Machine learning-based numerical model for water-heat dynamics in soil under freezing conditions

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Abstract: Frost heave significantly impacts performance of the critical infrastructure such as the foundations, pavements, and tunnels in frozen soils. The phase transitions between water and ice alter the soil structure, affecting the thermo-hydro-mechanical (THM) properties of frozen soils. In recent years, researchers have focused on developing machine learning-based models to predict frozen soil behavior, leveraging the advantages of machine learning in handling complex problems, integrating diverse datasets, and enhancing prediction efficiency. This study employs a previously developed least square boosting (LSB) model, an ensemble learning algorithm, to predict the thermal conductivity of frozen soils using easily measurable soil parameters. The LSB model is integrated into numerical simulations of frozen soils, combining governing equations for water and heat transfer. Fourier's and Richard's equations are incorporated to construct a robust numerical model for simulating frozen soil behavior under freezing conditions. By elucidating these relationships, especially the interplay between soil temperature, water-ice content and thermal parameters, new insights can be gained into the simulation of the THM behavior of frozen soils. The proposed model is used as a tool to predict trends of the freezing front movement, the volumetric ice contents, and the soil displacement with respect to time in a soil column.

Introduction

Seasonal frozen soils are subjected to annual cycles of freezing in winter and complete thawing in summer; these soils are predominantly distributed in mid- to high-latitude regions of both the northern and southern hemispheres. The frozen soil depth thickness decreases progressively from the poles toward the equator, following climatic gradients [1]. In these regions, the freezing process significantly influences various geotechnical properties throughout the year, creating numerous challenges for the design of civil infrastructure such as highways, railways, and pipelines. Reliable frost heave estimation is one of the major challenges in frozen soil areas. Notable examples of infrastructure affected by such conditions include the Trans-Alaska Pipeline System (TAPS), spanning 1,287 kilometers through Alaska's permafrost and seasonal frozen regions, and the Dempster Highway, a 740-kilometer route crossing permafrost and seasonal frozen soils in Canada [2, 3]. While these projects have facilitated regional economic growth and resource development, frost heave related to the freezing process remains a persistent geotechnical challenge. This phenomenon causes severe soil deformation, compromising the stability of engineering structures, endangering transportation safety, and leading to substantial economic losses. A comprehensive understanding of the coupled water-heat dynamics is required for heave estimation in frozen soils to predict and mitigate their impact on engineering stability and safety.

In low-temperature environments, water in the soil migrates from the warmer region towards the freezing front, where the phase transition from liquid water to ice, combined with water migration, leads to frost heave. Researchers have developed approaches to model this process. Based on water migration and heat transfer, the gradient of matric suction has been identified as the driving force for water migration in the soil, and the capillary model is widely used as a tool for frost heave estimation [4]. The ice formation process occurs at a relatively slow pace, allowing enough contact between phases to establish local thermal equilibrium. The transport equations for water and ice can be formulated using a moving boundary finite difference method when freeze-thaw hysteresis is not considered. The concept of segregation potential was introduced to model the formation of the final ice lens when soil freezes under constant temperature boundary conditions. Theoretical background associated with the frost heave due to temperature variations is strongly related to the ice lens formation. More recently, thermodynamic equilibrium models are proposed considering the water balance, heat, and stress fields for establishing a dynamic relationship between water migration and ice crystal growth. These approaches incorporate the Clapeyron equation to describe the equilibrium state of water and ice in frozen soil, capturing the interplay between temperature, pressure, and water migration [5].

Based on different theoretical foundations, numerical models for frozen soils have evolved from single-field simulations (e.g., thermal or moisture fields) to multi-field coupling simulations. Common multi-field models include heat-water coupling, thermo-hydro-mechanical (THM) coupling, heat-water-vapor-mechanics coupling, and thermo-hydro-mechanical-chemical (THMC) coupling models. These models comprehensively consider the interactions between temperature variations, water migration, ice formation, and mechanical stresses, providing a more realistic representation of the frost heave process. Yang et al. [6] presented a coupled analysis model for water freezing, temperature, and stress fields, validated through numerical simulations and field measurements of ground freezing in underground excavation. Li et al. [7] conducted centrifuge modeling and numerical simulations to study frost heave mechanisms in cold-region canals. The study revealed that frost heave deformation is driven by a temperature gradient, with significant vertical displacement at the canal top and horizontal deformation in the middle-lower slope, making these zones more susceptible to frost damage. Teng et al. [8] developed a numerical model to simulate ice formation and frost heave in coarse-grained soils, incorporating the processes of vapor transfer and desublimation.

