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Calculating water saturation from passive temperature measurements in near-surface sediments: Development of a semi-analytical model

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ABSTRACT

A novel semi-analytical model for the calculation of water saturation levels in the near subsurface using passive temperature measurements is derived. The amplitude and phase of dominant natural diel temperature variations are exploited, although the solution is general so that a cyclical temperature signal of any period could be used. The model is based on the first-principles advection-conduction-dispersion equation, which is fully general for porous media. It requires a single independent soil moisture estimate, but directly considers the spatially variable saturation dependency of thermal conductivity which has been avoided in previous studies. An established empirical model for the thermal conductivity of variably saturated porous media is incorporated and two solutions for saturation are derived. Using data from numerical models, a spatially sequential implementation of one of these solutions is shown to predict the vertical saturation profile to within 2% for a hydraulically stable case and to within the saturation range observed over a single day for percolation rates up to 10 cm/day. The developed model and methodology can aid in the analysis of archived temperature data from the vadose zone and will serve as a powerful tool in future heat-tracing experiments in variably saturated conditions.

1. Introduction

Accurate transient measurements of soil moisture levels are of vital importance to investigations in the areas of agronomy [e.g., 1,2], geochemistry [e.g., 3,4], and near-surface hydrogeology [e.g., 5,6]. Many indirect methods of soil moisture measurement have been developed and are applicable at a large range of spatial and temporal scales [7]. Methods such as neutron probes [8], ground penetrating radar [9], cosmic rays [10], and time-domain transmissometry/reflectometry [11] all offer benefits and disadvantages and no single method is applicable for all types of studies. At the sub-meter scale, time-domain reflectometer (TDR) and time-domain transmissometer (TDT) probes offer accurate measurements of water content in a variety of conditions and their use is widespread [e.g., 3,12]. However, the cost of the multiple sensors needed to measure moisture content to a high degree of spatial resolution with these probes can be prohibitive. Furthermore, the probes also fail in environments with high pore water electrical conductivity, limiting their use in studies of coastal, estuarine or saline arid zones. Many TDT/TDR probes do not offer a spatial resolution on the scale of <10 cm due to the volume-averaging principle of the measurement. Temperature measurements, which are routinely performed during vadose zone studies, can provide another indirect method to measure soil moisture on the sub-meter scale with the potential for centimetre-scale vertical resolution.

The use of heat-as-a-tracer in surface water and groundwater studies has seen a large amount of interest over the past decade [see the reviews of 13–15]. Temperature offers the advantage of being relatively straightforward and inexpensive to measure automatically. High spatial resolution or large-scale measurements can be made through the use of fibre-optic distributed temperature sensing (FO-DTS) [16], which can be deployed in a coiled configuration for fine ($\sim$1 cm) vertical resolution measurements [e.g., 17–19]. Through analysis of the hydrothermodynamics of a system, time-series measurements of temperature can be used as a proxy for estimating other physical quantities, such as thermal diffusivity or vertical water exchange rates [20–23].

Thus far, the majority of work on heat-tracing in subsurface research has been limited to saturated conditions, although some

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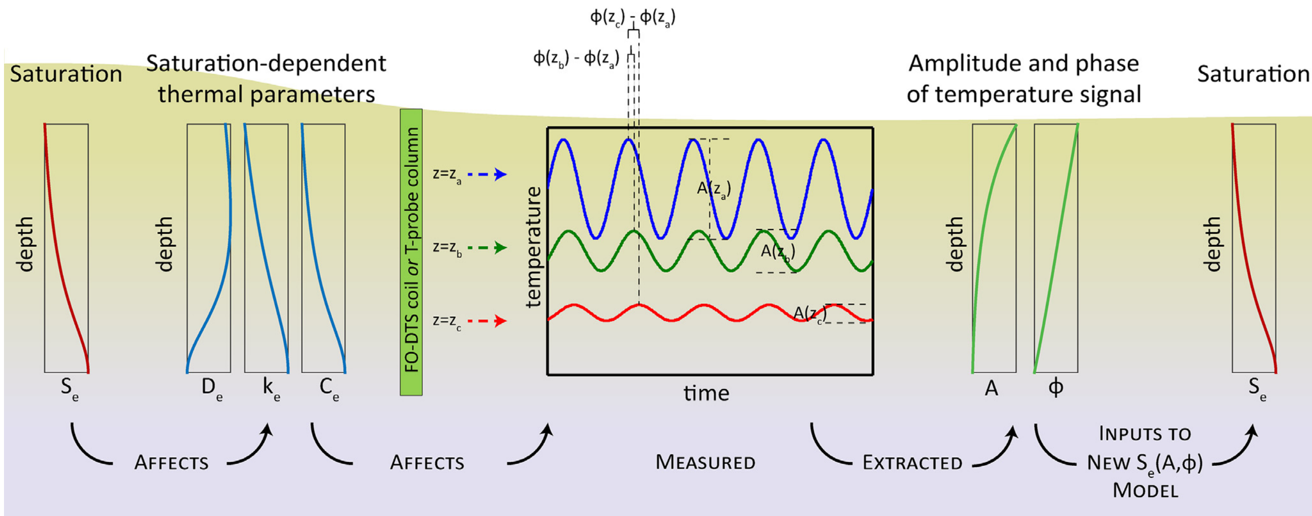

