



# In situ measured and simulated seasonal freeze–thaw cycle: A 2-year comparative study between layered and homogeneous field soil profiles



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## SUMMARY

Annual freeze–thaw cycles of soil significantly impact agricultural and ecosystem services in cold regions. For advancing our understanding of freeze–thaw process, both improved measurements and simulations of coupled-heat-water-transfer (CHWT) phenomenon are needed under different field conditions. This paper focused on a comparative study between a CHWT-model simulation versus in situ measurements of liquid soil water content (LSWC) and soil temperature (ST) at two agricultural field sites. The first site consisted of a layered soil profile with sandy silt loam (0–60 cm) and clay loam (60–130 cm) layers, and the other site was a uniform sand profile (0–110 cm). Measurements were made over two winters between 2011 and 2013, i.e. the first winter is 2011–2012 (year 1) and the second winter is 2012–2013 (year 2), in the northeast of China employing an access-tube dielectric sensor combined with a temperature measurement array. During the freezing period of the year 1 winter, the soil freezing characteristic curves (SFCCs) were determined in situ in relation to the site-specific data of LSWC and ST and subsequently used for the model calibration. For the thawing process of year 1 and the freeze–thaw process of year 2, the resulting ST simulation time series were well-correlated with field measurements. In terms of the resulting LSWC, the numerical simulations also correlated well ( $R^2 > 0.895$ ,  $RMSE < 0.0381 \text{ cm}^3 \text{ cm}^{-3}$ ) with the in situ observations of freezing and quasi-steady-state conditions at depths of 50- and 100-cm. The reasons for relatively reduced agreement between simulated and measured LSWC during the thawing stage (i.e.,  $R^2 > 0.702$ ,  $RMSE < 0.0468 \text{ cm}^3 \text{ cm}^{-3}$ ) are discussed. The resulting time series simulations confirm the model's capability for describing freeze- and thaw-front migration in layered and homogeneous freezing soils.

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## 1. Introduction

In cold regions, both temporal and spatial variations of the soil freeze–thaw process are important for optimizing agricultural field management. For instance, water management through irrigation in early winter may be indispensable for addressing the physiological needs of winter cereals, while on the other hand inaccurate irrigation time could lead to excessive leaching or may cause surface runoff. Transitioning from winter to spring, farmers need information regarding the soil thawing process to time field activities and to avoid additional fuel costs associated with the high tillage resistance in partially frozen soil.

Unlike pure water, which freezes at 0 °C under atmospheric pressure, soil water remains partially unfrozen over a range of sub-zero temperatures because the soil matric force lowers the energy status of the soil water, which, consequently, depresses the freezing point of that water (Spaans and Baker, 1996). Modeling soil freeze–thaw process is complicated by the intertwined relationships of heat transfer, water flow and phase change occurring within a porous medium comprised of a distribution of soil pore sizes. To formulate this appropriately, soil temperature (ST), liquid soil water content (LSWC) and soil ice content (SIC) are three key variables that must be considered.

One of the initial attempts to model coupled-heat-water-transfer (CHWT) in partially frozen soil was proposed by Harlan (1973) and subsequently modified by others (e.g. Guymon and Luthin, 1974; Fuchs et al., 1978; Zhao et al., 1997). Flerchinger and Saxton (1989) presented a comprehensive model (SHAW) to

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compute the coupled heat, water and solute transfer associated with climatic factors (net radiation, air temperature and precipitation) and site-specific field conditions. They suggested optimizing model parameters using part of the predetermined data in the field. These contributions have been developed into a software package for frozen soil simulations (<ftp://ftp.nwrc.ars.usda.gov/public/ShawModel/>).

