Theoretical Basis for Modeling Porous Geomaterials under Frost Actions: A Review

Zhen Liu
Dep. of Civil Engineering
Case Western Reserve Univ.
2104 Adelbert Rd., Bingham 256
Cleveland, OH 44106

Ye Sun
Dep. of Electrical Engineering and Computer Science
Case Western Reserve Univ.
2104 Adelbert Rd., Bingham 203C
Cleveland, OH 44106

Xiong (Bill) Yu*
Dep. of Civil Engineering
Case Western Reserve Univ.
2104 Adelbert Rd., Bingham 206
Cleveland, OH 44106

We review the theoretical basis for modeling the behaviors of porous materials under frost actions. An attempt is made to categorize the previous research to understand the frost-induced coupled processes. The importance of the coupled processes between the thermal, hydraulic. and mechanical fields in porous materials is emphasized. Methods to describe such coupling actions are classified into basic governing mechanisms as well as the explicit and implicit relationships among individual parameters. Analytical models developed from soil science, civil engineering, and engineering mechanics are summarized. Various terminologies and expressions from different disciplines are discussed in relationship to the general physical mechanisms. From this, models can be selected for implementing holistic simulations of porous geomaterials under frost actions. We also discuss problems deserving further investigation.

Abbreviations: PDE, partial differential equation; SWCC, soil water characteristic curve; TH, thermo-hydraulic; THM, thermo-hydro-mechanical.

Porous materials (or media), which consist of a solid (often called the frame or matrix) permeated by an interconnected network of pores (voids) filled with fluid (liquid or gas), have been the subject of a wide range of interests (Coussy, 2004). Such materials are frequently found as civil construction materials, i.e., soils, concrete, asphalt concrete, and rock. The applications of porous materials, however, also include areas such as catalysis, chemical separation, tissue engineering, and microelectronics (Davis, 2002; Cooper, 2003).

There is growing interest in studying the behavior of porous materials under frost actions (Sliwinska-Bartkowiak et al., 2001; Fen-Chong et al., 2006). This topic has been studied by researchers in civil engineering, soil science, and agricultural science due to the common interest in frost impacts (Anderson and Morgenstern, 1973; O'Neill, 1983). The term *geomaterials* refers to porous materials such as soils, rocks, cement, and concrete (Murton et al., 2006; Coussy and Monteiro, 2007, 2008). This review focuses on the various aspects related to modeling porous materials under frost actions, with recognition of the similarities among different disciplines.

The substantial amount of published literature tends to leave a false impression that there has been little consensus among researchers about how to analyze the physical processes involved in frost actions (Newman and Wilson, 1997). As pointed out by Newman and Wilson (1997), civil engineers are more concerned about the mechanical behavior of freezing or frozen soils, such as failure and deformation (e.g., frost heave or creep), while soil scientists usually focus on predicting the temperature and water content profiles in agricultural soils. The divergence in goals is responsible for the use of different terms, definitions, and expressions for similar or even the same relationships. Besides this, different ways to formulate the mathematical models can

Soil Sci. Soc. Am. J. 76:313–330
Posted online 27 Dec. 2011
doi:10.2136/sssaj 2010.0370
Received 29 Sept. 2010
*Corresponding author (xxy21@case.edu)

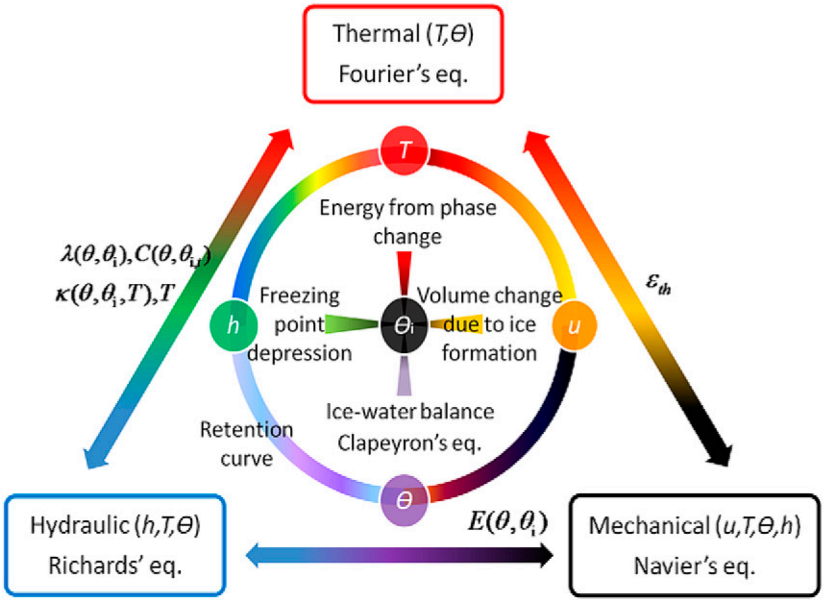


Fig. 1. Structure of a typical coupled thermo-hydro-mechanical model. (State variables: *h*, total water head; *T*, temperature; *u*, total suction; θ, volumetric water content; θ_i, volumetric ice content. Thermal and transport properties: λ, thermal conductivity; *C*, heat capacity; *k*, hydraulic conductivity. Other coupling factors: ε_{th}, strain caused by thermal expansion; *E*, modulus of the soil.)

also lead to distinct models. This seeming discrepancy can be reconciled by studying the origins and basic assumptions of the commonly used models in different disciplines.

The behavior of porous materials under frost action can be studied by experimental, analytical, or numerical approaches. The existing literature has focused on the parameters of porous materials, e.g., the hydraulic conductivity (Gardner, 1958; Mualem, 1976, 1986; van Genuchten, 1980; Lundin, 1989; Fredlund et al., 1994, Šimůnek et al., 1998), or the relationship between different parameters, e.g., the soil water characteristic curve (SWCC) (Koopmans and Miller, 1966; van Genuchten, 1980; Fredlund and Xing, 1994; Schofield, 1935; Mizoguchi, 1993; Reeves and Celia, 1996). Previous works have also investigated the mechanisms (Horiguchi and Miller, 1980; Gilpin, 1980; Dash, 1989; Philip and de Vries, 1957; Cary, 1965, 1966) or discussed the forms of the governing equations (Celia et al., 1990; Celia and Binning, 1992).

Previous research has contributed to the ultimate goal of holistically modeling the processes in unsaturated soils that involve the coupling of more than one physical field, e.g., TH (thermo-hydraulic) or THM (thermo-hydro-mechanical) models. The structure of a typical THM model is shown in Fig. 1. The governing equations and auxiliary relationships are demonstrated. Such models, together with boundary conditions, are usually solved by numerical methods (the finite difference method, finite element method, or finite volume method) and independently verified by experimental data.

Progress in modeling multiphysical processes in unsaturated soils has been made by researchers in different areas. For example, there have been a substantial number of studies designed to study the coupled TH, THM, or thermo-hydro-mechanico-chemical field for rocks and soils from the fields of soil science (Kay and Groenevelt, 1974; Sophocleous, 1979; Flerchinger and Pierson, 1991; Nassar and Horton, 1992, 1997; Scanlon and Milly, 1994; Noborio et al., 1996a; Jansson and Karlberg, 2001) and civil engineering (Milly, 1982; Thomas, 1985; Thomas and King, 1991; Thomas and He, 1995, 1997; Sahimi, 1995; Noorishad et al., 1992; Noorishad and Tsang, 1996; Stephansson et al., 1997; Bai and Elsworth, 2000; Rutqvist et al., 2001a,b; Wang et al., 2009). Most of these models are free from water phase changes (or free from freezing–thawing processes). These models were developed either from the theory of nonisothermal consolidation of deformable porous media or from extending Biot's phenomenological approach with a thermal component to account for thermally induced hydraulic flow (Biot, 1941). They can be extended to accommodate the influence of a phase change for water (at freezing or thawing).

The purpose of this review is to summarize the theoretical basis for modeling frozen porous materials, with an emphasis on the coupling of physical fields. For a better understanding of the coupling actions, the interactions among physical fields in porous materials subjected to frost actions are grouped into three layers. The first layer is the basic mechanisms. The formulation for this layer of coupling actions is usually straightforward, and the relevant actions (e.g., the influence of energy carried by a convective fluid mass on a thermal field) can be readily taken into account by adding the corresponding terms into the governing partial differential equations (PDEs). The second layer is the explicit relationships, i.e., the relationships among the state variables that may be treated as the independent variables of the governing equations. The third layer is the implicit relationships, i.e., the dependence of material properties on the state variables and other parameters. Figure 2 illustrates the focus of this review and its role in developing multiphysics simulations and field applications. As illustrated in Fig. 2, the multiphysics models of porous media under frost actions can be categorized based on the types of physical fields considered as well as their interactions (circles on the left). These models can be utilized to solve different engineering problems (on the right side of this figure). The degree of complexity is dependent on the major factors involved. A common pool of knowledge serves as the theoretical basis of the computational models. Understanding these basics is necessary for a sound model simulation. The focus of this review is to summarize and categorize the technical bases of different models. Additionally, contributions from different disciplines are summarized to reconcile seeming discrepancies and to identify the similarities.