In recent years, machine learning methods have been incorporated into modeling the behavior of frozen soils. Chen et al. [9] suggested a method that considers the interface behavior between frozen soil and structures taking account of the combined effects of temperature, moisture content, and normal pressure. Ren et al. [10] estimated the unfrozen water content in frozen soil under various conditions using artificial neural networks. Li et al. [11] proposed a data-driven model that incorporates uncertainty to simulate the stress-strain behavior of frozen soils. Machine learning methods demonstrate advantages in handling highly nonlinear relationships and enabling rapid computation for complex multivariable problems. However, the integration of machine learning with numerical models to study frozen soils under multi-field coupling conditions remains highly limited.

For this reason, in this study a novel water-heat coupled numerical model is introduced extending the integration of a machine learning-based thermal conductivity model using the ensemble learning algorithm for frost heave analysis. The proposed model incorporates the heat convection induced by water migration and the effects of latent heat during phase transitions by combining the governing equations of the water and temperature fields. The model is validated by successfully simulating the freezing front movement and predicting the volumetric ice content, and displacement within the soil column. In summary, the incorporation of machine learning methods is promising for reliable estimations of thermal conductivity, water migration, ice-water phase transitions, and soil deformation, offering a more robust framework for analyzing frost heave dynamics.

Numerical modeling

Song et al. [12] developed ensemble learning methods based on thermal conductivity models for frozen soils. They used seven physical parameters of the frozen soil that include the water content, dry density, temperature, and the fractions of gravel, sand, silt, and clay as input parameters. The output of the model is the thermal conductivity of the frozen soil. Among the ensemble learning methods, the Least-Square Boost (LSB) model from their study was adopted for the numerical simulations presented in this paper.

In modeling simultaneous heat and mass transfer in soil columns under freezing/thawing conditions, the following assumptions are made to simplify calculations: (1) heat and water transfer are considered only in the vertical direction; (2) the system is simplified into a plane strain model for frost heave and freeze-thaw processes in a closed soil column; (3) moisture migrates solely as liquid water under the influence of capillary and cryogenic suction forces, without vapor migration or phase change; (4) the compressive deformation of the porous medium skeleton and ice, as well as changes in internal stress fields affecting thermal and hydraulic properties, are neglected; and (5) the soil is assumed to be isotropic. Furthermore, due to the slow velocity of liquid water migration during freezing, convective heat transfer is negligible compared to conduction, as supported by typical thermal diffusivity values observed in frozen soils [13, 14].

Governing equations

1. Water field

Even at extremely low temperatures, soil undergoing freezing process retains a certain amount of liquid water. The migration of this unfrozen water follows Darcy's law. The governing differential element equation for unfrozen water migration in unsaturated frozen soils can be expressed based on the Richards equation, while accounting for the obstructive effect of pore ice on unfrozen water flow, changes in water and ice content, and the influence of gravitational forces, using equation (1) [13].

$$\frac{\partial\theta_u}{\partial t} = \nabla[D(\theta_u)\nabla\theta_u + k(\theta_u)] - \frac{\rho_i}{\rho_w}\frac{\partial\theta_i}{\partial t} \tag{1}$$

where θ_u is the volumetric unfrozen water content of the soil, t is time, $D(\theta_u)$ is the water diffusion coefficient, $k(\theta_u)$ is the hydraulic conductivity of unsaturated soil, ρ_i, ρ_w are the density of ice and water respectively, θ_i is the volumetric ice content in the soil.

The formation of ice can act as an obstacle for the migration of water in a frozen soil. A passage resistance factor, I, is typically introduced to account for the influence of ice on water migration, as shown in equation (2) [15]. Consequently, the hydraulic parameters of frozen soil can be related to those of unsaturated soil using the resistance factor (equation (3)).

$$I = 10^{10\theta_i} \tag{2}$$

$$D(\theta_u) = \frac{k(\theta_u)}{\varphi(\theta_u)} I \tag{3}$$

where $\varphi(\theta_u)$ represents the change in water content caused by the change in matric suction, determined by the Van Genuchten model, as expressed in equation (4).

$$\varphi(\theta_u) = \frac{a_0 m}{1-m} {S_r}^{1-m}\left(1 - {S_r}^{1-m}\right)^m \tag{4}$$

where a_0 and m are parameters, S_r represents the saturation of soil.

