Coupled THM mechanical model for porous materials under freezing condition

Modèle mécanique couplé THM pour les matériaux poreux dans des conditions de congélation

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ABSTRACT: Recent growing interests associated with frozen ground have required to advance fundamental theories and to precede systematic researches of soil behavior under freezing conditions. Unlike the well-established soil mechanics' theory, temperature variation and phase change of pore-water cause water migration to cold side, ground heaving, sharp increase in earth pressure, etc., and they bring about serious problems to freezing geotechnical structures. Elasto-plastic mechanical constitutive model for frozen/unfrozen soil subjected to fully coupled THM phenomena is formulated based on a new stress variable that is continuous in frozen and unfrozen regions. Numerical simulations are conducted to discuss numerical reliability and applicability of the developed constitutive model. The numerical results show that developed model can efficiently describe complex THM phenomena of frozen soil, and it can be utilized to analyze and design the geotechnical structures under freezing conditions, and predict long-term behavior of them.

RÉSUMÉ : Récentes intérêts croissants associés à un sol gelé ont besoin pour faisons avancent des théories fondamentales et de pour précédent recherches systématiques du comportement du sol sous des conditions glaciales. Contrairement à la théorie de la mécanique des sols bien établis , les variations de température et de changement de phase de l'eau interstitielle migration de l'eau à cause de côté froid, soulèvement du sol, forte augmentation de la pression de la terre, etc, et ils produisent de sérieux problèmes à geler les structures géotechniques. Élasto-plastique modèle mécanique constitutive d' frigorifié / soluble sol à charge des phénomènes parfaitement couplés THM est formulé à partir d'une variable nouvelle contrainte qui est continue dans les régions frigorifizé et soluble. Des simulations numériques sont accomplies pour discuter de fiabilité numérique et l'applicabilité du développé constitutif modèle. Les résultats numériques montrent que le constitutif modèle peut décrit des phénomènes complexes de THM sol gelé, et cela utilisé pour analyse et dessiné les structures géotechniques dans des glaciales conditions, et de prédire le comportement à long terme d'entre eux.

KEYWORDS: frozen soil, mechanical constitutive model, THM coupling, heaving pressure.

1 INTRODUCTION

Soil behavior during a freezing process has been intensively studied mainly in Canada, the United States, Russia, and Japan from the 1920s. In Korea, a recent Antarctic bases and gas-pipeline negotiations to introduce Russia's natural-gas line with 1100km long have attracted attention to understand fundamental phenomena of natural or artificial frost ground.

Typically, freezing region within soil is divided into frozen zone, frozen fringe, and unfrozen zone in Figure 1. New ice lens formation occurs on the boundary between frozen zone and frozen fringe, called a freezing front. The frozen fringe is the very thin layer with 1mm ~ 10mm thick, and soil type and freezing rate control its thickness. Cryogenic suction due to temperature gradients within the frozen fringe absorbs water from unfrozen zone, and form ice crystals onto the freezing front to separate between the soil particles, called segregation freezing. Konrad and Morgenstern (1981) defined the ratio of a thermal gradient within the frozen fringe to liquid inflow rate as segregation potential, and empirical correlations between segregation potential and basic properties of the soil were proposed to evaluate freezing susceptibility (Konrad, 1999).

Silty soil with relatively high hydraulic conductivity and triggering high suction is prone to freeze and form an ice-lens due to temperature drop. Slowing freezing and resulting low temperature gradient forms thicker ice crystals in the soil (Lawrence, et al., 2005). Konrad and Morgenstern (1982) suggested segregation potential function to consider the effect of an external load on the inflow rate into the freezing fringe due to a thermal gradient. It was known that overburden pressure limits the amount of heaving, but the presence of shut-off pressure restraining further expansion is still debating (Arvidson & Morgenster, 1977). Electrolyte in the soil pore water reduces total suction, and plays a role to decrease the amount of frost heaves of the soil.

