Abstracts

from session B
SUMMARY

Recent models propose the prediction of permeability for spectral induced polarization (SIP) data using estimates of formation factor and a hydraulic length scale related to fluid flow based on either a dominant relaxation time (τ) or a representative imaginary conductivity (σ′). We acquired SIP and supporting petrophysical data on two sandstone fractured rock sites in the United States. The time constant based model describes the permeability reasonably well from one site that is characterized by relatively low values of pore volume normalized surface area (Spor). However, the fitting is poor for the samples from the second site that are characterized by higher values of Spor and a wider variation in Spor. We find that imaginary conductivity is related to Spor and that our samples are consistent with a previously defined empirical relation determined for a wide range of samples spanning multiple datasets. We also find that imaginary conductivity of our samples is correlated with permeability, supporting the application of models based on the formation factor (F) and σ′. However, such models involve F raised to a large exponent, meaning that highly accurate estimates of the formation factor are needed for reliable permeability prediction.

INTRODUCTION

Contamination of fractured rock remains a long-term, persistent problem. The pore space that controls the mass transfer rates of contaminants into and out of the lower permeability matrix is currently difficult to characterize from borehole logs. Field technologies that non-invasively characterize the matrix are needed to estimate pore space (i.e. effective porosity, diffusion coefficients and hydraulic properties) controlling mass transfer rates. Spectral induced polarization (SIP) is a promising technology to non-invasively acquire such information and the spatial variability e.g. from a borehole geophysical logging survey.

Revil et al. (2015) propose the prediction of intrinsic permeability (k) from a measurement of a characteristic relaxation time (τ) and the electrical formation factor (F).

\[ k = \frac{D_{(s)} \tau}{4F} \] (1)

where \( D_{(s)} \) is the diffusion coefficient of the charge transport of ions in the Stern layer. Equation 1 is based on the premise that \( \tau \) is an indirect measure of effective pore radius controlling fluid flow. The objective of this work was to determine whether this relaxation time-based estimation of permeability is applicable to laboratory datasets acquired on fractured rock sandstone formations from two sites in the United States (US).

METHOD AND RESULTS

Samples were acquired from two fractured rock sites referred to as [1] Santa Susana, and [2] Hydrite. Santa Susana is a deep sea sandstone turbidite deposit whereas Hydrite is composed of fine grained quartzose sandstones. Eighteen Santa Susanna samples and fifteen Hydrite samples were acquired. Pore geometrical properties characterization conducted on all samples to date includes specific surface area using nitrogen gas adsorption, gas permeability (with Klinkenberg correction), total porosity and electrical formation factor, estimated from real part of complex conductivity measurements with an empirically derived correction for surface conductivity described in Weller et al. (2013). Spectral induced polarization measurements were acquired between 0.001-1000 Hz using the LSIP instrument (Ontash & Ermac, USA). All samples were fully saturated with a synthetic groundwater (660 µS/cm) using a vacuum/pressure saturation method.

Specific surface area of the Santa Susana cores varied from 0.7-2.8 m²/g whereas Hydrite cores showed a larger variation from 0.19-5.6 m²/g. Permeability varied from 0.15-14.9 mD in the Santa Susana cores, and the Hydrite cores again showed a larger variation from 0.09-367 mD, in part due to measurements in the vertical and horizontal directions. Phase spectra for one borehole at each site are shown in Figure 1. Nearly all samples are characterized by a clear peak in the spectrum, making the dataset well suited to application of the relaxation time-based model given in equation 1. Some exceptions are noted for the Hydrite samples, i.e. those samples with a small phase angle below 0.005 rad (a phase peak may still be estimated). Many of the Hydrite samples show a sharper peak in the phase response than in the Santa Susana samples. Despite over three orders of magnitude of
variation, the phase peaks only vary by approximately an order of magnitude.

Figure 1. Phase spectra for all samples in the study: Santa Susana samples (left) and Hydrite samples (right). Samples colour coded by pore normalized surface area ($S_{por}$)

Figure 2 shows the predictions of equation 1 for both sets of samples assuming a single value of $D_{1,1}$ equal to $3.8 \times 10^{-12}$ m$^2$/s that has been proposed for clayey materials (Revil, 2013). The colours of the symbols in the two plots represent variations in pore volume normalized surface area ($S_{por}$). The solid line represents the 1:1 relation and the dashed lines represent one order of magnitude variation on either side of the 1:1 relation.

Figure 2. Phase spectra for all samples in the study: Santa Susana samples (left) and Hydrite samples (right).

Most of the $k$ predictions (21 out of 25 samples) from equation 1 fall within +/- one order of magnitude of the measurements for the Santa Susana samples. These samples have a narrow range of $S_{por}$. The samples cluster well around the 1:1 line, suggesting the applicability of the model. In contrast, Hydrite samples do not cluster around the 1:1 line and show no correspondence with the model. Most Hydrite samples (14 out of 22 samples) fall outside of the range of one order of magnitude bounds from the 1:1 line. Unlike the Santa Susana samples, Hydrite samples show a broad range in $S_{por}$.

The pore volume normalized surface area provides an alternative effective hydraulic length scale to the pore radius and can be estimated from the imaginary part of the complex conductivity ($\sigma''$) (e.g. Weller et al., 2010). The relationship between $\sigma''$ and $S_{por}$ is shown overlain on the database and relationship described in Weller et al. (2010) in Figure 3. To be consistent with the data reported in Weller et al. (2010), our sample imaginary conductivities are plotted at a frequency of 1 Hz. The Santa Susana samples fall very close to the 1:1 line of the relationship $\sigma'' = 0.01 S_{por}$ with $S_{por}$ in $\mu$m$^{-1}$ and $\sigma''$ in mS/m. The Hydrite samples fall within +/- one order of magnitude of the measurements with the exception of one sample. However, the high $S_{por}$ samples cluster well below the 1:1 line.

Figure 3. Samples from this study plotted with the database of Weller et al. (2010). The solid line shows the relationship.

Permeability, $k$, has been shown to be related to imaginary conductivity, $\sigma''$ and $F$ with a relationship of the form (Weller et al., 2015):

$$ k = \frac{a}{b F (\sigma'')^c} $$  \hspace{1cm} (2)

where $a$, $b$, and $c$ are fitting parameters. Weller et al. (2015) found the best fitting value of $b$ to equal 5.35 indicating a strong influence of $F$ on the $k$ estimate and the need for extremely accurate estimates of $F$ for accurate $k$ estimation from such a model. Given that we currently only have $F$ estimates from the IP correction for surface conductivity procedure proposed by Weller et al. (2013), we do not apply this model here (note in contrast equation 1 includes $F^{-1}$ making uncertainty in $F$ less of a concern). However, analysis of the relationship between imaginary conductivity and permeability on our database encourages the use of a model with the form of equation 2 that uses $\sigma''$ instead of $\tau$ (equation 1) to predict permeability (Figure 4).
DISCUSSION

The two sandstone datasets exhibit distinctly different SIP behaviour that appears to be related to $S_{\text{por}}$. The Santa Susana samples are characterized by low $S_{\text{por}}$ values and a relatively narrow range of $S_{\text{por}}$ variation. These samples all show a phase peak in the complex conductivity spectrum, although the spectra are much broader than those observed for most of the Hydrite samples. Given the clear peaks in the complex conductivity spectra for the Santa Susana samples, the time constant based model for $k$ prediction can readily be applied. Figure 2 shows that these samples satisfy the model (equation 1) well.

The Hydrite samples show a greater variation in pore geometric properties and numerous samples have a relatively high $S_{\text{por}}$. These high $S_{\text{por}}$ samples show sharp phase peaks (Figure 1) and are therefore in theory very well-suited for application of the time constant based permeability model. However, these samples do not satisfy the model well (Figure 2) with fourteen of the samples falling outside of +/- one order of magnitude from the 1:1 line.

![Figure 4: Relationship between permeability and imaginary conductivity Santa Susana and Hydrite samples combined.](image)

An alternative way to estimate $k$ from SIP data is through the link between imaginary conductivity and $S_{\text{por}}$ (Weller et al., 2015). Figure 3 demonstrates that the samples from both sandstone formations comply with the empirical relation between $\sigma''$ and $S_{\text{por}}$ identified by Weller et al. (2010). Figure 4 shows empirical evidence for a dependence of $k$ on $\sigma''$ in the combined sample database, supporting the application of a model based on $\sigma''$ (equation 2) instead of $\tau$ (equation 1). However, equation 2 requires high confidence in the $F$ estimate that may make it inapplicable using $F$ estimates based on the correction for surface conductivity using IP data proposed by Weller et al. (2013) and applied here to date. High salinity experiments are currently underway to determine the true formation factor.

CONCLUSIONS

Examination of SIP data from two new sandstone formations where spectra are characterized by a distinct peak in the phase spectra indicate challenges with the application of permeability estimation models based on a relaxation time. The model performance is degraded for samples from a sandstone formation characterized by higher variations in $S_{\text{por}}$, and overall higher $S_{\text{por}}$ relative to samples from a formation where $S_{\text{por}}$ values are low and vary over a narrow range. Alternative models that use the imaginary conductivity (instead of $\tau$) as proxies of length scales controlling fluid flow may be more robust. A dependence of permeability on imaginary conductivity is observed in support of this approach. However, such models are highly sensitive to errors in the formation factor.

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SUMMARY

The main objective of this study is to examine SIP as a tool for identifying and quantifying the presence of organic and inorganic pollutants in the soil. Several experiments were performed in this study. First the influence of a free-phase organic liquid on the SIP signature was examined on an unsaturated sandy loam soil. The added non-aqueous phase liquid (NAPL; decane) caused a decrease of the imaginary part of the soil’s complex conductivity as well as the relaxation frequency. We suggest that membrane polarization is the main polarization mechanism responsible for these results. Altering the characteristic pore throat length, due to the interaction between water and decane, controls the SIP response when a free-phase compound is added to the system. Further, we used loess soil (calcium rich) to investigate the SIP effect of several different organic pollutants and their mixtures, in order to examine the ability to distinguish them by the SIP method. The same trend of decreasing polarization was observed. However, the real part of the conductivity had a clear decrease when decane was added. The calcium rich environment had apparently contributed to the formation of different surface interactions of the polar organic compounds in the presence of decane. Furthermore, we present an artificial neural network classification with preliminary satisfying ability to indicate the existence of a specific contaminant. Third, the soil solution and adsorbed phase inorganic composition influence on the SIP signature was examined. A clear influence on the soil’s electrical signature was observed. Coherent changes exist in the relaxation time and chargeability when the chemical composition of the soil was changed. Addition of divalent cation to the porous media causes an instantaneous shift in the relaxation frequency, while the polarization magnitude is affected in a more gradual way. Three types of data driven models to potentially predict inorganic species are introduced. Dominant species were fairly well predicted.

Key words: organic contaminants, pollution identification, soil solution composition, polarization mechanism.

INTRODUCTION

As soil and groundwater resources become scarcer and more vulnerable there is a pressing need to manage their usage. Therefore, a great need exists to develop tools and approaches for monitoring and characterizing the variety of processes in the subsurface, preferably in a useful non-invasive manner. Geophysical methods can fulfill that need, specifically the spectral induced polarization (SIP) method. SIP measures the frequency dependent electrical conductivity and soil’s polarization by applying an alternating current field. In the induced polarization method the resultant electrical field (due to current injection) is known to show a phase lag $\phi$ with respect to the applied electrical current. The complex electrical conductivity relationship to the phase lag and conductivity (or resistivity) magnitude and the imaginary ($\sigma''$) and real ($\sigma'$) components is expressed by:

$$\sigma = \sigma' + i\sigma'' = \sqrt{\sigma'^2 + \sigma''^2} e^{i\phi}$$

The SIP response is a complex function of pore solution volume and chemistry, microgeometry and grain surface chemical properties. Hence, it is greatly affected by the presence of pollutants. The interactions of pollutants with the soil influence the soil’s electrical properties which are reflected in the SIP signature.

In the low frequency range ($<100$Hz), used throughout this work, the polarization phenomenon is attributed to polarization processes taking place at the electrical double layer (EDL). This polarization may be due to the Stern layer and membrane polarization processes. Stern layer polarization refers to the polarization of this layer at the EDL, which is in close vicinity to the grain and therefore relates mainly to tangential movement of counter-ions in the Stern layer. Membrane polarization takes place in the diffuse layer and the pore space (in certain distance from the grain surface), and mainly refers to accumulation of charge in the pore throat as a result of ion migration in an applied electric field. Most existing models that describe SIP are involved with the Stern layer polarization, connecting spectral induced polarization to the electrochemistry and the Stern layer polarization model on the grain surface (Leroy and Revil 2009; Leroy et al. 2008; Jougnot et al. 2010; Revil and Florsch 2010; Vaudelet et al. 2011). Few studies (Titov et al. 2002; Titov et al. 2004; Bucker and Hordt 2013) developed the IP membrane polarization model, originally presented by Marshall and Madden (1959). Both models account for the chemo-physical properties of co-ions and counter-ions in EDL, however the developed Stern layer model refers to the chemistry more explicitly. The Stern layer model considers polarization occurring at the Stern layer alone, where the different species occupying the layer closest to the grain surface, can create outer or inner-sphere complexes with the surface (with or without intermediate water molecules, respectively). As membrane polarization does not explicitly refer to the grain surface chemistry, the Stern layer model is commonly used when dealing with chemical surface processes. The measured complex conductivity is greatly dependent on the composition of the surface counter-ions and their properties. Therefore, the
Identifying pollutants with SIP

Spectral induced polarization method has the potential to identify and distinguish different species in the subsurface in a non-invasive manner.