To arrange the modeling basis for coupling actions in a logical way, the terminology is discussed first. The presentation of the basic mechanisms is intended to be concise and comprehensible, highlighting the contributions from different disciplines.

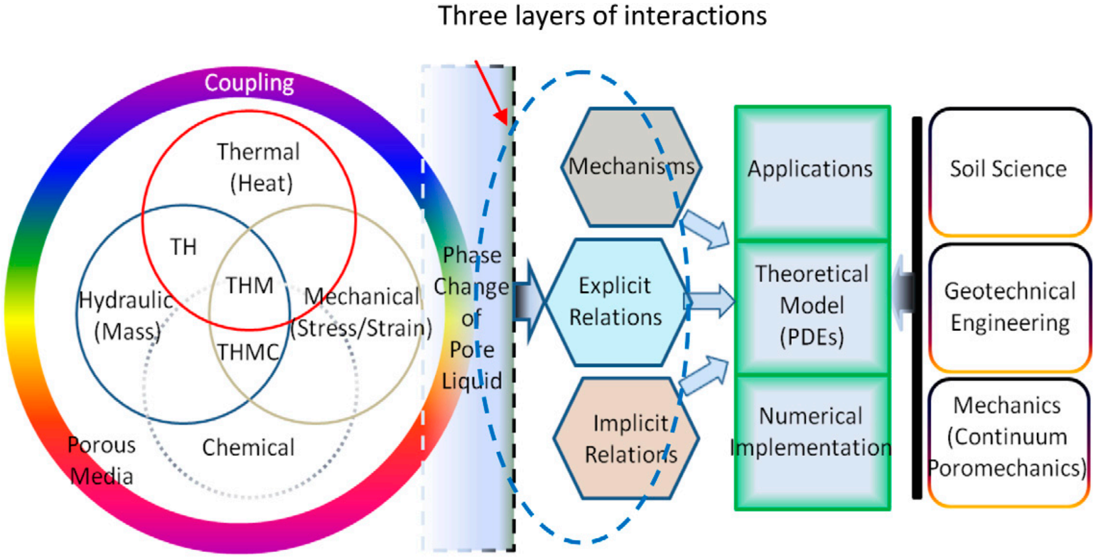


Fig. 2. Schematic overview of this review.

The other two layers of interactions, i.e., the explicit relationships and the implicit relationships, are then discussed sequentially.

BASIC TERMINOLOGY

Among the few terms that can serve as the independent variables of an individual physical field (e.g., suction, water pressure, temperature, water content, ice content, and displacement), suction and water pressure are the ones that tend to cause confusion and therefore require special attention. The concept of suction, which is also known as moisture suction or tension, was first introduced by agricultural researchers at the end of 19th century (Briggs, 1897) and then by Buckingham (1907) and Schofield and da Costa (1938). *Suction* in agricultural research refers to any measured negative pore pressure, which is now widely referred to in soil science. In civil engineering, however, where the effects of applied stress on the suction of soil carry practical significance, another term, *negative pore pressure*, was reserved for any pressure deficiency (below atmospheric pressure) measured under loading conditions (Croney and Coleman, 1961). The term *suction* in the sense of civil engineering, as commented by Cooling (1961), was rather vague and can be alternatively replaced by the currently used term *matric suction*. Matric suction, which was originally expressed in terms of the free energy of the water system with reference to a standard energy level, was defined as the amount of work per unit mass of water for the transport of an infinitesimal quantity of soil solution from the soil matrix to a reference pool of the same soil solution at the same elevation, pressure, and temperature (Campbell, 1985). In the mathematical form, the matric suction (s) can be obtained from

$$s = p_a - p_w \quad [1]$$

where p_a is the pore air pressure and p_w is the pore water pressure.

Matric potential is sometimes used in the place of matric suction (or suction). This is due to the fact that the unit of pressure (N m^{-2} or Pa) can also be expressed in the form of energy (J m^{-3}). Matric potential (ψ_m) has an identical absolute value to matric suction; the only difference lies in the sign:

$$\psi_m = -s \quad [2]$$

If a solute exists in the pore water, the *osmotic potential*, which also contributes to the total potential (or suction), needs to be taken into account. Osmotic potential indicates the additional energy required to equilibrate the solution with pure water across a perfect semipermeable membrane (Campbell, 1985). Among the terms composing the total potential, osmotic potential, and matric potential are those that are affected by the liquid water content. They are therefore frequently combined as the (soil) water potential. In civil engineering, soil matric suction is frequently used for issues such as frost heave because the effect of solution is negligible; however, we must keep in mind that soil water potential is more accurate under saline solution conditions. In the following context, soil water potential, which has been frequently used, is more accurately matric potential.

Some other factors, such as the overburden pressure, pneumatic pressure, and gravitational force can also have certain influences on the behavior of porous materials under frost actions. Taking the overburden pressure as an example, many researchers, e.g., Konrad and Morgenstern (1982b), Gilpin (1980), O'Neill and Miller (1985), and Sheng et al. (1995), have noticed its effects on the rate of frost heave and proved this tendency by both modeling and experiments. Even for the gravitational force, which has been neglected by most researchers in their models for simplification, has proved to be considerable under some circumstances (Thomas, 1985). Therefore, the total potential, ψ, in a porous medium can be written in complete form as (Campbell, 1985; Mizoguchi, 1993; Scanlon et al., 1997; Hansson, 2005)

$$\psi = \psi_m + \psi_o + \psi_g + \psi_e + \psi_a \quad [3]$$

where ψ_o is the osmotic potential, ψ_g is the gravitational potential, ψ_e is the envelope potential resulting from overburden pressures, and ψ_a is the pneumatic potential.

The matric potential (or matric suction), is usually believed to result from the combination of surface tension and absorption. In soils that have a relatively small amount of colloidal mineral substance, the influence of absorption is negligible. In this case, matric suction can be considered as an absolute product of the air–water interface and given by the capillary rise equation:

$$\psi_m = -\frac{\sigma_{wa}}{r\rho_w} \qquad [4]$$

where σ_{wa} is the water–air surface tension, r is the radius of curvature of the interface, and ρ_w is the density of water. Schofield (1935) stated that surface tension theories should be applicable down to particle sizes of 20 µm (Miller and Miller, 1955).

Differences also need to be pointed out in the usage of water content and ice content terms. In soil science, volumetric water content, θ, is conventionally used; in geotechnical engineering, gravimetric water content, w, is commonly used. The degree of saturation or water saturation, expressed as the ratio of water volume to pore volume, is usually used in soil mechanics and petroleum engineering. The term *effective saturation* (also called *normalized saturation*) is frequently adopted in the formation of the SWCC as

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad [5]$$

where Θ is the effective saturation, θ_r is the residual water content as the ratio of the volumetric water gradient to suction approaches zero, and θ_s is the saturated water content, which is approximately equal to the porosity.

A few important terms are involved in describing the transport processes in porous materials. The transport of heat and mass in porous materials can be formulated in the same form as Fick's first law:

$$\vec{J} = -D_0 \nabla u \qquad [6]$$

In heat transfer, $\vec{J}$ is the flux of heat transfer, D_0 is the thermal conductivity and equals the thermal conductivity (λ), and u is an independent variable such as temperature, T. In mass transfer, $\vec{J}$ is the flux of mass transfer, D_0 is the hydraulic conductivity, and u is the independent variable, i.e., the water potential.

The properties of hydraulic conductivity under drying or freezing conditions have been investigated by many researchers (Richards, 1931; Brooks and Corey, 1964; Campbell, 1974; Fredlund et al., 1994). The intrinsic permeability is a fundamental hydraulic property of porous materials:

$$K = k_i \frac{\rho_w g}{\mu} \qquad [7]$$

where K is the hydraulic conductivity, µ is the viscosity of the liquid, k_i is the intrinsic permeability (or *permeability* for short), and g is gravitational acceleration. It therefore can be seen that k is an intrinsic materials property of the solid matrix while K depends additionally on the properties of fluids, such as the density and viscosity.

Another important parameter for describing frozen unsaturated materials is the concept of the apparent specific heat capacity (gravimetric), C_a. Instead of the actual specific heat capacity, C_p, the term is usually adopted when a phase transition occurs. The only difference is that the apparent heat capacity includes the heat released or adsorbed by the phase change of water. More details are provided below.

BASIC MECHANISMS

The basic mechanisms governing the coupled processes in freezing porous materials include three major components, i.e., the mechanisms for the thermal process, the hydraulic process, and the mechanical process. Figure 2 gives a schematic of the relationships among these mechanisms. The external excitation and the way it induces the coupled processes are the basis of various models. Typical TH or THM processes are triggered by a disturbance at the thermal boundary. The resultant thermally induced fluid flow or change in the microstructure of porous materials has been an area of interest to the research and practical application communities.

In fact, among the theories describing the basic mechanisms, the ones concerning thermally induced moisture transfer have received the most attention because such models are the key components of the multiphysical interaction processes.

