Numerical Modelling of Vapour-Ice Desublimation Process in Unsaturated Freezing Soils

Jidong Teng[1(✉)], Feng Shan[1], Sheng Zhang[1], and Daichao Sheng[1,2]

[1] Central South University, Changsha 410075, China
jdteng@csu.edu.cn
[2] The University of Newcastle, Callaghan, NSW 2308, Australia

Abstract. Recent studies reveal that ice formation via vapour-ice desublimation in unsaturated freezing soils can lead to damage to infrastructures. Actually, the role of vapor flow in a freezing soils is unclear, and it is usually ignored when analyzing water migration process. In this study, a theoretical framework is established to formulate the coupled thermal and hydrological process, where the vapour diffusion governs the mass transfer process. The new model is designed to avoid using the local equilibrium assumption and the hydraulic relations that accounts for liquid water flow. This model contains 6 undetermined variables that are interacted in the 6 governing equations. In order to validate the numerical formulations/codes, a series of laboratory experiments are performed on a coarse sand which is not considered as frost susceptibility soil. The computed results show that the proposed model can indeed reproduce the unusual moisture accumulation observed in relatively dry soils, while the result agree well with the experimental date. This model provides an explanation for coupled movement of heat and moisture in cold and arid regions.

Keywords: Vapour-ice desublimation · Unsaturated soil · Diffusion Numerical model

1 Introduction

Freezing and thawing processes are of great importance in cold regions as it may cause many engineering problems, including cracking of pavements, damage to the foundation of structures, and fracture of piplines (Lai et al. 2014; Sheng et al. 2014). Much attention initially focused on the problem of frost heave that is caused by the liquid water migration from warm to cold region in freezing soils (Konrad 1999). Nevertheless, recent studies have showed that vapour transfer in unsaturated freezing soils could lead to a large amount of ice formation, which may cause damage to infrastructures (Eigenbrod and Kennepohl (1996); Zhang et al. (2016a); Niu et al. (2017)).

When using the existing models to analyze the unusual frost damage as mentioned above, it is found they are always incapable of revealing the mechanism. The reason can be as follows. Firstly, in the earlier studies, vapour flow is usually assumed to make negligible contribution to the overall moisture transfer in a freezing soil (Harlan 1973). Secondly, in the case that water content of soil is relatively low, for example near to the

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residual water content, liquid water flow may be insignificant comparing to vapour flow at this stage (Zhang et al. 2016b). It is inaccurate to describe mass flow by using soil water retention curve and the derived unsaturated permeability function (Fredlund and Rahardjo 1993). Thirdly, the mechanism of multi-phase flow in unsaturated freezing soils have been less understood (Pauwels and Wood 1999; Decker and Zeng 2006). Since a number of empirical equations are used in the existing models to clarify the role of ice phase, but these empirical relations are hard to validate in laboratory test. Therefore, although many existing models have been reported to deal with soil freezing issue, few of them can truly describe the vapour flow process in unsaturated freezing soils.

In this study, to better understand the mechanism of vapour-ice desublimation in unsaturated freezing soils, a theoretical framework is established. The new model is designed to avoid using the local equilibrium assumption and the hydraulic relations that accounts for liquid water flow. The coupled model was solved by finite element method. A series of laboratory experiments are performed to validate the proposed model. Finally, some conclusions are drawn based on the numerical and experimental results and discussion.

2 Materials and Methods

2.1 Theory

(1) Physical process and basic assumption

The physical system is depicted as a vertical, one-dimensional soil profile that is covered by an impermeable plate (see Fig. 1). The soil is considered as a homogeneous porous media. Vapour will diffuse from the warmer and more humid end to the colder and dryer end. When the vapour reaches the cold and impervious cover, it will change into ice directly through desublimation, causing the ice lens forming just beneath the impervious cover. In vapour transfer zone, the vapour flow is governed by the vapour density in soil and will condense into liquid water. If the soil temperature at a certain depth drops below than 0 °C (freezing front, as shown in Fig. 1), the condensed water will solidify into pore ice.

In order to simplify the quantitative description of coupled process with phase change, some assumptions are made as follows:

a. The deformation of the soil matrix due to variations of temperature and pore water pressure or ice formation can be neglected.
b. The freezing front is always located at the depth where the soil temperature is 0 °C.

