



Heat and mass transfer effects of ice growth mechanisms in a fully saturated soil



Daoyong Wu^{a,b}, Yuanming Lai^{a,c,*}, Mingyi Zhang^a

^a State Key Laboratory of Frozen Soil Engineering, Cold and Arid Regions Environmental and Engineering Research Institute, Chinese Academy of Sciences, Lanzhou 730000, China

^b University of Chinese Academy of Sciences, Beijing 100049, China

^c School of Civil Engineering, Lanzhou Jiaotong University, Lanzhou, Gansu 730070, China

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ABSTRACT

To control heat and mass transfer during freezing, it is essential to understand the phase change behavior of ice crystals. However, limited research has been performed on the coupling effects involved in the kinetics of ice crystal nucleation and growth with fluid flow and heat transfer in porous media. In this paper, the conditions of nucleation and crystal growth, which must be met during the ice crystallization process, were studied. In the process of water freezing, we thought water activity is the inducing factor of the ice-water phase transformation. Based on the 'water-activity criterion', a macro kinetic model of ice crystal growth was established, which is useful to quantify the processes of nucleation and growth coupled with fluid flow and heat transfer. The driving force of moisture migration is the chemical potential gradient under different temperatures based on thermodynamics, which is different from the conventional form obtained from Darcy's law. In addition, a mathematical model coupling the heat-fluid transport in a fully saturated soil with phase change was proposed. Because the problem is significantly nonlinear, a numerical method for its solution was applied, and the temperature, moisture and frost heave of a soil column during the freezing process were calculated. Validation of the model is illustrated by comparisons between the simulation and experimental results. From this study, it is found that temperature has a great influence on the distribution of the total water content during ice crystallization and moisture migration, and the relationship between water velocity and temperature can be used to explain the distribution of the water content. The predicted values are consistent with the experimental data and verify the accuracy of the crystallization kinetics approach that couples heat and mass transfer in porous media.

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1. Introduction

Studies on the freezing processes of porous media play an important role in environmental, energy, biological and industrial systems. For example, the natural freeze–thaw cycle in cold areas, food storage, thermal energy storage and refrigerated storage of biological tissues all involve the freezing phenomenon. In addition, frost heave and thaw settlement in frozen soil during the freeze–thaw cycle in cold regions have a significant impact on foundation and road engineering [1–3]. Numerous studies [4–6] have investigated the phenomena of heat and mass transfer in porous media, and the phenomena are strongly coupled [7–8]. Harlan [9],

Guymon et al. [10] and other scholars have correlated the water transport mechanisms in partially frozen soil with the water transport mechanisms in unsaturated soil and then built a hydrodynamic model coupled the heat–fluid transport in porous media. Based on the secondary frost heave model presented by Miller [11], O'Neill [12] advanced the rigid ice model. Konrad and Morgensten [13] proposed the concept of segregation potential and then established the segregation potential theory. Masami and Seiti [14] verified this model and applied it to the prediction of field frost heaving. Another theory [15,16] based on the mixture model has been widely adopted to describe heat and mass transfer in porous media. However, Tani [17] suggested that the axiomatic theory of mixtures can lead to a temperature with no lower bound. Thus, the development of an accurate model of heat and mass transfer in porous media remains a challenge, particularly for immiscible solid–fluid mixture.

These above mentioned models only produce rough predictions of the overall variation in the temperature and moisture fields,

* Corresponding author at: State Key Laboratory of Frozen Soil Engineering, Cold and Arid Regions Environmental and Engineering Research Institute, Chinese Academy of Sciences, Lanzhou 730000, China. Tel.: +86 931 4967288; fax: +86 931 8279968.

E-mail addresses: wdy123456@yeah.net (D. Wu), ymlai@lzb.ac.cn (Y. Lai), myzhang@lzb.ac.cn (M. Zhang).