Theoretical Perspectives of Thermally Induced Moisture Transfer

Philip and de Vries (1957) developed a theory based on thermodynamics to explain the movement of moisture in porous materials under temperature gradients:

$$\begin{aligned}\vec{J}_v &= -Dv\alpha\theta_a \nabla\rho_a \\ &= -Dv\alpha\theta_a \frac{d\rho_a}{dT}\nabla T - \frac{Dv\alpha\theta_a g\rho_a}{RT}\frac{\partial\psi}{\partial\theta_a}\nabla\theta_a\end{aligned} \qquad [8]$$

where $\vec{J}_v$ is the gravimetric vapor flux, D is the molecular diffusivity of water vapor in air, v is the mass-flow factor, α is a tortuosity factor allowing for extra path length, θ_a is the volumetric air content of the medium, ρ_a is the density of water vapor, and R is the gas constant. The density of saturated water vapor is related to that at a reference temperature by $\rho_a = \rho_{a,0}\exp(\psi g/RT)$ (Edlefsen and Anderson, 1943), where $\rho_{a,0}$ is the density of saturated water vapor and T is the temperature.

The migration of moisture under gravimetric potential is given by

$$\vec{J}_l = -\rho_w K \frac{\psi}{\sigma}\frac{d\sigma}{dT} - \rho_w \frac{\partial\psi}{\partial\theta}\nabla\theta - \rho_w K\vec{i} \qquad [9]$$

where $\vec{J}_l$ is the gravimetric liquid flux, σ is the surface tension of soil water that is temperature dependent, and $\vec{i}$ is the unit vector in the direction of gravity.

Cary (1965, 1966) summarized that surface tension, soil moisture suction, and kinetic energy changes associated with the H bond distribution, as well as thermally induced osmotic gradients, should be responsible for the thermally induced moisture flow. Based on this recognition, he made modifications to Philip's theory (Philip and de Vries, 1957). Dirksen and Miller (1966) used similar concepts but with an emphasis on the mechanical analysis. Studies from physical chemistry emphasized the influence of surface tension (Nimmo and Miller, 1986; Grant and Salehzadeh, 1996; Grant and Bachmann, 2002) and kept calling for attention to the role of water vapor adsorption processes (Or and Tuller, 1999; Bachmann and van der Ploeg, 2002; Bachmann et al., 2007). Coussy (2005) described the transport of water and vapor as the result of density differences, interfacial effects, and drainage due to expelling, cryo-suction, and thermomechanical coupling. Most of the hydrodynamic models were developed from these thermodynamics theories or theories in similar forms (Harlan, 1973; Guymon and Luthin, 1974; Noborio et al., 1996a; Hansson et al., 2004; Thomas et al., 2009).

A few researchers, however, described the transport of water in response to a temperature gradient and the transport of heat in response to a water pressure gradient using the theory of nonequilibrium thermodynamics (Taylor and Cary, 1964; Cary, 1965; Groenevelt and Kay, 1974; Kay and Groenevelt, 1974). Kay's theory, for example, was developed by exploiting the appropriate energy dissipation equation and the Clapeyron equation for the three-phase relationship. Transport equations were then obtained from the energy dissipation equation and the Clapeyron equation:

$$TS=-J_q{}'\frac{\nabla T}{T}-J_l\overline{V_l^e}\nabla p \qquad [10]$$

$$\vec{J}_q{}'=-L_T\frac{\nabla T}{T}-L_{Tw}\overline{V_l^e}\nabla p \qquad [11]$$

$$\vec{J}_l=-L_{Tw}\frac{\nabla T}{T}-L_w\overline{V_l^e}\nabla p \qquad [12]$$

where S is the entropy product; $\overline{V_l^e}$ are the volume and pressure of the "extramatric liquid," which refers to the water outside of the direct influence of the matrix but in equilibrium with the water within the direct influence; and p is the pressure of the "extramatric water." The variable $\vec{J}_q{}'$ is the so-called reduced heat flux; L_T, L_{Tw}, and L_w are coefficients of transport that have been deduced as functions of other parameters such as vapor conductivity, latent heat, and the volume of vapor. Theories from nonequilibrium thermodynamics have been seldom adopted due to the difficulties in numerical implementation (Kay and Groenevelt, 1974).

Thermo-hydraulic coupling theories based on either thermodynamics or nonequilbrium thermodynamics, as described above, are applicable for both saturated and unsaturated porous materials. Cases have been reported where both types of theories have been used successfully for unsaturated soils, but they failed to describe the freezing or thawing process when the phase transition between ice and water occurred. Dirksen and Miller (1966) found that the rate of mass transport within frozen soil exceeded by several orders of magnitude what could be accounted for as vapor movement through the unfilled pore space. They therefore concluded that the flux must have taken place in the liquid phase (by a factor at least 1000 times faster than that predicted by Philip and subsequent researchers). That is to say, a mechanism other than the ones mentioned above is responsible for the process of mass transfer, at least at the zones experiencing frost heave.

To reconcile the paradox, Miller (1978) proposed the "rigid ice model." In this model, ice pressure is nonzero (opposite to that assumed in the hydrodynamic model) and is related to water pressure through the Clapeyron equation. Moreover, a *mean curvature* variable was adopted. Hence, the change in the ice content (which is a function of the mean curvature and was determined by the water content, hydraulic conductivity, and stress partition function) that happened in the form of ice regulation (Horiguchi and Miller, 1980) was obtained. The liquid flux was assumed to obey Darcy's law. In summary, the "rigid ice model" assumed nonzero ice pressure and introduced the relationship between the mean curvature and other variables. This, together with the Clapeyron equation and Darcy's law, set the basis of the multiphysical model:

$$\vec{J}=\vec{J}_l=\rho_w\frac{kr_{ave}}{\mu}\left(\vec{i}+\nabla\psi\right) \qquad [13]$$

where the hydraulic permeability k is a function of the mean curvature, r_{ave}.

Starting from a nonzero ice pressure, Gilpin (1980) developed a theory by assuming that the movement of water in the liquid layer is totally controlled by normal pressure-driven viscous flow. As illustrated in Fig. 3A, water is "sucked" toward the base of an ice lens because of the existence of the curvature. This curvature of the interface, which inherently varies in porous material, leads to nonequilibrium between the pressure and temperature in a local freezing zone such as the freezing fringe. Consequently, unfrozen water has to move toward the ice lens to reach equilibrium, described by the Clapeyron equation. The thermal-induced liquid flow is calculated by

$$\vec{J}=\vec{J}_l=-\rho_w\frac{k}{\mu}\frac{V_s}{V_l}\nabla\left(p_s+\frac{L_fT}{V_sT_0}\right) \qquad [14]$$

where L_f is the gravimetric latent heat of melting or freezing, V_s and V_l are the specific volumes of solid and liquid, respectively, p_s is the pressure of the solid, and T_0 is the freezing point of bulk water (K). A similar interpretation was given by Scherer in the interfacial energy term (Scherer, 1999).

Dash (1989) proposed an explanation that appears similar to Gilpin's but actually differs. The driving force was attributed to the lowering of the interfacial free energy of a solid surface by a layer of the melted material (Fig. 3B), which occurs for all solid interfaces that are wetted by the melted liquid. Without a substrate, mass flow occurs due to the difference in the thickness of the melted layer (liquid) along the interface of the liquid and solid layers. This results in a thermomolecular pressure to reach equilibrium:

$$\delta P_{\mathrm{m}} = -\rho_{\mathrm{l}} L_{\mathrm{m}} \delta T \qquad [15]$$

where δP_{m} is the thermomolecular pressure, ρ_{l} is density of bulk liquid, L_{m} is the latent heat of melting per molecule, and $\delta T = (T_0 - T)/T_0$.

There are other models, such as Konrad's model (Konrad and Morgenstern, 1980, 1981, 1982a). In these models, the coupling has been simplified by introducing an experimental relationship where the rate of water migration is proportional to the temperature gradient in the frost fringe.

Common Types of Models for Coupling Processes in Porous Materials under Frost Effects

When a porous medium is subjected to freezing conditions, the thermal disturbance will lead to a change in the state variables (i.e., temperature, water contents, and displacements) and the parameters related to material properties (i.e., thermal and hydraulic conductivities and mechanical moduli). The variations in these variables with time characterize the coupled processes. In general, the purpose of the various coupling models is to simulate these variations. The distributions of temperature and water content as well as the associated volume changes have been the focus of investigations. Hydrodynamic models and rigid ice models are two of the most common types of models for this purpose.

