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Improvements of Soil Dielectric Mixing Model for Inversion Analysis of Time Domain Reflectometry Measurements

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Abstract

A mixing model for soil dielectric spectra is needed for inversion analysis of Time Domain Reflectometry measurements to obtain soil electrical and physical properties. Soils are multi-phased systems whose overall dielectric spectra are commonly described by a dielectric mixing formula. Three-phased mixing models, and more recently four-phased power law mixing models (including soil solids, air, bound water, and free water), have been utilized to study soil dielectric properties from TDR measurements. These models refer to models originally developed in optics and incorporate a factor related to particle orientation.

The mixing models used in current research have certain ambiguities or shortcomings for describing soil dielectric spectra. These include: 1) the result of mixing causes a shift of the effective relaxation frequencies in the overall dielectric spectra compared with those of the individual components; 2) the electrical conductivities (both free water and bound water) have an influence on both the real and imaginary parts of the overall dielectric spectra; and 3) the relaxation frequency of bound water was assumed to be smaller than the lower end of TDR measurement frequency range, which makes its real part essentially constant over the TDR frequency range. Most models do not distinguish between soils with low water content where most of the water is in the form of bound water.

This paper describes some approaches to improving the current dielectric mixing models for soils. The model considered here introduces the concept of bulk electrical conductivity and separates the electrical conductivity term from the mixing process. This model also keeps the relaxation frequencies of bound water and free water as the characteristic relaxation frequencies in the overall dielectric spectra. The relaxation frequency of bound water is set to be a fitting parameter to reflect the extent of restraints by the soil particles. The new mixing formula is theoretically validated and the predicted spectra are found to be consistent with those from independent measurements over a large frequency range.

Keywords: Dielectric mixing model, Time Domain Reflectometry, Inversion Analyses

Introduction

Time Domain Reflectometry (TDR) is increasingly used for a variety of applications to measure material properties. In addition to the commonly utilized information of the apparent dielectric constant and electrical conductivity that can be obtained from directly analyzing the time domain TDR signals, information on the material dielectric spectrum can also be determined. Compared with instruments that make measurement in the frequency domain, such as network analyzer or spectrum analyzer, Time Domain Dielectric Spectroscopy based on TDR technology has advantages in terms of lower cost and faster testing speed. The dielectric spectrum of a material can be determined by the joint time and frequency domain analyses of TDR signal. The process generally requires incorporating the model for the electromagnetic wave propagation in the TDR system. Directly solving the dielectric permittivity of a material at individual frequencies is possible. However, this approach becomes unstable at high frequencies (above 200 MHz for commonly used TDR system, Heimovaara 1994[1]). Causes are attributed to the non-ideal measurement probe configuration and the deviation of the electromagnetic wave propagation mode in the actual TDR system from the TEM mode assumptions (Lin 2003a[2]). A more practical approach incorporates a model for the material dielectric spectrum. The model parameters are then determined by matching the predicted signal by the model and the actual measured signal. The dielectric spectra can be determined from the model with the optimized parameters. Results by this model-based approach have been found to be reasonably stable.

An important issue of using the model-based approach for soil dielectric properties is the soundness of the soil dielectric model. A properly designed model can also be used to obtain soil physical properties. A few models have been utilized in the previous studies. These include the commonly used models such as the Debye's model (Debye 1929[5]), the Cole-Cole model (Cole and Cole 1941[6]) and more recently the volumetric mixing models. These models were found to obtain similar material spectra in the TDR frequency range (Yu et al. 2005[3]). However, Debye's model or Cole-Cole model does not bear direct relationship to the physical properties of soils. The use of dielectric mixing models for soil is advantageous as their parameters are directly related to the soil physical parameters. Incorporation of an appropriate mixing model for soils will enable the determination of soil properties with engineering significance such as the water content, density, electrical conductivity and the important information related to the specific soil type, such as the specific surface, plasticity index, etc. A sound dielectric mixing model is needed for this purpose.

Soils are mixtures consisting of soil solids, air and water. The overall dielectric spectra of soils are typically described by three-phased dielectric mixing model. More recently four-phased mixing model are introduced to account for the distinctive behaviors of the bound water. The complexity of soil behavior largely comes from the interactions between the soil solids and the bound water. This paper discusses some issues with the existing mixing formula and incorporates several ideas for an improved dielectric mixing model for soils.

Volumetric Mixing Models for Soils

The electric responses of soils to an external electromagnetic field excitation are decided by their dielectric properties, which are subsequently dependent upon the properties of the constituent

phases and the extent of their mutual interactions. Physical properties such as the relative portions of soil components, soil types, particle topography, and pore water characteristics are the most important factors determining overall the soil dielectric responses. The soil dielectric properties and dependency of dielectric properties on the soil physical properties have been utilized for geologic and geotechnical investigations by technologies such as Satellite or Airborne Remote Sensing, Ground Penetration Radar (GPR), and Time Domain Reflectometry (TDR). Information of soil dielectric spectra is important for these applications.

Due to the heterogeneity and non-uniform characteristics of soils, as well as the complex microscopic electrochemical phenomena, the complete description of true soil dielectric properties is practically impossible. In most instruments, the dielectric properties of soils are assumed to be homogeneous and isotropic, which is valid when the relative ratio of soil particle sizes and electromagnetic wave wavelength satisfies a certain scaling rule.

The dielectric behaviors of a mixing are described by dielectric mixing formula. Most mixing formulae are developed from analyses of the bulk dielectric behaviors to those of individual phases. Although various models have been used to describe the mixtures, no complete model is available that can describe the dielectric properties of soil (Hilhorst et al. 2000[4]). Most of the models used for research on soils refer to the research results of liquids, solid materials or simple mixtures. This includes many famous formulations such as Debye's model (Debye 1929[5]), Cole-Cole's model (Cole and Cole 1941[6]), Maxwell Garnett formula (1904)[7], Schwarz formula (1962)[8], etc. All these models are applicable to explain phenomena due to certain relaxation mechanisms or within a certain frequency range. In addition to these models, the semi-empirical power-law volumetric mixing model also is frequently used for soils (Birchak et al. 1974 [9]). Friedman (1997)[10] introduced a mixing model based on statistical concepts. The effects of particle size on the bulk dielectric constant of soil mixture have also been investigated (Jones and Friedman 2000)[11]. Robinson et al. (2003)[12] provided a very comprehensive review that covers the mixing model development for soils.