Several studies investigated the effect of organic pollutants on the SIP signature of different contaminants. Schwartz et al. (2012) observed an increase of the real part of the complex conductivity with NAPL addition for both diesel and motor oil, and a decrease of the imaginary part with increasing NAPL saturation. Their proposed mechanism was cation exchange with charged compounds within the NAPL. Further investigation of the charged NAPL (Schwartz and Furman 2012) showed that its low surface mobility, decreased the bulk soil polarization. Blondel et al. (2014) showed that free-phase oil caused an increase of the resistivity and phase lag for saturated conditions. However, according to the authors no prominent change was noticeable for quadrature conductivity (\(\sigma''\)) measurements between clean and contaminated nor before and after biodegradation. On the other hand, Personna et al. (2013) showed that ethanol depressed quadrature conductivity when added to saturated sand-clay mixtures and attributed it to suppressed charge movement at the EDL due to interactions with ethanol molecules.

In addition to organic pollutants, the composition of inorganic species in soils has a well-known influence on the soil's chemo-physical properties. This greatly affects the use and practices of the soil, from agricultural and environmental perspectives. The characteristics of soils are greatly affected by the elements composing their solution (Anderson and Rubin 1981). Therefore, the need to identify the composition of these inorganic species is an important part of appropriate soil usage.

Not many IP studies dealt with the influence of ionic composition of the soil solution and adsorbed species on the soil electrical signature. Lesmes and Frye (2001) have studied the pore fluid chemistry effect on the complex conductivity of sandstone. In another work, the SIP signature for adsorption of hydroxides and mineral precipitation on sand and silica gel was investigated (Zhang et al. 2012).

Leroy and Reivil (2004; 2009) proposed an electrical triple layer chemical complexation model (TLM) to describe electrochemical properties of clay minerals or clay rich soils and groundwater. Optimized surface site densities were able to reproduce the SIP response thus indicating the connection between the Stern layer surface species and the SIP signature of soil particles such as clays. The literature suggests that different species have their unique electrical signature.

In order to understand the mechanism controlling the SIP response of the contaminated soil, the possible chemical interactions between the contaminants and the soil solids (i.e. as part from adsorption process) should be considered (Underwood et al. 2015). The surface interactions influence the formed electric field at the double layer and the presence of charge particles in the pore space, which eventually affect the SIP response.

The main goal of this study is to examine SIP as a tool for identifying and quantifying the presence of organic and inorganic pollutants in the soil. This goal was achieved through a series of laboratory-scale experiments. First the influence of a free-phase organic pollutant on the SIP signature was examined. Second, we investigate the effect of several different organic pollutants and their mixtures, in order to examine the ability to distinguish them by the SIP method. Third, the soil solution and adsorbed phase inorganic composition influence on the SIP signature was examined.

**EXPERIMENTAL METHODS**

In this work we have explored the SIP signature of different soils with various contaminants using the SIP ZEL-SIP04 impedance spectrometer (Forschungszentrum Juelich, Germany) (Zimmermann et al. 2008). All electrical measurements were conducted with four electrodes in a Wenner or Schlumberger arrangement. We executed three main sets of experiments. The first experiment was conducted on an unsaturated red sandy loam soil in horizontal columns (Shefer et al. 2013). In this experiment the SIP signature of soil contaminated with three different concentrations of decane aside a clean treatment were examined. In addition timely SIP measurements were conducted on one of the treatments. The following set of experiments involved unsaturated calcium rich Loess soil. SIP measurements were taken for different treatments with varying combinations of organic contaminants (decane, TBP, aniline hexadecyltrimethylammonium bromide) in glass boxes. The third set of experiments was conducted in vertical flow columns with red sandy loam soil. Various different solutions that included chloride salts of Ca\(^{2+}\), Na\(^{+}\), Mg\(^{2+}\), NH\(_4\)\(^{+}\) and K\(^{+}\) (a single Ba\(^{2+}\) treatment was also conducted at the end of the experiment) and different combinations of them were measured with the SIP measurement system. The total salt concentration was set to 0.01N. All experiments were accompanied with complementary chemical measurements and in the last two sets the data was also fitted to the Cole-Cole model. Further, we present preliminary data driven models for pollutants identification and predication.

**RESULTS AND DISCUSSION**

Our results show that adding free-phase NAPL to the soil causes a decrease of the imaginary part of the complex conductivity as well as the relaxation frequency. We suggest that the polarization mechanism responsible for these results is the membrane polarization model. Since no change was observed in solution major ion composition we conclude that no ion exchange process took place and therefore no change in Stern layer composition. Together with the fact that the soil's grain size did not change, the Stern layer model cannot support our findings. Hence, by elimination, membrane polarization is, the responsible mechanisms for the observed results. We imply that the pore throat characteristic length is the length scale controlling the SIP response when a free-phase compound is added to the system, altering this length and affecting polarization and relaxation time (as demonstrated in Figure 1).

In the second set of experiments, where on top of the free-phase compound (decane) we added to a calcium-rich soil other organic compounds, the same trend of decreasing polarization was observed when soil was contaminated. However, the real part of the conductivity had a clear decrease (due to a decline in Ca\(^{2+}\) solution concentration) when decane was added, as opposed to no significant change in the previous study. The calcium rich environment had apparently contributed to the formation of different surface (mineral or OM surface) interactions of the organic compounds (polar or charged with different functional groups) in the presence of decane. These interactions affect the electrical properties of the soil either through specific interactions with the surface (Stern layer model) or through changing the pore throat length scale. The effect of calcium carbonate presence is also
considered, as its crystallization might have been encouraged in the presence of the organic solvents. Due to its insulating nature, it can greatly affect the soil conductivity and polarization.

In addition, an artificial neural network classification was presented, that showed a preliminary satisfying ability to indicate the existence of a specific contaminant (see Figure 2).

When examining the SIP method ability to identify and distinguish inorganic pollutants we see a clear influence of the chemical composition of the soil solution and the adsorbed phase on the soil’s electrical signature. Coherent changes in the relaxation time and chargeability (or phase values) when the chemical composition of the soil is changed. Furthermore, we note that divalent cations have a unique influence on the electrical signature: addition of divalent cation to the porous media (consisting mainly of monovalent cations) causes an instantaneous shift in the relaxation frequency, while the polarization magnitude is affected in a more gradual way (see Figure 3). This raises the idea that perhaps the changes in relaxation time and in polarization values are independent, however it should thoroughly examined.

Additionally, we have presented three types of data-driven models to potentially classify the presence or predict the concentration of inorganic species in the soil, based on the SIP measurements. The first model was an ANN model that based on the SIP signature of the different treatments can predict the adsorbed concentrations in the soil. The second model is a simplified chemical model that enables the prediction of species mobility, as a first step for their identification. The last model is a linear regression optimization to find the coefficients which relate the concentrations of species to chargeability and relaxation time. Even though the models were based on a limited amount of data, they were able to classify or predict fairly well the concentrations of the primary soil species.

(1) Membrane polarization model is the dominant mechanism to explain the findings of free-phase contaminant that are primarily related to the temporal relaxation of pore scale liquid arrangement. (2) Calcium cations play an important role in surface interactions with soil mineral and OM in the presence of hydrocarbons, affecting both membrane and Stern layer polarization mechanisms. (3) Classification of organic contaminants can be potentially achieved using SIP and data-driven models. (4) The properties (mobility, valance, radii, and affinity) of the adsorbed cations affect the electrical signature of the soil. (5) The measured spectra has the potential to reveal adsorbed concentrations of dominant species at the solid surface.

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**Figure 1.** Solution of the Young-Laplace equation (courtesy of Dr. Leonid Fel) for the described multiphase system, (a) the clean soil-water air interface (the border of the blue color and white background), before decane was added, (b) after decane was added: water-decane interface (the border of blue and red colors), and the decane-air interface (border of red color and white background).

**Figure 2.** Neural network classification for the binary presence of the examined pollutants in the soil. Each rectangle represents a specific contaminant: 0-for not present and 1-present in the soil. Blue dots are for the original measurements, green and red circles are trained and tested data by the ANN respectively. A successful prediction is indicated by a dot within a circle. The bottom axis indicates the type of treatment.
However, there still remains drawbacks for the spectral TDIP waveform, without current off-time, for TDIP measurements. Attempts have been made to achieve faster acquisitions and better signal-induced polarization (IP) response curves. Furthermore, efforts also consider the spectral information and inverting for the full moving from only inverting for the integral changeability to induced polarization (TDIP) data has changed. Research is aimed at doubling the spectrum of time-domain induced polarization, removing non-linear self-potential drift, harmonic noise and spikes, tapered gating, and uncertainty estimation.

SUMMARY

This paper presents an advanced signal processing scheme for time-domain induced polarization full waveform data. The scheme includes several steps with an improved induced polarization (IP) response gating design using convolution with tapered windows to suppress high frequency noise, a logarithmic gate width distribution for optimizing IP data quality and an estimate of gating uncertainty. Additional steps include modelling and cancelling of non-linear background drift and harmonic noise and a technique for efficiently identifying and removing spikes. The cancelling of non-linear background drift is based on a Cole-Cole model which effectively handles current induced electrode polarization drift. The model-based cancelling of harmonic noise reconstructs the harmonic noise as a sum of harmonic signals with a common fundamental frequency. After segmentation of the signal and determining of noise model parameters for each segment, a full harmonic noise model is subtracted. Furthermore, the uncertainty of the background drift removal is estimated which together with the gating uncertainty estimate and a uniform uncertainty gives a total, data-driven, error estimate for each IP gate. The processing steps are successfully applied on full field profile data sets. With the model-based cancelling of harmonic noise, the first usable IP gate is moved one decade closer to time zero. Furthermore, with a Cole-Cole background drift model the shape of the response at late times is accurately retrieved. In total, this processing scheme achieves almost four decades in time and thus doubles the available spectral information content of the IP responses compared to the traditional processing.

Key words: Spectral induced polarization; Time-domain; Signal processing; Uncertainty estimate; Electrical properties;

INTRODUCTION

Recently, the interpretation and inversion of time-domain induced polarization (TDIP) data has changed. Research is moving from only inverting for the integral changeability to also consider the spectral information and inverting for the full induced polarization (IP) response curves. Furthermore, efforts have been made to achieve faster acquisitions and better signal-to-noise ratio (SNR) by using a 100% duty cycle current waveform, without current off-time, for TDIP measurements. However, there still remains drawbacks for the spectral TDIP measurements, especially its limited spectral information content compared to for example laboratory frequency-domain spectral IP measurements (Revil et al., 2015). To date, only limited work has been done on increasing the spectral information content in TDIP measurement data even though recent developments in TDIP acquisition equipment have enabled access to full waveform recordings of measured potentials and transmitted current (e.g. the Terrameter LS and the Elrec pro). This paper presents a full waveform processing scheme for handling multiple issues limiting the spectral information quality and content. These issues are handled separately starting with background drift removal which is followed by identifying spikes, harmonic denoising, spike removal, tapered gating and uncertainty estimation.

DATA ACQUISITION

To be able to apply the processing scheme described in this paper it is necessary to use an instrument that is capable of recording full waveform data of the measured potentials. The required sampling rate for the full waveform depends mainly on the desired width of the shortest gate, how close it should be to the current switch and avoiding of aliasing. The data presented in this paper were acquired with a 50% duty cycle current waveform and 4s on-time using a Terrameter LS instrument for transmitting current and measuring potentials. The instrument operates at a sampling rate of 30 kHz and applies digital filtering and averaging depending on selected data rate. A data rate of 3750 Hz, corresponding to approximately 0.267 ms per sample, was used for the measurements presented in the paper. The sampling rate was chosen for being able to have the first IP gate one millisecond from the current pulse, considering that earlier gates would certainly suffer from EM-effects which we at present want to avoid, it was not judged meaningful with earlier gates. The instrument input filters were modified with a 4th order Butterworth filter with cutoff frequency of 1.5 kHz to avoid aliasing.

Two TDIP profiles (74 meter, 38 electrodes with spacing of two meter) were acquired on a grass field in Aarhus University Campus, with presence of multiple noise sources common in urban environments. The profiles were acquired with the instrument and settings as described in the previous paragraph, a multiple gradient protocol (364 quadrupoles) and acid-grade stainless steel electrodes.

IP GATE DISTRIBUTION

For retrieving spectral information close to the current pulses there is a need for gates which are shorter than the time-period of the harmonic noise (i.e. shorter than 20 ms for 50 Hz). This
is achieved by applying a log-increasing gating scheme that compensates for changes of signal-to-noise ratio throughout the IP response (Gazoty et al., 2013). When the gates are wide enough they are rounded off to multiples of the time period of the harmonic noise (Table 1, seven gates per decade). Thus, this gate distribution gives access to the IP response information more than one decade closer to the current pulse but still makes use of the efficient noise suppressing gate widths when possible.

Figure 1 shows the resulting IP response (green) after gating according to Table 1 and stacking according to the standard procedure (Fiandaca et al., 2012) when using a linear background drift estimate and the IP response retrieved from the instrument (magenta). The re-gated IP response shows similar magnitude as the instrument supplied when the gates are multiples of 20 ms. Contrastingly, it exhibits an erratic behaviour until the gate widths for both responses are multiples of 20 ms and suppress the 50 Hz harmonic noise (approximately at 60 ms). Clearly, the harmonic noise needs to be assessed to enable the use of gates shorter than 20 ms. Furthermore, the tail of both IP responses is increasing at the end as a result of the poor performance of the background drift removal when applying a linear drift model. Thus, to accurately retrieve the shape and spectral content of the IP response it is crucial to improve the drift removal by applying a more flexible drift model.