If there is no ice lens in the porous medium, the process of transport and deformation of the soil matrix can be formulated with the same method as for a continuous solid medium. That is, the heat and mass transfer can be described by a parabolic PDE; the displacement of the skeleton can be described by an elliptic (Poisson's) PDE. By solving the equation system, the transient thermal and hydraulic fields as well as the mechanical field at every point of the medium can be obtained:

Parabolic PDE:

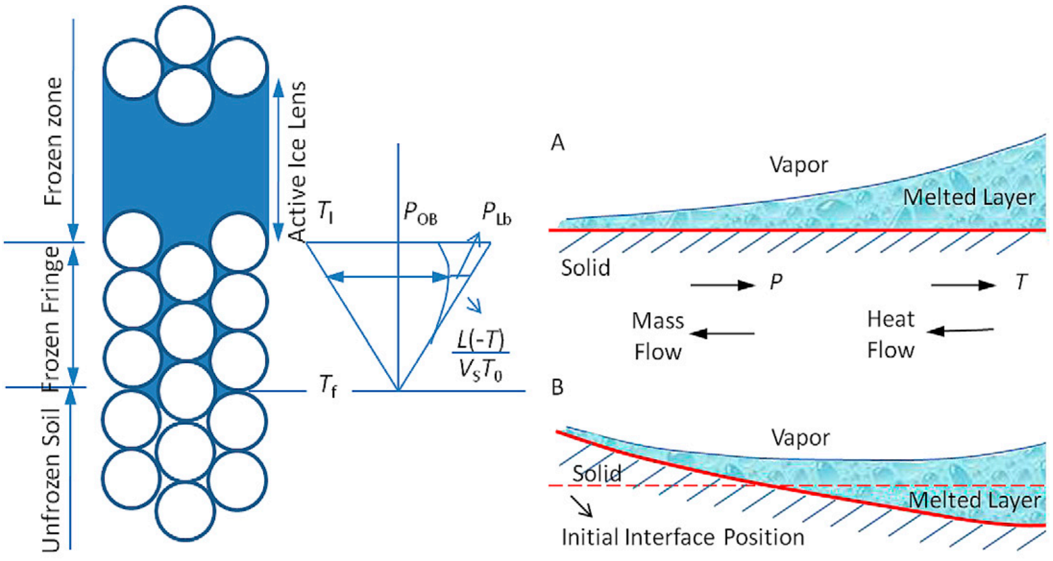
$$d_{\mathrm{C}} \frac{\partial u}{\partial t} = -\nabla\left(K_{\mathrm{C}} \vec{J}\right) + f, \quad \vec{J} = -\nabla u \qquad [16]$$

$$\text{Elliptic PDE:} \quad -\nabla(\nabla \mathbf{u}) = f \qquad [17]$$

where d_{C} and K_{C} are constants, f is the source or sink term, $\mathbf{u}$ is a tensor if two- or three-dimensional geometry is considered, and t is time. The Fick-type parabolic PDE (Eq. [16]) is written in its simplest form. The elliptic PDE used in the mechanical field is actually Navier's equation in mechanics. It can appear in a more complicated form when dealing with the plastic behavior of unsaturated porous media. In such cases, the form with deviatoric tensors regarding surface state theory is necessary (Alonso et al., 1990). On the other hand, under certain circumstances, it is not necessary to incorporate all the PDEs above for a complete form because a specific governing equation for an individual field can be simplified or even omitted under certain assumptions.

Hydrodynamic Model

The hydrodynamic models, in general, include the various models developed by soil physicists to predict water and temperature redistribution in unsaturated soils. Most of these models are TH models. There are emerging tendencies within the geotechnical engineering community to establish a THM model by importing the TH framework (Nishimura et al., 2009; Thomas et al., 2009). The characteristic of these models is that the ice



(a) Gilpin (1980) (b) Dash(1989)

Fig. 3. The mechanisms proposed by (A) Gilpin (1980) and (B) Dash (1989) (T, temperature profile; P, pressure profile; L, latent heat; V_s, specific volume of solids; T_0, freezing temperature at standard atmospheric pressure).

pressure is usually assumed to be zero or changes in the ice pressure are ignored. This assumption is seldom questioned except in cases such as ground heaving (Miller, 1973; Spaans and Baker, 1996; Hansson et al., 2004).

One early TH model that is widely referenced is the coupled heat–fluid transport model developed by Harlan (1973). The key factors for this coupled model include the analytical expression for the Gibbs free energy (equivalent to the SWCC), an assumed unique relationship between the soil-water potential and liquid water content, and the similarity between freezing and drying processes (Harlan, 1973):

$$\frac{\partial\left(\rho_{\mathrm{l}}C_{\mathrm{a}}T\right)}{\mathrm{d}t}=\nabla\left(\lambda\nabla T\right)-\rho_{\mathrm{l}}C_{\mathrm{a}}\nabla\left(\frac{\vec{J}}{\rho_{\mathrm{l}}}T\right) \qquad [18]$$

$$\frac{\mathrm{d}\left(\rho_{\mathrm{l}}\theta_{\mathrm{l}}\right)}{\mathrm{d}t}+\frac{\mathrm{d}\left(\rho_{\mathrm{i}}\theta_{\mathrm{i}}\right)}{\mathrm{d}t}=\nabla\left(\frac{K}{g}\nabla\psi\right) \qquad [19]$$

where θ_{i} is the volumetric ice content and ρ_{i} is the density of ice. Equations [18] and [19] create a coupled hydrodynamic model. The subscript l, for liquid, can be exchanged for w when the pore liquid is water.

As pointed out above, θ_{l} is a function of ψ (the definition of the SWCC). The original one-dimensional equation system of Harlan (1973) is written in three-dimensional form here. Besides this, the change in ice per unit volume per unit time is rewritten as the function of the ice content. By comparison with Eq. [17], the only substantial difference in Harlan's equations is the additional convection term in the heat transfer equation.

Later researchers, such as Guymon and Luthin (1974), confirmed that soil moisture and thermal states are coupled, particularly during freezing and thawing processes. Based on this, models similar to Harlan's were developed. The differences lie in the different correlations used to fit the relationships among parameters such as the hydraulic conductivities and other independent variables. Guymon and Luthin (1974) estimated the ice content by an empirical relationship suggested by Nakano and Brown (1971) instead of combining the SWCC and the Clapeyron equation. Other researchers, e.g., Taylor and Luthin (1978), Jame and Norum (1980), Hromadka and Yen (1986), Noborio et al. (1996a), Newman and Wilson (1997), and Hansson et al. (2004), established other models in a similar way that could be regarded as modifications to Harlan's model. Taking the more recent model presented by Hansson et al. (2004) for example, the governing equations are in exactly the same form if vapor terms are neglected. The various modifications mainly updated the models on more recently proposed relationships and numerical strategies (Celia et al., 1990). The results of simulations compared well with experimental results (Mizoguchi, 1990).

One important divergence in different modeling approaches is the choice of water content or pressure as the independent variable. This has repeatedly been the subject of discussion. Dirksen and Miller (1966) seemed to favor the pressure-type Richards equation for the reason that Briggs (1897) had pointed out, i.e., flow could actually be contrary to the water content gradient but would not be contrary to a pressure or tension gradient. Celia et al. (1990) supported the mixed-type Richards equation because of its advantage in avoiding large errors in mass balance usually resulting from the pressure-type model. This viewpoint won popularity among many researchers in the choice for the mixed-type Richards equation.

Rigid Ice Model (Miller Type)

This type of model assumes that the ice pressure is not necessarily zero. A great amount of research has been conducted since late 1970s, when engineering problems such as frost heave began to receive more and more attention. This kind of problem cannot be described by directly applying the governing equations in the thermodynamic model due to the existence of an ice lens.

The Miller type of rigid ice model is, in fact, similar to thermodynamic models with a nonzero ice pressure. The breakthrough of Miller's model lies in the dependence of the ice pressure on a newly introduced term, that is, the mean curvature (Miller, 1978). With relationships derived from this dependence, ice lens initiation can be investigated by analyzing the force balance:

$$\frac{\partial\left(\rho_{\mathrm{w}}C_{\mathrm{a}}T\right)}{\partial t}+\frac{\partial\left(\rho_{\mathrm{w}}L_{\mathrm{f}}\theta\right)}{\partial t}=\nabla\left(\lambda\nabla T\right) \qquad [20]$$

$$\nabla\vec{J}_{\mathrm{l}}=\left[\rho_{\mathrm{i}}v_{\mathrm{i}}+\frac{\left(\rho_{\mathrm{l}}-\rho_{\mathrm{i}}\right)}{\rho_{\mathrm{i}}}\vec{J}_{\mathrm{i}}\right]\nabla\theta \qquad [21]$$

where v_{i} is the rate of frost heave. Miller (1980) applied the model to simulating a very simple quasi-static state with a simplified set of equations. O'Neill and Miller (1982) provided a strategy for obtaining numerical solutions of the full set of equations for simple boundary conditions. The physical basis of the formulation, mathematical expression, and implementation was expanded by O'Neill and Miller (1985).

The model proposed by Gilpin (1980) was conventionally categorized as a rigid ice model; however, it actually differs significantly from Miller's model. The Gilpin (1980) model was based on a new perspective in the coupling mechanism. It is not really a coupled model because of the quasi-static strategy that has been introduced. Aiming at an overall prediction but with local information obtained by continuum mechanics, a freezing sample is divided into a frozen zone, a frozen fringe, and an unfrozen zone. A solution is obtained by ensuring that the energy and mass balance across individual zones. The model succeeded in explaining the formation of discreet ice lenses and predicting the rate of frost penetration and the extent of frost heave. The idea behind this model was used by subsequent researchers in studying frost heave, i.e., Sheng et al. (1995).

Semiempirical Model

The type of model originally proposed by Konrad and Morgenstern (1980, 1981, 1982a) won a lot of respect in the

1980s and early 1990s. Starting from a practical standpoint, these models provided good prediction of experimental observations. The models are constantly regarded as rigid ice models in some literature because of the use of nonzero ice pressure. It should be noted, however, that the role of ice pressure was negligible in the original model (Konrad and Morgenstern, 1980, 1981). Ice pressure was introduced later for the purpose of considering the effects of applied pressure on freezing soils (Konrad and Morgenstern, 1982b). These models, which had been calibrated from experimental data, have allowed engineering frost-heave calculations (Kujala, 1997). For example, these models were extended for applications such as the estimation of frost heave beneath pipelines (Nixon, 1991). This is the main reason that we introduce this type of model as an independent group of models.

