevance of research to Missouri needs, regional/national significance and potential users

Hydraulic conductivity is the fundamental property governing groundwater flow and advective solute transport. Consequently, knowledge of the magnitude of subsurface hydraulic conductivity and its spatial variability is crucial in the investigation and prediction of contaminant transport and the quality and safety of groundwater resources. Many incidents of groundwater contamination occur in the immediate subsurface (e.g. leaks from storage tanks, highway spills, landfill leachates, etc.) which in Missouri can be composed of many meters of unconsolidated sediments. Improvements in the modeling of solute transport will only come about with more comprehensive measurements of hydraulic conductivity than are currently available from measurements based on flow tests.

The unconsolidated sediments of northwestern Missouri contain a number of potable aquifers. Sources of groundwater include the Missouri river alluvium, glacial drift (variable) and the alluvium of tributary streams. The Missouri river/alluvial flood plain is the most abundant source of groundwater in the area. The Lower Grand and Thompson River basins are included in the are and offer potential for groundwater development (Skelton et al., 1982). More comprehensive estimates of hydraulic conductivity are required to model such aquifers. Water quality issues also exist in northwestern Missouri.

The mineralization of groundwater has been impacted by coal mining (acid mine drainage). Iron, manganese and nitrate concentrations in the Quaternary deposits are in excess in some instances (Detroy et al., 1983). Furthermore, much of the area is farmland and non-point source pollution issues arise. In particular, increasing nitrate concentrations from fertilizer use is another water quality concern (Detroy et al., 1983; Wilkison et al., 1994). These water resources and water quality issues highlight the need for methods that can assist estimation of hydraulic conductivity.

Direct measurement of hydraulic conductivity is often problematic. Standard field methods (flow tests) for the measurement of *K* are direct, invasive, and consequently both time consuming and expensive. Invasive sampling can cause disruption of the natural state resulting in *K* measurements not truly representative of the *in-situ* condition. In addition, issues regarding the scale of the measurement arise. Pumping tests typically provide lumped *K* values (an integrated response from a large aquifer volume) whereas borehole logging can provide *K* estimates representative of the material in the immediate vicinity of the borehole. Characterization of *K* at the intermediate scale, however, is problematic.

An electrical geophysical method for the estimation of *K* could be an attractive complimentary/alternative approach to *K* estimation. Field electrical methods typically provide densely sampled, spatially continuous information. Techniques are minimally invasive and the measurement scale can be controlled through consideration of field survey parameters. In order to develop an electrically based field method of *K* estimation, a thorough understanding of the relationship between electrical properties and *K* is required. This project would develop that understanding and identify models that would allow *K* to be predicted from low frequency (spectral induced polarization) electrical measurements.

Hydraulic conductivity estimation is clearly important at both the regional and national level. Any potential methods that can assist the measurement of this elusive property must be developed as the implications for groundwater resources and water quality are so obvious. Potential users of this research would include all government agencies and private companies involved in water resources evaluation and water quality protection.

Potential of future research & funding

The proposed study is considered the initial step in the development of an electrical method for the determination of *K* of unconsolidated sediments. Following the results of this study, down-borehole and field scale measurements are anticipated. This would incorporate both an element of instrumentation development as well as site characterization. The application of the method to assist *K* characterization at a Superfund site in Missouri is also anticipated. Ultimately, research into the incorporation of the electrical data into a 3D flow and transport model is expected. Using the data collected in this study as a proof of concept, proposals to the NSF Hydrologic Sciences Program are anticipated.

Student involvement

The primary student involvement is in the form of a full-time graduate (Masters) student dedicated to this project. Student responsibility includes data collection, analysis and interpretation. Student presentation of the results of the project at an international conference is expected.

The author is a beginning investigator in the Department of Geosciences at the University of Missouri Kansas City (as of the fall 1999). His responsibilities include the development of a teaching and research program in Applied Geophysics and Hydrogeology. This project would initiate student involvement in these fields at UMKC. The indirect result of such a funded laboratory research project in Hydrogeology/Geophysics would be the growth of student interest in these disciplines.

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