Soils have been physically described as a three-phased system made of soil solids, water and air. More recently, it has been increasingly realized that the portion of water close to the soil particle surfaces behaves differently from bulk free water. To describe the influence of bound water on the soil dielectric spectrum, Heimovaara et al. (1994)[1] proposed a four-phased (soil solids, air, bound water, free water) power law dielectric mixing model.

$$\varepsilon_m^{*\alpha} = \frac{\rho_d}{\rho_s}\varepsilon_s^{*\alpha} + \left(\theta - \delta\rho_d A_s\right)\varepsilon_{fw}^{*\alpha} + \delta\rho_d A_s \varepsilon_{bw}^{*\alpha} + \left(1 - \frac{\rho_d}{\rho_s} - \theta\right)\varepsilon_a^{*\alpha} \qquad (1)$$

where ε_i^* is the dielectric permittivity, subscripts *m, fw, bw,* and *a* stand for measured, free water, bound water and air respectively; ρ_d is the dry density of soil, ρ_w is the density of water, θ is the volumetric water content; A_s is the specific surface, δ is the thickness of layer of bound water, α is the orientation index that describe the orientation of the particles related to the electromagnetic field, typically α is assumed to be 0.5.

The dielectric permittivity of free water is described by Debye's model, Eq. (2).

$$\varepsilon_{fw}^{*} = \varepsilon_{s,fw} + \frac{\varepsilon_{\infty,fw} - \varepsilon_{s,fw}}{1 + i\left(\frac{f}{f_{rel,fw}}\right)} - i\frac{\sigma_{fw}}{2\pi f \varepsilon_0} \tag{2}$$

where $\varepsilon_{s,fw}$ is the static dielectric constant of free water, which is around 81. The term $\varepsilon_{\infty,fw}$ is the dielectric constant at infinite frequency, which is assumed to be around 4, the relaxation frequency of free water $f_{rel,fw}$ is assumed to be around 17 GHz (Haste 1974[13]), σ_{fw} is the electrical conductivity of free water.

The dispersion of the bound water is mostly attributed to electrical conductivity. There is no contribution to the dispersion term by the dielectric relaxation, i.e., the model for bound water is as shown in Eq. (3),

$$\varepsilon_{bw}^{*} = \varepsilon_{s,bw} - i\frac{\sigma_{bw}}{2\pi f \varepsilon_0} \tag{3}$$

This mixing formula refers to those used in optics, where materials generally do not show significant dispersion behavior. This four-phased model is also adopted in a subsequent study by Lin (2003a[2], 2003b[11]). The bound water term is assumed to follow Debye's model as well, Eq. (4).

$$\varepsilon_{bw}^{*} = \varepsilon_{s,bw} + \frac{\varepsilon_{\infty,bw} - \varepsilon_{s,bw}}{1 + i\left(\frac{f}{f_{rel,bw}}\right)} - i\frac{\sigma_{bw}}{2\pi f \varepsilon_0} \tag{4}$$

where $f_{rel,bw}$ is the relaxation frequency of bound water and is assumed to be 9 kHz.

Figure 1 shows a comparison of the dielectric spectrum predicted for free water and that by Eq. (4). The parameters for free water use those from the literature and those for bound water assumes the relaxation frequency is 9 kHz. The electrical conductivity terms are assumed to be zero in order to facilitate observing the dielectric relaxation phenomena. From the figure it can be seen that by assuming a relaxation frequency of 9 kHz, the dielectric spectrum of bound water is essentially a constant in the TDR frequency range (Eq. (5)). This is because the relaxation frequency of 9 kHz assumed for the bound water is much lower than the frequency range measured by TDR device, which typically covers from megaHertz to gigaHertz range. Thus the model by Lin (2003a[2], 2003b[14]) are equivalent to that used by Heimovaara (1994)[1]

$$\varepsilon_{bw}^{*} \approx \varepsilon_{\infty,bw} - i\frac{\sigma_{bw}}{2\pi f \varepsilon_0} \tag{5}$$

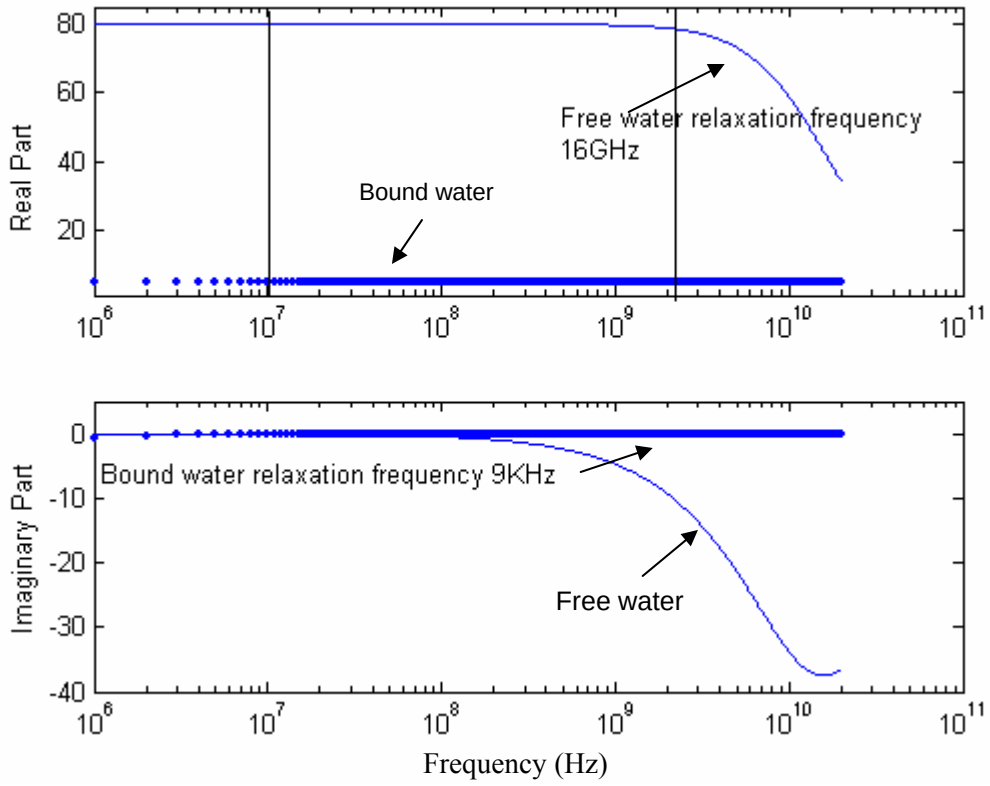


Figure 1. Dielectric spectrum of deionized water and bound water (a relaxation frequency of 9 kHz is assumed for bound water)