### SIGNAL PROCESSING

During TDIP measurements the potential response of the injection needs to be determined. However, the potential measured in the field is composed of the sum of multiple, known and unknown, sources. The known noise sources are handled separately in the processing scheme described in this paper and applied in a sequential manner. The first processing scheme step is drift removal which is followed by identifying spike samples, harmonic denoising, spike removal, tapered gating and uncertainty estimation.

**Cole-Cole model-based drift removal**

The background drift removal is normally done by approximating the drift as a linear trend (Dahlin et al., 2002). The background drift caused by current-induced electrode polarization is known to be orders of magnitude larger than the signal (Dahlin, 2000) and is common during field surveys due to difficulties of designing meaningful measurement sequences that account for all recent current injections. Electrode contact tests performed before initiating the TDIP measurements is also source for current induced electrode polarization. This background drift is caused by a depolarization phenomenon which is well described by the Cole-Cole model, thus this model is especially suitable for estimating the background drift. Two background drift estimates are used in this paper: the first with a linear estimate and the second with a Cole-Cole estimate.

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**Figure 2.** Top: full waveform potential (grey) and current (black), subset of the signal used for finding the drift model (orange x-marker) and background drift models (green: linear model, blue: Cole-Cole model). Bottom: resulting gated IP-response curves. Negative values are marked with circles.
To reduce the risk of any harmonic noise or IP response interfering with the drift model data, the fit is conducted for a subset of a down-sampled signal, taken at the end of the off-time period for the 50% duty-cycle and on-time period if applying a 100% duty-cycle current waveform. Fig. 2 show examples of generated drift models, as well as the resulting IP responses after gating and stacking the signal. Clearly, the linear model is not sufficient for accurately describing the drift in the full waveform potential and as a result it gives unrealistic increasing chargeability values for late gates of the IP response. Contrasting, the Cole-Cole model shows a good fit to drift data and consequently the resulting IP response does not exhibit the erroneous behavior at late gates. In total, it is clear that a linear drift model gives incorrect IP responses, especially at late times when signal-to-noise ratio is smaller and that a more advanced drift model such as the Cole-Cole is needed.

Model-based cancelling of harmonic noise

The processing approach applied in this paper is similar to the processing successfully applied on data from other geophysical methods, for example magnetic resonance soundings (Larsen et al., 2013) and seismoelectrics (Butler and Russell, 1993) but it has in this case been adapted to be applicable for data from TDIP measurement. The method takes a model-based approach for processing the TDIP full waveform potential by describing the harmonic noise in terms of a sum of harmonic signals. The different harmonic signals have frequencies given by a common fundamental frequency \( f_0 \) multiplied with an integer \( (m) \) to describe the different harmonics but have independent amplitudes \( (a_m \) and \( b_m) \) for each harmonic \( m \):

\[
\nu_{\text{harmonic noise}}(n) = \sum_{m} a_m \cos\left(2\pi f_0 \frac{m}{f_s} n\right) + b_m \sin\left(2\pi f_0 \frac{m}{f_s} n\right)
\]

for sample index \( n \) and sampling frequency \( f_s \). The reader is referred to the mentioned references for details.

Removal of full waveform spikes

Despiking of the measured full waveform signal is done for two main reasons. The first reason is that spikes in the full waveform data can corrupt the integrated values for IP gates, especially for short gates consisting of a few samples when only part of the spike falls within the gate thus having large effect on the integrated value. The second reason is related to the modelling of the harmonic noise and how the finding of noise model parameters is implemented in this paper which is known to be sensitive to spikes in data (Larsen et al., 2013).

The method for finding the spikes used in this paper employs several steps to enhance the spikes in the signal and defines a data-driven, automatic threshold limit based on a Hampel filter (Pearson, 2002) to determine if a sample index is to be considered as spike or not. By applying the filters in this manner an automatic data-driven threshold variable along the full-waveform acquisition is defined. All the samples above the threshold are marked as spikes and are neglected when performing the calculations for the residual energy in the harmonic denoising procedure. After harmonic denoising are the spike sample values replaces by the mean of their non-spike neighbours in the denoised signal.

Tapered gate design and error estimation

Today, the standard procedure for gating IP is to average the data within the predefined IP gates, corresponding to a discrete and normalized convolution with a rectangular window. In other geophysical methods (e.g. electromagnetics) a gate method applying different kinds of tapered windows have been used since decades (Macnae et al., 1984). Tapered window functions are superior in suppressing high frequency noise compared to the rectangular counterpart. Furthermore, the tapered windows allow the use of wider gates which has higher noise suppression, without distorting the signal. This paper, a Gaussian window with 3.5 times the width of the traditional rectangular window width was applied before evaluating the IP gate values. With this window, the main frequency response lobe of both windows cuts at approximately the same normalized frequency but the side lobes of the Gaussian window have around 40 dB higher frequency suppression.

Uncertainty estimation of the data for individual IP gates cannot be retrieved by directly comparing the individual IP stacks because each individual stack is different due to superposition from previous pulses (Fiandaca et al., 2012), hence other approaches are needed. It is also desirable that an uncertainty estimate make use of the advantage of applying the convolution with tapered gates as described in this paper. If enough gates per decade are used for gating the data, the signal variability is almost linear within the gates and for IP signals the linearity is more evident in lin-log space. Thus, it is possible to use a linear fit of the convoluted gate in lin-log space for estimating the gate uncertainty by taking the difference between the fit and the convoluted gate data. The difference gives a measure of the noise content within the gate after the convolution.

FULL FIELD PROFILE PROCESSING EXAMPLE

The processing scheme presented in this paper has been successfully applied to the entire test datasets with substantial improvements in spectral information content, data reliability and quality. One of the datasets is presented here as an illustration. Figure 4 shows IP responses from instrument processing and the redesigned processing scheme presented by this paper. The spurious IP increase present at late times in the response retrieved by the instrument is removed in the reprocessed IP response as a result of the improved drift removal. At the same time, the harmonic denoising processing enables to retrieve reliable IP data already 2.2 ms after the current switch, one decade closer to time zero compared to instrument IP processing.

![Figure 4. IP responses from instrument processing (magenta, instrument output) and the redesigned processing scheme presented by this paper (light blue) with error bars corresponding to one STD. Gates rejected by processing for containing spikes are marked in grey.](image-url)
Figure 5 shows pseudosections for a full data set acquired on the same profile as the previous data example was extracted from. It shows gates for IP responses generated by the full signal processing routine and corresponding pseudosections for the same gates but only applying the linear background drift removal. For the early gates which are not a multiple of the time period of the harmonic noise there is a clear improvement with much smoother pseudosection from gate 3 and higher. Contrastingly, IP gate number 18 which is little affected by the background drift removal shows very similar pseudosections for the two processing examples. However, the pseudosections for the last IP gate (25) show some difference due to the sensitivity of the late gates for background drift estimates where the linear drift model sometimes causes the IP responses to increase at late times. Again, the improved processing with Cole-Cole drift estimate shows smoother variation in the pseudosection, especially on the left side.

CONCLUSIONS

The TDIP signal processing scheme described in this paper significantly improves the handling of background drift, spikes and harmonic noise superimposed on the potential response in the measured full waveform potential. The Cole-Cole background drift removal substantially increases the accuracy of the drift model for non-linear drift cases and recovers the shape of the IP response at late times. The reliability of early IP response times, down to a few ms, is generally increased with a flexible data-driven despiking algorithm and model-based harmonic denoising. Furthermore, the improved gate distribution and tapered design gives access to early spectral IP response information and overall increases the signal-to-noise ratio by applying tapered and overlapped gates without distorting the IP response. Additionally, the data driven uncertainty estimates of the individual IP gate values provides valuable information for assessing data quality and for succeeding spectral inversion. In total, this processing moves the first gate one decade closer to time zero, recovers the late gates with reduced bias and supplies valuable estimates of IP gate uncertainty. These improvements double the usable spectral information of the IP response, achieving almost four decades in time, compared to instrument processing procedure.

### Table 1. Duration of delay time and IP gates for the processed field data corresponding to seven gates per decade. Note that the width of the gates from 13 and higher are multiples of 20 ms.

<table>
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<th>Delay</th>
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<th>2</th>
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<th>5</th>
<th>6</th>
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<td>1</td>
<td>0.26</td>
<td>0.53</td>
<td>0.80</td>
<td>1.06</td>
<td>1.33</td>
<td>2.13</td>
<td>2.93</td>
<td>4</td>
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An analysis of Cole-Cole parameters for IP data using Markov chain Monte Carlo

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SUMMARY

The Markov chain Monte Carlo (MCMC) method is used to invert time-domain induced polarization (TDIP) data. A novel random-walk algorithm samples models from a probability distribution based on a realisation of the model covariance matrix, allowing the algorithm to vary step lengths according to parameter uncertainty. The algorithm was found to converge to the posterior distribution over one hundred times faster than a standard Gaussian distributed model proposer. Synthetic TDIP data, simulating homogenous half spaces and three-layer models, are inverted using the MCMC method. The results show bell-shaped posterior distributions for all spectral Cole-Cole parameters with clear correlations between the parameters. Small values of the frequency exponent ($C_j$) are found to decrease the resolution of the model parameters. A comparative analysis between the standard deviations of the MCMC posterior distributions and the results of a linearized inversion shows that the linearized approach works well with well-resolved model parameters. We have compared inversion results of different acquisition ranges and current waveforms. We found that as the time range decreases the parameter correlations become nonlinear and the parameters become poorly resolved or completely unresolved. Combined, the inversion results show that it is possible to extract the spectral Cole-Cole parameters from time-domain IP data and that a linearized approach is justified for a sufficient acquisition range.

Key words: Time-domain induced polarization, Inverse theory, Markov chain Monte Carlo, Electric properties, Hydrogeophysics.

INTRODUCTION

Recently, the interpretation and inversion of TDIP data has changed from only inverting for the integral changeability to also consider the spectral information contained in the IP response curves (Fiandaca et al., 2012, 2013). Several examples of spectral TDIP applications have been presented, for landfill delineation (Gazoty et al., 2012b, 2013), lithotype characterization (Chongo et al., 2015; Gazoty et al., 2012a; Johansson et al., 2015), time-lapse monitoring of CO2 injection (Doetsch et al., 2015a; Fiandaca et al., 2015) and freezing of active layer in permafrost (Doetsch et al., 2015b). Furthermore, efforts have been made to achieve a wider time-range in TDIP acquisition, up to four decades in time (Olsson et al., 2016), for enhanced spectral content.

The spectral inversion of TDIP data is a high dimensional nonlinear problem. Ghorbani et al. (2007) argued that the problem is too nonlinear to be solved with least-squares methods, and that Cole-Cole parameters cannot be resolved from TDIP data.

The aim of this study is to analyse the uncertainty and correlation of spectral Cole-Cole parameters retrieved from TDIP data. This is done using the Markov chain Monte Carlo (MCMC) method with a novel model proposer.

MCMC ALGORITHM

A new MCMC algorithm is developed to sample the posterior probability distribution of the model space of the Cole-Cole parameters (Pelton et al., 1978) for the 1D TDIP forward mapping described in Fiandaca et al. (2012):

$$
\chi_j(\omega) = \rho_j \left[ 1 - m_{\theta j} \left( 1 - \frac{1}{1 + (\omega \tau_j)^C_j} \right) \right] 
$$

(1)

Where $\rho_j$ is the DC resistivity and $m_{\theta j}$, $\tau_j$, and $C_j$ are the IP parameters of the $j$'th layer with thickness $th_k$.

The Markov chain follows a random walk through the model space, where the next model in the chain only depends on the current model. Our MCMC algorithm is based on the Metropolis-Hasting sampling algorithm, which includes the following two steps (Metropolis et al., 1953; Hastings 1970): (1) A new model ($m_{\text{new}}$) is proposed from a proposal distribution $q(m_{\text{new}}|m_{t})$, where $m_{t}$ is the current model. The model proposer used here is introduced in the next section. (2) The proposed model is accepted or rejected based on an acceptance criterion, which is also described later. These two steps are repeated to generate a Markov Chain of models.

Model proposer

The computations are carried out in a logarithmic space to enhance linearity, with the model vector defined by:

$$
\mathbf{m} = \{\log(\rho), \log(m_{\theta}), \log(\tau), \log(C), \log(th_k)\}; \hspace{1cm} i=1:N_{\text{layers}}, \ j=1:N_{\text{layers}}-1
$$

(2)

Where $\rho$ is the resistivity [Ωm], $m_{\theta}$ is the chargeability [mV/N], $\tau$ is the time constant [sec], $C$ is the dimensionless frequency exponent, and $th_k$ is the layer thickness [m].
The new model, \( m_{\text{new}} \), is drawn from a normal distribution. The new proposed model is defined by:

\[
m_{\text{new}} = m_c + A
\]

Where \( m_c \) and \( A \) are the current model and the perturbation in the Markov chain, with \( A \) computed as:

\[
A = L \cdot n \cdot k
\]

The vector \( n \) contains random numbers drawn from a normal distribution and the constant \( k \) is the step length. \( L \) is the Cholesky decomposition of the linearized covariance matrix \( C_{\text{est}} \) of the initial model:

\[
C_{\text{est}} = LL^T
\]

This realisation of the model covariance matrix allows the proposer to take larger steps for poorly defined parameters. This makes the Markov chain convergence faster towards the target distribution. The covariance matrix, \( C_{\text{est}} \), is defined as in Auken et al. (2005).