The development of the methods were based on the assumption that the rate of heaving (water intake velocity) was directly related to the temperature gradient at the frost front in either a steady state (Konrad and Morgenstern, 1981) or a transient state (Konrad and Morgenstern, 1982a). The corresponding proportionality was called *segregation potential*. The segregation potential was treated as an important property for characterizing a freezing soil. The segregation potential depends on pressure, suction at the frost front, cooling rate, soil type, and so forth (Nixon, 1991). Frost heave can be calculated once the segregation potential and other parameters of temperature gradients are available. The mathematic representation of the segregation potential is

$$\mathrm{SP}(t)=\frac{v_{\mathrm{w}}(t)}{\nabla T(t)} \qquad [22]$$

where SP is the segregation potential, v_{w} is the water intake velocity, and ∇T is the temperature gradient at the frost front. All three of the quantities are functions of time. The original equation in one dimension was extended to three dimensions for a general description.

Poromechanical Model

The development of poromechanics offers a new perspective on modeling porous materials exposed to freezing conditions. Poromechanics was developed from Biot's theory of dynamic poroelasticity (Biot, 1941), which gives a complete and general description of the mechanical behavior of a poroelastic medium. One representative poromechanical model was developed by Coussy (2005) and Coussy and Monteiro (2008). The dependence of saturation and temperature at freezing temperature was obtained by upscaling from the elastic properties of the solid matrix (Dormieux et al., 2002), pore access radius distribution, and capillary curve. This model also has the advantage that the microscopic properties are linked to the bulk properties, such as the bulk modulus and thermal volumetric dilation coefficient of the solid matrix. The original Biot's theory consists of four distinct physical constants accounting for mechanical properties (Biot and Willis, 1957). Coussy (2005) and Coussy and Monteiro (2008) introduced other parameters to account for ice formation and thermal expansion, which can be reduced to four independent parameters. The micro–macro relationships extended from Biot's coefficients are determined as

$$\begin{aligned} b_{\mathrm{C}}+b_{\mathrm{L}} &= b \\ &= 1-\frac{K_{\mathrm{S}}}{k_{\mathrm{S}}} \end{aligned} \qquad [23]$$

$$\frac{1}{N_{jj}}+\frac{1}{N_{\mathrm{LC}}}=\frac{b_j-\Phi_0 S_j}{k_{\mathrm{S}}} \qquad [24]$$

$$a_j=\alpha_{\mathrm{s}}\left(b_j-\Phi_0 S_j\right) \qquad [25]$$

where K_{S} is the drained bulk modulus, b and N are the Biot coefficient and the Biot modulus, respectively, and a_j is the thermal volumetric dilation coefficient of the true porous solid. These macroscopic properties are linked to the bulk modulus of solid particles, k_{S}, and the thermal volumetric dilation coefficient of the solid matrix, α_{s}. In addition, Φ_0 is the initial Lagrangian porosity and j is a dummy index for the jth phase, The subscripts C and L indicate solid and liquid phases, respectively. The generalized Biot coupling moduli N_{jk} satisfy the Maxwell symmetry relations: $N_{\mathrm{LC}} = N_{\mathrm{CL}}$.

This poromechanical model provides comprehensive quantitative predictions of the mechanical behavior while accounting for the multiscale physics of the confined crystallization of ice. The constitutive relationship of Coussy's poromechanical theory was developed from Biot's general theory of consolidation (Biot, 1941). It is therefore safe to infer that the model accounted for the existence of air bubbles. Coussy used the term *unsaturated*, however, to stress the difference between this air-entrained state and a fully saturated state, which was adopted in the model of Powers (1949). This modification was based on the fact that Powers' model (Powers, 1949) may lead to unrealistic predictions of pressure and shrinkage by neglecting the entrained air bubbles. With the assistance of poroelasticity, the volume change attributed to a different mechanism can be analyzed with the constitutive relation. It must be noted, however, that theoretical extension from a saturated condition to an unsaturated condition in the mechanical field is still far from well developed, although several methods based on experiments are available (Alonso et al., 1990; Lu and Likos, 2006). Some other challenges for poromechanical models include information about the porous media such as the morphology and surface chemistry of constituents, which are obviously difficult to obtain and formulate.

There are also other types of models such as thermomechanical models (Duquennoi et al., 1989; Fremond and Mikkola, 1991; Li et al., 2000, 2002). As summarized in Li et al. (2002), the thermomechanical modeling by Fremond and Mikkola (1991) took deformation factors and phase-changing behavior into account. The behavior of the thermal–moisture-induced deformation of freezing soils are described using the mechanical theory of mixtures in such models.

EXPLICIT RELATIONSHIPS

The second layer of interactions, the explicit relationships, has a strong influence on the coupling processes. Although it does not affect the process as directly as the first layer does, it turns out that the solution to the PDEs is very sensitive to these explicit relationships. The existence of these relationships has been repeatedly proved, while the way to interpret them is continuously improving. The SWCC and the Clapeyron equation are two of the most frequently referenced explicit relationships, which are categorized in the second layer of interactions.

Soil Water Characteristic Curve

The soil water characteristic curve (water retention curve or soil moisture characteristic curve) is the relationship between the water content (volumetric, gravimetric, or saturation) and the soil water potential (or suction; Williams and Smith, 1989). This curve is the characteristic of different types of soils and is commonly used for investigating drying–wetting processes in soils. Because of the analogy between drying and freezing processes (Koopmans and Miller, 1966), this relationship was also widely used in the analyses of freezing processes in porous materials. In the past decades, numerous empirical equations have been proposed for SWCCs, which are summarized in Table 1 (Brooks and Corey, 1964; van Genuchten, 1980; Fredlund and Xing, 1994; Fayer, 2000; Vogel et al., 2000).

Table 1. A few frequently used equations for soil water characteristic curves.

Reference	Equation†
Gardner (1958)	$\Theta = 1/(1 + \alpha\psi^{n})$
Brooks and Corey (1964)	$\Theta = (\psi_{e}/\psi)^{\lambda}$
Haverkamp et al. (1977)	$\Theta = a/(a + \psi^{b})$
van Genuchten (1980)	$\Theta = \{1/[1 + (\alpha\psi)^{n}]\}^{m}$
Williams et al. (1983)	$\theta = \exp[(1/b)\ (\ln\psi - a)$
Bond et al. (1984)	$\theta = a + b\log(\psi) + c\log^{2}(\psi) + d\log^{3}(\psi) + e\log^{4}(\psi)$
McKee and Bumb (1984)	$\Theta = \exp[-(\psi - a)/b]$
Bumb (1987)	$\Theta = 1/\{1 + \exp[(\psi - a)/b]$
Fredlund and Xing (1994)	$\theta = \theta_{s}\{1/\ln[e + (\psi/a)^{n}]\}^{m}$

† Θ, relative degree of saturation; ψ, soil water potential; *a*, *b*, *m*, *n*, and α are empirical constants; θ, volumetric water content; θ_{s}, saturated water content.

Van Genuchten's function has gained popularity. The functional form was obtained by van Genuchten (1980) when he was trying to derive a closed-from equation for hydraulic conductivity. It came from functions similar to Haverkamp's that had been successfully used in many studies to simulate the SWCC (Ahuja and Swartzendruber, 1972; Endelman et al., 1974; Haverkamp et al., 1977). Fredlund and Xing (1994) commented that the assumed correlation between *m* and *n* in van Genuchten's equation reduces the flexibility of the equation. Therefore, Fredlund and Xing (1994) derived a new relationship for SWCCs.

In terms of thermodynamics, the SWCC is attributable to the chemical thermodynamics of interfacial phenomena (Morrow, 1970; Hassanizadeh and Gary, 1993; Grant and Salehzadeh, 1996). In other typical materials such as cement-based materials, three main mechanisms can be identified for an equivalent relationship to the SWCC (Baron, 1982). These include the capillary depression, the surface tension of colloidal particles, and the disjointing pressure (Powers, 1958; Hua et al., 1995; Lura et al., 2003; Slowik et al., 2009). The capillary effect on SWCCs has been the most frequently studied for soils; however, the effect of adsorption on SWCCs is receiving more and more attention in the high matric suction range (the dry region) (Fayer and Simmons, 1995; Webb, 2000; Khlosi et al., 2006). The influence of the latter two mechanisms can be dominant in pores of smaller size.

For practical applications, it is still acceptable to use a pore size distribution together with the capillary law for the purpose of obtaining SWCCs. Zapata et al. (2000) presented the empirical relationships between the coefficients in Fredlund's function (Fredlund and Xing, 1994) and soil properties such as the plastic index. The study by Reeves and Celia (1996) also shed light on the SWCC by analyzing an idealistic network model. A hypothesis was developed to predict the functional relationship between capillary pressure, water saturation, and interfacial area.