Considerations in Developing an Improved Dielectric Mixing Formula

While the existing four-phased dielectric mixing model considers the differences between the dielectric spectra of bound water from that of the free water, there are several characteristics of this model that brings undesirable effects for describing the dielectric spectrum of soils. As mentioned earlier and shown in Fig. 1, the parameter assumptions in these dielectric mixing models treat the bound water as non-dispersive or non-dispersive in the TDR frequency range. The actual behavior of bound water, however, can be much more complex. From microscopic aspects, the bound water is electrically attracted to the negatively charged surface of clay minerals. This influence can extend up to about 4 layers of water molecules (Sun and Young 2001[15]). The intensity of the electrical attraction is dependent upon the charge density on the clay surface as well as the distance of the water molecules to the surface of the solid particles. These determine the properties of bound water layers, i.e, their relaxation frequencies and their apparent dielectric constants. Because of the variations of the intensity of the electrical attractions, the properties of bound water layers change with the increasing distance to the mineral layers. The bound water layer closest to the clay surface behaves similar to ice with low dielectric relaxation frequency (in low kHz range). The outer layer, however, has increasingly higher dielectric relaxation frequencies due to lower restraints by the clay particles. Friel and Or (1999)[16], for example, has observed that bound water in soils has relaxation frequency in the

low megaHertz range. The bulk behavior of bound water thus varies with the soil type and the water content. Figure 2 is a schematic plot of the variation of apparent dielectric constant of bound water with the distance from the surface of a clay mineral. The bound water properties vary until about 4 molecular layers where the water molecules start to behave like bulk free water. Bound water is a polar molecule and thus always shows dielectric relaxation phenomena. The polar water molecules interact with (are bound to) also electrically negative surfaces. The variation of the measured dielectric constant is ultimately due to the variation of the relaxation frequencies (Lin 2003[2]).

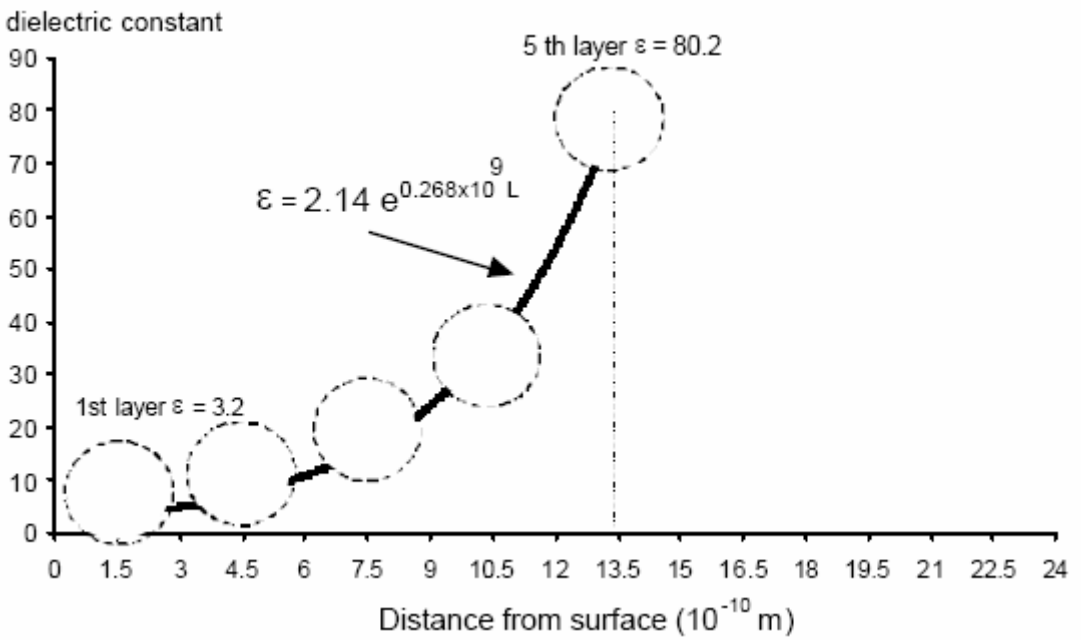


Figure 2. The dielectric constant increases exponentially with the distance from the surface of soil particles (after Sun and Young 2001[15])

The discussion above indicates that the relaxation frequency of bound water is influenced by a variety of factors. Treating the dielectric constant of bound water as a constant ignores the variation in the interactions between soil and water. It is anticipated that the relaxation frequency could provide important information on bound water behavior that is related to soil properties. In the new model the relaxation frequency of bound water is defined as a variable to properly account for the differences in the soil water interactions among different soils. This can be subsequently used to study different soil behaviors.

The existing dielectric mixing formula also introduces a few undesirable effects on the overall dielectric spectrum of the soil mixture, i.e., 1) there is a shift of the relaxation frequency in the overall dielectric spectrum compared with those of the individual phases; and 2) the electrical conductivity (of both free water and bound water) have cross influence on the real part of the dielectric spectrum. Figure 3 shows an example to illustrate the shift of the relaxation frequency during the mixing process. The volumetric mixing model (Eq. (1)) is used to simulate a mixture consist of a dispersive phase described by Debye's model with a relaxation frequency of 1.6 GHz together mixed with non-dispersive phases. The electrical conductivities of all phases are assumed to be zero. Both the bulk dielectric spectrum and the dielectric spectrum of the

dispersive phase are plotted in Figure 3. This figure shows that Eq. (1) predicts that the bulk mixture also shows dielectric relaxation. The predicted relaxation frequency of the bulk mixture, however, is smaller than that of the individual phase. This implies that if spectrum measurement is taken on the mixture, a dielectric relaxation will be observed at a frequency lower than 1.6 GHz. This is perplexing since there is no mutual influence of the mixture phases, the dielectric relaxation should be observed at the same frequency by the dispersive phase.