Field evaluation of CHWT models is challenging given the need for independent measurements of in situ ST, LSWC and SIC. To address this challenge, [Flerchinger and Saxton \(1989\)](#) employed a neutron probe together with an array of temperature sensors yielding measurements of total soil water content (TSWC) and ST. Thereafter, [Xu et al. \(1992\)](#) evaluated the same CHWT model (SHAW) in an agricultural field subjected to variably-saturated and variably-frozen soil using a single season winter-time dataset collected with multiplexed time-domain reflectometry (TDR) probes for the LSWC profile and a neutron probe for the TSWC profile. Although the LSWC profile is measurable using multiple TDR-probes, the installation of these probes involves excavating a pit for probe insertion at different depths, which inevitably disturbs the soil structure surrounding the probes ([Whalley et al., 2004](#)). [Xu et al. \(1992\)](#) suggested that better-characterized soil hydraulic properties and more accurate LSWC measurements were critical for improving agreement between model simulated LSWC and measurements. Rather than using multiple TDR probes, [Li et al. \(2012\)](#) tested the SHAW model with multiple winter-time temperature profile datasets ranging from 10 to 250 cm and gravimetric soil water content data collected using an auger. Besides, [Kojima et al. \(2013\)](#) proposed a sensible heat balance method to determine rates of soil freezing and thawing, consequently the freeze-thaw process was simulated using the SHAW model.

One of the ideal in situ soil moisture profiling approaches involves a dielectric tube sensor, which has been used in unfrozen soils for many years ([Dean et al., 1987](#); [Evelt et al., 2012](#)). Compared to the use of multiple TDR probes, the dielectric tube sensor facilitates profiling soil moisture content in situ without the inherent error associated with sensor-to-sensor variability. Field installation of access tubes has been improved with specialized kits resulting in minimal disturbance of the soil profile. Moreover, tube-access sensors allow repeated in situ measurements across multiple locations at the field scale. Based on these merits, [Sun et al. \(2012\)](#) tested its feasibility for in situ profile monitoring of LSWC in frozen soil. As a continuation of these previous efforts, we set out to expand our research into freezing soils using a combination of measurements and numerical simulations. The major objective of this frozen soil research was to present a 2-year comparative study between a CHWT-model simulation and in situ measurements of LSWC and ST in two different agricultural field locations, one with a two-layer soil of contrasting textures and one with homogeneous soil condition. Importantly, the in situ measurements can provide valuable profile data for testing the model, and on the other hand the numerical results can support interpreting the measured data in relation to the freeze-thaw process.

## 2. Materials and methods

### 2.1. Coupled heat- and-water-transfer model (CHWT)

To fully simulate water flow and heat transfer in frozen and unfrozen soils, a pair of one-dimensional partial differential equations (PDEs) has been presented as (e.g. [Hansson et al., 2004](#)):

water flow equation:

$$\frac{\partial \theta_l}{\partial t} + \frac{\rho_v}{\rho_l} \frac{\partial \theta_v}{\partial t} + \frac{\rho_i}{\rho_l} \frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial z} \left( D \frac{\partial \theta_l}{\partial z} - K + K_{LT} \frac{\partial T}{\partial z} + K_{vh} \frac{\partial \psi}{\partial z} + K_{vT} \frac{\partial T}{\partial z} \right) - U \quad (1)$$

heat transfer equation:

$$C_m \frac{\partial T}{\partial t} - \rho_i L_f \frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial z} \left( \lambda_m \frac{\partial T}{\partial z} \right) - c_l \rho_l \frac{\partial q_l T}{\partial z} - c_v \rho_v \frac{\partial q_v T}{\partial z} - L_{lv} \left( \frac{\partial \theta_v \rho_v}{\partial t} + \frac{\partial q_v}{\partial z} \right) - S \quad (2)$$