Phase change between liquid water and solid ice in porous material intimately affects deformation characteristics, as water and heat flow do. Thus, fully coupled THM (Thermo-Hydro-Mechanical) phenomena in the porous material require well-established governing equations, and necessitate solving nonlinear equations and complex numerical correlation between constitutive models. Up to date, many numerical studies have been conducted to imitate fundamental characteristics of frozen soil. However, most cases performed combined TH analysis without considering mechanical effects (Tan, et al., 2011; Painter, 2011). Lately mechanical analyses based on the total stress was attempted for frozen soil (Michalowski and Zhu, 2006), and frozen ground was assumed as a linear elastic material and interpretations was carried out (Liu & Yu, 2011; Thomas, et al., 2009), except for the case of Nishimura et al. (2009).

In this paper, THM elasto-plastic mechanical constitutive model is presented to reproduce freezing action in porous material consisted of soil particles, unfrozen water, and ice. The adopted new stress variable represents the sum of ice and soil skeleton stress to maintain continuity across the frozen-unfrozen transition regions, and stress-strain relationship is derived as the form of incremental formulation. After conjunct with pre-developed THM finite element program, THM numerical analyses for freezing process in porous materials were performed to evaluate the performance of the mechanical model.

2 GOVERNING EQUATIONS

2.1. General assumptions and mass balance equations

The governing equations for porous materials under freezing action were assumed the following to define deformation characteristics associated with THM phenomena.
First, the void of soils is fully saturated with water or water/ice. That is, ice and unfrozen water fill the pore under frozen condition, and the void is fully saturated with liquid water above freezing temperature.
Second, porous material consisted of soil particles, water, and ice is under local thermal equilibrium conditions.
Finally, a freezing porous medium, in the context of theory of mixtures, is viewed as a mixed continuum of three independent overlapping phases of solid and liquid (Bear & Bachmat, 1991). For every phase, its mass conservation equations can be obtained according to the principles of continuum mechanics and mixture theory.

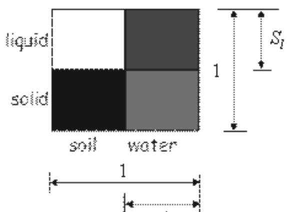

Figure 1. Phase diagram for frozen soil

The macroscopic balance of any species or property per unit volume in a continuum can be expressed by the following generalized partial differential equations (Lewis & Schrefler, 1998).

$$\frac{\partial \rho^{\psi}}{\partial t} + \nabla \cdot \underset{\sim}{j}^{\psi} = 0 \tag{1}$$

where ψ is a species in porous material (e.g. soil, water), and ρ^{ψ} is mass per unit volume of each species. $\underset{\sim}{j}^{\psi}$ is mass flux of each species which can include advective and non-advective components.

2.2. Soil mass balance equation

Soil particles only exist in solid-state, so mass balance equation can be summarized as follows: mass density $\rho^{\psi} = \rho_s(1-\phi)$, mass flux $\underset{\sim}{j}^{\psi} = \rho^{\psi} \dot{\underset{\sim}{u}} = \rho_s (1-\phi)\dot{\underset{\sim}{u}}$ in Equation 1.

$$\frac{\partial}{\partial t}\left[\rho_s(1-\phi)\right] + \nabla \cdot \left[\rho_s(1-\phi)\dot{\underset{\sim}{u}}\right] = 0 \tag{2}$$

where ρ_s 는 is mass density of soil particles, ϕ is soil porosity, and $\dot{\underset{\sim}{u}}$ is velocity of soil particles.

2.3. Water mass balance equation

Since water can exist in liquid water or solid ice, the governing equation was derived from generalized law of mass conservation ($\rho^{\psi} = \rho_i^w \phi(1-S_l) + \rho_l^w \phi S_l$). Solid ice is assumed to be an immobile substance which can make phase change from solid to fluid.

$$\frac{\partial}{\partial t}\left[\rho_i^w \phi(1-S_l) + \rho_l^w \phi S_l\right] + \nabla \cdot \left[\rho_i^w \phi(1-S_l)\dot{\underset{\sim}{u}} + \rho_l^w \phi S_l \dot{\underset{\sim}{u}} + \rho_l^w \underset{\sim l}{q}\right] = 0 \tag{3}$$

where ρ_l^w is mass density of liquid water, S_l is degree of liquid saturation in the void of material. $\underset{\sim l}{q}$ is flow rate of liquid water from Darcy's law.