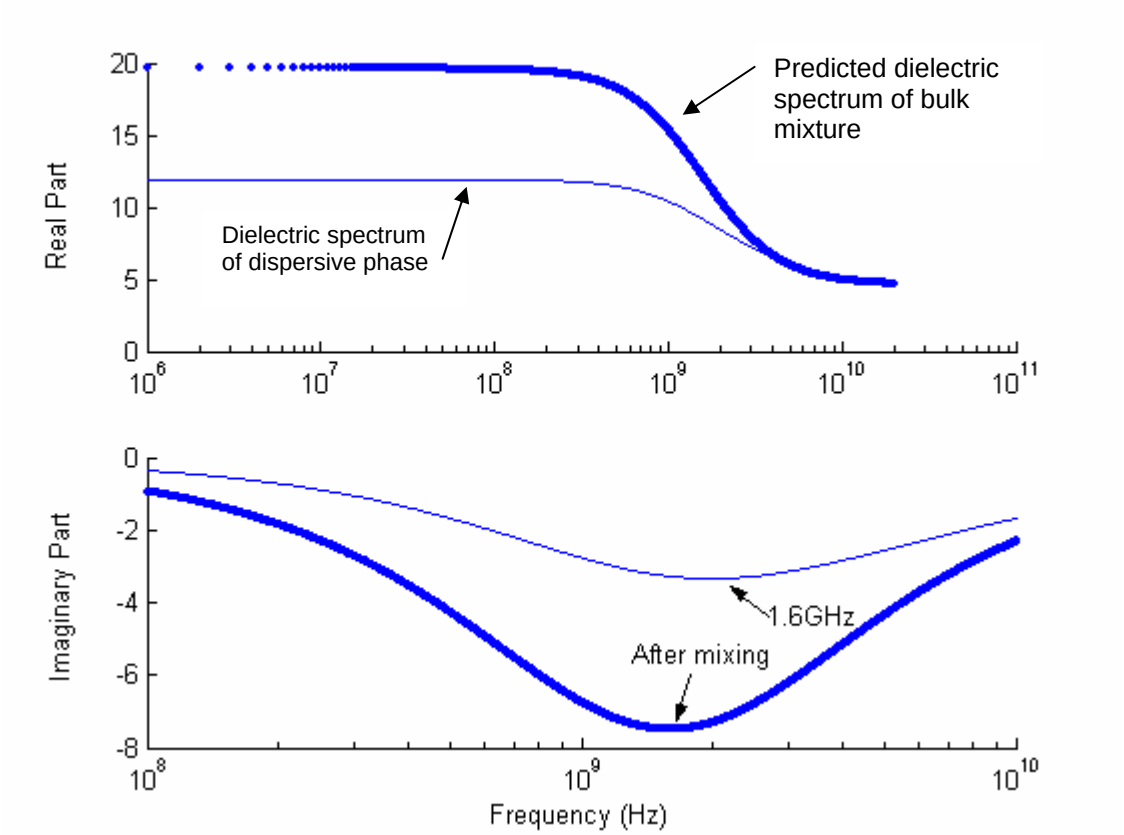


Figure 3. Dielectric spectrum of the dispersive phase and the predicted bulk dielectric spectrum of the mixture.

Figure 4 is generated to illustrate the cross effects of the electrical conductivity in the existing mixing formula. To isolate the effects of dielectric relaxation, it is assumed that all the constituent phases are non dispersive. If all the phases are non-conductive, both the real and imaginary part of the bulk soil dielectric spectrum predicted by the model will be a flat line. However, by assuming a finite electrical conductivity for one of the mixture phase, the resultant dielectric spectrum behaves significantly different. As shown in figure 3, both the predicted real and imaginary part of the bulk soil dielectric spectrum increases with decreasing frequency. This can be misinterpreted as Maxwell-Wagner effects. Since the Maxwell-Wagner effects are physical phenomena stemming from conductivity/permittivity contrast at the interfaces, it is irrelevant to the dielectric mixing process. From the physics concepts, the dielectric mixing formula, which accounts for the interactions between the soil phases, should not implicitly imply the existence of another type of dielectric phenomena.

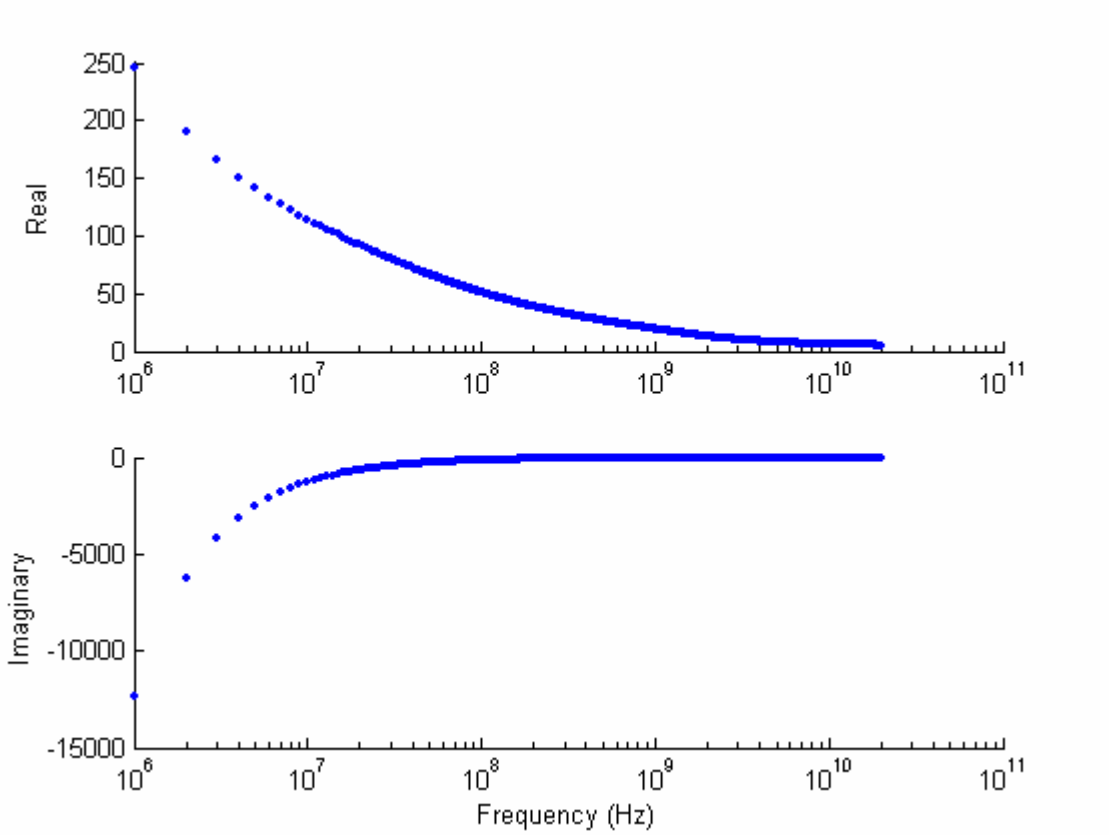


Figure 4. Predicted dielectric spectrum by the existing mixing formula for non-dispersive mixture with electrical conductivity

In addition to those discussed, the existing dielectric mixing formula does not distinguish the different number of phases at low water content versus high water content for a cohesive soil. Most water in cohesive soils is in the form of bound water at low water content. At this stage, the soil system can be regarded as three phases made of soil solids, bound water and air. As water is gradually added, the portion of water farther away from the surface of soil solids start to show behaves like bulk water. This however is not accounted for in the existing formula. Thus it can be physically wrong when the water content is relatively low. To correctly embrace the different situations, it is necessary to differentiate the cases with three phases and four phases.