The step length is adjusted for each Markov chain, so that the acceptance rate of new models is approximately 20-35%. A value of five is chosen as a maximum for the perturbation in order to confine the distance between \( m_{\text{new}} \) and \( m_c \).

**Model acceptance criterion**

The next step of the Metropolis-Hastings algorithm is to determine whether a proposed model should be accepted or rejected. If \( m_{\text{new}} \) is accepted, the model becomes the next model \( m_c \) in the Markov chain. If \( P(m) \) is the probability distribution of the model \( m \), then the acceptance probability of the new model is given by:

\[
\alpha = \min \left[ 1, \frac{P(m_{\text{new}}) \cdot q(m_c|m_{\text{new}})}{P(m_c) \cdot q(m_{\text{new}}|m_c)} \right]
\]

As the proposal distribution is symmetric in the logarithmic space, the equation reduces to:

\[
\alpha = \min \left[ 1, \frac{P(m_{\text{new}})}{P(m_c)} \right]
\]

So, the model \( m_{\text{new}} \) is always accepted if its probability is larger than the probability of the current model. If its probability is smaller, then the model is accepted with probability \( \alpha \).

**SYNTHETIC DATA**

Given a layered medium described by the Cole-Cole model, the 1D forward TDIP response is calculated using the algorithm presented by Fiandaca et al. (2012).

Single quadrupolar measurements (geometric factor of approximately 470 m) and Schlumberger soundings (20 quadrupoles) are simulated for homogenous half spaces and three-layer models, respectively. The Cole-Cole parameters range between \( \rho = 10 - 1000\ \Omega m \), \( m_0 = 5 - 800 \text{ mV/V} \), \( \tau = 0.001 - 10 \text{ sec} \) and \( C = 0.1 - 0.6 \). Three stacks are considered for each quadrupole, with both 50% duty cycle and 100% duty cycle waveforms (Olsson et al., 2015). Two different distributions of gates are used to simulate varying acquisition range. The minimum range has 20 gates generated with increasing widths of 20-200 msec, a current on-time of 2 sec and a measurement delay of 20 msec as used by Ghorbani et al. (2007). The maximum range has 22 gates generated with approximately log-distributed widths from 1.06 to 1300 sec. The on- and off-time of the current is 4 sec, and the measurement delay is 2.59 msec.

A Gaussian noise model is added to resistivity and chargeability values with a standard deviation equal to 2% for the resistivity and 10% for the chargeability. Additional a voltage threshold of 0.01 V is added to the data. The noise is added to give the best simulation of the noise level in the field (Gazoty et al., 2013).

In the following the results of a homogenous half space with model parameters \( \rho = 100\ \Omega m \), \( m_0 = 200 \text{ mV/V} \), \( \tau = 0.01 \text{ sec} \), \( C = 0.6 \) and a maximum acquisition range with 50% duty cycle is presented as an example.

**CONVERGENCE**

We have tested the convergence of the covariance-scaled MCMC model proposer in comparison to the basic Gaussian model proposer. For the Gaussian proposer Eq. (4) reduces to:

\[
A = n \cdot k
\]

It is found that the covariance-scaled proposer and the Gaussian proposer find approximately the same posterior model distribution (Figure 1), but the covariance-scaled proposer convergences towards the target distribution much faster. For the previous defined homogenous half space, the proposers analyse 5,000 and > 500,000 models, respectively, before reaching convergence. Using the scaled model proposer reduces the computation time for simple models from approximately one hour to 20 sec on 10 cores.

**RESULTS**

![Figure 1: The normalised posterior distributions of Cole-Cole parameter \( \tau \) resulting from two different model proposers: A covariance-scaled proposer (A) and a Gaussian proposer (B). The figure illustrates the faster convergence rate of the covariance-scaled model proposer, where we see convergence after just 5000 model proposals.](image-url)
Figure 2 (last page) shows the posterior distribution of the DC resistivity and the IP parameters for the homogeneous half space defined earlier. 100,000 models are proposed and 33 % are accepted and added to the posterior distribution. The histograms along the diagonal show the distributions of parameter values in log space with the true model values indicated in red. The off-diagonal are cross-plots of all combinations of the four parameters.

The distributions are all bell-shaped, which means they are all approximately log-normal. The parameters show a single maximum and are resolved to a different extent. However skewness is evident for $m_0$ and $\tau$.

The DC resistivity is almost uncorrelated to the Cole-Cole parameters. The chargeability shows a negative correlation to $\tau$ and $C$ with a Person’s correlation coefficient of 0.77 and 0.70 respectively. The correlation between to $\tau$ and $C$ is positive with a correlation coefficient of 0.86.

It is possible to compute the standard deviation (STD) on the model parameters from the posterior distributions. A relative standard deviation factor (STDF) is used here, where the 68% confidence interval for parameter $p$ then lies between:

$$\frac{p}{\text{STDF}} < p < p \cdot \text{STDF}$$

A perfect resolution will give STDF = 1. Using the terminology from Auken et al., 2005, STDF < 1.2 is a well-resolved parameter, 1.2 < STDF < 1.5 is a moderately resolved parameter, 1.5 < STDF < 2 is a poorly resolved parameter and STDF > 2 is an unresolved parameter. For the MCMC posterior distribution the standard deviation is calculated over all accepted models.

The STDF values are shown in Figure 3 for a varying value of the frequency exponent $C$. Together with the MCMC STDFs, we show the STDFs obtained from the linearized approach. Figure 3 shows that the uncertainty increases if the value of $C$ is decreased. This holds for both the MCMC- and the linearized approach. For $C = 0.6$ all parameters, except $\tau$, is well resolved with STDF < 1.2 for both MCMC- and linearized inversion. For $C = 0.2$, only the resistivity value is well resolved. The linearized estimations of the STDFs are reasonable for well resolved parameters, but are underestimated for poorly resolved parameters. As the $C$-value decreases the posterior distribution of the Cole-Cole parameters resulting from the MCMC analysis become more non-loglinear and the correlation between the model parameters becomes stronger.

More complex three-layer models verify the results with resolved bell-shaped posterior distributions for all the Cole-Cole parameters and linear correlations. Synthetic data are simulated on the same homogenous half space with a minimum acquisition range. The MCMC result shows nearly bell-shaped posterior distributions, but with nonlinear correlations between the parameter $C$ and $m_0$ and between $C$ and $\tau$. The STDFs of the DC resistivity and $C$ are almost unchanged compared to the result of the maximum range, but $\tau$ and $m_0$ are unresolved. The maximum of the posterior distribution and the true model is not consistent as well. Similar results are obtained for the 100% duty cycle data, confirming the equivalence of the 50% and 100% duty cycle waveforms for spectral resolution.

CONCLUSIONS

The results of running a MCMC inversion of synthetic TDIP data show that it is possible to extract the spectral Cole-Cole parameters from time-domain data.

The sampled posterior probability distributions of the Cole-Cole parameters are all bell-shaped with one maximum. Strong correlations are present between the IP parameters and for more complex models correlations can also been seen between these and the DC resistivity.

The uncertainties of the model parameters increase with decreasing values of $C$, which makes it more difficult to resolve parameters. This holds for the MCMC and the linearized approach. However the linearized standard deviations work well for well resolved parameters.

If the acquisition range is too short (2 decades or less), then the Cole-Cole parameters become poorly- or completely unresolved, and the correlations become nonlinear.

In general, all the results justify the linearized inversion of TDIP data for resolved Cole-Cole parameters, when the necessary acquisition range is used.

REFERENCES


Figure 2: The posterior probability distribution of the Cole-Cole parameters for a homogenous half space: $\rho = 100 \Omega m$, $m_0 = 200$ mV/V, $\tau = 0.01$ sec, $C = 0.6$. The diagonal shows histograms of the distribution of each Cole-Cole parameter. The off-diagonal shows the correlation between the parameters. The true model parameters are indicated in red. Note the figure is symmetric about the diagonal.
Simulation of membrane polarization for 2D and 3D pore networks

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INTRODUCTION

The characterization of porous media (e.g. unconsolidated sediment or rocks) by geophysical methods is a research topic of fundamental importance in environmental and economic issues like the investigation of water reservoirs or the evaluation of waste deposits. The spectral induced polarization (SIP) method is supposed to have big potential to provide useful information based on relationships between electric and hydraulic parameters. Several empirical approaches for the interpretation of the measured SIP response exist. Attempts have been made to correlate a characteristic time scale, derived from the phase-shift spectra, with measured material parameters like hydraulic conductivity or pore radii (Titov et al., 2010; Binley et al., 2005). Another approach is to compare the imaginary conductivity at a single frequency (Weller et al., 2010) to the specific surface of the pore space. Although both methods are based on different assumptions they are supported by examples of reasonable agreement with laboratory experiments.

The formulation of a comprehensive theoretical model is difficult because the underlying physical processes on the pore scale are not yet fully understood. The two main models, the theory of electrochemical polarization, first suggested by Schwarz (1962), and subsequently extended by several authors (e.g. Leroy et al. 2008; Revil and Florsch 2010), and the theory of membrane polarization, first suggested by Marshall and Madden (1959) and extended by Bücker and Hördt (2013), are both based on the ion movement in the electrical double layer. The fundamental difference between the both models is expressed in the definition of the mineral geometry. The electrochemical polarization is based on mineral grains where the polarization effect is based on a local concentration of charge on the grain. The membrane polarization is based on sequences of narrow and wide pores where the polarization effect is caused by narrow throats between the pores (FIGURE 1).

SUMMARY

We extend an existing membrane polarization model to 2D and 3D pore combinations networks, which are numerically solved to obtain an overall SIP response. We investigate the behaviour of these networks by varying the distribution function of the pore combinations and the size of the network.

Equally distributed pore combinations show a dominance of high phase shifts. For empirically distributed combinations, obtained from measured pore radii distributions, high phase shifts tend to dominate only in big 3D networks. Our simulations show that for networks, which are comparable to real rocks, higher maximum phase shifts than the mean of the original pore combinations are possible. The results suggest that networks may allow a simulation of more realistic pore geometries than the original 2-pore system.

Key words: membrane polarization, pore networks, measured pore radii distribution.

Figure 1: Marshall and Madden polarization. Overlapping cation layers in pore throats (grey) lead to decreased anion mobility. An applied electric field causes concentration gradients which relax with a characteristic time after switch-off.

Figure 2: 2D-extension of the model. Parameterizing the narrow and wide pores through pore radii allows to...
calculate the Marshall and Madden ion mobilities by taking into account the electrical double layer (dark-blue layers).

The combination of a narrow and a wide pore is a simplified model that does yet not account for the complexity of macroscopic porous media. A basic study on geometrical parameters of the model showed generally reproducibility of phase shifts and characteristic time scales in the range typically measured with natural sandstones (Hördt et al., 2016b). As a next step towards the simulation of realistic pore space geometries, we present an approach to merge different pore combinations to 2D and 3D network grids. The aim of this work is to examine possible differences of the response behaviour of such networks in comparison with the simplified model and to determine minimum size and necessary complexity requirements.

METHODS

Each pore combination of a narrow and a wide pore (e.g. FIGURE 2) can be treated as an impedance component which we merge to a resistor network (FIGURE 3). We obtain the SIP response of this network by numerically solving a linear equation system corresponding to the finite differences method.

In a first approach, we use equally distributed pore combinations to obtain an overview over the behaviour of such networks. In order to match realistic pore space geometries, we use measured pore radii distributions of real rocks (e.g. Weller et al. 2011). First, we approximate the distributions by a fractal relationship. Then, we chose the pore combinations such that the overall radii distribution in our model matches the fractal distribution.

RESULTS

In FIGURE 4, we investigate 100 equivalent random 2D networks constructed from 4 representative pore combinations. The simulations show unexpected behaviour. The total maximal phase shifts of the networks concentrate in two bins. The higher one (~70 mrad) corresponds with pore combination 2 and the lower one (~30 mrad) with pore combination 3. Both bins are higher than the weighted mean of the 4 pore combinations (red line in figure 4). The two pore combinations 1 and 4 with very small maximal phase shifts (< 1 mrad) are not represented at all. This dominance of high phase shifts is more pronounced in 2D networks but can also be observed in 3D networks.

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Simulation of membrane polarization for 2D and 3D pore networks

Figure 5: Maximum phase shift of 100 equivalent random 3D networks (each of 125 nodes), constructed from empirically distributed pore combinations. Red line: Mean of the maximum phase shifts of the empirical combinations, weighted with the appearance in the network.

CONCLUSIONS

In order to get closer to a realistic description of real rocks we extended an existing membrane polarization model to impedance networks. We investigated the behaviour of 3D and 2D networks of different size and different pore combination distributions. The choice of the distribution function influences the SIP response behaviour. While equally distributed pore combinations in small networks (<100 nodes) show dominance of high phase shifts, this behaviour cannot be confirmed with empirically distributed combinations. In big networks (>1000 nodes) the behaviour tends to split between the dominance of high phase shifts for 3D and low phase shifts for 2D networks.

Our results show that for impedance networks, higher maximum phase shifts than the mean are in general possible. This is more pronounced with equally distributed combinations, but can also be shown, although with much smaller evidence, for big 3D networks with empirically distributed combinations. Big empirically distributed networks are most comparable to real rocks, which allows us to get closer to realistic SIP response modelling than with the simplified 2-pore model only.

