



Numerical Modeling of Water-Vapor Migration and Phase Transformation in Unsaturated Freezing Soils

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Abstract. Because of ignoring the vapor migration in freezing soils, coarse-grained soils have long been deemed not susceptible to frost heave. However, recent studies reveal that vapor migration can increase the total water content and lead to remarkable frost heave hazards in coarse-grained soils. In this paper, a new numerical model is developed based on the coupled thermal and hydrological processes. The soil water characteristic curve and the soil freezing characteristic curve are taken into account in this model. The model is established by using COMSOL Multiphysics which contains 5 equations and 5 variables. In order to validate the numerical model, laboratory experiments were performed in coarse-grained soils. The result shows that there are sharp increases in water content at the top of samples and the freezing front. A good match between measured and computed results indicates that the new model can make a good explanation for the coupled movement of heat and moisture in coarse-grained soils.

Keywords: Water-vapor migration · Moisture accumulation · Numerical model

1 Introduction

The freezing and thawing processes are important factors in the engineering in cold and arid regions, including destruction of roadbed hazards, foundation damage, and pipeline cracking, etc. (Sheng et al. 2014; Lai et al. 2014). Recently, many studies reveal that vapor migration can increase the total water content of coarse-grained soils and lead to remarkable frost heave (Niu et al. 2017). For example, in the cold and arid regions of northwest China, the silt area under the airport runway plate often presents high water content or frost heave hazards (Li et al. 2014).

Based on the traditional hydrothermal coupling theory, Zhang et al. (2016) and Teng et al. (2019) reproduced a series of laboratory experiments in terms of water-vapor migration phenomena in unsaturated freezing soils. These studies qualitatively explained the phenomenon of water accumulation and revealed the mechanism of

water-vapor migration under the impermeable covering. However, the coupling effect of water-vapor migration and phase transformation has not been clarified.

In this paper, through theoretical analysis of water-vapor migration and phase transformation, a new numerical model is developed based on the coupled thermal and hydrological process by using COMSOL Multiphysics. The soil water characteristic curve (SWCC) and the soil freezing characteristic curve (SFCC) are taken into account in this model.

2 Theory and Methods

2.1 Physical Process and Basic Assumption

The physical process is depicted as a vertical, one-dimensional soil profile that is covered by an impermeable cover (Fig. 1). Initial water in soil flows downward because of gravity. After that, water flows upwards and becomes pore ice owing to the temperature gradient in the freezing zone, and vapor diffuses from the warmer layer to the colder layer. When vapor reaches the cold and impervious cover, it will change into ice directly through desublimation, forming the ice lens just beneath the impermeable cover. Meanwhile, there are mixtures consisting of ice and soil particles at the freezing front.

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

- a. The deformation of the soil due to variations of temperature, pore water pressure, and ice formation can be neglected.
- b. The hysteretic effect of SWCC is not considered.
- c. Assuming the density of pore ice in soil is constant.

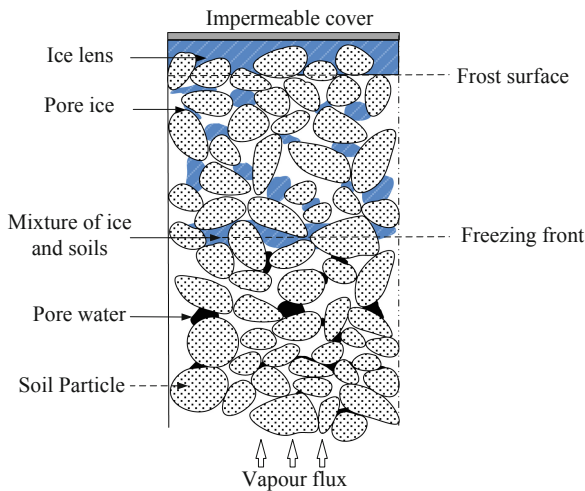


Fig. 1. Schematic diagram of the water-vapor migration process in soil

2.2 Governing Equation

(1) Mass governing equations

Water migrates under the action of matrix potential, temperature potential and gravity potential in unsaturated freezing soil. The mass governing equation for one-dimensional moisture migration is given as follows:

$$\frac{\partial \theta_w}{\partial t} + \frac{\partial \theta_v}{\partial t} + \frac{\rho_i}{\rho_w} \frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial x} \left[K'_{wh} \left(\frac{\partial h}{\partial x} + 1 \right) + K_{wT} \frac{\partial T}{\partial x} + K_{vh} \frac{\partial h}{\partial x} + K_{vT} \frac{\partial T}{\partial x} \right] \quad (1)$$

where x and t represent soil depth (m) and time (s) respectively, h is water head (m) and T is temperature (K). θ , ρ and q are volumetric water content (%), density (kg m^{-3}) and flux (m s^{-1}), and the subscripts w , v , i and s denote the water, vapor, ice and soil respectively. K'_{wh} , K_{wT} represent the hydraulic conductivity by matrix potential at negative temperature (m s^{-1}) and temperature potential ($\text{m}^2 \text{s}^{-1} \text{K}^{-1}$), while K_{vh} , K_{vT} represent the diffusivity coefficient by matrix potential (m s^{-1}) and temperature potential ($\text{m}^2 \text{s}^{-1} \text{K}^{-1}$).