Nomenclature

A	frequency factor	p_w	water pressure
a_w	water activity	Q_T	heat source
C_i, C_w	concentrations of ice and water	r, r_{crit}	crystal radius and critical radius
$C_{p,eff}$	effective specific heat capacity	r_p	radius of a cylindrical pore
$C_{p,\alpha}$	specific heat capacity of α -phase	S_w	saturation degree of water
ΔC_p	specific heat capacity difference	ΔS_{fv}	entropy of fusion per unit volume crystal
e	total enthalpy per unit volume porous medium	$T, \Delta T$	temperature, supercooling degree
e_α	enthalpy of α -phase	$T^*, T_0^*, \Delta T^*$	freezing point of pore water, bulk water, and increment of freezing point
F_m	body force of per mole water	u_w	water velocity in unit volume porous medium
f_m	body force of unit volume	v	velocity of unit volume water
$\Delta G_V, \Delta G_S, \Delta G_C$	free energy variation in volume, surface and crystal	$V_{m,w}$	molar volume of water
$\Delta G_{crit}, \Delta G_0$	nucleation work, activation energy	Ω	volume of a single molecule
Δg_v	single molecule free energy decrease	γ_{sf}	surface tension between ice and water
$\Delta_m H_1$	molar latent heat	ν	molecule collision frequency
H	frost heave	ν_0	pre-exponential factor of collision frequency
h_c	convective heat transfer coefficient	$\mu_w, \mu_{w,0}$	chemical potential of water and pure water
q_h	heat flux at boundary	θ_α	volume content of α -phase
I	probability of forming supercritical embryos	θ_{tw}	total volumetric water content
J_e	enthalpy flux	ρ_α	density of α -phase
J_T	heat flux	λ_α	thermal conductivity of α -phase
K	crystallization rate	λ_{eff}	effective thermal conductivity
K_f, K_r	forward and reverse rate constants	η_w	dynamic viscosity of water
$\mathbf{k}_{int}, \mathbf{k}_0$	permeability tensor and its initial value	ε_v	volumetric strain
k_{rw}	relative permeability	κ_{sf}	curvature of crystal/liquid interface
L_{cl}	latent heat	φ	angle between crystal and pore wall
M	migration rate	Θ	volume of soil sample
\dot{m}	phase change rate	Ψ	cross-sectional area of soil sample
$N(t)$	number of nuclei formed at time t		
n, n_e, n_0	porosity, effective porosity and initial porosity	Subscripts α	
n_{w0}, n_{cr}, n_s	number of supercooled water molecules, critical nuclei and molecules on nucleus surface	s	solid skeleton
n_{wi}, n_{iw}	material parameter	w	water
		i	ice

which do not have a direct relationship with the nucleation process [18]. Limited studies [19,20] have modeled the kinetics of ice crystal nucleation and growth. In particular, the coupling of fluid flow, heat transfer and ice crystal nucleation and growth has been neglected, and there are even fewer studies on the coupling effects in porous media [1]. Therefore, developing an model understanding the phase change behavior of ice crystals during freezing is essential for the control of heat and mass transfer during ice crystallization [21,22].

In this paper, a physical model was developed to study the heat and mass transfer effects of the ice growth mechanisms in porous media. A numerical method was applied to calculate the temperature, moisture and frost heave of a freezing soil column, and the predicted values are consistent with the experimental data and verify the accuracy of the crystallization kinetics approach that couples heat and mass transfer in porous media. This theory not only provides a possible method of describing the actual process of crystallization and studying the coupled heat and mass transfer during phase change in porous media, but it also provides a theoretical basis for the prevention of damage during nucleation and growth in porous materials.

2. Nucleation and kinetics of crystal growth

2.1. Critical radius and nucleation work

In thermodynamic terms, the nucleation process is correlated to a change in the Gibbs free energy, which consists of two

counteracting parts [23–25]: the variation in the Gibbs free energy related to the volume of the growing crystals, which is known as the volume free energy ΔG_V , and the variation in the free energy related to the formation of an interface between the two phases, which is defined as the surface free energy ΔG_S .

$$\Delta G_C = \Delta G_V + \Delta G_S \quad (1)$$

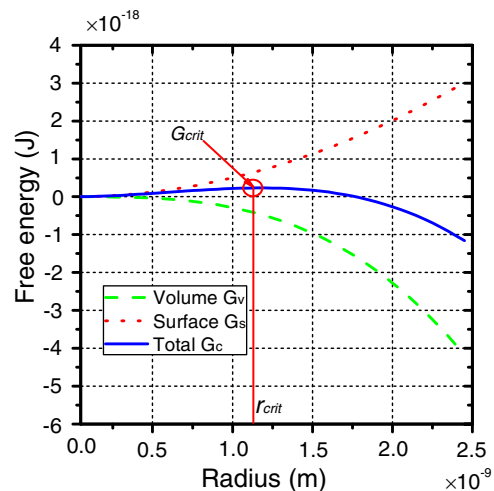


Fig. 1. Relationship between the work of nucleation and crystal size. To quantify the change in free energy, the following parameters are used: $\Delta_m H_1 = 6010$ J/mol, $V_m = 1.8 \times 10^{-5}$ m³, $\Delta T = 1$ K, $\gamma_{sf} = 0.04$ J/m², and $T^* = 273.15$ K.

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