2.4. Energy balance equation

Although the energy balance is expressed by enthalpy balance in most cases, it is preferable to express it in terms of internal energy (Olivella, et al., 1996; Lewis, et al., 1998). If thermal equilibrium between phases is assumed, the temperature is the same in all phases and only one equation of total energy is required. Adding the internal energy of each phase, the total internal energy per unit volume of the porous medium becomes,

$$\begin{aligned}
&\frac{\partial}{\partial t}\left[(1-\phi)\rho_s E_s + \phi(1-S_l)\rho_i^w E_i^w + \phi S_l \rho_l^w E_l^w - \phi(1-S_l)\rho_i^w L_f\right] \\
&+ \left[(1-\phi)\rho_s E_s + \phi(1-S_l)\rho_i^w E_i^w + \phi S_l \rho_l^w E_l^w - \phi(1-S_l)\rho_i^w L_f\right]\nabla \cdot \underset{\sim}{u} \\
&+ \nabla \cdot \left[\underset{\sim c}{i}\right] + \nabla \cdot \left[\rho_l^w E_l^w \underset{\sim}{q_l}\right] = 0
\end{aligned} \tag{4}$$

where E_s is internal energy of soil per unit mass, and E_i^w is internal energy of water in solid phase per unit mass. Energy transfer by heat conduction in porous materials was estimated using from the Fourier's law ($\underset{\sim c}{i} = -\lambda \underset{\sim}{\nabla} T$). Last term $-\phi(1-S_l)\rho_i^w L_f$ in first partial derivative represents internal energy loss due to water phase change (Thomas, 2009; Tan, 2011; Jane, 1980).

2.5. Static equilibrium equation

Neglecting the inertial effects over all phases, the momentum conservation equation reduces to the static stress equilibrium based on the total stress.

$$\underset{\sim}{\nabla} \cdot \underset{\sim}{\sigma} + \rho_m \underset{\sim}{g} = 0 \tag{5}$$

where $\underset{\sim}{\sigma} = \sigma_{ij}\ (i,j=1,3)$ is total stress, average mass density is $\rho_m = (1-\phi)\rho_s + \phi(1-S_l)\rho_i^w + \phi S_l \rho_i^w$, and gravity direction is $g_i = [0,0,-1]$.

2.6. Numerical implementation

Substituting Eq. 2 into Eq. 3 and 4, the differential equation governing non-isothermal liquid flow through frozen-nonfrozen porous material is obtained. The primary variables are displacement components $\underset{\sim}{u}$, liquid pressure P_l , and temperature T from fully coupled governing equations. The material derivative with respect to the solid velocity field will be very useful to obtain the final expressions for balance equations and equilibrium equation. The material derivative relative to the a phase is given by

$$\frac{d}{dt}(\bullet) = \frac{\partial}{\partial t}(\bullet) + \underset{\sim}{\nabla}(\bullet)\cdot \dot{\underset{\sim}{u}} \tag{6}$$

Generalized trapezoidal rule (Eq. 7) is used to perform time integration between $t^{(n)}$ and $t^{(n+1)}$ of coupled governing equations, and they use discrete approximations to take advantage of Newton's iterative process.

$$\begin{aligned}
&\int_{t^{(n)}}^{t^{(n+1)}} P_l\, dt \approx (t^{(n+1)} - t^{(n)})\left[\theta P_l^{(n+1)} + (1-\theta)P_l^{(n)}\right] \\
&\approx \Delta t\left[\theta P_l^{(n,i+1)} + (1-\theta)P_l^{(n)}\right] = \Delta t\left[P_l^{(n)} + \theta \Delta P_l + \theta dP_l\right]
\end{aligned} \tag{7}$$

where θ is an integration parameter to govern stability and accuracy of the solution, and the solution is unconditionally stable if $\theta \geq 1/2$.