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Lithological characterization of a contaminated site using Direct current resistivity and time domain Induced Polarization

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**SUMMARY**
Characterization tools for contaminated sites have become advanced with the continued development of geophysical methods. Resistivity methods and time-domain induced polarization methods have proven their capability to delineate the subsurface properties by complementing each other. In the present study a large contaminated site in Denmark was investigated using direct current resistivity and time domain induced polarization (DCIP). For this purpose 14 profiles were collected alongside a stream in order to investigate the contamination and delineate the lithological units. 2D inversion using a cole-cole model of two selected profiles are presented. They show that the resistivity model alone cannot depict the geology as inferred in the borehole. However, when including the models of chargeability and mean relaxation time the geological units are clearly defined, which helps in identifying the possible contaminations.

**Key words:** Time Domain Induced Polarization, Cole-Cole model

**INTRODUCTION**
Groundwater and surface water can be contaminated due to various types of human activities e.g. waste from residential, commercial, industrial, and agricultural activities. Especially in cities with an industrial history this is often a severe problem. In order to evaluate the risks, characterization of the contaminated sites in terms of geology and contaminant leachate is needed. This characterization is often carried out using limited drill hole information, but a much more detailed picture of the subsurface can be obtained by dense surface-based geophysical methods.

Multi-electrode direct current (DC) resistivity and induced polarization (DCIP) methods have proven their capability to delineate the contaminant mass from the host geology, as contamination strongly influences the resistivity and chargeability of the subsurface (Gazoty et al., 2012). The method has recently advanced in terms of data acquisition techniques (Dahlin et. al., 2002) and processing and inversion optimizations (Auken et. al., 2009).

In this study we investigated a contaminated site using DCIP measurements along a stream in the city of Grindsted (southern part of Denmark) where a pharmaceutical industry deposited massive amounts of chemicals on a number of sites.

**METHODS AND RESULTS**

**DCIP Methodology**
Direct current resistivity and Induced polarization methods (DCIP) have been extensively used in environmental studies. The resistivity method is based on the fact that distribution of electrical potential in the subsurface depends on the resistivities around a current injecting electrode. In normal practice two electrodes are used for injection and another pair of electrodes measures the potential. The IP method is based on the chargeability effects of the subsurface. When measuring in the time-domain and when the subsurface is chargeable, the voltage does not drop immediately to zero following the current shut down, but rather it decays slowly over a few seconds. The magnitude of the polarization and the shape and length of the decay depend on subsurface parameters such as ion content and type, clay content, and pore structure to mention a few. Time-domain IP data are recorded along with the traditional DC data using the same measurement setup.

Recent developments in the field of data acquisition such as multichannel measurements (Dahlin et al., 2002) have made the time-domain DCIP method more robust, faster and more convenient to perform in the field. Combined with advancements in the numerical modelling of IP data including modelling of transmitter waveform and low-pass filters enable us to retrieve the Cole-Cole parameters from time-domain measurements of the entire decaying IP signal (Fiandaca et al., 2012). The cole-cole model (Pelton et al., 1978) is a commonly used empirical model which involves the parameters resistivity, chargeability, relaxation time, and frequency exponent.

**Field Site and Geological Settings**
The investigated study area is located in the region of southern Denmark, Grindsted. Two of Denmark’s 122 locations classified as “large contaminated sites” are located here (Grindsted factory and Grindsted landfill). Contamination from the landfill and factory site is posing great risks to Grindsted stream and a large impact from contaminations have been observed in the stream (Nielsen et al., 2014). The geology of the Grindsted area consists of an upper 10-12 m quaternary sand layer and a lower tertiary sand layer, locally separated by silt and clay layer (Heron et al., 1998). Below this layer, we have a regional micaceous sandy layer approximately 65 m thick, which is underlain by a clay layer at 80 m depth.

Data Acquisition

The site was investigated with the collection of 14 DCIP profiles (Figure 1) covering both the north and the south bank of the river. The profiles are will be treated in a full 3D framework, but here we will present selected 2D results. Out of the 14 profiles, seven profiles were 410 m long with 5 m electrode spacing and other seven profiles were 126 m long with 2 m electrode spacing. The survey was performed using the gradient array (Dahlin and Zhou, 2006) and we used the ABEM Terrameter LS for the data acquisition.

Results

The processing and inversion of the DCIP data were carried out using Aarhus Workbench (Auken, 2009). Processing of DCIP data involves removal of outliers from apparent resistivity data and culling of disturbed IP decays. Data were inverted using the 2D DCIP inversion code developed by Fiandaca et al. (2013). This inversion routine uses the cole-cole model to invert the DCIP data, which gives four model parameters namely resistivity ($\rho$), chargeability ($m_0$), relaxation time ($\tau$) and frequency exponent ($C$). The inversion code also models the full waveform and stack sizes. Figure 2 presents the inversion results of two representative profiles (profile 3 and 6) located at the northern bank of the river. The cole-cole parameters shown from top to bottom are resistivity ($\rho$), chargeability ($m_0$), relaxation time ($\tau$) and frequency exponent ($C$). The borehole located on profile 6 (shown as blue dot in figure 1) is presented as a bar with the different geological units indicated. The bar colour code represents major lithological unit identified in borehole (Brown: sand, light blue: sand mixed with clay, blue: clay). It can be seen that the low resistivity anomaly in both profiles does not clearly represent the clay rich layers seen in the borehole. This could be attributed to the combined response of clay layer and the contamination present in the sandy aquifer above and below the clay layer in the north western part of the profile.

However, in the chargeability section a high chargeability layer agrees very well with the clay layers. This layer clearly stands out also in the tau section. The bottom of the high chargeable layer indicates the lower boundary of the clay layer.

To show this boundary in the resistivity section, a red dashed line is drawn in both profiles. We can see that in the northwestern part of both profiles the low resistivity signature is continuing in the sandy aquifer, which possibly indicates the presence of contaminations.

These observations indicate that the IP response is mostly dominated by the clay rich layers, which helps in identifying the lithological units more adequately than the resistivity section alone.

In the presentation we will show results in 3D combining the results of all the lines to visualize the delineation of a possible contamination.

CONCLUSIONS

DC resistivity and the time domain induced polarization method were used at a contaminated site for characterizing the contaminants and lithology. The results are presented in terms of Cole-Cole parameters.

The major lithological unit could not be interpreted from the resistivity section alone, but the chargeability section clearly delineate the major lithological boundaries observed in a borehole. Identification of the geological units allows for speculations on possible contaminations identified in the resistivity section.

ACKNOWLEDGMENTS

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Figure 1 Location of DCIP profiles. Location of the borehole is shown as blue dot on profile 6.

Figure 2 DCIP inversion results from profile 3 and 6. Cole-Cole parameter shown from top to bottom are resistivity ($\rho$), chargeability ($m_0$), relaxation time ($\tau$) and frequency exponent($C$). DOI is shown by continuous black lines and dotted line in resistivity section shows the interpreted lower boundary of the clay layer.
**Spectral induced polarization of sand-biochar mixtures: experiments and modeling**

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**SUMMARY**

Biochar attracts increasing research interest due to its potential for agricultural and environmental purposes such as soil amendment and greenhouse gas reduction. To better monitor and investigate biochar in soil, non-invasive measurement approaches that can be applied in the laboratory and at field scale are needed. The goal of this work is to examine the sensitivity of the spectral induced polarization (SIP) method to the presence of disseminated biochar in sand. We investigate the complex electrical conductivity of saturated mixtures of sand and sieved biochar, and use a mechanistic SIP model that accounts for the redox reactions at the surface of the polarized particles to invert the measured data. The magnitude of the measured complex electrical conductivity showed a positive correlation with the mass fraction of biochar, while the peak frequency of the imaginary part showed a negative correlation with the particle size of the biochar. The model provides reasonable fitting results for low mass fraction of biochar in the mixtures.

**Key words:** SIP, biochar, electrochemical model

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**INTRODUCTION**

Biochar is the by-product of biomass pyrolysis and gasification. It is derived from a wide variety of sources, including wood (Cheng et al., 2014), green waste (Chan et al., 2007), poultry litter (Chan et al., 2008), agricultural residues (Demirbas et al., 2006), and a wide range of additional sources. The application of biochar to farmland can increase plant growth, reduce leaching of nutrients, and increase water retention and microbial activity (Hunt et al., 2010). Furthermore, biochar seems to be a promising option for long-term sequestration of carbon to offset CO2 emissions (Sohi et al., 2009). Long-term effects of biochar in soil, however, are not yet sufficiently investigated. Therefore suitable methods of monitoring and investigating biochar in soil are still required to better evaluate the true agronomic and environmental value of biochar as a soil amendment.

The physical and chemical properties of biochar vary largely owing to different feedstocks and production processes. Characterizing biochar and its properties in soil media by using traditional physico-chemical methods is therefore difficult and time consuming. SIP is a promising method to overcome these problems due to its real-time and non-invasive features and the relatively large monitoring volumes or areas in the field. However, modeling and understanding the SIP signal related to the physical nature of the samples are still challenging. Existing mechanistic models are mostly based on the theory of the polarization of the charges in the electrical double layer (EDL) at the solid-liquid interface. These models, however, cannot be directly applied to the polarization that is observed in the presence of disseminated materials with electronic conductance (Gurin et al., 2013). Wong (1979) developed a model that we refer to as the electrochemical SIP model in the following. This model was originally proposed to describe the SIP response of disseminated sulfide ores, which show similar electronic conductance as particles of biochar. In this work, we study the spectral induced polarization of disseminated biochar in sand media, and test the ability of the electrochemical SIP model to describe the measured SIP data.

**METHOD AND RESULTS**

**SIP Measurement**

We used the SIP method to measure the complex electrical conductivity \( \sigma = \sigma^+ + i\sigma^- \) of mixtures of sand and sieved biochar. The experimental set-up is shown in Figure 1. The sample holder has a height of 18 cm and an inner diameter of 3 cm. Water can flow through the sample from the bottom to the top of the sample holder. Flushing with electrolyte solution was used to saturate the material inside the column and to remove excess salts released from the biochar after sample preparation. Two porous bronze plates were used as current electrodes at the top and bottom of the column to inject current. Two metal potential electrodes were used at a distance of 6 and 12 cm from the bottom of the sample holder. To avoid electrode polarization, the potential electrodes were retracted about 1.2 cm (2 times of the diameter of the potential electrodes) into their borings.

---

**Figure 1. Sketch of the experimental set-up. A water tank is connected with the bottom of the column for flushing the sample.**
We investigated two sets of samples (Table 1). In both sets, the biochar was obtained from pine woodchips by slow pyrolysis at 400 °C. Biochar of various particle diameter (d) and mass fractions (ξ) was added to a well-sorted sand. All samples were flushed with 4 mM NaCl solution.

Table 1: Mass fraction and particle size of biochar in samples

<table>
<thead>
<tr>
<th>Set A</th>
<th>Fraction of biochar (ξ)</th>
<th>Particle size of biochar (d) (mm)</th>
<th>Set B</th>
<th>Fraction of biochar (ξ)</th>
<th>Particle size of biochar (d) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1%</td>
<td>0.5-1</td>
<td>1</td>
<td>2%</td>
<td>0.25-0.5</td>
</tr>
<tr>
<td></td>
<td>2%</td>
<td>0.5-1</td>
<td>2</td>
<td>2%</td>
<td>0.5-1</td>
</tr>
<tr>
<td></td>
<td>3%</td>
<td>0.5-1</td>
<td>3</td>
<td>2%</td>
<td>1-2</td>
</tr>
<tr>
<td></td>
<td>4%</td>
<td>0.5-1</td>
<td>4</td>
<td>2%</td>
<td>1-2</td>
</tr>
</tbody>
</table>

**Modeling Method**

The electrochemical SIP model is based on a combination of electrochemical principles and electrical potential theory. In Wong’s model, the complex electrical conductivity of the particles is determined by the sum of surface conductivity and the conductivity produced by the redox reaction. We used an extended form of the model that is able to consider the particle size distribution:

\[
\sigma_\alpha(\omega) = \frac{\omega}{\sigma_0} \sum_{l=1}^{n} v_l T_l(\omega c_l + \sigma_0),
\]

where \( \omega \) is the angular frequency, \( v_l \) is the volume fraction of spheres with radius \( a_l = 0.5 \ d_l \), \( \sigma_0 \) is the complex electrical conductivity of the sample and \( \sigma_\alpha \) is the electrical conductivity of the electrolytic medium. In addition, the reflection coefficient (\( r(\omega) \)) is given by:

\[
f(\omega) = 1 + \frac{\left(1 + \frac{\sigma_0}{\omega c_l} f_1\right) + \frac{\sigma_0}{\omega c_l} (2 - 1)}{\left(1 + \frac{\sigma_0}{\omega c_l} f_1\right) + \frac{\sigma_0}{\omega c_l} (2 - 1)},
\]

with

\[
f_1 = \frac{\lambda_2 a_2 z_2 a_2 z_2}{\lambda_1 a_1 z_1 a_1 z_1}, \quad f_2 = \frac{\lambda_2 a_2 z_2 a_2 z_2}{\lambda_1 a_1 z_1 a_1 z_1}, \quad f_3 = \frac{\lambda_2 a_2 z_2 a_2 z_2}{\lambda_1 a_1 z_1 a_1 z_1},
\]

\[
\lambda_2^2 = 2 \chi^2 + \omega D / \lambda_2^3 = \omega D / \lambda_2^3, \quad \chi_2 = \sigma_0 (\sigma D),
\]

where

- \( \chi \) - electrochemical reaction parameter (A s\(^{-1}\) kg\(^{-1}\) mol\(^{-1}\))
- \( \beta \) - electrochemical reaction parameter (m\(^{-1}\) s\(^{-1}\))
- \( c \) - concentrations of active cations (n/(m\(^3\)))
- \( c_0 \) - total concentration of cations and anions (n/(m\(^3\)))
- \( D \) - diffusivity of cations and anions (m\(^2\)/s)
- \( \varepsilon \) - dielectric constant (F/m)
- \( \mu \) - mobility of ions (m\(^2\) V\(^{-1}\) s\(^{-1}\)).