The shortcomings of the existing dielectric mixing formula were considered in developing an improved mixing model. These include: 1) treat the relaxation frequency of bound water as a variable. (This accounts for the differences between soil-water interactions); 2) separate the electrical conductivity term from the dielectric mixing process. (The effects of electrical conductivity are represented with a bulk electrical conductivity term. This avoids the crossing effects of the electrical conductivity of constituent phases on the bulk dielectric spectrum); and 3) account for the different number of dielectric phases for cohesive soils under low or high water content. (A critical water content θ_{cr} is introduced to differentiate the cases with three or four constituent phases.)

The formula of this new dielectric mixing model is shown in the equation below:

$$\varepsilon_m^{*n} = \begin{cases} \dfrac{\rho_d}{\rho_s}\varepsilon_s^{*n} + \theta\varepsilon_{bw}^{*n} + \left(1 - \dfrac{\rho_d}{\rho_s} - \theta\right)\varepsilon_a^{*n} + i\dfrac{\sigma}{2\pi f\varepsilon_0} & \text{for } \theta < \theta_{cr} \\ \dfrac{\rho_d}{\rho_s}\varepsilon_s^{*n} + (\theta - \theta_{cr})\varepsilon_{fw}^{*n} + \theta_{cr}\varepsilon_{bw}^{*n} + \left(1 - \dfrac{\rho_d}{\rho_s} - \theta\right)\varepsilon_a^{*n} + i\dfrac{\sigma}{2\pi f\varepsilon_0} & \text{for } \theta \geq \theta_{cr} \end{cases} \quad \text{for clay} \quad (6a)$$

$$\varepsilon_m^{*n} = \frac{\rho_d}{\rho_s}\varepsilon_s^{*n} + \theta\varepsilon_{fw}^{*n} + \left(1 - \frac{\rho_d}{\rho_s} - \theta\right)\varepsilon_a^{*n} + i\frac{\sigma}{2\pi f\varepsilon_0} \quad \text{for sand} \quad (6b)$$

where the terms bear similar meaning as in Eq. (1) with the exception that the dielectric permittivity of individual phases, $\varepsilon_s^*, \varepsilon_{fw}^*, \varepsilon_{bw}^*, \varepsilon_a^*$, does not include the electrical conductivity component, θ_{cr} is the critical water content below which all the water in the clay is in the form of bound water, σ is the bulk electrical conductivity.

The threshold water content in the mixing formula (Eq. (6)) is calculated by

$$\theta_{cr} = \delta\rho_d A_s \quad (7)$$

where δ is the thickness of bound water layer.

From Figure 2, the thickness of bound water layer varies and is based on a variety of factors. An average distance of 2 molecule layers can be assumed for theoretical analyses, which corresponds to 6×10^{-10} nm in terms of the distance from the center of the molecule to the surface of the solids. This assumed thickness of bound water layers is larger than those used by previous studies. The assumed values of 3×10^{-10}m by Lin (2003)[2] and 1.5×10^{-10}m by Heimovaara (1994)[1] corresponding to water layers that are more closely bound to the surface of solids and exert lower relaxation frequencies. For typical clay minerals, the range of specific surface area is 400-800 m^2/g for montmorillonite, 80-100 m^2/g for illite and 10-20 m^2/g for kaolinite (Mitchell 1993)[17]. Assume a bulk density of around 1500 kg/m^3, this corresponding to a bound water content of 27%-54%, 5.4%-6.75%, and 1.35%-0.675% for montmorillonite, illite, and kaolinite, respectively. The thickness of bound water layer can also be estimated from a calibration test.

The dielectric spectra of both free water and bound water are assumed to follow Debye's model. This is similar to that presented in Eq. (4) with the exception that the relaxation frequency of bound water is no longer a constant. The parameters for free water can be easily obtained from literature. The parameters for bound water deserve more deliberation. As discussed in the earlier part of this paper, the dielectric properties of bound water varies slightly depending on its distance from the surface of the solid particles. Low (1976) [18] has shown that for water bound to the surface of solid particles, the relaxation time is related to the size and viscosity of water molecules as well as the distance of the water molecule from the surface of the solid particle, Eq. (8).

$$\tau(x,T) = \frac{4\pi r^3\eta_0(T)\exp\left(\dfrac{a}{xT}\right)}{kT} \quad (8)$$

where $\tau(x,T)$ is the relaxation time, which is related to the relaxation frequency by $f_{rel}=1/\tau(x,T)$, x is the distance of the bound water molecule to the surface of solid particles, T is the temperature, r is the diameter of the molecule, a is a coefficient used by Low (1976) [18] and Wraith et al. (2001)[19] to represent the strength of interactions between molecules and the surfaces of solid particles, k is the Boltzmann constant, $\eta_0(T)$ is the viscosity at temperature T.

Taking logarithm of equation (8) and substitute the concept of relaxation frequency, the follow equation can be obtained:

$$\log f_{rel} = A - \frac{B}{x} \tag{9}$$

where A and B are two constants reflecting the effects of the terms in equation (8). A is related to factors such as radius of molecules, viscosity and temperature, B is related to the temperature and the intensity of interactions between the water molecule and the surface of the solid particles.

Equation 9 indicates the bound water, strictly speaking, needs to be represented by layers with different relaxation frequencies. Accurately accounting for this will make the bulk model extremely complex. The use of the dielectric model in Equation (4) significantly simplifies the representation of the dielectric properties of bound water. This representation treats the properties of bound water as a single phased material with a given relaxation frequency. The parameters, including the relaxation frequency, thus need to be viewed as equivalent parameters. Equation (9) can be analyzed by integration to determine an equivalent relaxation frequency and the corresponding equivalent distance based on the average value of enclosed area by the curve it specified. The results of manipulation are shown in equation (10) and the steps of analyses are not elaborated here:

$$\begin{aligned} x_{eq} &= \frac{A}{2B} \\ f_{rel,eq} &= \frac{A^2 - 2B^2}{A} \end{aligned} \tag{10}$$

Equation (10) indicates the equivalent relaxation frequency is influenced by properties of water molecules (size and viscosity) and temperature. It is also dependent upon the interactions between water molecules and surface of solid particles. The latter dependency indicates that the equivalent relaxation frequency of bound water is related to the soil types. This prediction is consistent with experimental observations.