(2) Energy governing equations

The energy governing equation of moisture migration is shown as follows:

$$C_p \frac{\partial T}{\partial t} + L_w \rho_w \frac{\partial \theta_v}{\partial t} - L_i \rho_i \frac{\partial \theta_i}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} - C_w \frac{\partial q_w T}{\partial x} - C_v \frac{\partial q_v T}{\partial x} - L_w \rho_w \frac{\partial q_v}{\partial x} \quad (2)$$

Equivalent specific heat capacity C_p is the cumulative sum of the proportions of each component (De Vries 1958). L_l and L_i are latent heat of water (2.50 kJ kg^{-1}) and ice (0.334 kJ kg^{-1}), and λ is the coefficient of thermal conductivity (Chung and Horton 1987).

(3) The soil water characteristic curve

The soil water characteristic curve is a functional curve describing the constitutive relationship between matric suction and water content. This paper adopts Fredlund et al. (1994) model (abbreviated FX model):

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\{\ln[e + (h/a)^n]\}^m} \quad (3)$$

where θ_s and θ_r are saturated volumetric water content (32%) and residual water content (0%), FX model is determined by three empirical shape parameters a , n , m by measuring the inflection point of SWCC (-0.05, 1.6, 1.8, unitless).

(4) The soil freezing characteristic curve

The soil freezing characteristic curve describes the relationship of temperature and unfrozen water content in soil, and water content decreases rapidly and forms pore ice below the freezing point. Unfrozen water content θ_u (%), based on FX model, has the same fitting parameters to express:

$$\theta_u = \theta_r + \frac{\theta_s - \theta_r}{\{\ln[e + (h_i/a)^n]\}^m} \tag{4}$$

Based on the thermodynamic theory and the Clausius–Clapeyron equation, the relationship of water head in frozen soil h_i and temperature, referred to as the freezing-point depression equation, can be derived as $h_i = L_i(T - T_0)/gT_0$ (Zhang et al. 2007).

(5) The relationship among water, ice and vapor content

Based on the relationship of SWCC and SFCC, water, ice and vapor content are given as follows:

$$\theta_w = \begin{cases} \theta_u & T \leq T_0, \theta > \theta_u \\ \theta & \text{else} \end{cases} \tag{5}$$

$$\theta_i = \frac{\rho_w}{\rho_i} (\theta - \theta_w) \tag{6}$$

$$\theta_v = \rho_{vs} H_r \frac{\theta_s - \theta}{\rho_w} \tag{7}$$

2.3 Establishing the Numerical Model

In the one-dimensional model, two physics of coefficient form of partial differential equation (PDE) are added, corresponding mass governing equations and energy governing equations. There are 50 fixed elements in the 13.5 cm interval (it differs a little if the meshes are more than 30 elements). The top and bottom boundary are set as $-5\text{ }^\circ\text{C}$ and $10\text{ }^\circ\text{C}$ respectively and initial volumetric water content is 7%. This study calculates 1, 3, 5, and 7 days in time dependent. Table 1 gives the values of the related parameters and variates in this model.

