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Thermo-hydro-salt-mechanical coupled model for saturated porous media based on crystallization kinetics

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ABSTRACT

Crystallization is generally considered as the most destructive factor of porous material, but few studies have reported the coupling effects among fluid flow, heat transfer, crystallization and deformation in porous media. In this paper, the driving forces of phase transition were studied initially and then the crystallization kinetics models were established. Moreover, constitutive relations related to saline frozen soil were discussed, and the expression of unfrozen water content in non-equilibrium state was improved. Finally, a thermo-hydro-salt-mechanical coupled model for fully saturated saline frozen soil with phase change was proposed. Validation of the model is illustrated by comparisons between the simulation and experimental results. The predicted values of frost heave, temperature and moisture distribution are consistent with the experimental data, and it is demonstrated that the presented crystallization kinetics approach is valid for studying heat and mass transfer coupled problem with phase change in porous media.

1. Introduction

The issue of porous media involves mutual coupling among deformation, seepage, heat transfer, mass migration and chemical reaction, which has been recognized gradually in engineering practice. The earlier hydrothermal models included hydrodynamic model (Harlan, 1973; Guymon and Luthin, 1974; Taylor and Luthin, 1978; Jame and Norum, 1980), rigid ice model (O'Neill and Miller, 1985; Sheng, 1994) and segregation potential model (Konrad and Morgenstem, 1980, 1981). The coupling of moisture and temperature can be obtained accurately from the hydrothermal models, but the variations of stress and corresponding deformation are difficult to describe. Therefore, researchers paid more attention to thermo-hydro-mechanical coupled model. Initially, the researchers (Glipin, 1980; Hopke, 1980; Mu and Ladanyi, 1987; Nixon, 1991) took into account the impact of external loads on the hydrothermal model, and then established their own models respectively. In recent years, with the development of mixture theory, many scholars (Fremond and Mikkola, 1991; Hartikainen and Mikkola, 1997; Lu et al., 2011) proposed the thermo-hydro-mechanical coupled model for frozen soil based on mixture theory. This THM model can well simulate water, temperature and stress in frozen soil, but cannot describe the mechanism of ice crystallization. Additionally, numerous complicated parameters limit the development and application of the THM model.

Dissolved salt can penetrate into building materials through the porous matrix and existing cracks (Derluyn, 2012). Salt crystallization in pore spaces generated high stress on the pore walls can also causes degradation of building materials (Nicolai, 2008). At present, mechanism of salt heave for saline frozen soil is not well understood; especially the multi-field coupled theory, involving salt crystallization and dissolution, is inadequate. Furthermore, large number of assumptions or approximations ignored the interaction between various conditions (Niu, 2006).

Many models mentioned above only present a theoretical framework, but lack corresponding numerical calculations. The others only performed numerical simulations without appropriate experimental verification. Therefore, providing a more complete thermo-hydro-salt-mechanical coupled model and the corresponding experimental verification is extremely important in theory. This paper studied the driving forces of phase change, and then established the crystallization kinetics models for crystal growth. Furthermore, constitutive relations related to saline frozen soil were discussed in detail. Based on crystallization kinetics, a thermo-hydro-salt-mechanical coupled mathematical model for fully saturated saline frozen soil with phase change was proposed. Finally, experimental and numerical calculation results were used to verify the accuracy of the model.