The SWCC or similar relations has been widely adopted in most of the simulations of freezing soils involving thermal and hydraulic fields; however, the direct introduction of the SWCC to freezing porous materials to relate suction to saturation (unfrozen water content) is questionable. According to Koopmans and Miller (1966), a direct relationship between the moisture characteristic and the freezing characteristic can be drawn only for adsorbed water. For capillary water, a constant parameter is required to apply SWCCs to partially frozen soils. This constant is equal to the ratio of the surface tension of the water–air interface and that of the water–ice interface. The matric suction in the capillary-controlled range develops at the water–air interface in unsaturated soil or the water–ice interface in partially frozen soils; however, the surface tensions of the two surfaces are different (Bittelli et al., 2003). Experimental results have indicated that the SWCC can be directly applied to frozen soil at suctions >50 kPa (Spaans and Baker, 1996). This has been confirmed by a few other investigators (e.g., Stähli et al., 1999).

Clapeyron Equation

The Clapeyron equation describes the pressure–temperature relationship. This relationship has been discussed since the beginning of the 20th century (Kay and Groenevelt, 1974), i.e., by Hudson (1906) and Edlefsen and Anderson (1943). The Clapeyron equation, which describes the relationship between two phases along an interface, has a unique form, although it can be expressed in different ways and with different notations. The Clapeyron equation can be derived from the equilibrium of the interface between two phases by applying the Gibbs–Duhem equation (de Groot and Mazur, 1984). Its application in freezing porous material is not strictly valid because the Clapeyron equation assumes a closed system while a porous medium is an open system. It is reasonable to assume that the liquid, solid, and air phases in pores tend to reach equilibrium near the interface. Moreover, such equilibrium in the quasi-static sense can only be confidently ensured near the interfaces. Using the Clapeyron equation across the whole region (for every infinitesimal point) needs to be done with care, especially in the presence of a rapid transient transport process.

One common form of the Clapeyron equation, which also considers the effects of a solute on freezing, is (Hansson, 2005)

$$p_{\mathrm{l}} = \rho_{\mathrm{l}} L_{\mathrm{f}} \ln\frac{T}{T_0} + \frac{\rho_{\mathrm{l}}^2}{\rho_{\mathrm{i}}^2} p_{\mathrm{i}} + icRT \qquad [26]$$

where L_f is the gravimetric latent heat of the pore liquid, i is the osmotic coefficient (van't Hoff), c is the concentration of the solute, R is the universal gas constant, and p_{l} and p_{i} are the water pressure and ice pressure, respectively, and T_0 is the freezing point of bulk water at normal pressure (K).

Relationships between the water content and temperature have also been developed for freezing porous media. The essence of such relationships is the combination of the SWCC and the Clapeyron equation. One example is the thermodynamic state function proposed by Coussy (2005). It was based on similar thermodynamics theory as the SWCCs and Clapeyron equation are, but was expressed in the form of a saturation–temperature relationship. This verified the postulation of Harlan (1973) that at subzero temperature, the energy state of liquid water in equilibrium with ice is a function of temperature (except for very dry conditions) and is independent of the total water content.

IMPLICIT RELATIONSHIPS

The third layer of interactions describes changes in material properties with changes in the state variables. These parameters include thermal conductivity, heat capacity, permeability (or hydraulic conductivity), and others. Other parameters, such as the hydraulic conductivity of the vapor phase, the coefficient of convective conduction, and various moduli, are also functions of state variables. Interactions in this layer can also have considerable influence on the coupling processes and are partially responsible for the high nonlinearity of the PDE system for freezing porous media.

Thermal Conductivity

It is known that the thermal conductivity of soil is affected by its density, water content, mineral composition (i.e., the quartz content), particle size distribution, texture, and organic matter content, among others (Kersten, 1949; Penner, 1970; Côté and Konrad, 2005). The air space controls the thermal conductivity at low water content, while solid phase becomes more important at higher water content (Campbell, 1985). Efforts have been made to simulate the thermal conductivity by means of physics-based models, by empirical models for unsaturated soils, and by extension to partially frozen soils.

The early attempts at physically based models usually adopted a geometry in which inclusions in different shapes, e.g., cubic, spherical, ellipsoid, or lamellar, are well arranged in a cubic lattice (Russell, 1935; Woodside, 1958; de Vries, 1963). Among them, the model proposed by de Vries (1963) was designed for unsaturated soils. It is now widely used, for example, in the SHAW model (Flerchinger, 2000). De Vries' model stemmed from the formulae for the electrical conductivity of a two-phase system consisting of uniform spheres of one material arranged in a cubic array of another material. According to Woodside (1958), de Vries (1963) adopted and extended the form of Burger (1915) to the case of ellipsoidal particles and a multiphase medium. The equation was later applied to partially frozen soils by Penner (1970) in the following form:

$$\lambda = \frac{\lambda_{\mathrm{w}}\theta_{\mathrm{w}} + \lambda_{\mathrm{i}}\theta_{\mathrm{i}} + \sum_{j=1}^{M}\lambda_j\theta_j F_j}{\theta_{\mathrm{w}} + \theta_{\mathrm{i}} + \sum\theta_j F_j} \qquad [27]$$

where F_j is the ratio of the average temperature gradient in the jth particles to the average temperature gradient in the continuous medium and M is the number of types of granules. Particles with the same shape and the same conductivity are considered as one type. The quantity F_j depends only on the shape and the orientation of the granules and on the ratio of the conductivity, $\lambda_j/\lambda_{\mathrm{w}}$. It can be calculated as

$$F_J = \frac{1}{3}\sum_{a,b,c}\left[1+\left(\frac{\lambda_j}{\lambda_{\mathrm{w}}}-1\right)g_{\mathrm{a}}\right]^{-1} \qquad [28]$$

where g_a (g_b or g_c) is the depolarization factor of the ellipsoid in the direction of the a (b or c) axis. The quantities g_a, g_b, and g_c depend on the ratios of the axes a, b, and c. Penner (1970) supported the use of $g_a = g_b = 0.125$ and $g_c = 0.75$ obtained by de Vries on a trial-and-error basis. As mentioned by Lu et al. (2007), however, the model requires many input parameters (Bachmann et al., 2001; Tarnawski and Wagner, 1992) and proper selection of the shape factors (Horton and Wierenga, 1984; Ochsner et al., 2001) to accurately predict the thermal conductivities.

Johansen (1975) proposed an empirical relationship for the thermal conductivities, which was later modified by Côté and Konrad (2005) and Lu et al. (2007). The key concept in these models is the unique relationship between the normalized thermal conductivity and normalized saturation. The differences among the models are mainly the use of different empirical equations to describe the relationships. In the reviews of Farouki (1981, 1982), Johansen's model was regarded as the one that gave the best prediction of thermal conductivities for sands and fine-grained soils among those available in the literature. The later modification by Côté and Konrad (2005) was developed based on a large pool of data (220) and was believed to be applicable to a wide range of soils and construction materials. The subsequent study of Lu et al. (2007) indicated that Côté's model (2005) does not always perform well at low water contents, especially on fine-textured soils. Lu's improved model led to comparatively smaller root mean square errors (Lu et al., 2007). The basic relations in these models are expressed by

$$\lambda_{\mathrm{r}} = \frac{\lambda - \lambda_{\mathrm{dry}}}{\lambda_{\mathrm{sat}} - \lambda_{\mathrm{dry}}} \qquad [29]$$

$$\lambda_r = f(\Theta) \quad [30]$$

where λ_r is the normalized thermal conductivity, and λ, λ_{dry}, and λ_{sat} are the actual thermal conductivity and the thermal conductivities of dry and saturated soils, respectively; Θ is called *normalized saturation*, which is equivalent to the effective saturation mentioned above. The relationship between normalized thermal conductivity and normalized saturation (function *f*) can be different for different materials such as fine sands and fine-grained soils. Therefore, for the same soil, the function can be much different if freezing occurs. The functions for frozen soils can be found in Johansen (1975) and Côté and Konrad (2005).

One empirical relationship for the thermal conductivity of partially frozen soils that has been successfully applied in TH modeling is the one presented by Hansson et al. (2004):

$$\begin{aligned}\lambda = {} & C_1 + C_2\left[\theta_w + \left(1 + F_1\theta_i^{F_2}\right)\theta_i\right] - \left(C_1 - C_4\right) \\ & \times \exp\left(-\left\{C_3\left[\theta + \left(1 + F_1\theta_i^{F_2}\right)\theta_i\right]\right\}^{C_5}\right) \\ & + \beta_t C_w \left|\vec{J}\right|\end{aligned} \quad [31]$$

where θ_w is the volumetric water content, C_1, C_2, C_3, C_4, and C_5 are constants for curve fitting, β_t is the longitudinal thermal dispersivity, and C_w is the heat capacity of water. This equation is a modification of the empirical equation proposed by McInnes (1981) from experimental data. This original equation was verified by Cass et al. (1981), who succeeded in using the modified equation to express the thermal conductivity of a soil from the Hanford site.

Many other simple empirical ways for predicting the thermal conductivity as a function of the state variables of frozen porous materials, i.e., temperature and water content, are available, such as the relationships suggested by Sawada (1977):

$$\lambda = AT^B \quad [32]$$

$$\lambda = C\exp(Dw) \quad [33]$$

where *w* is the gravimetric water content and *A*, *B*, *C*, and *D* are constants from curve fitting.