Table 1. The input used in the numerical computation

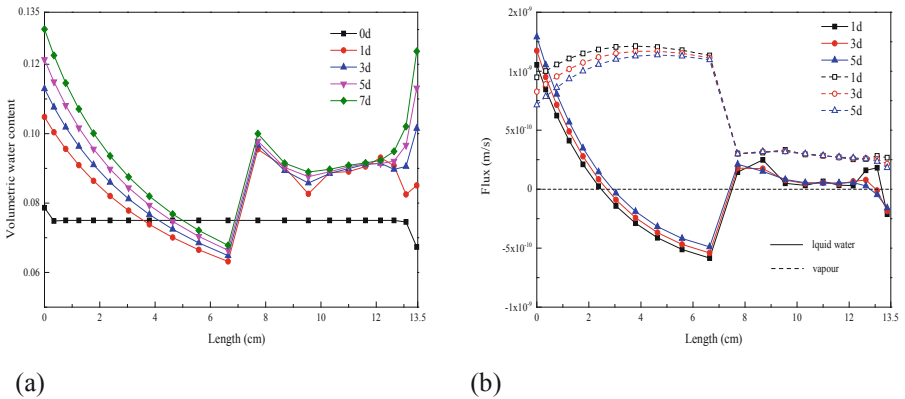
Symbol	Value	Symbol	Value
T_0 (K)	273	k_s (m s ⁻¹)	3.47×10^{-5}
ρ_i (kg m ⁻³)	913	ρ_d (kg m ⁻³)	1400
ρ_w (kg m ⁻³)	1000	ρ_s (kg m ⁻³)	2700
C_n (MJ m ⁻³ K ⁻¹)	2.16	C_w (MJ m ⁻³ K ⁻¹)	4.18
C_v (kJ m ⁻³ K ⁻¹)	6.3	C_i (MJ m ⁻³ K ⁻¹)	1.74
D_v (m ² s ⁻¹)	$2.12 \times 10^{-5} \left(\frac{T}{T_0}\right)^2$	D (m ² s ⁻¹)	$\frac{(\theta_s - \theta)^{10}}{\theta_s^{10}} D_v$
K_{wh} (m s ⁻¹)	$k_s \left(\frac{\theta_w}{\theta_s}\right)^N$	K_{wT} (m ² s ⁻¹ K ⁻¹)	$K_{wh} \left(HG_{wT} \frac{1}{\gamma_0} \frac{d\gamma}{dT} \right)$
K_{vh} (m s ⁻¹)	$\frac{D}{\rho_w} \left(\rho_{vs} H_r \frac{Mg}{RT} \right)$	K_{vT} (m ² s ⁻¹ K ⁻¹)	$\frac{D}{\rho_w} \left(\eta H_r \frac{d\rho_{vs}}{dT} \right)$
K'_{wh} (m s ⁻¹)	$10^{-10\theta_i} \times K_{wh}$	H_r	exp(HMg/RT)
C_p (J K ⁻¹ m ⁻³)	$C_n(1 - \theta_s) + C_w\theta_w + C_v\theta_v + C_i\theta_i$		
ρ_{vs} (kg m ⁻³)	exp(31.37 - 6014.79/T - 7.92 × 10 ⁻³ T)/1000T		
λ (W K ⁻¹ m ⁻¹)	0.228 - 2.406(θ _w + Fθ _i) + 4.909√(θ _w + Fθ _i)		

Notes: Saito et al. (2006) gave the equations of the hydraulic conductivity (K_{wh} , K_{wT}) and the diffusivity coefficient (K_{vh} , K_{vT})

3 Results and Discussion

3.1 Volumetric Water Content

The computed water content profiles for the case of 7% initial volumetric water content are presented in Fig. 2a. In the freezing zone, it can be shown that peak water content appears at the top surface and the freezing front. Pore ice content increases with the increase of the time at the top from 7% to 12.5%, while it changes a little at freezing front around 10%. In the unfrozen zone, water content decreases with the increase of the height in space.


Fig. 2. (a) Volumetric water content curve and (b) Migration flux curve

3.2 Migration Flux

Figure 2b compares the change over time between water migration flux (full line) and vapor migration flux (imaginary line). In the unfrozen zone, water flows upwards at the range of 0–2.5 cm and flows downward at the range of 2.5–7.5 cm. In the freezing zone, water migration becomes negative at the top surface, which means water flows downward. Vapor diffuses upwards in unfrozen zone, while vapor migration flux remains almost the same in time in freezing zone.

Upward vapor migration flux is much higher than that of water both in unfrozen zone and freezing zone. It is concluded that vapor migration is the main mechanism of pore ice formation during the process of water-vapor migration and phase transformation in porous media.

3.3 Comparison Between Computed Results and Experiment Data

Teng et al. (2019) have performed a series of freezing tests on unsaturated quartz sand based on a newly developed device. The computed and measured water content profiles are presented in Fig. 3. It can be shown that the predicted results fairly agree with the measured data. Two peak water contents at the top surface and the freezing front can be simulated by the proposed model. However, the measured data are higher than computed results in these two areas. In the unfrozen zone, water content decreases with the increase of height both in experiments and computed models.

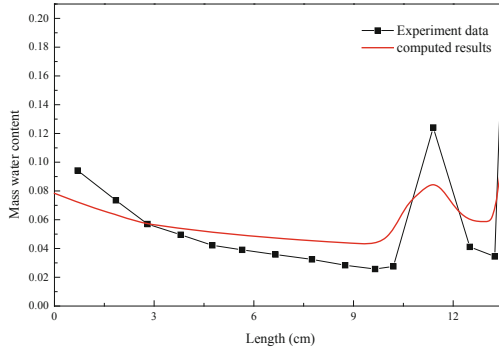


Fig. 3. Comparison between computed and measured water content

4 Conclusion

The mechanism of water-vapor migration and phase transformation in unsaturated freezing soils has been less understood. In this paper, a mathematical model for describing the vapor flow and heat transfer is presented and applied by COMSOL. Comparison of experimental data and simulation results shows that:

- (1) In freezing zone, peak water content appears at top surface and freezing front. In unfrozen zone, water content decreases with the increase of the height in space.

- (2) Vapor migration flux is much higher than that of liquid water both in unfrozen zone and freezing zone, so vapor migration is the main mechanism of pore ice formation.
- (3) There are two peak water contents at top surface and the freezing front. Water content curve trend fairly agree with the measured data in unfrozen zone, decreasing with the increase of height.

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