(2) Governing equations

The governing equation for one-dimensional vapour flow in an unsaturated freezing porous medium is given as follows:

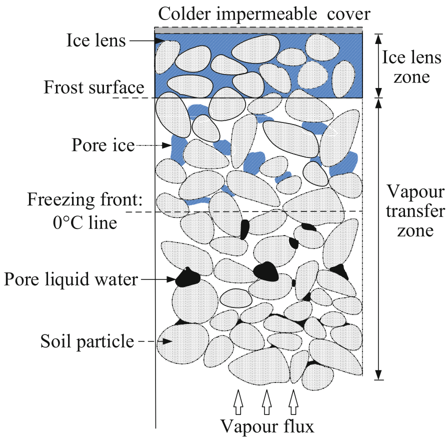

Fig. 1. Schematic diagram of the vapour-ice desublimation process in soil.

$$\frac{\partial(n(1-S)\rho_v)}{\partial t} + \frac{\partial(nS\rho_w)}{\partial t} = \frac{\partial}{\partial z}\left(K_T \frac{\partial T}{\partial z} + K_s \frac{\partial S}{\partial z}\right) \tag{1a}$$

$$K_T = \frac{K}{\mu_v} R \rho_v^2 \tag{1b}$$

$$K_S = \left[\frac{K}{\mu_v} R \rho_v T + \frac{(1-S)n}{\tau} D\right] \frac{\partial \rho_v}{\partial S} \tag{1c}$$

Where z(m) and t(s) represent soil depth and time, respectively, n is the porosity of soil (dimensionless), S is the saturation of liquid water and pore ice (dimensionless), here $S = S_w + S_i\rho_i/\rho_w$. T is temperature (K). ρ is the mass concentration in soil (kg m^{-3}). The subscripts w, v, and i denote the liquid water, vapour and pore ice, respectively. K_S and K_T are the effective diffusivity by saturation gradient (kg m^{-1} s^{-1}) and the effective mass conductivity by temperature gradient (kg m^{-1} s^{-1} K^{-1}), respectively. R is the specific gas constant of water vapour (461.89 J kg^{-1} K^{-1}). μ_v is dynamic viscosity of vapour (kg m^{-1} s^{-1}). D is vapour diffusivity in soil (m^2 s^{-1}), τ is the tortuosity factor (unitless), which indicates ratio of the real length of transfer path to the apparent length.

It has been found that the sensible heat associated with vapour movement is insignificant because it is two orders of magnitude smaller than the heat conduction (Zhang et al. 2007). Therefore, the heat balance equation with water phase change in soil can be written as

$$\rho C \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[(\lambda + K_T L_{i,v}) \frac{\partial T}{\partial z}\right] + \frac{\partial}{\partial z}\left(K_S L_{i,v} \frac{\partial S}{\partial z}\right) - L_{i,w} \frac{\partial(nS_w\rho_w)}{\partial t} \tag{2a}$$

$$\rho C = (1-n)\rho_s C_s + nS_i\rho_i C_i + nS_w\rho_w C_w + n(1-S)\rho_v C_v + n(1-S)L_{i,v}\frac{\partial\rho_v}{\partial T} \quad (2b)$$

$$\lambda = (1-n)\lambda_s + nS_i\lambda_i + nS_w\lambda_w + n(1-S)\lambda_v \quad (2c)$$

Where ρ is the total density of soil, C is the volumetric heat capacity as expressed by Eq. (2b). λ is the thermal conductivity (W m^{-1} K^{-1}) as expressed by Eq. (2c). L represents the latent heat changes between different phases. The subscripts s and v in above equations indicate the solid phase and vapour phase in soil.

When ice phase forms in an unsaturated freezing soil, the saturation of the remained unfrozen water can be expressed as a function of temperature. Anderson and Morgenstern (1973) found that the relationship between the unfrozen liquid water content and temperature of freezing soils can be reasonably approximated with a power law:

$$S_{uw} = \frac{\rho_s}{\rho_w}\frac{(1-n)}{100n}\alpha(T_0 - T)^{\beta} \qquad T \le T_0 \quad (3)$$

Where T_0 is the freezing point of free water (273.15 K), α and β are empirical fitting parameters that is dependent on the specific surface area of soil.

The variable S_{uw} in Eq. (3) indicates the maximum liquid water content that will not freeze at a subzero temperature T. Base on the computed values of S and S_{uw}, the criteria for determining the saturations of pore ice and liquid water can be obtained as follows

$$S_i = \begin{cases} 0 & T > T_0 \\ 0 & T \le T_0 \text{ and } S \le S_{uw} \\ \rho_w(S - S_{uw})/\rho_i & T \le T_0 \text{ and } S \le S_{uw} \end{cases} \quad (4a)$$

$$S_w = S - S_i\frac{\rho_i}{\rho_w} \quad (4b)$$

It has been recognized from chemical engineering that an adsorption-desorption equilibrium relationship should be replaced to describe the desublimation or sublimation process of a hygroscopic porous media with bound moisture (Liapis and Bruttini 1994). Such a relation is adopted here to describe the equilibrium state among vapour, pore ice and liquid water in an unsaturated freezing soils, as follows

$$\frac{P(T,S)}{P_{vs}(T)} = e^{\frac{-\gamma(1-S)}{SRT}} \quad (5)$$

Where $P(T, S)$ is the equilibrium vapour pressure in unsaturated freezing soil (Pa), it is a function of temperature T and saturation S. $P_{vs}(T)$ is the saturated vapour pressure at temperature T (Pa). γ is an empirical parameter.