Fig. 1. Conceptual illustration showing the parameters dependent on saturation level, S_e, that govern thermodynamics in the vadose zone: effective saturation level, S_e; thermal diffusivity, D_e; thermal conductivity, k_e; and volumetric heat capacity, C_e. These parameters affect the behaviour of the temperature signal induced by the diurnal heating cycle at the surface. The amplitude, A, and phase, ϕ, of this signal are used to reconstruct S_e by the method developed in this study.

investigations showing the potential for the expansion of the techniques to the unsaturated zone have been published. Béhaegel et al. [24] extracted water content and saturation boundary depth from surface and 60 cm depth temperature time-series by two modelling approaches, finding acceptable results using monthly data and employing the Johansen [25] model for effective thermal conductivity as a function of effective saturation, $k_e(S_e)$. Steele-Dunne et al. [26] demonstrated the feasibility of using passive FO-DTS measurements to estimate soil moisture levels and, in turn, compared the performance of $k_e(S_e)$ models from Johansen [25] and Campbell [27]. The simplified diffusion-only heat-transfer model used in the Steele-Dunne et al. [26] study assumes that k_e is spatially uniform. Ciocca et al. [28] provided a method for estimating S_e using active heating and coiled fibre-optic distributed temperature sensing cables. Bechkit et al. [29] presented a study comparing TDR data and finite difference calculations based on time-series from platinum thermistors which confirmed the utility of heat tracing in estimating soil moisture. Research in the field of unsaturated zone heat-tracing is accelerating as evidenced by recent works [30,31] that investigate the use of the Hydrus-1D model and data assimilation including a particle batch smoother to estimate soil moisture from temperature measurements.

A key aspect in estimating effective saturation (S_e), the degree of water saturation between 0 and 1, with temperature data is the dependence of thermal conductivity and heat capacity on temperature. While the dependence of volumetric heat capacity ($C_{v,\,e}$) can be calculated as a simple volumetric average of the materials present (i.e., the sediment, water and air), the relationship between temperature and thermal conductivity (k_e) is non-linear and material-dependent and must be investigated empirically. Much research exists in this field [e.g., 25,27,32–37] and multiple models have been proposed for various material classes. The $k_e(S_e)$ model proposed by Johansen [25] saw widespread uptake since its formulation, but it did not accurately describe the relationship at low saturation levels. More recently, Côté [36] provided a generalized empirical model that can be inverted to obtain an explicit expression for effective saturation as a function of thermal conductivity.

Temperature in combination with the full heat transport equation offers an indirect and passive approach for measuring soil moisture content. The aim of this paper is to develop a new method for the quantification of soil moisture content in near-surface sediments by building on the fundamental physics that govern heat transport in the variably saturated subsurface (Fig. 1). Previous efforts in determining soil moisture from natural temperature variations have primarily avoided an analytical approach and have not treated the thermal conductivity term as a quantity that varies spatially due to moisture content, leading to an incomplete consideration of the physics governing the coupling of soil moisture and temperature. We develop and propose a closed-form solution for soil moisture as a function of the amplitude and phase of cyclic temperature variations in the subsurface, akin to SW-GW exchange velocity solutions proposed by others [21–23]. A first-principles approach is taken and, by incorporating the empirical model for thermal conductivity of Côté [36], we derive two explicit soil moisture solutions that depend on the spatial and temporal behaviour of the amplitude and phase of naturally occurring cyclical temperature signals. We then illustrate that our new method accurately predicts saturation profiles for certain implementations using numerically modelled temperature data. The developed method is a robust tool for estimating water saturation levels using natural temperature variations and avoids the assumption of constant thermal conductivity that prior studies have made. The semi-analytical model and outlined method of sequential implementation will aid future field studies in the near-surface vadose zone.

2. Method development

Throughout, parameters are defined as they are introduced. For quick reference, definitions of parameters and mathematical notation symbols can be found in Appendix A.

2.1. Advection-conduction-dispersion equation with sinusoidal temperature

The advection-conduction-dispersion heat equation describes the behaviour of thermal energy propagation in a porous medium [38]:

$$C_{v,e}(t,\vec{x})\frac{\partial T(t,\vec{x})}{\partial t} + C_{v,f}(t,\vec{x})\vec{v}\cdot\nabla T(t,\vec{x}) = \nabla\cdot[k_e(t,\vec{x})\nabla T(t,\vec{x})] \tag{1}$$

where T is temperature; $C_{v,\,e}$, the total effective volumetric heat capacity; $C_{v,\,f}$, the fluid (water) volumetric heat capacity; $\vec{v}$, the