Soundness of the Mixing Formula

A major difference of this new dielectric mixing formula from the existing formula is that the effects of electrical conductivity are treated separately from those of dielectric relaxation. The soundness of this manipulation needs to be justified. All valid formulae for material dielectric spectrum need to satisfy the Kramer-Kronig relations. Kramer-Kronig relations establish causality. The term causality means that the response to an excitation should not come before

the excitation is applied. For dielectric permittivity of a material represented as $\varepsilon = \varepsilon^{'} - j\varepsilon^{"}$, the Kramer-Kronig relationship implies the real and imaginary part of the dielectric permittivity must satisfy the following relationships:

$$\varepsilon^{'}(\omega)) = \varepsilon_{\infty} + \frac{2}{\pi}\int_0^{\infty} \varepsilon^{"}(\omega)\frac{\omega^{'}}{\omega^{'2} - \omega^2}d\omega^{'}$$
$$\varepsilon^{"}(\omega) = \frac{2}{\pi}\int_0^{\infty} \varepsilon(\omega)\frac{\omega^{'}}{\omega^{'2} - \omega^2}d\omega^{'} \qquad (11)$$

It can be shown that if dielectric permittivity $\varepsilon = \varepsilon^{'} - j\varepsilon^{"}$ satisfy the Kramer-Kronig relationship, with an added term of electrical conductivity to the dielectric permittivity, i.e., $\varepsilon = \varepsilon^{'} - j\varepsilon^{"} - j\frac{\sigma}{\varepsilon_0\omega}$, the Kramer-Kronig relationship still holds. This can be verified by substituting the expanded expression into Eq. (11). It can be shown that the term related to the electrical conductivity becomes zero after integration. Thus inclusion of a separate electrical conductivity term will not influence its compliance to the Kramer-Kronig relation. On the other hand, since the dipolar relaxation and dc conductivity are two independent processes, it might also be justified to include separate treatment for these effects. That is, to use the dielectric mixing formula to represent the dielectric dispersion and to use the bulk electrical conductivity to represent the effects of the electrical conductivities of constituent components.

Dielectric Spectrum by the New Mixing Formula

Figure 5 shows an example of dielectric spectrum predicted by the new dielectric mixing model. Plots are generated to simulate the dielectric spectra of clay with levels of water content. The plots shows that at low water content (below the threshold water content level), all the soil water is in the form of bound water. Only one dielectric relaxation can be observed in the dielectric spectrum. With increasing water content, two relaxation mechanisms can be observed that corresponds to the relaxation of bound water and free water, respectively. Hoekestra and Delaney (1974) [20] showed that the dielectric spectrum of wet soils is best described by a sum of two different Cole-Cole parameter sets having closely spaced relaxations (one for bound water and one for bulk water). The high end of spectrum, which is indicative of bulk water, is not sensitive to soil's microstructure and soil-water interactions. The low end of spectrum, which includes the responses of bound water, is indicative of solid-liquid interactions.

Since the electrical conductivity term is not included in the mixing process, the influence of the electrical conductivity can be separated in the imaginary part of the dielectric permittivity. This electrical conductivity corresponds to the bulk electrical conductivity of soils that can be easily determined from a measured TDR signal (Yu and Drnevich 2004[21]).

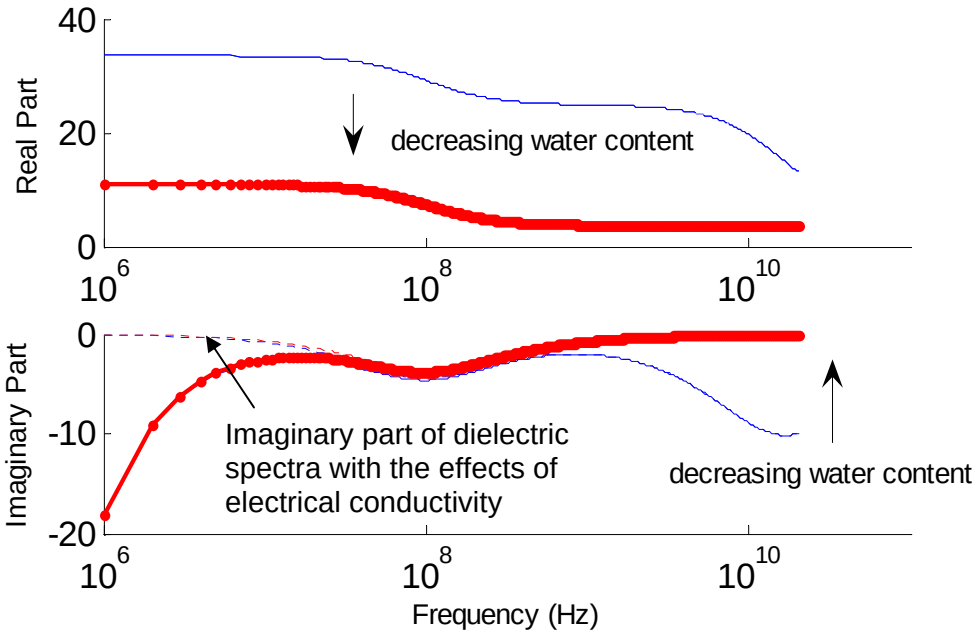


Figure 5. Example dielectric spectrum by the new mixing model for soils (blue lines are dielectric spectrum when the water content is above threshold level, red lines are dielectric spectrum when the water content is below the threshold level, dashed lines are the imaginary part of dielectric spectrum with the contribution of electrical conductivity term removed)

Steps in Applying the New Dielectric Mixing Formula for Inversion Analysis

A few issues need to be resolved before proceeding to apply this new dielectric mixing formula to the inversion analysis of TDR system. Firstly, the dielectric mixing formula needs to be used together with a model for a general model for the TDR system. A few models have been developed and refined including those by Heimovaara et al. (1994)[1] and Jones and Or (2004)[19] for a matched TDR probe, Yanuka et al. (1988)[23] for an unmatched TDR system with no dielectric dispersion, Feng et al. (1999)[24] and Lin (2003a)[2] for a non-uniform TDR system. The model by Lin (2003a)[2] for a general non-uniform TDR system is refined and applied in this study.

The new mixing model includes quite a few parameters related to the physical and electrical properties of soil components. It is necessary to reduce the number of parameters for the results of inversion analyses to be stable. This also alleviates the issue of non-uniqueness. A few parameters in the model can be determined by referring to values in the literature. These include the dielectric properties of the air (1) and free water. All the parameters for Debye's model (ε_s , ε_∞ , $f_{rel,fw}$) can be obtained from the literature or from standard calibration tests). The bulk electrical conductivity σ can be determined from the measured TDR signal.

Experimental signals on reference materials were then used to further screen the parameters in the model. Parameters slight variation of which cause the results to be unrealistic are left out. Default values of a few model parameters are obtained from literature of from calibration tests. From the screening analyses, the specific gravity is left out as a parameter for inversion due to

the low sensitivity. The orientation index is left out due to the significant uncertainty these parameters induce on the other parameters. Parameters like the thickness of bound water layer and static dielectric constant of bound water are calibrated from measured signals on reference samples.