**Measurement Results**

The SIP spectra of sand-biochar mixtures were analyzed in terms of the real part \( \sigma'(\omega) \) and the imaginary part \( \sigma''(\omega) \). Figure 2 presents the frequency-dependent complex electrical conductivity as a function of frequency for different mass fraction (\( \xi \)) and particle size (\( d \)) of biochar, respectively. Figure 2a shows that \( \sigma'(\omega) \) increases with the whole frequency range, and this increase is stronger when the amount of biochar increases. Figure 2b shows that \( \sigma''(\omega) \) first increases and then decreases with increasing frequency. A peak with an increasing maximum value related to the increasing fraction of biochar is observed for each of the spectra in a similar frequency range. Figures 2c and 2d show that there is no obvious influence of the particle size distribution on the magnitude of \( \sigma'(\omega) \) and \( \sigma''(\omega) \). The larger biochar particles show the increase of \( \sigma''(\omega) \) at lower frequency. The peak frequency of \( \sigma''(\omega) \) clearly moves to lower frequencies for increasing particle size.

**CONCLUSIONS**

We investigated the SIP response of sand-biochar mixtures with varying particle sizes and different amounts of biochar. The results show that biochar in sand shows significant polarization and a characteristic SIP response. The particle size and fraction of biochar have an influence on the characteristics of the SIP signal. The reasonable modelling results show that the electrochemical SIP model has some potential to characterize the SIP signal in the presence of electronic conductors such as biochar. Next, we will extend the model to elliptical particles rather than spherical particles to improve the accuracy of the model for the visibly non-spherical biochar particles.
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Figure 3. Measured SIP spectra (dotted lines) and best fitting results for the electrochemical SIP model (green continuous lines).
Numerical correction of phase errors due to leakage currents in wideband EIT measurements

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SUMMARY
Advanced model-based data correction methods are needed in order to determine the small phase response of low-polarizable soils and rocks in the higher frequency range up to 10 kHz. Methods have been developed to correct several system-dependent errors, such as amplification errors, signal drift, current measurement errors, potential measurement errors due to high electrode impedances, propagation delay of the signal due to the long cables, and phase errors introduced by inductive coupling between the electrode cables. However, measurements at test sites with high resistivity have shown a new dominating phase error, which was found to be related to capacitive leakage currents between system ground and the soil. In order to correct this error, we enhanced the FEM modelling used for the reconstruction of the electrical conductivity distribution. Using this new formulation of the FEM forward model, this source of error was reduced by a factor of five or more. This enables an electrical conductivity reconstruction for frequencies up to 10 kHz. In future work, it will be investigated whether the capacitive leakage currents can be reduced by optimization of the cable layout. In any case, it is helpful to use the leakage current as a proxy for data error during data filtering, and it can also be used to decide if the enhanced FEM model presented here should be used.

Key words: electrical impedance tomography, leakage current, capacitive coupling, inductive coupling.

INTRODUCTION
Impedance measurements on low-polarizable soils and rocks in the mHz to kHz range require advanced data correction methods and a sophisticated EIT measurement system to achieve the necessary phase accuracy. For data acquisition, a prototype spectral EIT system optimized for measurements with high phase accuracy has been developed. In addition to the system design, model-based numerical correction methods are used to remove several errors introduced by amplification errors, signal drift, current measurement errors, potential measurement errors due to high electrode impedances, the propagation delay of the signal due to the long cables, phase errors introduced by inductive coupling between the electrode cables and other system or cable dependent sources (Zimmermann et al. 2008, Kelter et al. 2015, Zhao et al. 2015).

The use of model-based corrections enables accurate impedance measurements for frequencies up to some kHz. However, at test sites with high resistivity the correction methods were not sufficient to provide accurate measurements, which is a clear indication that an additional phase error not yet considered in our corrections is affecting measurement accuracy. Close inspection of the errors showed that the remaining errors are related to capacitive leakage currents between system ground and the soil. In this paper, we will present a new correction method based on an enhanced FEM model, and verify the efficiency of the new model-based correction using impedance measurements at resistive and conductive test sites for frequencies up to 10 kHz.

METHOD AND RESULTS
Impedance measurements were made using 30 surface electrodes with an electrode separation of 1 m at one conductive and one resistive field site in the vicinity of Milano, Italy. A simple fan-shaped cable layout was used to connect the electrodes to the measurement system. This allows a relatively straightforward calculation of the inductive coupling between the cables, and a subsequent correction following the methods outlined in Zhao et al. (2015). At the conductive test site, previously developed model-based phase corrections worked well. However, the corrections were not sufficient at the more resistive test site. After analysis of the measured data, we found that there was a strong correlation between the capacitive leakage currents between system ground and soil and the phase response of the measured transfer impedances. In a first attempt to correct this error, we developed a correction method based on a simple electrical model. However, this method did not work well due to the inhomogeneous electrical conductivity of the soil and the unknown and variable potential distribution at the surface for different electrode configurations. Therefore, it became necessary to enhance the forward FEM model to directly consider leakage currents during the inversion of the data. Our starting point was the following enhanced FEM model that uses an additional admittance matrix $Y_t$ to...
consider the capacity between the cable shield and the surface of the soil

\[(Y + Y_A) U = I\]  \(1\)

where Y is the admittance matrix of the soil, U is the potential distribution at the nodes of the used mesh, and I the current source (Zimmerman 2011, Zhao et al. 2013). The total capacity between system ground potential, which is also the shield potential of the cable, and the soil is measured with the EIT system. At the resistive test site, it was found to be 10.5 nF. This capacity is considered in the admittance matrix Y_A by assuming that the capacity is equally distributed along all cable paths. In order to consider the effect of leakage current, we modify the source term of the FEM model:

\[I = I_s + I_l\]  \(2\)

where the vector I_s represents a symmetric current injection (normal case) and the vector I_l represents leakage currents. Using this modified FEM model, we calculate the transfer impedance according to:

\[Z = Z_s + Z_L\]  \(3\)

where Z_s is the impedance for symmetric current injection (normal case), and the impedance Z_L for excitation with the leakage current. The leakage current is calculated from the measured current at the two used current electrodes for all configurations.

The modified forward FEM model is included in the inversion in order to reconstruct the complex soil conductivity using a 3D mesh for the forward model and a 2D mesh for the inversion. After inversion, we calculated the corrected impedance Zc using

\[Z_c = Z_M - Z_L\]  \(4\)

in order to verify the effect of the model-based correction on the imaginary part of the measured impedance Z_M.

Figure 1 shows the impedance spectra for different correction steps. It can be seen that the correction for inductive coupling has the biggest effect at the conductive site, whereas the correction for capacitive leakage currents has the biggest effect at the resistive site. After correction, the imaginary part of the impedance is consistently negative as expected, and the spread of the impedance values at high frequencies is minimized. As illustrated in Figure 2, the additional model-based correction developed in this study allows the reconstruction of the soil conductivity for frequencies up to 10 kHz for both conductive and resistive test sites.

**CONCLUSIONS**

In this study, we could show that the new model-based correction that relies on FEM modelling enables the correction of measured impedances of resistive test sites where leakage currents cause a strong phase error in the data. This correction is important for wideband spectral EIT measurements. However, it requires the measurement of the leakage current and the total parasitic capacity between system ground and the soil in addition to a well-defined cable layout. Based on our current understanding, it is likely that the cable layout can be optimized to reduce errors in measurements of the phase of the impedance. However, the optimal lay-out will depend on the dominating error source (inductive coupling or capacitive leaking currents). In addition, capacitive leaking currents increase with increasing contact impedance of the electrodes, which thus need to be as low as possible in order to minimize phase errors in the impedance measurements. In any case, it is helpful to use the leakage current as a proxy for data error during data filtering, and it can also be used to decide if the enhanced FEM model presented here should be used.

**ACKNOWLEDGMENTS**

We are grateful to Silvia Inzoli and Mauro Guidici for support during the field measurements.

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Figure 1. Impedance spectra of the measured and corrected transfer impedances of a more resistive (a … e) and a more conductive (g … j) test site with the real (a, f) and imaginary part (b, g) of the uncorrected data, the imaginary part (c, h) after correction for inductive coupling, the imaginary part after additional correction due to the capacitive leakage current (d, i) and after additional removal of impedances with a ratio $I_I/I_S > 10\%$. It should be noted that the scale can change from step to step.
Figure 2. Magnitude (a, c, e, g) and phase image (b, d, f, h) of the reconstructed conductivity distribution of the more resistive (a ... d) and the more conductive (e ... h) test site in Milan at the frequencies 164 Hz and 10 kHz.
Comparison of Cole-Cole and Constant Phase Angle modeling in time-domain induced polarization

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SUMMARY

The Cole-Cole model and the constant phase angle (CPA) model are two prevailing phenomenological descriptions of the induced polarization (IP), used for both frequency domain (FD) and time domain (TD) modeling. The former one is a 4-parameter description, while the latest one involves only two parameters. Choosing between a Cole-Cole description and a CPA one to invert a specific frequency domain data set is easy, since a look at the data is enough to estimate their spectral content. This is, however, not the case with TDIP data. This work aims at understanding how the spectral content is reflected in TDIP data, and therefore, at identifying (1) if and when it is possible to distinguish, in time domain, between a Cole-Cole description and a CPA one, and (2) if features of time domain data exist in order to know, from a simple data inspection, which model will be the most adapted to the data. Synthetic forward responses were computed for homogeneous Cole-Cole models, varying both time range of the modeled IP data and Cole-Cole parameters. Subsequently, CPA inversions were carried out on the Cole-Cole data. The inversion results show that it is generally possible to distinguish CPA and Cole-Cole models in time domain, except when the Cole-Cole frequency exponent is small (below 0.1) or for specific combinations of the Cole-Cole parameters. The distinctness increases with the time range of the IP data, but usually two decades in time are sufficient to distinguish the two models. Furthermore, forward modeling of quadrupolar sequences on 1D and 2D heterogeneous CPA models shows that the CPA decays differ among each other only by a multiplication factor. Consequently, the inspection of field data in log-log plots gives insight on the modeling needed for fitting them: the CPA inversion cannot reproduce the shape variability of the IP decays. Field examples of this latter result are presented.

Keywords: Cole-Cole, CPA, time-domain, spectral inversion

INTRODUCTION

The Induced Polarization of rocks and soils can be described with a frequency-dependent complex resistivity. Several models are used to describe the induced polarization of geomaterials, but the most used are the Cole-Cole model presented by Pelton et al. (1978) and the constant phase angle model (CPA), as described for instance in Van Voorhis et al. (1972).

The CPA model is suitable if no or negligible variation of the phase shift is observed in the complex resistivity data. Thus, the choice of using the Constant Phase Angle (CPA) model instead of the Cole-Cole model to describe a specific set of frequency domain IP data is straightforward. This is, however, not the case with time domain IP data. Being able to understand how the Cole-Cole description differs from the CPA description in time domain will allow us to judge more easily, which description will manage best to describe the induced polarization of a specific studied area.

TDIP forward responses of homogeneous half-spaces have been computed, using the Cole-Cole modeling and varying the acquisition time ranges. Each synthetic decay has then been inverted using the CPA modeling, in order to test to what extent the CPA inversion is able to fit Cole-Cole data. Finally, a field data set has been inverted using both models, to assess in a real 2D situation their ability to explain data.

METHOD AND RESULTS

The Cole-Cole and CPA models are the two principal phenomenological models used to describe the induced polarization of rocks and soils. The complex resistivity $\xi_{\text{Cole-Cole}}$ of the Cole-Cole model takes the form:

$$\xi_{\text{Cole-Cole}} = \rho \left(1 - m_0 \left(1 - \frac{1}{1 + (i\omega \tau)^{m}} \right) \right)$$  (1)

where $\rho$ is the direct current resistivity, $m_0$ is the intrinsic chargeability, $\tau$ is the time constant, $C$ is the frequency exponent and $i$ is the imaginary unit.

The CPA model is much simpler, and describes the complex resistivity using only two parameters:

$$\xi_{\text{CPA}} = K (i \omega)^{-b}$$  (2)

where $b$ is a positive fraction, $\varphi = -\frac{\pi}{2} b$ represents the phase shift and completely defines the IP response, $K$ is a constant and $i$ is the imaginary unit. In the CPA model the DC resistivity cannot be defined, because the complex resistivity increases indefinitely at low frequencies. For this reason Van Voorhis et al. (1973) introduced the Drake model:

$$\xi_{\text{Drake}} = K (i \omega + \omega_0)^{-b}$$  (3)

where in comparison with the CPA model a low frequency pole $\omega_0$ is introduced and the DC resistivity can be defined as $\rho = K \omega_0^{-b}$. In our implementation of the time-domain forward response, we used the Drake model of equation (3) with a fixed value for the low frequency pole $\omega_0 = 10^{-5}$ Hz. In this way, the inversion is set up in terms of the model parameters $\rho$ and $\varphi$.