Due to the differences in the physical properties of water and ice, for instance, at 0 °C at standard atmosphere, water has a thermal conductivity of 0.57 W/(m·K) and a density of 1.0 g/cm^3, whereas ice has a thermal conductivity of 2.28 W/(m·K) and a density of 0.92 g/cm^3[16, 17]. The amount of unfrozen water (or ice) is a key factor in calculating thermal convection processes and the mechanical behavior of frozen soils. The unfrozen water content in a soil can be inferred from the relationship between temperature and unfrozen water content that is typically referred to as the soil-freezing characteristic curve (SFCC) [18]. The empirical model (i.e., equation (5)) developed by Zhang et al. [19] is used in this study to determine the unfrozen water content.

$$w_u = \begin{cases} w_0\left[1 - \left(\dfrac{T_f - T}{273.15 + T_f}\right)^{\omega}\right], -273.15 < T < T_f \\ w_0, \quad T \geq T_f \end{cases} \tag{5}$$

where, w_u refers to the unfrozen water content, w_0 is the initial water content of the soil, T_f is the freezing point of the soil, ω is a fitting parameter related to soil physical properties.

The unfrozen water content, volumetric water content, and ice volumetric content in frozen soil are expressed in equation (6).

$$\theta = \theta_u + \frac{\rho_i}{\rho_w}\theta_i \tag{6}$$

Assuming a 10% volume expansion during the phase change from water to ice, the relationship between the volumetric ice content and the unfrozen water content is shown in equation (7). The volumetric changes induced by the water–ice phase transition is introduced as thermal strain applied to the soil skeleton. This strain serves as a coupling mechanism between the thermal and mechanical fields, where the temperature-dependent evolution of unfrozen water content governs the extent of ice formation, and consequently, the induced deformation in the soil matrix. By incorporating this phase-change-induced strain into the mechanical equilibrium equations, the model enables the simulation of frost heave behavior driven by thermal gradients.

$$\frac{\theta_i}{\theta_u} = \begin{cases} \dfrac{1.1}{1 - \left(\dfrac{T_f - T}{273.15 + T_f}\right)^{\omega}} - 1.1, & T < T_f \\ 0, & T \geq T_f \end{cases} \tag{7}$$

2. Heat transfer

Typically, heat radiation is neglected in frost heave experiments involving a soil column tested in a closed system. The convective heat transfer is much smaller than heat conduction and can be ignored during the heat transfer process in the soil [19]. According to Fourier's heat conduction equation and the principle of energy conservation, the amount of heat conducted into a unit of soil is equal to the sum of the latent heat from phase change and the heat generated by temperature change. The heat transfer in the soil can be described by equation (8). Based on the energy conservation law for an infinitesimal element of frozen soil and Fourier's law of heat conduction, the first term on the left side of this equation represents the heat increment within the soil element. The first term on the right side of the equation represents the heat change within the soil element caused by heat conduction, with higher-order terms being neglected. During the freezing process of soil, pore water undergoes a phase change from liquid to ice, which is an exothermic process. The second term on the right side of the equation represents the heat change due to this phase transition.

$$\rho c \frac{\partial T}{\partial t} = \lambda \nabla^2 T + L \cdot \rho_i \frac{\partial \theta_i}{\partial t} \tag{8}$$

where ρ is the density of soil, c is the specific thermal capacity of soil, T is temperature, λ is the thermal conductivity of soil, L is the latent heat of transition if ice and water.

The volumetric heat capacity of a frozen soil is calculated as the sum of the heat capacities of each component, weighted by their corresponding volumetric fractions, as presented in equation (9) [20].

$$\rho c = C_w\theta_w + C_i\theta_i + C_s(1-n) \tag{9}$$

where C_w, C_i, C_s are the volumetric heat capacity of water, ice, soil particles, respectively, n is the porosity of the soil.