The problem of inversion for the parameters of the new dielectric mixing model was described as unconstrained nonlinear minimization problem using the predicted time domain signal as the target signal to match. The optimization problem was solved by Nelder-Mead simplex algorithm provided by MATLAB®. Since some parameters cover a large range (for example, the relaxation frequency and the area of specific surface), the logarithms of their values input for inversion. Although taking the logarithms is not a perfect solution, it was found it significantly improved the sensitivity of these parameters in the inversion analyses.

Additional considerations taken to make the results more reliable include: 1) setting realistic constants for fixed parameters; 2) providing range constrains for certain parameters; and 3) setting accurate initial guess of water content and dry density.

Selection of proper fixed parameters is achieved by referring to literature values or by measurement on given material. The authors believe that measurements on given material is better in that they partly account for the imperfect nature of the TDR system. In this study the TDR measured signal for dry Ottawa sand was used to obtain the soil properties such as the specific gravity and dielectric constant of soil solids. The measured TDR signal in water is used to determine the dielectric parameters for water. Figure 6 shows an example of TDR signal from inversion analyses on dry Ottawa sand.

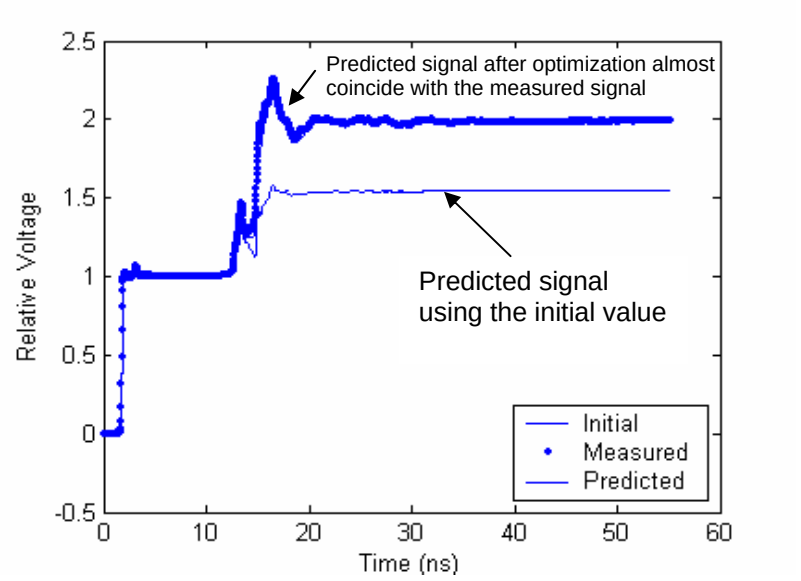


Figure 6. Example of TDR signals during the calibration using dry Ottawa sand

Estimating the of range for parameters to be inverted utilizes results that can be obtained from directly analyzing the TDR signals. The apparent dielectric constant and bulk electrical

conductivity from the TDR signal can be used to estimate the volumetric water content via Topp's equation (Topp et al., 1980)[25] for example.

Results and Analysis

Figure 6a shows an example of using the new volumetric mixing model together with the general model of a non-uniform system to invert for model parameters from a test signal acquired on a clay soil with low plasticity (CL). The plots show that the predicted TDR signal by the new dielectric mixing model closely matches the actual measured TDR signal. Figure 6b shows the predicted dielectric spectra from the new dielectric mixing model using the model parameters from the inversion analyses.

The dielectric spectra of the low plastic clay (CL) directly measured using HP Network Analyzer was shown in Figure 7a and was compared with the dielectric spectra from the inversion analyses using this new model in Figure 7b. The comparison indicates the predicted dielectric spectrum using the new dielectric mixing model with inverted parameters closely matches that from the direct measurement. Similar results were observed for other types of soils. The preliminary conclusion is that the new dielectric mixing model is capable of describing the dielectric spectrum of soils. The time domain signal predicted using this model closely describes actual measurements.

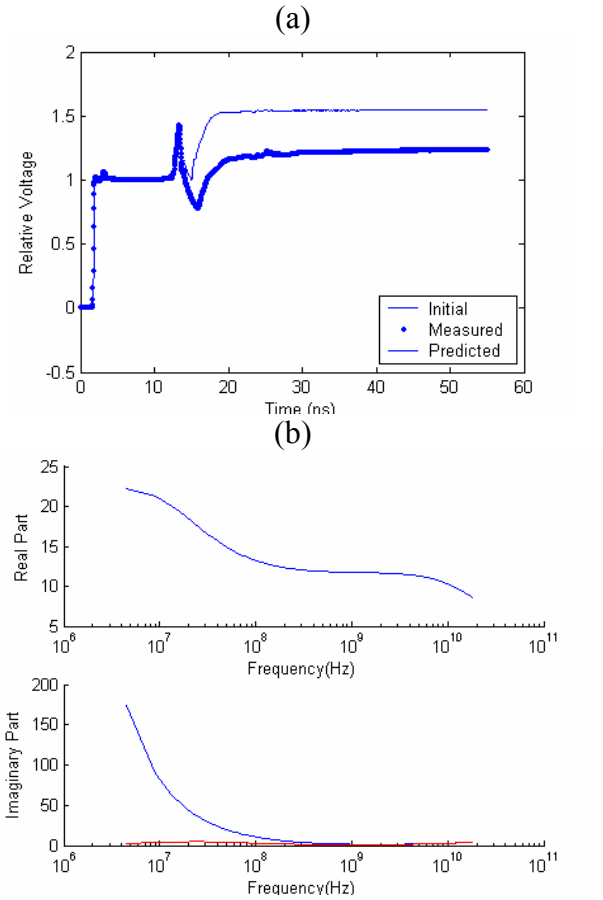
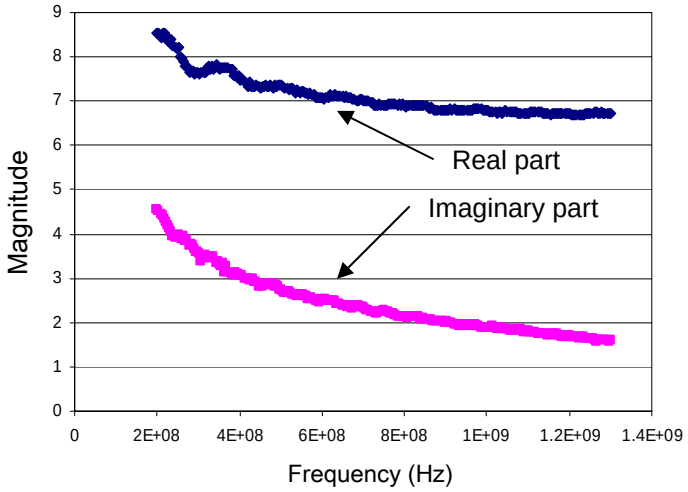