We computed synthetic time domain data using the Cole-Cole description of the induced polarization, and tested for different types of acquisition to what extent the CPA inversion was able
to fit the synthetic data. We chose to simulate data from homogeneous half-spaces, to be able to interpret the results of the tests easily. The computations of forward responses and inversions have been realized using the algorithm presented in Fiandaca et al. (2012). We simulated different data, changing the Cole-Cole model parameters $C$ and $\tau$, at fixed $m_0$ and $\rho$ values. In particular, we chose as synthetic models every possible combination of the following parameters: $\rho = 100 \, \Omega \cdot \text{m}$, $m_0 = 40 \, \text{mV/V}$, $C = [0.1, 0.3, 0.5]$, $\tau = [0.001, 0.01, 0.1, 1, 10] \, \text{s}$. Different acquisition ranges have been investigated, starting from a reference acquisition with 40 log-increasing gates ranging from 1 millisecond to 10 seconds. The reference acquisition range has been reduced (Figure 1): decreasing the $T_{\text{on}}=T_{\text{off}}$ values ($T_{\text{on}}$ and $T_{\text{off}}$ being the current on-time and off-time, respectively), and consequently the time of the last gate (range-type 1); increasing the delay after the current turn-off $m_{\text{dy}}$, and consequently by increasing the time of the first gate (range-type 2); increasing $m_{\text{dy}}$ and decreasing $T_{\text{on}}$ at the same time (range-type 3).

Figure 1. Definition of the three acquisition range-types. Range-type 1: the time length of the decay is increased by adding gates at the end of the acquisition time, keeping $m_{\text{dy}} = 1 \, \text{ms}$ (red lines). Range-type 2: the time length of the decay is increased by adding gates at early times and keeping $T_{\text{on}}=T_{\text{off}} = 10 \, \text{s}$ (blue lines). Range-type 3: the length of the decays is increased by adding gates both at the late and at the early times (yellow lines).

Figure 2 shows exemplary fits of Cole-Cole decays with CPA modeling when only 10 gates (one decade in time) are used in the acquisition range for all the three different range-types. The CPA inversion manages to explain the 10 gates-long curves for any $C$ values, and it is not possible to distinguish CPA and Cole-Cole modeling. Figure 3 presents the CPA fits of three different 40-gates Cole-Cole decays, for different $\tau$ values (0.01 and 1 seconds) and $C$ values (0.3 and 0.5). The shape of the Cole-Cole forward responses changes significantly when varying $\tau$ and $C$, while the shape of the CPA modeling in log-log scale remains practically unchanged, the only difference being a translation along the y axis. Practically, the shape of the CPA decays in log-log scale is univocally defined by the current waveform (in terms of current on-time $T_{\text{on}}$, current off-time $T_{\text{off}}$ and stack size). For specific combinations of $\tau$ and $C$ parameters (e.g. $\tau=1 \, \text{s}$ and $C=0.3$) the CPA and Cole-Cole decays are really similar, but in general the decays differ significantly.
Figure 4. Complete results of the synthetic tests in terms of inversion residuals ($\chi$ values, 5% error bars). The results have been sorted according to the acquisition range-type (row), the frequency exponent (column) and the time constant (line color). For each case, the inversion residuals are displayed as a function of the number of gates in the synthetic data.

Figure 5. Examples of field decays, along with their Cole-Cole and CPA fits obtained through a 2D inversion.

Figure 4 shows the inversion residuals ($\chi$ values, 5% error bars) of the CPA inversions carried out on Cole-Cole forward decays, when varying model, range-type and number of gates. All the models with $C=0.1$ present misfit below/equal to one, regardless of the number of gates. This is easily understood considering that the Cole-Cole model tends to the CPA model when $C$ goes to zero. On the other hand, with $C=0.5$ the two modeling are almost always distinguishable, except for specific models when less than two decades are used in the acquisition time range. In particular, it is more difficult to distinguish the CPA and Cole-Cole models for high $\tau$ values and range-type 1 when too few gates are used (i.e. when we miss the late times). With range-type 2 the CPA and Cole-Cole models are more difficult to distinguish with low $\tau$ values. The results with $C=0.3$ are similar to the results with $C=0.5$, except that the inversion misfits is smaller. Interestingly, with $\tau=1$ s the CPA and Cole-Cole models are more difficult to differentiate, and the CPA inversion often fits the Cole-Cole data within 5% also with 40 gates.

Finally, Figure 5 shows the comparison of CPA and Cole-Cole modeling of field data, inverted in 2D following Fiandaca et al. (2013). The field data were acquired at Grindsted, Denmark, with a Terrameter LS (ABEM Instrument). We used an on-time and an off-time of 8 s both, and 10 gates per decade (re-gating the full-waveform data and applying the de-noising scheme described by Olsson et. al (2016)). The data quality was generally good, and after processing, most of the decay curves had still ~30 gates. As for the synthetic modeling for homogeneous halfspace, the shape of the CPA forward responses does not change in log-log plots. Consequently, the CPA description cannot explain the variety of shapes present in the data. On the contrary, the Cole-Cole modeling is able to retrieve the shape of the field decays.

CONCLUSIONS

The synthetic results show that it is generally possible to distinguish CPA and Cole-Cole models in time domain, except when the Cole-Cole frequency exponent is small (below/equal to 0.1) or for specific combinations of the Cole-Cole parameters. The distinctness increases with the time range of the IP data, but usually two decades in time are sufficient to distinguish the two models. Furthermore, the shape of the CPA forward responses in log-log plots is univocally defined by the current waveform, also for 2D modeling. Consequently, the
inspection of field data in log-log plots gives insight on the modeling needed for fitting them: the CPA inversion cannot reproduce shape variability of the IP decays, as verified on field examples.

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SUMMARY

Negative transients in coincident loop airborne time domain electro-magnetic (ATEM) data have often been observed when exploring for kimberlite deposits. It is usually supposed that the negative transients arise from chargeable material such as surficial clays or ice in permafrost. As such, this EM signal is generally regarded as a “problem” in mineral exploration because it distorts the EM signals from the conductive kimberlites, and if not corrected for, results in an incorrect conductivity. However, chargeability could be reflective of the kimberlite, hence the induced polarization (IP) effects can be valuable “signal”. The ATEM surveys at the Tli Kwi Cho (TKC) kimberlite complex have been a testbed for illustrating the existence of negative transients and we focus on that region. The two pipes that constitute TKC have been extensively drilled and the resultant geologic models can be used to validate our inversion results. In addition, the complex impedance of TKC core samples have been measured in the laboratory and the results showed that the kimberlites can be chargeable and that different kimberlite units have different IP characteristics. In this paper, we first address the important issue about depth of resolution of buried chargeable bodies relevant to kimberlite exploration. After showing its potential we remove the EM effects from the IP data and invert them to recover 3D distributions of pseudo-chargeability at multiple time channels. The recovered pseudo-chargeability at different times provides meaningful information about the diamondiferous portion of the pipe and distinguishes it from other kimberlithic rocks.

Key words: airborne EM, Induced polarization, Kimberlite, and 3D inversion

INTRODUCTION

Figure 1(a) shows a typical geologic model of a kimberlite composed of three different parts: crater, diatreme, and hypabyssal facies. Physical properties of those three facies are shown in Figure 1(b). Kimberlite exploration has focused on looking for high magnetic susceptibility, low density and high conductivity (Power and Hildes, 2007). The high conductivity is often associated with lake bottom sediments as well as the pyroclastic units at depth. The conductivity of the kimberlites is usually found using airborne EM (AEM) surveys, and in particular airborne time domain EM (ATEM) systems. Often however, negative transients observed (Jansen and Witherly, 2004) indicating there is chargeable material (Weidelt, 1982). Ice and near surface clays are known to be chargeable (Smith and Klein, 1996), and these materials distort the AEM signals and impede ability to extract good information about the conductivity. As such, the existence of chargeable materials is usually considered to be a “problem” and it is referred to as IP contamination. The possibility exists however, that the chargeability is reflective of the kimberlite and it is therefore “signal” that we want to interpret.

Figure 1. (a) General structure of kimberlite pipe. (b) Physical properties of geological units in the kimberlite pipe

The Tli Kwi Cho (TKC) kimberlite complex is located approximately 360 km northeast of Yellowknife, NWT, Canada within the Archean Slave craton. The complex is part of the larger Lac de Gras kimberlite field. The TKC kimberlites are composed of two main pipes called DO-18 and DO-27, and they are respectively located at northern and southern part of the region as shown in Figure 2(a). There are four rock units of importance: XVK (Xenolithic kimberlite), VK (volcaniclastic kimberlite), HK (hypabyssal kimberlite) and PK (pyroclastic kimberlite). DO-18 pipe is mostly XVK and DO-27 is a combination of PK and HK. The PK unit is the sought diamondiferous portion of the pipe. An east-west geological section at DO-27, generated from drilling results (Harder et al., 2006) is shown in Figure 2(b). Petrophysical data including density, susceptibility, Koenigsberger, complex conductivity have been measured from core samples at both pipes. Figure 3 shows the measured complex impedance from TKC core samples corresponding to PK (green), HK (red), and XVK (purple) units.

Figure 2. Geological background of Tli Kwi Cho (TKC) Kimberlites. (a) Plan maps of TKC with kimberlite units: PK, HK, VK, and XVK. (b) East-west geological section of DO-27 pipe. The map showing PK is at a shallower depth than the map showing HK.

The impedence plots indicate that the kimberlites are chargeable, and analysis shows that the estimated time constants are different; PK has a much slower decay than HK and XVK. This raises two important questions: a) Can we invert ATEM data for chargeability? and b) Can this provide some meaningful information about the kimberlite?
A major challenge for extracting IP information from airborne data arises from the $1/r^3$ decay of signal away from the surface and the fact that the top few tens of meters often include permafrost and clay (Macnae, 2015). AIP is thus often thought of as a ‘clay mapper’. Investigation of the depth resolution on AIP is therefore crucial. We will use the geometry of TKC pipes to address this question and then carry through an analysis to extract geologic information from the AIP data. To investigate depth resolution for AIP data we generate synthetic AIP data sets with a chargeable target at different depths and apply a 3D IP inversion to them. To proceed, we briefly outline essential definitions and procedures. Detailed information can be found in Kang and Oldenburg (2016).

**Figure 3.** Complex impedance measured from core samples from PK (green), HK (red), and XVK (purple) units. Left and right panel shows real and imaginary parts of the impedance.

**COMPLEX CONDUCTIVITY**

Complex conductivity in the frequency domain can be expressed as

$$\sigma(\omega) = \sigma_\infty + \Delta\sigma(\omega)$$

(1)

where $\sigma_\infty$ is conductivity at infinite frequency, and $\omega$ is angular frequency $(rad/s)$. Different descriptive models exist but, following Smith et al. (1988), we use the Cole-Cole model from Pelton et al. (1978):

$$\Delta\sigma(\omega) = -\sigma_\infty \frac{\eta}{1 + (1-\eta)(\omega\tau)^c},$$

(2)

where $\eta$ is intrinsic chargeability, $\tau$ is time constant, and $c$ is frequency dependency.

**LINEAR FORM OF IP RESPONSE**

An ATEM observation, $d^{obs}$, includes both EM and IP effects and can be expressed as

$$d^{obs} = d^F + d^{IP},$$

(3)

where the fundamental response is $d^F \equiv F(\sigma_\infty)$, which does not include any IP effects, and $d^{IP}$ is the IP response. Here $F[-]$ indicates Maxwell’s operator which takes conductivity and computes a TEM response. The IP datum can be expressed as

$$d^{IP} = d^{obs} - d^F,$$

(4)

This procedure can be considered as EM-decoupling because we are removing EM induction effects from the observations. The IP responses can be written in a linear form:

$$d^{IP}(t) = G\tilde{\sigma}(t),$$

(5)

where $G$ is the sensitivity function and $\tilde{\sigma}(t)$ is the pseudo-chargeability. Note that this pseudo-chargeability is time-dependent, but the intrinsic chargeability is not. This linear form will be the forward function that we use to invert IP data.

**DEPTH INFORMATION IN AIP**

The depth resolution of AIP data is limited because of the geometric decay of the IP signal from a chargeable target. It is often expected that the resolution is only a few tens of meters for a compact target at the surface and about 90 m for chargeable layers (Macnae, 2015). We systematically treat this issue in the context of kimberlite exploration. We consider a circular-shaped chargeable target, which is moderately conductive and embedded in a resistive background. This could correspond to a PK unit or a crater facies (Figure 1a).

Depth resolution of the AIP data includes two important items: detection and delineation. For the first item, using an ATEM survey geometry shown in Figure 1(a), we perform forward modelling and compute $d_b/dt$ (Figure 1b) using the EMTDIP code (Marchant et al., 2014). The half-space earth $(10^4 S/m)$ includes a conductive and chargeable cylinder and Cole-Cole parameters of the chargeable unit are $\sigma_\infty=10^1 S/m$, $\eta=0.1$, $c=0.5$ and $t=10^3$ micro-s. With fixed thickness (75 m) and radius (100 m) of the cylinder, we alter the depth from the surface to 0, 75, and 150 m. Although the amplitude of the observation decreases with increasing depth, the time at which the negative value appears is almost constant (~700 micro-s) for all three depths. Assuming a noise level of $10^{-3}$ pV/A-m, the detectability level is about 150 m. The cylinders at depths of 75 or 100 meters have numerous time channels of negative values that are well above this threshold. The main difference of the responses at the three depths is just an amplitude factor so it is not likely that depth information can be obtained from a single sounding. In practice, however, we obtain ATEM data from a number of sounding locations.