A volume integration of all governing equations then leads to a weighted residual approximation to the governing equations, based on the Galerkin method. After all governing equations are discredited, the final system of algebraic equations can be expressed in matrix form with respect to primary variables $\mathbf{D}(\underset{\sim}{u}, P_g, P_l, T)$.

$$\mathbf{K}^{(n,i)} d\mathbf{D}^{(n,i+1)} = (\mathbf{F_{EXT}})^{(n+1)} - \mathbf{F_{INT}}(\mathbf{D}^{(n,i)}) \tag{8}$$

where $\mathbf{K}^{(n,i)}$ is non-symmetric tangential stiffness matrix at $t^{(n,i)}$, and the right term is residual load vectors.

3. MECHANICAL CONSTITUTIVE MODEL

The proposing mechanical constitutive model is based on the following assumptions to define deformation characteristics associated with THM phenomena.

First, the void of soils is fully saturated with water or water/ice. That is, ice and unfrozen water fill the pore under frozen condition, and the void is fully saturated with liquid water above freezing temperature.

Second, porous material consisted of soil particles, water, and ice is under local thermal equilibrium conditions

Based on these assumptions, this study proposes a mechanical constitutive model for two-phase porous materials, with a similar framework of BBM (Barcelona Basic Model) for unsaturated soils (Alonso, et al. 1990). Stress and strain are positive value for compression.

3.2. Stress variables

Mechanical constitutive law to describe deformational behavior can be expressed by various stress variables. In saturated soils, only effective stress is a stress variable to determine soil behavior (Terzaghi, 1936). However, selection of stress variables in unsaturated soils is still critical issue (Shin, 2011). The most previous studies for frozen soils performed TH coupled analysis so that alteration of hydraulic and thermal properties from deformation cannot be considered, or performed simple linear-elastic analyses for frozen soil. Recently, Nishimura et al. (2009) used net stress $p_n = p - \max(P_l, P_i)$ and suction $s = \max(P_i - P_l, 0)$ to simulate nonlinear deformation behavior of frozen ground. However, ice pressure P_i below freezing temperature shows such a rapid increase that it could be greater than the sum of surface loads, soil skeletal force and water pressure. These stress variables can lose physical meaning and become discontinuous across freezing temperature, and it inhibits numerical stability, along with emission of latent heat of fusion.

In the developed model, a new stress variable $\underset{\sim}{\overline{\sigma}}$ defines the sum of soil skeletal stress and ice stress in Eq. (9), and internal variable suction s (difference between ice pressure and fluid pressure) only affect the pre-consolidation stress.

$$\underset{\sim}{\sigma} = \underset{\sim}{\sigma}' + (1-\chi) P_i \underset{\sim}{1} + \chi P_l = \underset{\sim}{\overline{\sigma}} + \chi P_l \underset{\sim}{1} \tag{9}$$

where $\underset{\sim}{\sigma} = \sigma_{ij}\ (i, j = 1{,}3)$ is total stress, $\underset{\sim}{\sigma}'$ is effective stress carrying soil skeletal force, P_i is ice pressure from Clausius-Clapeyron equation, and P_l is fluid pressure. $\underset{\sim}{1} = \delta_{ij}$ is Kronecker's delta tensor, and χ is Bishop's coefficient of effective stress which can be simplified to degree of liquid water saturation. The new stress variable $\underset{\sim}{\overline{\sigma}} [= \underset{\sim}{\sigma}' + (1-\chi) P_i \underset{\sim}{1}]$ is the same as effective stress above the freezing temperature. It can be useful stress variable to develop mechanical constitutive model for unsaturated freezing soils including air and gas phase.

3.3. Yield surface and plastic potential function

New stress variable $\underset{\sim}{\overline{\sigma}}$ is used to define yield surface and plastic potential function which describe deformational behavior of frozen and unfrozen soils. The proposed yield function is based on MCC (Modified Cam Clay) model which has an oval shape of yield surface, taking account of bonding strength due to ice (Figure 2).