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Nomenclature

A Frequency factor (−)
a_s, $a_{s,\,start}$ Supersaturation ratio and its trigger value (−)
a_w Water activity (−)
$\boldsymbol{b}$ Body force (N/m^3)
c, c_{sat} Mass concentration of dissolved salt and its saturated value (kg/m^3)
$\Delta C_{p,wi}$ Specific heat capacity difference between water and ice (J/kg/K)
$C_{p,\alpha}$ Specific heat capacity of α-phase (J/kg/K)
C_α Apparent concentration of α-phase (kg/m^3)
$[D]$ Matrix of elastic constant (MPa)
D_{sd} Diffusion coefficient of dissolved salt (m^2/s)
E_s Compression modulus (MPa)
$F(\sigma', \varepsilon^{vp})$ Yield function
F_s Surface force (N/m^2)
Δg_v Single molecule free energy decrease (J)
G Gibbs free energy (J)
ΔG_{crit}, ΔG_0 Nucleation work, activation energy (J)
ΔG_{iw}, ΔG_{sc} Free energy differences of phase change (J)
H_{sc}, H_{wc},H_{wi} Enthalpy differences of phase change (J/kg)
$\Delta_m H^*_{iw}$ Standard molar enthalpy of ice-water (J/mol)
$\boldsymbol{I}$ Unit tensor (−)
$\boldsymbol{J_s}$,$\boldsymbol{J_w}$ Flux of dissolved salt and water (kg/m^2/s)
$\boldsymbol{J_T}$ Heat flux (J/m^2/s)
k Boltzmann constant (J/K)
$K(T)$ Kinetics function (s^{-1})
K_{wi}, K_{iw}, K_{sc}, K_{cs} Rate constants (s^{-1})
$\boldsymbol{k}_{int}$, $\boldsymbol{k}_0$ Intrinsic permeability tensor and its initial value (m^2)
k_{int} Intrinsic permeability coefficient (m^2)
k^r Relative permeability (−)
L_{sc}, L_{wc}, L_{wi} Latent heats of phase change (J/kg)
m_s Molality of salt solution (mol/kg)
$\dot{m}_\alpha$ Production rate of α-phase (kg/m^3·s)
M_{H_2O}, Ms Molar mass of water and salt (kg/mol)
n, n_e, n_0 Porosity, effective porosity and initial porosity (−)
n_m Mole number of solute (mol)
N Avogadro's number (mol^{-1})
p_α Pressures of α-phase (Pa)
Δp_{iw}, Δp_{cs} Pressure difference at crystalline and amorphous interface (Pa)
Q_T Heat sources and sinks (W/m^3)
$Q(\sigma', \varepsilon^{vp})$ Viscoplastic potential function
R Ideal gas constant (J/mol·K)
s_k $(k = i,w)$ Molar entropy of species k (J/mol·K)
Δs_{fc} Fusion entropy per unit volume crystal (J/m^3·K)
Δs_{iw} Fusion entropy of ice-water (J/mol·K)
S_T Energy variation caused by phase change
S_α Saturation degree of α-phase (W/m^3)
T, ΔT Temperature and supercooling (K)
T^*,T^*_0,ΔT^*_0 Freezing point of pore water, bulk water, and freezing point depression (K)
T_{ref} Reference temperature (K)
$\boldsymbol{u}$, u_x, u_y, u_z Displacement vector, and its component in x, y and z direction (m)
V_c Salt crystal volume in the system (m^3)
$\boldsymbol{v_l}$ Absolute velocity of liquid (m/s)
$\boldsymbol{v}^r_\alpha$ Relative velocity of α-phase (m)
$v_{m,\,\alpha}$ Partial molar volume of α-phase (m^3/mol)
v_M, v_X, v_w Stoichiometric number for positive ions M, negative ions X and molecules of water (−)
Z_{M^+}, Z_{X^-} Charges of positive ion M and negative ion X
β Linear thermal dilatation coefficient (K^{-1})
γ_{sf}, γ^0_{sf} Surface tensions of solution and pure water (N/m)
γ_{vp} Viscosity parameter (1/MPa·s)
ε, ε_0, ε^T, ε^{vp} Total,initial,thermal,viscoplastic strain(m/m)
ζ Supersaturation degree (−)
η Dynamic viscosity of fluid (Pa·s)
θ^*_w Residual unfrozen water content (m^3/m^3)
θ_α Volumetric content of α-phase (m^3/m^3)
κ_{sf} Curvature of solid-liquid interface (m^{-1})
λ_e Effective thermal conductivity (W/m·K)
λ_α Thermal conductivity of α-phase (W/m·K)
μ Chemical potential (J/mol)
ξ Experimental parameter of surface tension related to type of salt J·kg/(m^2·mol)
ρ_α Density of α-phase (kg/m^3)
σ, σ' Total stress and effective stress (N/m^2)
σ_0 Macroscopic crystallization stress (N/m^2)
$\varphi(F)$ Scalar function (−)
χ_s, χ_w Ratios of solute and water in solution (−)
Ω Volume of a single molecule (m^3)
ω, ω_{sat} Mass fraction of dissolved salt and its saturated value (kg/kg)

Subscripts α
c Salt crystal
i Ice
l Liquid
m Material matrix
p Pore
s Dissolved salt
w Water

2. Components in saturated saline frozen soil

The saline frozen soil is described as a multiphase continuous porous medium. In saturated condition, the gaseous phase is neglected, and the components are assumed to be comprised partly of liquid phase and solid phase. In reality, different types of salt and salt crystal forms may co-exist in the pore solution (Castellazzi et al., 2016). However, the main object of study in this paper is sodium sulfate because its destructivity is larger than that of other salts. Thus, only one type of salt and salt crystal (c) was considered, i.e., mirabilite ($Na_2SO_4 \cdot 10H_2O$), which greatly simplified this issue and established the foundation for further study on the situation that a variety of salt and salt crystals are co-exist in the soil. Thus, the liquid solution consists of liquid water (w) and dissolved salt (s). Ice crystals (i) may exist in the supercooling soil. The impact of material matrix (m) deformation on mass transfer cannot be neglected.

The total porosity, defined as the volume of voids per unit volume of porous medium, is denoted by n. The content of each component can be described by apparent concentration C_α, defined as the mass of α in per unit volume of porous medium, or by the corresponding saturation degree S_α, defined as the pore volume occupied by α:

$$C_\alpha = \theta_\alpha \rho_\alpha = n S_\alpha \rho_\alpha \tag{1}$$

where ρ_α is the mass density of α, and $\theta_\alpha = nS_\alpha$ is volume of α in per unit volume of porous medium, which satisfy the following relation:

$$\theta_m + \theta_w + \theta_s + \theta_i + \theta_c = 1 \tag{2}$$

The saturation degrees of all the components satisfy:

$$S_w + S_s + S_i + S_c = 1 \tag{3}$$