The developed LSB model was used to determine the thermal conductivity of frozen soil in a closed system, which can be expressed as a function of water content (w), unfrozen water content (w_u), dry density (ρ_d), temperature (T), fraction of gravel (f_{gravel}), sand (f_{sand}), silt (f_{silt}), clay (f_{clay}), as shown in equation (10).

$$\lambda = \Phi(w, \rho_d, T, f_{gravel}, f_{sand}, f_{silt}, f_{clay}) \tag{10}$$

Model Implementation

The theoretical framework for the water and heat transfer model consists of multiple partial differential equations and several unknown variables. Commercial software COMSOL Multiphysics was used to solve these equations as outlined in the preceding sections. To simulate the freezing process, a numerical model was developed using a soil column with a height of 0.1 m (H_y) and a width of 0.055 m (D). The initial temperature of the soil column was uniformly set to 5°C. The bottom of the soil column was maintained at a constant temperature of 5°C, while the upper boundary was subjected to a time-dependent temperature gradient, as illustrated in Figure 1. The temperature drop rate was set to 1°C per hour within specific temperature intervals, and the entire freezing process lasted for 120 hours. In this closed system, no water was allowed to enter or exit through the boundaries. Furthermore, the left and right sides of the soil column were thermally insulated, with no heat flux across them. The bottom of the soil column was fixed, while the upper boundary was set to allow free deformation in vertical direction.

For a specific soil with a water content of 24%, a dry density of 1.467 g/cm^3, and fractions of gravel, sand, silt, and clay of 0.36%, 22.16%, 57.67%, and 19.86%, respectively, the relationship between soil thermal conductivity and temperature was obtained using the LSB model for a temperature gradient from 5 °C to -20 °C. The results are shown in Figure 2. This relationship was used as an input function for thermal physical parameters in the model establishment.

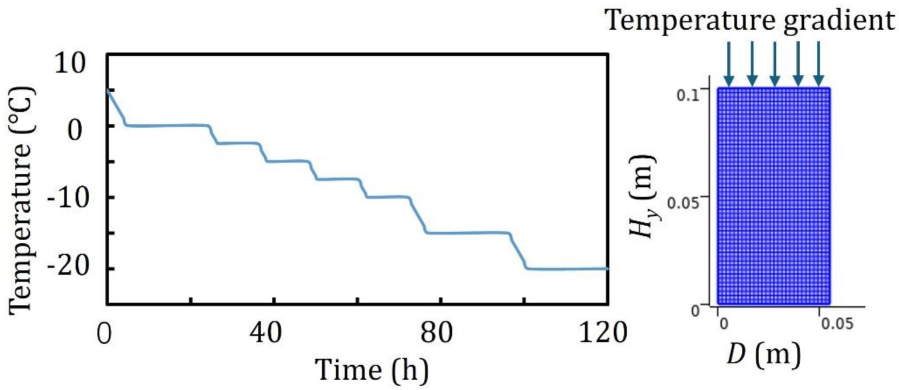

Figure 1: Temperature gradients and model sketch.

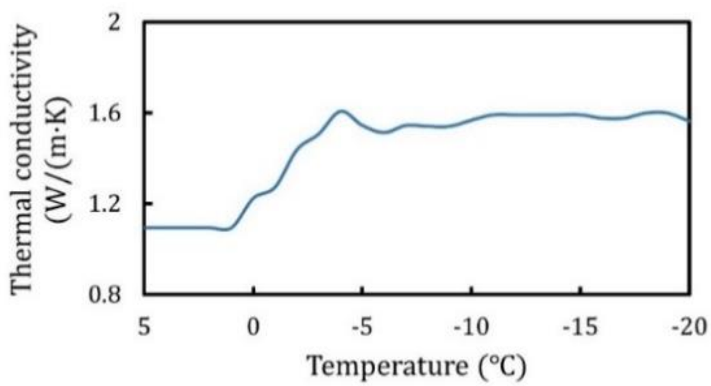

Figure 2: Thermal conductivity of the soil obtained from the LSB model.