It has been reported that the thermal conductivity of frozen soils may be lower than that of unfrozen soils at low degrees of saturation (Kersten, 1949; Penner, 1970; Côté and Konrad, 2005). This phenomenon generally can't be described by the physics-based models, yet it can be considered in empirical ones.

Heat Capacity

The heat capacity is usually formulated as the weighted sum of different components of the porous medium (de Vries, 1963; Campbell, 1985; Williams et al., 1983):

$$\rho C_p = \rho_w C_w \theta_w + \rho_i C_i \theta_i + \rho_s C_s \theta_s + \rho_a C_{air} \theta_a \quad [34]$$

where *C* is the gravimetric heat capacity; θ is the volumetric water content; the subscripts *w*, *i*, *s*, and *a* denote water, ice, solid, and air, respectively; and C_p is the actual gravimetric heat capacity. Difficulties arise from the heat released or absorbed during the phase transition of the pore liquid, a key factor to couple the thermal and hydraulic fields. Direct treatment of the heat phase transition is rare because heat release or absorption occurs near the freezing point of the pore liquid and gives rise to numerical instability (Hansson et al., 2004). Alternatively, the latent heat is typically accounted for by use of the concept of apparent heat capacity:

$$C_a = C_p + L_f \frac{d\theta_i}{dT} \quad [35]$$

where C_a is the apparent gravimetric heat capacity. This term was introduced by Williams (1964) and later used by Anderson et al. (1973) to ensure computational stability. In this method, the released or absorbed energy was incorporated into the heat capacity term. The same concept has been used by many researchers (e.g., Harlan, 1973; Guymon and Luthin, 1974; Hansson et al., 2004).

Permeability

Permeability, or hydraulic conductivity, is one of the most challenging soil properties. Because of this, great attention has been paid to its prediction by theoretical models (Fredlund et al., 1994). Brutsaert (1967) presented a review on this topic. Most of the early researchers used empirical methods and usually described the permeability as a function of soil suction, because soil suction was one of the two stress state variables controlling the behavior of unsaturated soils. The relationship between the volumetric water content and the relative permeability was also frequently used. Table 2 lists a few of these relationships (Fredlund et al., 1994),

Some of the equations listed in Table 2 were originally written in the form of hydraulic conductivity. They can be transformed into permeability only if viscosity does not vary with other parameters, e.g., temperature. This may not be true, however, because the variation of viscosity from −20 to 20°C is not negligible (Seeton, 2006).

Childs and Collis-George (1950) and Burdine (1953) developed statistical models to predict permeability. The permeability functions were determined by using the SWCC, or more directly, the variation in pore size. These models based on the pore size distribution represented by Childs and Collis-George (1950) were later improved by Marshall (1958) and Kunze et al. (1968). This kind of statistical model received the most attention in the past 30 yr. The first great breakthrough came from Mualem (1976), who derived and equation for predicting permeability based on a conceptual model similar to Childs and Collis-George (1950):

$$k_r = \left[\frac{\int_{\theta_r}^{\theta} d\theta/\psi(\theta)}{\int_{\theta_r}^{\theta_s} d\theta/\psi(\theta)}\right]^2 \quad [36]$$

Table 2. A few frequently used equations for intrinsic permeability (k_i).

Reference	Equation†
Richards (1931)	$k_i = a\psi + b$
Wind (1955)	$k_i = a\psi^{-n}$
Gardner (1958)	$k_i = \exp(-a\psi)$ and $k_i = k_S/(b\psi^n + 1)$
Brooks and Corey (1964)	$k_i = k_r, \psi < \psi_{aev}; k_i = (\psi/\psi_{aev})^{-n}, \psi > \psi_{aev}$
Rijtema (1965)	$k = k_r, \psi < \psi_{aev}; k_i = \exp[a(\psi - \psi_{aev})], \psi_{aev} < \psi < \psi_l$ $k = k_l(\psi/\psi_l)^{-n}, \psi > \psi_l$
Averjanov (1950)	$k_i = \Theta^n$
Davidson et al. (1969)	$k_i = k_r \exp[a(\theta - \theta_s)]$
Campbell (1974)	$k_i = k_r(\theta/\theta_s)^n$

† k_r, relative permeability, which denotes the ratio of permeability to the saturated permeability; ψ, soil water potential; ψ_{aev}, soil water potential close to saturation; ψ_l, soil water potential close to dry condition; k_l, intrinsic permeability close to dry condition; Θ, effective or normalized saturation; θ, volumetric water content; θ_s, saturated water content; *a*, *b*, and *n*, empirical curve-fitting parameters.

Van Genuchten (1980) developed a closed form for the model by using a particular form of the incomplete beta function:

$$k_r = \Theta^{1/2}\left[1-\left(1-\Theta^{1/m}\right)^m\right]^2 \qquad [37]$$

Fredlund et al. (1994) developed another similar form of equation by implying the SWCC proposed by Fredlund and Xing (1994):

$$\theta = C(\psi)\frac{\theta_s}{\left\{\ln\left[e+(\psi/a)^n\right]\right\}^m} \qquad [38]$$

where a is the air-entry value of the soil and $C(\psi)$ is a special correcting function defined by Fredlund et al. (1994).

From this introduction, one type of SWCC leads to one type of model for predicting permeability. This viewpoint has been accepted and used in some simulation studies (Fayer, 2000).

These models were originally developed for partially saturated soils. Their application was conventionally extended to frozen porous materials based on the similarity between the freezing–thawing process and the drying–wetting (desorption–sorption) process. A significant basis is Harlan's postulation that the permeability vs. suction relationship for a partially frozen soil is the same as that of the SWCC (Jame and Norum, 1980; Noborio et al., 1996b; Hansson et al., 2004). Some other relationships taking soil suction as an independent variable are also widely used in simulations (Guymon and Luthin, 1974; Noborio et al., 1996b). Many researchers have tended to use an impedance factor to account for the effects of ice on the permeability (Lundin, 1990; Hansson et al., 2004). A newer viewpoint, however, has stated that the impedance factor is not necessary when an accurate SWCC is available (Newman and Wilson, 1997; Watanabe and Wake, 2008). On the other hand, there are reports that the magnitude of the hydraulic conductivity increased by 1.5 to two orders of magnitude in compacted clays after being subjected to freeze–thaw cycles. Horizontal and vertical cracks were believed to be responsible for the increases in the bulk hydraulic conductivities (Benson and Othman, 1993; Othman and Benson, 1993). This phenomenon can have a major impact on the behavior of frozen soils.

CHALLENGES IN THE IMPLEMENTATION OF MODEL SIMULATION

Solving the coupling processes of freezing porous materials requires the relationships among temperature, unfrozen water content, soil water potential, and frozen water content to be determined. This is because there are two PDEs for the transport of heat and mass, while there are four independent state variables (i.e., the temperature, unfrozen water content, soil potential, and frozen water content). To solve the PDEs, explicit relationships such as the SWCC and Clapeyron equation or other similar relationships need to be incorporated. This usually causes difficulties in implementing numerical solutions for these models. Specifically, it is hard to solve the set of coupled PDEs, which are highly nonlinear and highly interdependent. For example, determining the freezing point depression requires the soil water potential and temperature to be known, which are in turn dependent on the estimation of the freezing point.

The couplings between the mechanical field and the other two fields have received less discussion in the literature because they have comparatively weak coupling effects, especially the coupling from the mechanical field to the thermal or hydraulic fields. Simplified methods based on mixture theories, poromechanics, or even direct coupling based on experimental relationships can reasonably account for such coupling effects in most cases. Close attention is required when the variations in stress or strain have a significant influence on other physical fields.

DISCUSSION

The aspects of frost action discussed here are not exhaustive. There are still other foci that have received substantial consideration. Understanding the basic mechanisms relevant to the freezing or frozen multiphase system of a porous medium is the prerequisite (Miller and Morgenstern, 1973). The following provides a brief discussion on a few salient points for selection and implementing simulation models for freezing effects on porous materials. We also point out a few important aspects that need to be further investigated.

The investigation of porous materials under frost action requires an integral approach. To increase the understanding of the fundamental mechanisms, people with different backgrounds have addressed the issue from different perspectives. The rich collection of viewpoints, while aiding the understanding of this complex phenomenon, can also cause confusion (e.g., due to the inconsistency in the terminology, deviations in the basic assumptions, and different interpretations of the underlying mechanisms). A holistic approach to categorize the theoretical basis for simulation model development is needed to reconcile the seeming inconsistencies. For this purpose, mechanisms responsible for coupling interactions in a porous material system need to be elucidated. One main issue is to unify our understanding of the process under saturated and unsaturated conditions. Phenomena such as frost heave, which is generally believed to happen in saturated soils, can occur when the degree of saturation reaches 80 to 90% rather than 100% (Dirksen and Miller, 1966). The study of Dirksen and Miller (1966) outlined a preliminary and interesting picture for integrating phenomena under both saturated and unsaturated conditions. There were, however, very rare follow-up investigations. As commented by Lundin (1990), efforts to extend models for freezing saturated porous materials into the partially saturated condition have been scarce (Lundin, 1990). This is also partially due to the complexity in solving the coupled nonlinear PDEs.