(3) Soil hydraulic properties

As for the unsaturated freezing state, an expression for K can be obtained by adding an impedance factor to the permeability function of air phase in soil (Brooks and Corey 1964; Zhang et al. 2016a).

$$K(S)= 10^{-cS_i} k_s (1-S)^2 (1-S^{\frac{2+b}{b}}) \tag{6}$$

Where b and c are fitting parameters. The term of 10^{-cSi} denotes the obstruction of pore ice to vapour flows.

Vapour transport in porous medium as described by Fick's law can be divided into two types due to the different mechanisms, molecular diffusion and Knudsen diffusion. The harmonic averaging method is used to calculate the vapour diffusivity D bases on the molecular diffusion coefficient D_m and the Knudsen diffusion coefficient D_k,

$$D = \frac{1}{1/D_m + 1/D_k} \tag{7a}$$

$$D_m = 0.66n(1-S)D_a \tag{7b}$$

$$D_k = 97.0\frac{d}{2}\sqrt{\frac{T}{m_w}} \tag{7c}$$

Where D_a is the diffusivity of water vapour in air (m^2 s^{-1}), d is the average pore diameter (m), m_w is the molecular wright of water (kg mol^{-1}).

The governing equations consist of mass conservation equation Eq. (1a, 1b, 1c), and energy balance equation Eq. (2a, 2b, 2c), which are highly non-linear and coupled. There are 4 undetermined variables in the two equations, S_w, S_i, T and ρ_v. While Eqs. (3) to (5) provide the other three additional relations by adding a new variable S_{uw}, such that the simultaneous equations can be solved mathematically.

2.2 Testing Program

Teng et al. (2018) have performed a series of freezing tests on unsaturated coarse sand on basis of a newly developed device. In the reported test, the soil sample was packed into a cylinder that was 13.5 cm long and 10 cm in diameter. The top and bottom of the soil sample was exposed to the temperatures of ″′+″ °C and 10 °C, respectively. The side wall of the cylinder was thermally insulated. Thus, the sample was subjected to freezing from the top down. The cylinder were taken from the freezing apparatus after 7 days, and then the soil samples were divided into 1-cm-thick slices and dried in an oven to obtain total water content (liquid water plus ice) distributions. 14 different conditions are reported in Teng et al. (2018), but here we adopted the two cases to verify the proposed model, their initial water content are 0%, and 5%, respectively.

3 Result and Discussion

The governing equations, combined with appropriate initial and boundary conditions, are solved numerically using the finite-element method for spatial discretisation and the finite-difference method for temporal discretisation. The solution procedure is facilitated by the Comsol Multiphysics package (5.3). Table 1 gives the values of the related parameters in this model.

Table 1. The input used in the numerical computation.

Symbol	Value	Symbol	Value
$\rho_w\left(\mathrm{kg\ m^{-3}}\right)$	1000	α	1.69
$\rho_i\left(\mathrm{kg\ m^{-3}}\right)$	913	β	−0.81
$\lambda_i\left(\mathrm{W\ m^{-1}K^{-1}}\right)$	2.22	$K_s\left(\mathrm{m^2}\right)$	4×10^{-12}
$\lambda_s\left(\mathrm{W\ m^{-1}K^{-1}}\right)$	2.68	$C_i\left(\mathrm{J\ kg^{-1}K^{-1}}\right)$	1930
$\lambda_v\left(\mathrm{W\ m^{-1}K^{-1}}\right)$	0.022	$C_s\left(\mathrm{J\ kg^{-1}K^{-1}}\right)$	800
$\lambda_w\left(\mathrm{W\ m^{-1}K^{-1}}\right)$	0.54	$C_v\left(\mathrm{J\ kg^{-1}K^{-1}}\right)$	1886
$L_{i,v}\left(\mathrm{J\ kg^{-1}}\right)$	2.839×10^6	$C_w\left(\mathrm{J\ kg^{-1}K^{-1}}\right)$	4180
$L_{i,w}\left(\mathrm{J\ kg^{-1}}\right)$	0.334×10^6	$C_i\left(\mathrm{J\ kg^{-1}K^{-1}}\right)$	1930
$\mu_v\left(\mathrm{kg\ m^{-1}s^{-1}}\right)$	$0.011 \times (T/273.15)^{1.5}/(T + 961)$	$T_0(\mathrm{K})$	273.15
$D_a\left(\mathrm{m^2s^{-1}}\right)$	$2.12 \times 10^5(T/273.15)^2$		

Figure 2a shows the measured profile of the gravimetric water content at 7 days for the initial dry soil. The tests are also simulated by using the proposed model, and the simulation results are also presented in Fig. 2a for comparison. It is shown that the computed results are close to the measured values. In particular, the rapid increase in the total water content immediately below the imperious cover is well captured by the numerical simulation. An evident increase in water content is observed in the top zone of the soil column, where the water is the mainly in ice phase that is feed by the vapour flow. The measured and simulated temperature profiles at different time are presented in Fig. 2b. A good agreement can be observed between the simulated and experimental values of the soil temperature at most times. The results also show that an approximately linear profile is obtained after approximately 1 day.