Simulation Results and Discussions

The dynamic region known as the freezing front is the boundary or transition zone within the soil mass where liquid water transitions into ice as the temperature drops below the freezing point. The freezing front generally moves downward into the soil as cold temperatures from the surface penetrate deeper into the soil column due to thermal conduction. As shown in Figure 3, during the freezing process, the freezing front progressively moved downward through the soil column over time as lower temperatures were applied to the upper boundary. Water migrates toward the freezing front due to cryogenic suction and freezes upon reaching it, leading to the formation of ice lenses and an increase in frost heave. At the freezing front, water undergoes a phase change from liquid to solid, releasing latent heat. This latent heat temporarily slows the freezing rate, as it must be conducted away before further freezing can occur. Over time, the freezing front may stabilize if the heat influx from below balances the heat loss from the surface.

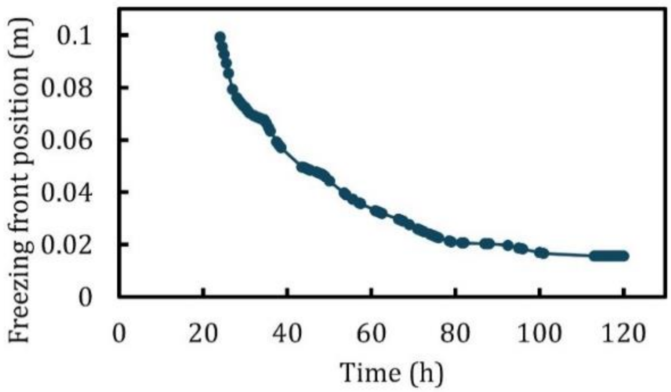

Figure 3: Movement of freezing front during the freezing process.

Figure 4 shows the changes in volumetric ice content at various H_y values over time, H_y represents the height along the central axis of the soil column, measured from the base. As the temperature at the upper boundary of the soil column decreases, the freezing front penetrates deeper into the soil. Water in the pores gradually turns into ice, increasing the volumetric ice content in the soil. The volumetric ice content at higher height is higher than that at lower height of the soil column. When the temperature is near the water-ice phase transition range, the change in volumetric ice content becomes significant, and the rate of increase in volumetric ice content with decreasing temperature is relatively high. Such a behavior may be attributed to a large amount of unfrozen water that gradually freezes into ice within this temperature range, leading to a noticeable rise in volumetric ice content. However, as the temperature drops further below -5°C, most of the unfrozen water in the soil at this temperature is already in a frozen state. The increase in volumetric ice content slows down for such a scenario with the slope becoming noticeably smaller. This phenomenon indicates that the impact of temperature on soil ice content is most pronounced near the phase transition temperature, while at extremely low temperatures, the changes are minimal.

The phase change from water to ice generates additional stress among soil particles, water, and ice. When this stress exceeds the initial consolidation pressure and the ice volume increment surpasses the tolerance of the soil pores, frost heave occurs. Figure 5 shows the displacement of points at different heights along the central axis of the soil column. Near the surface (the low-temperature region), displacement begins to increase once the temperature drops below the freezing point. As the temperature continues to decrease, the phase change causes significant volumetric expansion, leading to a noticeable increase in volumetric strain, while the rate of displacement growth slows down due to the reduction in unfrozen water available for ice formation. Meanwhile, frost heave near the lower boundary accumulates, contributing to the overall upward displacement of the soil column's upper surface.