Figure 7. Example of inversion analyses using the new dielectric mixing model: a) time domain signals; b) dielectric spectra predicted by the model parameters

(a)



(b)

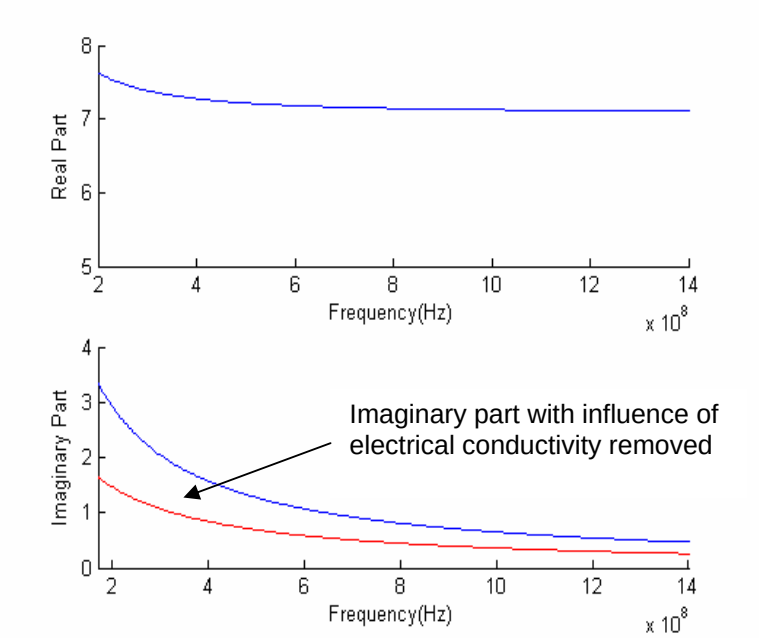
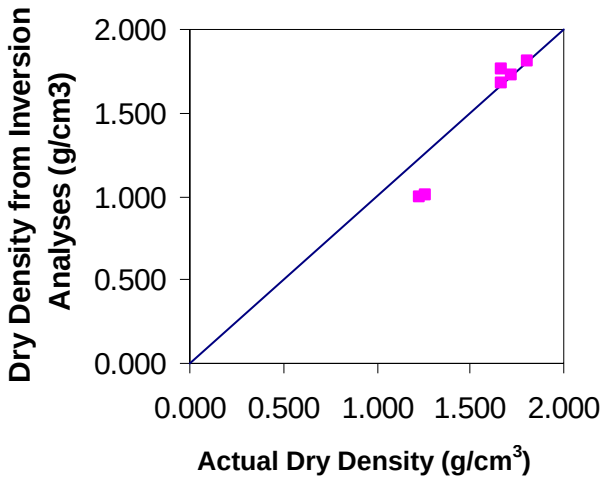


Figure 8. a) Dielectric spectrum measured by HP Network Analyzer; b) Dielectric spectrum predicted from the new dielectric mixing model with the parameters from the results of inversion analyses

The inversion analyses were also conducted on TDR signals measured on ASTM graded sand with different water contents. Since water is mostly in the form of free water, the dielectric mixing model can be simplified as a three phased mixing model with electrical conductivity term separated. The results of inverted soil water content and dry densities were compared with those from actual measurements and shown in Figure 9. The results of water content and dry densities reasonably match those of actual measurements.

(a)



(b)

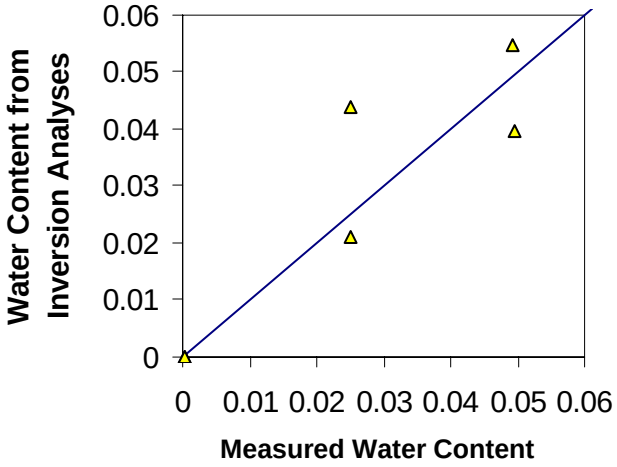


Figure 9. Comparison of water content and dry density of graded sand from inversion analyses: a) dry density; b) water content

Six parameters were needed for inversion analyses of a clayey material. These include the water content, the dry density, dielectric constant of soil solids, specific surface area, relaxation frequency of bound water and the bulk electrical conductivity. The specific surface area and relaxation frequency were represented using logarithm scale during the inversion analyses because of the much larger magnitude of the values compared with the other quantities. Table 1 summarizes the results of inversion analyses on the measured signals on samples of low plastic clays compacted using standard compaction energy. The results were found to be satisfactory compared with independent measurements. One advantage of this new dielectric mixing model is that most of the physical properties from the inversion analyses can be checked from independently measurement. This will be utilized in the future investigations.

Table 1 Example results of inverted model parameters for a low plastic clay

Dry Density (g/cm^3)	Volumetric Water Content	Dielectric constant of soil solids (ε_s)	Logarithm of the specific surface	Specific Surface, As (m^2/g)	Logarithm of the relaxation frequency	Relaxation Frequency, f_r (Hz)	Electrical Conductivity, σ (S/m)
1.889	0.097	6.924	1.699	50.003	7.310	2.040E+07	0.016
1.477	0.273	2.891	1.640	43.642	7.249	1.775E+07	0.043
1.526	0.292	3.272	1.600	39.783	7.268	1.852E+07	0.065
1.480	0.352	2.148	1.729	53.518	7.140	1.381E+07	0.054
1.483	0.353	2.202	1.699	50.038	7.172	1.486E+07	0.058

Conclusions

A new dielectric mixing model for soils was introduced. The motivations for this model development are to compensate for the limitations of existing volumetric mixing models, which are needed for inversion analyses of TDR systems to determine more information of soil dielectric properties. The new mixing model incorporates special terms for the treatment of the effects of bound water in the bulk mixture, which makes it possible to evaluate the accuracy of inverted model parameters from independent time domain measurements. The soundness of this new model is evaluated theoretically and results of experiments on two soils indicate that it has promise for determining the dielectric spectra and the physical properties for soil mixtures from TDR signals.

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