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Evaluation of five composite dielectric mixing models for understanding relationships between effective permittivity and unfrozen water content

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ABSTRACT

Accurate estimation of unfrozen/liquid water content (θ_l) of soils with time domain reflectometry (TDR) is important for understanding freezing and thawing processes and hydrology in cold regions. Empirical equations and composite dielectric mixing models are the two most commonly used methods to estimate water content in unfrozen soils from TDR-measured soil effective permittivity (ε_{eff}). However, empirical equations derived from unfrozen soil data always overestimate θ_l in frozen soils and few studies were found to examine the validity of composite dielectric mixing models for measuring θ_l. Therefore, the objective of this study was to evaluate the sensitivities and applicability of composite dielectric mixing models for modeling the $\varepsilon_{eff}(\theta_l)$ relationship. Five multi-phase, composite dielectric mixing models (i.e., power law model, de Loor model, Sihvola discrete model, Sihvola confocal model, and Sphere model) were evaluated with published dataset consisting of independently measured ε_{eff} and θ_l on the same samples. The results show that: (1) the power law model and de Loor models are independent of configurations of dielectric mixtures; (2) the Sihvola discrete model depends on the host medium and independent on the configurations of the other components; (3) different dielectric mixing models may end up with the similar $\varepsilon_{eff}(\theta_l)$ relationships by parameter adjusting to represent the same problem; and (4) the de Loor model, and Sihvola discrete and confocal models are most appropriate for modeling the $\varepsilon_{eff}(\theta_l)$ relationship of frozen soils based on the published dataset. This study will significantly contribute to the application of TDR method for liquid water measurement in frozen soils and facilitate the understanding of freezing/thawing processes.

1. Introduction

Soil water freezes over a few degrees below 0 °C due to a decrease of free energy of soil water resulting from surface forces of soil particles, pore geometry, and the existence of solutes (Cannell and Gardner, 1959; Miller, 1980). Phase change from soil water to ice takes place first in the large soil pores and followed by water in small capillaries, while soil water absorbed by soil particles or organic matter may remain unfrozen at very low subfreezing temperature (Ishizaki et al., 1996). The existence of solutes further decreases the freezing point of soil water. Generally more unfrozen water can be found in fine-textured soils than coarse-textured soils, and more in soil with high organic matter (OM) content/solute concentration than low OM content/solute concentration at a given temperature. Therefore, unfrozen/liquid water and ice coexist in soils at subfreezing temperatures (Cannell and Gardner, 1959; Anderson and Tice, 1972; Miller, 1980). This characteristic affects many frozen soil biological and environmental processes as well as cold regions engineering. For instance, unfrozen water content largely determines microbial respiration (Koponen and Martikainen, 2004; Öquist et al., 2009; Tilston et al., 2010); the amount of water and ice contents govern hydraulic and thermal properties that influence the mass and energy transport at the land surface (e.g., runoff, infiltration, erosion, freezing and thawing processes) (Andersland et al., 1996; Flerchinger et al., 2005; Christensen et al., 2013; He et al., 2015a,

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2015b); water and ice content also determines soil mechanical properties (Lai et al., 2008; Roman and Zhang, 2010).

The importance of accurate measurement of unfrozen/liquid water content (θ_l) has long been recognized and various techniques and methods (e.g., dilatometry, calorimetry, X-ray diffraction, heat capacity, and nuclear magnetic resonance) have been developed to measure θ_l. Among these methods, time domain reflectormetry (TDR) is easily multiplexed and automated (Spaans and Baker, 1995), it has become the most widely used technique for continuous and non-destructive measurements in both lab and field conditions (Patterson and Smith, 1980, 1981; Smith and Tice, 1988; Stahli and Stadler, 1997; Christ and Park, 2009; Watanabe and Wake, 2009; He and Dyck, 2013; Zhou et al., 2014; He et al., 2015a, 2015b). The TDR technique is based on the measurement of the travel time of an electromagnetic wave pulse (0.5–1.5 GHz) generated by a TDR cable tester through a TDR probe inserted in soil. The travel time of the wave through the probe is a function of the effective permittivity of soil (ε_{eff}), which in turn is a function of permittivities of the individual constituents in the soil (i.e., gas/air, water, solids, and ice), their volumetric fractions, and geometric arrangements. This permits estimation of θ_l through the relationship between the ε_{eff} and θ_l.