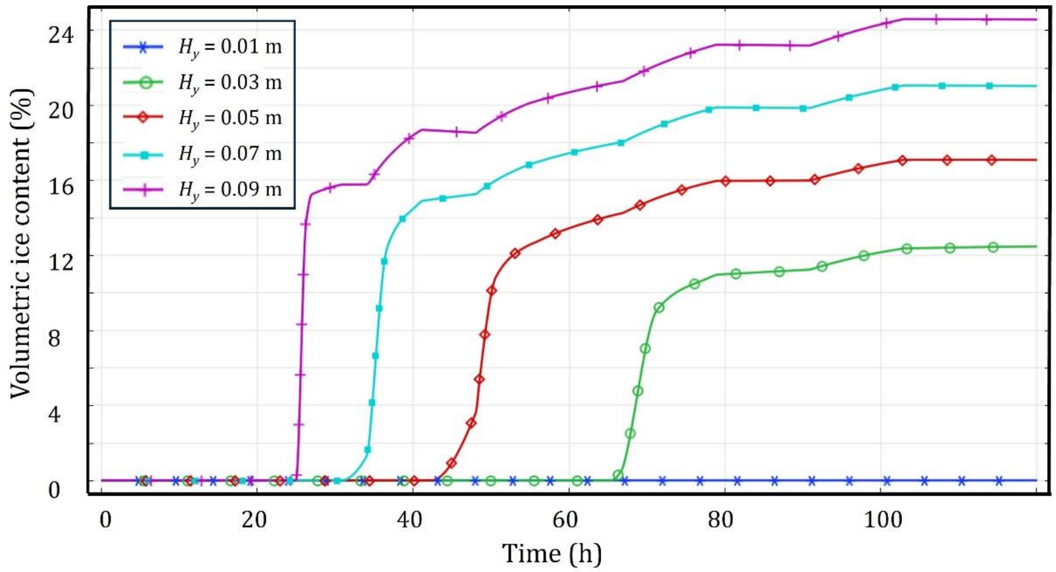

Figure 4: Variation of volumetric ice content over time at different heights in the soil column.

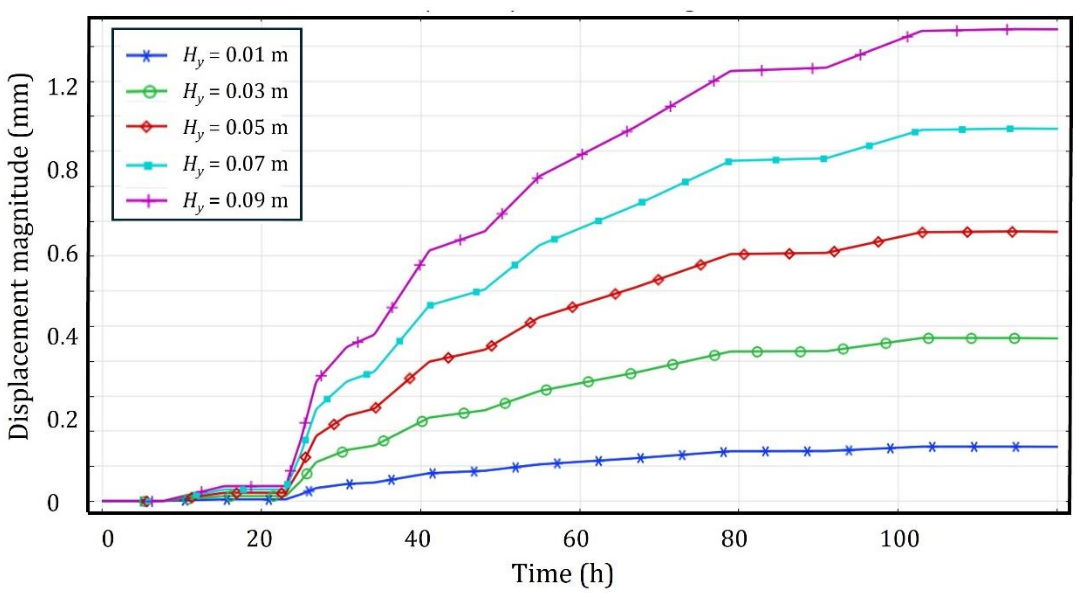

Figure 5: Displacement at different heights of the central axis of the soil column.

Conclusions

The numerical simulation of the freezing process in a closed-system soil column effectively captured the migration of the freezing front, changes in volumetric ice content, and soil displacement. This was achieved by integrating a machine learning approach, specifically an ensemble learning-based thermal conductivity model with simple input parameters.

During the simulation, the freezing front in the soil column, measured from the top boundary, progressively moves downward as cold temperatures penetrate deeper due to thermal conduction, with latent heat release temporarily slowing the freezing rate until thermal equilibrium is reached. As the freezing front advances, the volumetric ice content is higher at greater heights in the soil column compared to lower ones. The most significant changes in volumetric ice content occur near the water-ice phase transition range, where rapid freezing of unfrozen water leads to substantial ice formation. However, as the temperature drops below -5°C, the rate of change in volumetric ice content with temperature decreases. Displacement increases near the surface as the temperature falls below the freezing point, volumetric strain rises significantly near the freezing point due to rapid ice formation, while frost heave near the lower boundary accumulates, collectively causing an upward displacement of the soil column's upper surface.

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