**Figure 4.** (a) Geometry of an ATEM system, and a chargeable cylinder embedded in the half-space earth. (b) Observed vertical magnetic fields (dB/dt) with varying depths for the chargeable unit. Solid and dotted lines respectively indicate positive and negative data. We perform two forward modelling: $F[\sigma]$ (observation) and $F[\sigma_\infty]$ (fundamental) at 210 sounding locations. Then, using Eq. (4), we evaluate the IP data at 1300 micro-s as shown in Figure 5. As the depth increases, the IP responses get broader and smoother due to the geometric effects. Although not shown here, the spatial variation of the IP data hardly changes in time, hence, this is similar to potential field data. Similar to the inversion of magnetic data we apply a depth weighting to compensate for the $(1/r^3)$ decay. In the following we carry out 3D IP inversions with, and without, the depth weighting applied to IP data sets where the models had different depths ($z = 0$, 75, and 150 m). Forming the sensitivity function requires a 3D conductivity model, and we used the true conductivity model for each case. Figure 6 shows the recovered pseudo-chargeability models. Based upon these results, resolving depth information looks possible and the depth weighting seems to be advantageous, but not crucial.
Figure 5. True IP responses computed by subtraction using Eq. (4). Depth of the chargeable cylinder varies: a) 0m, b) 75 m, and c) 150 m depth. Dots indicate horizontal locations of soundings.

Figure 6. Sections of recovered pseudo-chargeability at different depths. (a) Without depth weighting and (b) with depth weighting. Top, middle, and bottom panel correspondingly indicate a chargeable target at 0, 75, and 150 m-depth.

FIELD EXAMPLE: TKC

TKC ATEM data

Airborne EM surveys flown over TKC include DIGHEM, AeroTEM, and VTEM systems. We focus on the VTEM data set because it illustrates the challenges we can encounter when handling AIP data. As shown in Figure 7(a), even at the earliest time (90 micro-s), VTEM data have negative values (dotted contours) over DO-18 and between DO-18 and DO-27. DO-27 shows a positive anomaly (solid contour) at this time, but data become negative at 680 micro-s as shown in Figure 7b. Easting profile lines over DO-18 and DO-27, respectively shown in Figure 7(c) and (d), show the transition.

Figure 7. TKC VTEM data. Maps of VTEM responses at (a) 90 micro-s and (b) 680 micro-s. Easting profile line data near (c) DO-18 and (d) DO-27.

3D ATEM and IP inversions

Our approach to invert AIP data is based upon Kang and Oldenburg (2016). The first step is to invert ATEM data to recover the conductivity. To exclude IP effects in the observations, we only use the first 6 time channels of the VTEM data (90-190 micro-s) near DO-27. This cannot be done for VTEM data near DO-18 since even the earliest channel is negative. Fortunately, DIGHEM data covers the entire TKC area and we assume it is not significantly affected by IP, so we cooperatively invert VTEM and DIGHEM data. The recovered 3D conductivity model is shown in Figure 8. At B-B’ section, we overlay the boundaries of different kimberlite units obtained from drilling results (Figure 2b). The two conductive pipes are imaged at depth. The pipe for DO-27 extends deeper than one for DO-18. The location of recovered conductive pipe at DO-27 matches well with the PK unit.

Figure 8. Recovered 3D conductivity model. Left panel shows plan view at 65.5 mbsf. Middle and right panels show section views at Northing 713445m and 7133595m.

Based upon the recovered conductivity, $\sigma_{est}$, we proceed with EM-decoupling:

$$d_{raw}^{IP} = d^{obs} - F[\sigma_{est}]$$

where $d_{raw}^{IP}$ is raw IP data, $F[\sigma_{est}]$ is estimated fundamental data. Figure 9 shows the observed, estimated fundamental response, and raw IP data at 130 and 410 micro-s where both EM and IP effects are substantial. Our EM-decoupling effectively removes EM induction effects due to the conductive pipe at DO-27 at both of the times evaluated here.
In this paper, we investigated the feasibility of the AIP technique for kimberlite exploration and used the TKC kimberlite region as an example. The area has been extensively drilled and four types of kimberlitic rocks have been found. Lab measurements on core samples showed TKC kimberlites are chargeable and that they have different IP parameters. This promoted two important questions: a) Can we invert ATEM data for chargeability at depth? and b) Can the results provide meaningful information about the kimberlite? Through the use of a synthetic model that emulates a TKC pipe, we analyzed the depth resolution issue and found that targets buried 75-100 meters might still be detectable and that inversion that included a depth weighting was beneficial, but might not be crucial.

We applied a 3D ATEM-IP inversion workflow to TKC VTEM data. To recover conductivity, we inverted early time channels of VTEM data (presumed to have insignificant IP-contamination) cooperatively with DIGHEM data. The details for that result will be published in a separate paper. The recovered conductivity includes two moderately conductive pipes near DO-18 and DO-27. The conductivity was used to estimate the fundamental EM response which was subtracted from the data to generate raw IP data at multiple time channels. 3D IP inversions were carried out and the pseudo-chargeabilities at multiple times were obtained. Four chargeable anomalies are imaged at depths (~70 m); A1-A4 possibly correspond to four different kimberlites: XVK, VK, HK and PK. These correspondences can be inferred by comparing the recovered chargeability with geologic logging in boreholes. The recovered pseudo-chargeability at different times suggests a distinction between the PK unit and the other three kimberlite units. Moreover, the outline of the inferred PK unit matches well with the boundaries of the PK unit obtained from drilling, but some of this is likely attributed to the conductivity model and the fact that IP sensitivities are enhanced in regions of higher conductivity. From a geologic perspective, the two main results might be the differentiation of rocks associated with the two pipes. The XVK unit comprising DO-18 is substantially different from the dominant PK unit at DO-27. On a smaller scale, we appear to be able to differentiate between the PK and HK units at DO-27. This is potentially important since PK is strongly diamondiferous and HK has minimal diamond showings. This discrimination might be further enhanced through the use of ground IP using either galvanic or inductive sources. Overall, our study of AIP shows the potential benefits in kimberlite exploration, and hence motivates further research and application in other geoscience problems.

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INTRODUCTION

In order to estimate hydraulic parameters of sediments from frequency-dependent electrical properties, theoretical models to simulate the electrical impedance depending on the geometrical properties of the material at the pore scale may be useful. Existing models are either based on the sedimentary grains (e.g. Leroy et al., 2008) or on the properties of the pore space (e.g. Titov et al., 2002). Here, we focus on geometrical parameters of the model, e.g. radii \( r \) and lengths \( L \) of two cylindrical pores.

In principle, a wide range of spectra can be generated, covering orders of magnitude in both maximum phase shift and characteristic time scales. One ingredient to obtain large phase shift is a small radius of the narrow pore in the range of tens of nm. Time scales are mainly controlled by pore lengths. Generating large time scales and phase shifts at the same time in principle requires large ratios between pore lengths and radii. However, within the four-dimensional parameter space, which exhibits regimes of different behaviour, examples can be found where moderate \( L/r \) ratios (10:1) can produce time scales in the range of seconds with phase shifts of a few mrad. The results encourage further attempts to combine impedances of 2-pore systems to approach the simulation of real rock systems.

Key words: membrane polarization, characteristic time, phase shift, pore space.

THE MODEL

The model suggested by Bücker and Hördt (2013a) consists of an infinite sequence of wide and narrow pores, the geometry of which is described by the pore length and pore radii (figure 1).

So far, the model is limited to a relatively simple sequence of two types of wide and narrow cylindrical pores. In order to simulate more realistic pore geometries, one possibility is to connect several such 2-type systems to a complex network (Stebner et al., 2016). However, since the model has many parameters and allows a huge number of parameter combinations, it is also essential to understand the model behaviour. Therefore, we review the properties of the model with a particular emphasis on the geometrical parameters, i.e. two pore lengths and pore radii. We investigate which range of parameters is necessary to obtain spectra that are typically obtained with laboratory data, and discuss whether these geometries are realistic to occur in real rocks.
Figure 2 illustrates that a wide range of spectra may be obtained by just varying geometrical parameters. Relatively large phase shifts of several tens of mrad with the maximum at low frequencies (in this case 0.01 Hz, curve 1), corresponding to long relaxation times, intermediate phase shifts and intermediate relaxation times (curve 3), and large phase shifts combined with small relaxation times (curve 2). These curves are just a few examples, a much wider range can actually be obtained by further variations. The phase spectra in these images are relatively sharp, i.e. there is a well-defined maximum. This is a typical feature of the model, but broader spectra may of course be obtained by combining several impedances in a network.

**MODEL STUDIES**

**Pore radii**

First, we investigate for which pore radii we obtain realistic phase shifts, typically in the range between at least 1 mrad up to several tens of mrad. Figure 3 shows the maximum phase shift, colour coded on a logarithmic scale vs. the radii of the two pores. There is a finite size zone where phase shifts are above 1 mrad. The radius of the small pore ($r_2$) is in the tens of nm range. It is constrained by the diffusive layer thickness, defined by the Debye length (e.g. Bücker and Hördt, 2013a). If the pore is large compared to the Debye length, the relative transport of anions and cations is approximately equal, and no membrane effect exists. The radius of the second pore is roughly 10 times larger. The optimum ratio between pore radii is related to the length ratio (in this case 100:1) by a square root relationship, consistent with findings of Bücker and Hördt (2013a).

The Debye length depends on several parameters, and the partition factor might also become important, such that general rules are difficult to derive. However, small pore radii in the range below 0.1 $\mu$m can be considered typical to generate measurable phase shifts.

Figure 3: Maximum phase shift extracted from the frequency-dependent spectra, colour coded vs. the radii of the two pores. The pore lengths are $L_1=5 \mu$m, $L_2=0.05 \mu$m, all other parameters as given in table 1.

Whether or not submicron pores are relevant in real rock is not trivial to decide from independent measurements. CT images hardly have a resolution below 1 $\mu$m. Mercury injection measurements provide data down to a few nm. Weller et al. (2011) show examples of different sandstones where pore radii below 100 nm constitute more than 20% of the pore volume. Recently, Weller et al. (2015) found that they obtained better correlation between imaginary conductivity and specific internal surface area ($S_{int}$) if they use a wet-state methylene blue (MB) method instead of the conventional BET to determine $S_{int}$. The reason is that the MB method is also sensitive to the small pores in Clay minerals and thus provides higher $S_{int}$ values. We take this as further evidence that pores in the range 0.1 $\mu$m and smaller, are indeed relevant in real rock.

In principle, almost any type of reasonable spectrum might possibly be simulated theoretically. In the following, we explore the parameter space to assess which geometrical parameters required to fit data are realistic and might represent real rock conditions.

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<td>Length of pore 2</td>
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</table>
Pore lengths

The pore lengths have a strong influence on the characteristic times, calculated here from the frequency \( f_{\text{max}} \) at which the maximum phase shift occurs:

\[
\tau_{\text{max}} = \frac{1}{2\pi f_{\text{max}}}
\]

The relationship is illustrated in figure 4. In general the characteristic time increases with the pore length. Two regimes can clearly be separated where \( \tau_{\text{max}} \) is either controlled by the length of the narrow or the wide pore. The regimes were defined more generally by Bücker and Hördt (2013b) and named “long narrow pore (LNP)” (top left in fig. 4) and “short narrow pore (SNP)” (bottom right) regime depending on the geometrical parameters.

Figure 4: Characteristic time, colour coded vs. the length of the two pores. The radius of the large pore \( r_1 \) was fixed to 500 nm, the radius of the small pore \( r_2 \) was fixed to 50 nm.

Figure 4 shows that by varying pore lengths, it is possible to obtain characteristic times that are usually obtained with real rocks, in the range between 0.001 s and 100s (e.g. Kruschwitz et al., 2010). However, to cover the upper end in the range around 10s, relatively long pores up to a mm seem to be necessary.

Length-to-radius ratios

We now have established that small pores are required to generate a sufficient phase shift, whereas long pores generally cause large characteristic times. This implies that in order to fulfil both criteria, large ratios between pore length and pore radius will be required. In figure 5, we investigate this relationship in detail for one particular example. Note that the figure was generated by fixing \( L_1 \) and \( r_2 \), and varying \( L_2 \) and \( r_1 \), which is one possibility to cut a plane out of the 4D parameter space, but not the only way, of course.

The figure shows that it is possible to obtain both large characteristic times and large phase shifts with moderate \( L/r \) ratios in the range of 10:1 (bottom left corner of the figure). This may be a particular situation, but at least the figure illustrates that large \( L/r \) ratios are not mandatory.

Figure 5: Top panel: Maximum phase shift, colour coded vs. the length-to-radius ratio of the two pores. The radius of the small pore \( r_2 \) was fixed to 50 nm, and the length of the large pore \( L_1 \) was fixed to 500 μm; \( r_1 \) and \( L_2 \) were varied to obtain the corresponding ratios. Bottom panel: same as top panel, for characteristic times.

CONCLUSIONS

We have carried out a model study to illustrate which geometrical parameters are required to obtain phase shifts and relaxation times in the range typically measured with natural sandstones. We focus on geometrical parameters and fix those describing the electrical double layer, but even then the parameter space is 4-dimensional and not trivial to explore. As general guidelines, a small (tens of nm) minimum pore radius in the range of the Debye length is required to obtain significant phase shifts. There is evidence, however, that these exist and are relevant in real rock. Relatively long pores are required if large characteristic times in the range of seconds need to be explained. Although these two conditions appear to
require large L/r ratios, parameter combinations exist where moderate ratios around 10:1 are sufficient.

Our results also show that speculations, membrane polarization might be particularly important at long characteristic time scales, which can sometimes be found in literature (e.g. Leroy and Revil, 2009) are not consistent with the conceptual model underlying the theory used here, as it covers a wide range of relaxation times. When attempting to match geometrical parameters typically found in real rock, it seems challenging to produce long time scales rather than short ones.

The considerations here are intended to provide a general understanding of membrane polarization. Another aim is to provide guidelines for combining impedances in networks, to get one step further towards the description of real rock geometries (Stebner et al. 2016).

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