where  $\theta_l$ ,  $\theta_i$  and  $\theta_v$  denote liquid (unfrozen) soil water content, soil ice content and water vapor content ( $\text{cm}^3 \text{cm}^{-3}$ ), respectively;  $\rho_l$ ,  $\rho_i$  and  $\rho_v$  denote the densities of liquid water, ice and water vapor ( $\text{g cm}^{-3}$ ), respectively;  $\psi$  is the soil water potential (Pa);  $K$  is the liquid water content-dependent unsaturated hydraulic conductivity due to a matric potential gradients ( $\text{cm h}^{-1}$ );  $K_{LT}$  is the unsaturated hydraulic conductivity due to a temperature gradients ( $\text{cm h}^{-1} \text{K}^{-1}$ );  $K_{vT}$  is equivalent hydraulic conductivity of vapor in response to a temperature gradient ( $\text{cm h}^{-1} \text{K}^{-1}$ );  $K_{vh}$  is equivalent hydraulic conductivity of vapor in response to a matric potential gradient ( $\text{cm h}^{-1}$ );  $D$  is the water diffusivity ( $\text{cm}^2 \text{h}^{-1}$ );  $q_v$  is the vapor flux ( $\text{kg m}^{-2} \text{s}^{-1}$ );  $T$  is the soil temperature (K);  $\lambda_m$  is the soil thermal conductivity ( $\text{W m}^{-1} \text{K}^{-1}$ );  $L_f$  is the latent heat of fusion ( $334 \text{ kJ kg}^{-1}$ );  $L_{lv}$  is the latent heat of evaporation ( $\text{kJ kg}^{-1}$ );  $q_l$  is the liquid water flux ( $\text{cm h}^{-1}$ );  $C_m$  is the volumetric heat capacity of soil ( $\text{J cm}^{-3} \text{K}^{-1}$ );  $c_l$  and  $c_v$  are the specific heat of liquid water and water vapor ( $\text{J kg}^{-1} \text{K}^{-1}$ ), respectively;  $U$  is the sink/source term associated with root water uptake and  $S$  represents the uptake of energy associated with root water uptake.

For soil conditions near freezing temperatures, liquid water flow is considerably larger than vapor flow, suggesting that the vapor flow component can be neglected ([Harlan, 1973](#); [Guymon and Luthin, 1974](#); [Fuchs et al., 1978](#)). The effect of temperature gradients on water flow can also be neglected because of its minor contribution to the redistribution of water ([Fayer, 2000](#)) under phase change conditions. Based on these assumptions, the CHWT model (Eqs. (1) and (2)) can be simplified with the following water flow equation:

$$\frac{\partial \theta_l}{\partial t} + \frac{\rho_i}{\rho_l} \frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial z} \left( D(\theta_l) \frac{\partial \theta_l}{\partial z} \right) - \frac{\partial K(\theta_l)}{\partial z} + U \quad (3)$$

And using the following heat transfer equation:

$$C_m \frac{\partial T}{\partial t} - \rho_i L_f \frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial z} \left( \lambda_m \frac{\partial T}{\partial z} \right) - c_l \rho_l \frac{\partial q_l T}{\partial z} \quad (4)$$

where  $\theta_i$  equals zero in unfrozen soil.

In terms of  $K$  and  $D$ , both are functions of  $\theta_l$ , described by ([Flerchinger and Saxton, 1989](#)):

$$K(\theta_l) = K_s \left( \frac{\theta_l}{\theta_s} \right)^{(2b+3)} \quad (5)$$

and

$$D(\theta_l) = K(\theta_l) \frac{\partial \psi}{\partial \theta_l} \quad (6)$$

where  $K_s$  is the saturated soil hydraulic conductivity ( $\text{cm h}^{-1}$ ),  $\theta_s$  is the saturated volumetric soil water content ( $\text{cm}^3 \text{cm}^{-3}$ , assumed equal to soil porosity),  $b$  is a parameter related to the soil pore size distribution. The parameter  $\psi$  is the soil water potential (Pa) and is commonly determined by the Campbell model ([Campbell, 1974](#)):

$$\psi = \psi_e \left( \frac{\theta_l}{\theta_s} \right)^{-b} \quad (7)$$

where  $\psi_e$  is the air entry potential (Pa).

Liquid water movement, which in frozen soil simultaneously induces heat convection, can be expressed in terms of  $q_l$ ,  $\theta_l$ ,  $K$  and  $D$  using Darcy's law as:

$$q_l = D(\theta_l) \frac{\partial \theta_l}{\partial z} + K(\theta_l) \quad (8)$$

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