ε_{eff}~θ_l relationships generally include (1) empirical regression equations and (2) physically-based composite dielectric mixing models. Empirical equations, in a form of a polynomial relationship $\theta_l = a + b \cdot \varepsilon_{eff} + c \cdot \varepsilon^2_{eff} + d \cdot \varepsilon^3_{eff}$ (a, b, c, d are parameters), estimate θ_l based on the fact that permittivity of water ($\varepsilon_l = {\sim}80$) is significantly greater than the other soil components (e.g., gas, $\varepsilon_g = {\sim}1$; solid, $\varepsilon_s = {\sim}5$; ice, $\varepsilon_i = {\sim}3$). Prevalent empirical equations used in unfrozen soils (e.g, Topp et al., 1980 equation) showed discrepancy in estimated and measured θ_l for frozen soil applications. The discrepancy is attributed to ice and temperature effects, because previous studies assumed ε_i to be equal to ε_g (or the amount of total water content prior to freezing does not place any effects on ε_{eff}) and ε_l is assumed to be a constant rather than temperature-dependent value (Seyfried and Murdock, 1996; Yoshikawa and Overduin, 2005). He and Dyck (2013) indicated that existence of ice may change the depolarization of liquid water that affects ε_l, and change the $\varepsilon_{eff}(\theta_l)$ relationship. Therefore, TDR-measured ε_{eff} has to be calibrated against other methods measured θ_l to establish empirical equations in order to get accurate θ_l (Patterson and Smith, 1981; Smith and Tice, 1988; Spaans and Baker, 1995), one of the examples is the Smith and Tice (1988) equation. However, the validity of such empirical equations has not been demonstrated for whole range of possible soil types and initial water contents (Seyfried and Murdock, 1996; Yoshikawa and Overduin, 2005; He and Dyck, 2013; Zhou et al., 2014).

Composite dielectric mixing models consider soil as a mixture of dielectric components (i.e, soil solid, water, air, and ice). The sizes of dielectric components are considerably smaller than the wavelength of the applied electric field. The macroscopic/effective dielectric properties of soil (ε_{eff}) is therefore related to dielectric properties of soil constituents, their volume fractions and the internal soil structure (Tinga et al., 1973; Roth et al., 1990; Sihvola, 1989, 1999). Compared to empirical equations, dielectric mixing models could provide a better description of the relationship among ε_{eff}, θ_l, θ_i, initial total water content prior to freezing (θ_{init}), temperature, soil structure, and interactions among soil constituents (Seyfried and Murdock, 1996; Watanabe and Wake, 2009; He and Dyck, 2013). It is more versatile and is promising to be used to fairly well estimate θ_l of a wide range of soils and θ_{init}. Because there is no exact solution for the electromagnetic problem with random parameters and boundaries, extensive mixing models based on different assumptions about the shape and distribution of soil constituents are available in literature. There remains a need for evaluation of their performance in θ_l estimation so as to select the most appropriate dielectric mixing model(s) for frozen soil applications.

One of the most reliable approaches to evaluate these models is to fit these models with TDR-measured ε_{eff} and independently measured θ_l. He and Dyck (2013) have showed ε_{eff} and θ_l measured on separate soil samples are prone to hysteresis effects due to the practical difficulties of maintaining both samples in the same conditions (e.g., same temperature to start freezing or thawing and the same rates of freezing/thawing). ε_{eff} and θ_l values then may actually be retrieved from different freezing/thawing curves and end with wrong ε_{eff} and θ_l relationship. Therefore, independent measurements of ε_{eff} and θ_l taken on the same soil sample are required, and only the dataset from Spaans and Baker (1995) meet this criteria after extensive literature search. The objective of this study was to evaluate performance of dielectric mixing models using dataset of Spaans and Baker (1995).

2. Material and methods

2.1. Published dataset

Literature datasets related to frozen soil and TDR was collected and analyzed, and were screened according to the following criteria: (1) θ_l was measured on frozen soil samples independently of TDR; (2) θ_l was measured on frozen soil samples with at least two unique θ_{init} prior to freezing; (3) ε_{eff} and θ_l were measured on the same soil sample simultaneously. This screen ended up with Spaans and Baker (1995) dataset with TDR-measured ε_{eff} and independently measured θ_l by gas dilatometer on the same soil sample. Two soil samples (Waukegan silt loam, two θ_{init}) in total were tested between −10 to 5 °C. The reader is referred to their paper for a complete description of methodology.

2.2. Dielectric mixing models

Five composite dielectric mixing models frequently appearing in literature are investigated. These mixing models differ in their assumptions of the geometrical arrangement of the soil constituents. Some of the models originally developed for unfrozen soil applications (3-phase model-soil solids, water and air) were extended for frozen soils (4-phase model- soil solids, unfrozen water, ice and air) by introducing an additional ice phase term into the models. A brief description of these mixing models is given below.

2.2.1. Power law model

It is a simple, semi-empirical approximation for a layered material without referring to its microstructure and it assumes the soil components to be perfectly layered (Birchak et al., 1974; Dobson et al., 1985; Roth et al., 1990; Robinson et al., 2003; Watanabe and Wake, 2009):

$$\varepsilon_{eff}^{\alpha} = \sum\nolimits_{j=0}^{3} \phi_j \varepsilon_j^{\alpha} \tag{1}$$

where ϕ_j, ε_j are the volumetric fraction ($m^3\ m^{-3}$) and permittivity of the j^{th} soil constituents, respectively, $\sum\nolimits_{j=0}^{3} \phi_j = 1$; α is geometric factor which