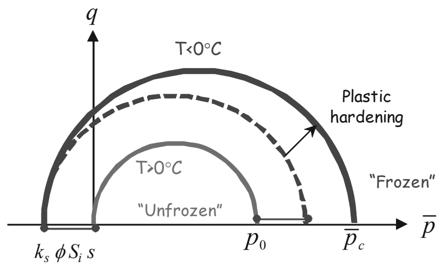

Figure 2. Yield surface of porous material in frozen and unfrozen regions

The increase in the bonding strength is assumed to be equal in the direction of compression and tension, and be proportional to strength ratio k_s (Nishimura, et al., 2009) and pore volume fraction of ice $\phi S_i = \phi(1 - S_l)$.

$$f = q^2 - M^2\left(\overline{p} + k_s \phi S_i s\right)\left(\overline{p}_c - \overline{p}\right) = 0 \tag{10}$$

where pre-consolidation pressure can be expressed as $\overline{p}_c = p_r \left(\frac{p_0}{p_r}\right)^{\frac{\lambda(0)-\kappa(0)}{\lambda(s)-\kappa(s)}} + k_s \phi S_i s$ (Alonso, et al. 1990). Above freezing temperature, $\overline{p}_c$ is the same as p_0, however it evolves nonlinearly below freezing temperature from suction and ice pressure P_i development. p_r is reference stress, and M is the slope of critical state line in $\overline{p}-q$ space. Compression index at various suction is $\lambda(s) = \lambda(0)\left[(1-r)\exp(-\beta s) + r\right]$, and swelling index $\kappa(s)$ is assumed to have the same function of suction as compression index for numerical stability.

Mechanical plastic potential function determining incremental direction of plastic deformation follows associated flow rule $g = f$, and strain-rate-dependent characteristic of frozen soil is not considered in this model.

3.4. Strain components

Total strain increment can be divided into mechanical strain from stress variable, thermal strain, and phase change between liquid water and solid ice in the pore. In addition, mechanical strain increment has elastic and plastic mechanical strain parts.

$$d\underset{\sim}{\varepsilon} = d\underset{\sim}{\varepsilon}^{<m>} + d\underset{\sim}{\varepsilon}^{<T>} + d\underset{\sim}{\varepsilon}^{<ph>} = d\underset{\sim}{\varepsilon}^{e<m>} + d\underset{\sim}{\varepsilon}^{p<m>} + d\underset{\sim}{\varepsilon}^{<T>} + d\underset{\sim}{\varepsilon}^{<ph>} \tag{11}$$

where elastic mechanical strain increment is $d\underset{\sim}{\varepsilon}^{e<m>} = \underset{\sim}{D}^{e^{-1}} : d\underset{\sim}{\sigma}$ (Sheng et al., 2008), and $\underset{\sim}{D}^e = (K - 2G/3)\underset{\sim}{1} \otimes \underset{\sim}{1} + 2G\underset{\sim}{I}$ is (elastic stiffness tensor). K and G are elastic buck and shear modulus, and $\underset{\sim}{1} \otimes \underset{\sim}{1} = \delta_{ij}\delta_{kl}$, $\underset{\sim}{I} = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$.

Temperature-dependent volumetric change in elastic region is determined from thermal elastic contractile coefficient (α_T), $d\varepsilon_v^{<T>} \approx d\varepsilon_v^{e<T>} = \frac{\partial \varepsilon_v^e}{\partial T} dT = 3\alpha_T dT$. And volumetric strain due to phase change is the following from conservation of water mass.

where ρ_l^w and ρ_i^w are mass density of water in liquid and solid phase, and strain due to phase change can be expressed as

$d\underset{\sim}{\varepsilon}^{<ph>} = \underset{\sim}{a}^{<ph>} dT + \underset{\sim}{b}^{<ph>}$ (Liu & Yu, 2011). Frost heave can be inhibited by overburden stress (Konrad, 2005; Michalowski & Zhu, 2006). This sensitivity of volumetric expansion to overburden stress can be expressed as $d\varepsilon_i^{<ph>} \propto \sigma_i^{-a}$, conserving increment of volumetric strain from Eq. (11).