The measured and computed water content profiles for the case of 5% initial water content are presented in Fig. 3. It can be shown that the predicted results fairly agree with the measured data. The two peak water contents at top surface and the freezing front can be simulated by the proposed model, but the measured water content profile at super-zero zone is fitted relatively poorly. The increase of measured water content at bottom is caused by the downward drainage of liquid water due to gravity, while the proposed model only considers the flow of vapour in soil and neglects the liquid water. It is noted that the proposed model reveals mechanism of the two usual peak water contents. The top peak water content represents the formation of clear ice between the soil specimen and the top plate. The second peak was caused by the vapour flow that impeded at freezing front.

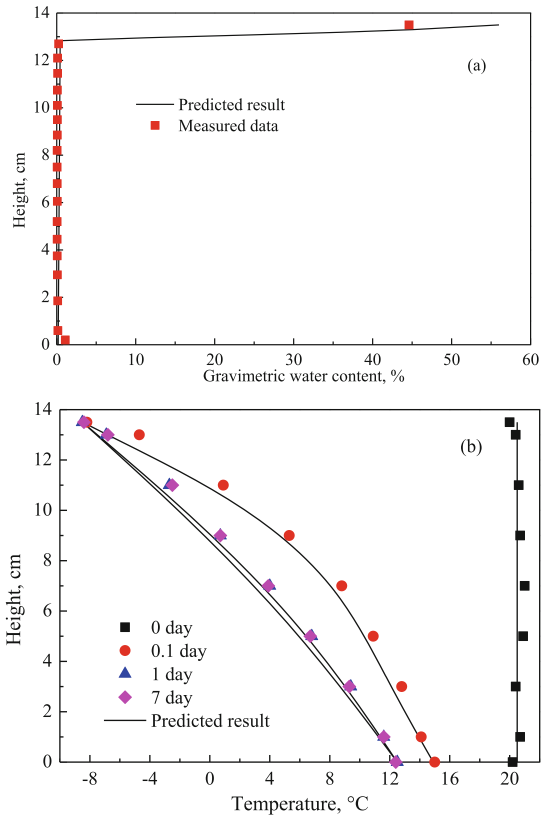

Fig. 2. (a) Comparison between measured and predicted water content after 7 days; (b) Measured and simulated temperature profiles. The initial water content is 0%.

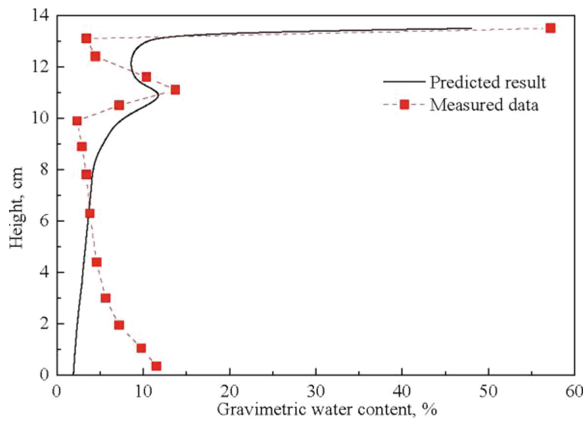

Fig. 3. Comparison between measured and predicted water content for the case that the initial water content is 5%.

4 Conclusions

The mechanism of vapor flow and its phase change in unsaturated freezing soils has been less understood. In this paper, a mathematical model for describing the vapour flow and heat transfer is presented and applied to the analysis of the unusual fluid transfer phenomena in unsaturated freezing soil. The model differs from the previous models, it avoids using the local equilibrium assumption and the hydraulic relations that account for liquid water flow. The vapour flow in this model is governed by vapour density or vapour pressure, which is more close to the physical situation.

A series of laboratory experiments are performed to validate the proposed model. The computed results show that the proposed model can indeed reproduce the unusual ice accumulation observed in unsaturated soils. Meanwhile the predicted result generally agrees with the experimental date, which indicates the proposed model is capable of describing the vapour-ice desublimation process. This model provides an explanation for coupled movement of heat and moisture in cold and arid regions.

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