Incremental relations of the effective stress and strain can be expressed as follows:

$$d\underset{\sim}{\overline{\sigma}} = \underset{\sim}{D}^e : [d\underset{\sim}{\varepsilon} - d\underset{\sim}{\varepsilon}^{p<m>} - d\underset{\sim}{\varepsilon}^{<T>} - d\underset{\sim}{\varepsilon}^{<ph>}] \tag{12}$$

Plastic flow rule determines increment of mechanical plastic deformation in a direction perpendicular to plastic potential function with a magnitude of non-negative scalar multiplier $d\lambda$.

$$d\underset{\sim}{\varepsilon}^{p<m>} = d\lambda \frac{\partial g}{\partial \underset{\sim}{\sigma}} \tag{13}$$

3.5. Hydraulic characteristics of frozen soils

Darcy's law using the slope of total head has been adopted to describe fluid flow in porous material. Many experimental results on frozen soils showed liquid flow in the direction to lower temperature even at the same total head (Hoekstra, 1966; Mageau & Morgenstern, 1980). Water flow due to thermal gradient could be estimated by introducing cryogenic suction from water-fluid interfacial tension (Thomas et al., 2009; Hansson et al., 2004; Liu & Yu, 2011) or segregation potential (Tan et al., 2011).

This study used segregation potential method which can directly calculate thermal water flow through the laboratory tests. And Darcy's law considering abundance of liquid water in frozen soils can be summarized as follows.

$$\underset{\sim}{q_l} = -\frac{k_l}{\gamma_l}\left(\underset{\sim}{\nabla P_l} - \gamma_l \underset{\sim}{g}\right) - \phi S_l SP_0 \underset{\sim}{\nabla T} \tag{14}$$

where SP_0 is segregation potential, the ratio of fluid velocity of unfrozen water to thermal gradient (Konrad & Morgenstern, 1981). The effect of applied stress is well considered in the variation of porosity as a function of mean stress (Konrad & Morgenstern, 1984).

The relationship between temperature and volumetric water content in frozen soil is called freezing characteristic function. It can be estimated from empirical equation through laboratory experiments (12a, Andersland & Ladanyi, 2004) and using similarity with SWCC in unsaturated soils (22b, van Genuchten, 1980; Nithimura et al., 2009; Tan et al., 2011). Empirical formula (22a) was partially modified due to inordinate prediction in temperature range $-1.0^\circ C < T < 0.0^\circ C$ (Thomas, et al., 2009).

$$S_l = [1 - (T - T_0)]^\alpha \tag{15a}$$

$$S_l = \left[1 + \left(\frac{P_i - P_l}{P_0}\right)^{\frac{1}{1-\lambda}}\right]^{-\lambda} \tag{15b}$$

where T_0 is freezing temperature of water, and α is determined from pore size and chemical composition of the pore fluid (Thomas et al., 2009). P_0 and λ are material parameters in van Genuchten model (van Genuchten, 1980), and .

Ice pressure P_i in frozen soil can be calculated from Clausius-Claperyron (Eq. 23), assuming that thermodynamic equilibrium is satisfied at the contact surface between ice and liquid water in the pore (Henry, 2000).

$$P_i = \frac{\rho_i^w}{\rho_l^w} P_l - \rho_i^w L_f \ln(T/273.15) \tag{16}$$

where L_f is specific latent heat of fusion of water, $3.34 \times 10^5 J/kg$.

4. CONCLUSIONS

Recent increasing interest in the frozen soil has raised the demand to advance theoretical establishment and numerical tools to interpret fully coupled thermal-hydro-mechanical phenomena in naturally or artificially freezing ground. However, previous numerical analysis of freezing soil usually disregarded mechanical characteristics or assumed freezing porous material as a linear elastic material.

In this paper, THM elastoplastic constitutive model for porous materials is derived for the frozen-unfrozen soil consisted of soil particles, unfrozen water, and ice. The new stress variable, the sum of skeletal stress and ice pressure, has continuity in the frozen-unfrozen transition condition, and it can easily be applicable to unsaturated freezing soil. Stress increment due to strain and temperature change was derived as the form of incremental formulation. Proposed mechanical model was implemented into THM FEM code, and it was applied to numerical examples to confirm stability of solution and applicability of the model. Numerical results effectively described complex THM phenomena related with frozen soil, where governing equations had high nonlinear and constitutive models were inter-coupled.

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