The influence of temperature on heat and mass transport in freezing porous materials requires further investigation. First of all, the temperature-induced liquid flow has been formulated by the theory of Philip and de Vries (1957) or its equivalent in most hydrodynamic models. The theory reflects the fact that solid–liquid surface tension is temperature dependent. This dependence can be directly considered in a temperature-dependent SWCC. Currently, however, we usually adopt a temperature-dependent permeability and isothermal SWCC (Jame and Norum, 1980). This strategy has been shown to be able to effectively reduce nonlinearity, but the rationality for such treatment requires further validation. Second, in addition to surface tension, the contact angle has been found to be more significantly influenced by temperature, causing two to 10 times variations in the gain factor, as observed in a few studies (Nimmo and Miller, 1986; Grant and Salehzadeh, 1996; Bachmann et al., 2002; Bachmann and van der Ploeg, 2002). To precisely predict the coupling between the thermal and hydraulic fields, a more thorough understanding of the variation in the contact angle with temperature is necessary. This effect is, by nature, another explicit relationship, which is between suction and temperature.

Poromechanics, which was developed from micromechanics, provides a robust approach to study phenomena in porous materials based on fundamental mechanisms. The definition of "unsaturated" in current poromechanics is still distinct, however, from the term used in geotechnical engineering. Theories developed from Biot's theory consider entrapped air bubbles (Biot, 1941) but have failed to cover all unsaturated conditions such as porous materials with an interconnected air phase. The assumption of Biot's theory, that all pores deform in the same way when subjected to the same pore pressure, needs to be further validated. Moreover, the current homogenization technology is still far from satisfactory to consider the complex morphology of a solid matrix and the variations caused by thermal and hydraulic fields.

The general concept of suction, rather than separate components such as matric suction or osmotic suction, was used here for a general introduction to this topic. This, however, reveals the fact that most studies have typically focused on certain components of suction. For example, the osmotic potential was generally ignored in simulations of frozen soil in civil engineering applications (Nishimura et al., 2009; Thomas et al., 2009). This approximation is acceptable only if one of the following conditions is satisfied: (i) the soil is free of soluble salts or the influence of osmotic suction is negligible in comparison with that of matric suction in the suction range of interest; and (ii) the SWCC is obtained with respect to soil water suction instead of matric suction. Otherwise, the osmotic suction needs to be considered because soluble salts are excluded from the ice phase and remain in the unfrozen water on freezing of moist soil (Banin and Anderson, 1974). Consequently, osmotic suction can increase considerably in a freezing process. This is similar to the role of osmotic suction in a drying process, which possibly prevails across most of the suction range (Krahn and Fredlund, 1972).

While there is significant progress in describing and simulating the coupling in freezing porous materials, understanding the fundamentals remains a major driving force for the development of unsaturated soil mechanics. One classic example is ice regelation transport (Horiguchi and Miller, 1980). The phenomena observed with an "ice sandwich" permeameter leads to a perspective that ice will not move due to its unmovable geometry but it can benefit the mass transport (or "apparent hydraulic conductivity") by melting on one side while regelating on the other side. The second example that can be cited is the phenomenon of secondary heave. This happens because both water expelled from a descending zone of freezing due to water expansion and absorption of water to freezing sites occur at the same time. In secondary heave, a flow may be in either direction and reverse, leading to discrete ice lenses that are not level and continuous. Another example is the shutoff pressure, which was observed be dependent on soil type, stress history, and freezing temperature. It was observed that water was expelled from the freezing front and ice lens creation ceased at overburden pressures greater than the shutoff pressure and vice verse. This macroscopic observation was deemed to be relevant to the Young–Laplace equation at the mesoscale and microscale (Arvidson and Morgenstern, 1977):

$$p_{\mathrm{i}}-p_{\mathrm{w}}=\frac{2\sigma_{\mathrm{wi}}}{r_{\mathrm{wi}}} \quad \text{(or a constant)} \qquad [39]$$

where p_{i} is the ice pressure, which is also the overburden pressure when an ice lens develops; σ_{wi} is the water–ice surface tension; and r_{wi} is the radius of the water–ice interface. It was confirmed by experiment that the pressure difference $(p_{\mathrm{i}}-p_{\mathrm{w}})$ was approximately equal to a constant for each soil type (Williams, 1967; Sutherland and Gaskin, 1973). This, however, needs to be further validated.

CONCLUSIONS

This review provided a general overview on the theoretical basis for implementing model simulations for freezing porous materials. It categorized the various model development efforts into a general framework and presents the theoretical foundations as three layers of interactions, i.e., the basic mechanisms, the explicit relationships, and the implicit relationships. For the basic mechanisms, representative theories and their basic assumptions were discussed for the coupling of thermo-hydraulic processes. The explicit relationships provide closure to the system of PDEs and ensure the uniqueness of the solution. These implicit relationships describe the dependencies of parameters on the state variables. The interactions of the three different layers results in highly coupled nonlinear processes associated with freezing effects on porous materials. Implementation of model simulations therefore requires deliberate and proper accounting for these interactions. A general framework categorizing the important bases for a simulation model, such given here, will help to address the challenging task of implementing such model simulations.

While the focus of this review was to summarize the existing accomplishments in understanding the freezing of porous materials, it also discussed a few aspects that require further deliberation. For example, the unification of existing theories for unsaturated soil and saturated soils is suggested. Progress in these areas will provide an even stronger foundation for simulation models and will lead to a general and holistic simulation platform for porous materials under frost actions.

VARIABLE DEFINITIONS

a_j	thermal volumetric dilation coefficient of the true porous solid
b	Biot modulus
C	specific heat capacity
C_w	heat capacity of water.
C_a	apparent specific heat capacity (gravimetric)
C_p	actual specific heat capacity (gravimetric)
c	concentration of the solute
D	molecular diffusivity of water vapor in air
D_0	general term of diffusion coefficient, the thermal conductivity for the heat transfer problem, and the hydraulic conductivity for the mass transfer problem
F_j	ratio of the average temperature gradient in the *j*th particles to the average temperature gradient in the continuous medium
f	source or sink term
$f(\Theta)$	relationship between normalized thermal conductivity and the normalized saturation
g	gravitational acceleration.
g_a (g_b or g_c)	depolarization factor of the ellipsoid in the direction of the *a* (*b or c*) axis
i	osmotic coefficient (van't Hoff)
$\vec{i}$	unit vector in the direction of gravity
j	dummy index
$\vec{J}$	flux; vector that represents either heat or mass flux
$\vec{J}_l$	gravimetric liquid flux
$\vec{J}_q{}'$	reduced heat flux
$\vec{J}_v$	gravimetric vapor flux
K	hydraulic conductivity
K_S	drained bulk modulus
k_i	intrinsic permeability (or permeability for short)
k	hydraulic conductivity
k_S	thermal volumetric dilation coefficient of the solid matrix
L_f	gravimetric latent heat of melting or freezing
L_m	latent heat of melting per molecule
L_T, L_{Tw}, L_w	coefficients of transport deduced as functions of other parameters such as vapor conductivity, latent heat, and volume of vapor
N	Biot modulus
p	pressure of the "extramatric water"
p_a	pore air pressure
p_i	ice pressure
p_s	pressure of solid
R	universal gas constant
p_w	pore water pressure
r	radius of curvature of the interface
r_{ave}	mean curvature
r_{wi}	radius of water–ice interface
S	entropy product
s	matric suction
SP	segregation potential
T	temperature
T_0	freezing point of bulk water at normal pressure (K)
t	time
u	independent variable in a governing equation (PDE)
$\mathbf{u}$	tensor of the independent variable in two or three dimensions
V_s, V_l	specific volume of solid and liquid, respectively
$\overline{V_l^e}$	volume of the "extramatric liquid"
v	mass-flow factor
v_i	rate of frost heave
v_w	water intake velocity
w	gravimetric water content
α	tortuosity factor allowing for extra path length
α_s	initial Lagrangian porosity
β_t	longitudinal thermal dispersivity
δP_m	thermomolecular pressure
Θ	effective or normalized saturation
θ	volumetric water content
θ_a	volumetric air content
θ_I	volumetric ice content
θ_r	residual water content
θ_s	saturated water content
θ_w	volumetric water content
λ	thermal conductivity
λ_r	normalized thermal conductivity
λ_{dry}, λ_{sat}	thermal conductivity of dry and saturated soils, respectively
μ	viscosity of the liquid
ρ_w	water density
ρ_a	density of water vapor
$\rho_{a,0}$	density of saturated water vapor
ρ_i	density of ice
ρ_l	density of bulk liquid
σ	surface tension of soil water
σ_{wa}	water–air surface tension
σ_{wi}	water–ice surface tension
ψ	total potential
ψ_a	pneumatic potential
ψ_e	envelope potential resulting from overburden potential
ψ_m	matric potential
ψ_o	osmotic potential
ψ_g	gravitational potential
Φ_0	initial Lagrangian porosity

Note: d_C and K_C are constants; C_1, C_2, C_3, C_4, C_5, *A*, *B*, *C*, and *D* are constants for curve fitting; The subscript *l*, *w*, *a*, *i*, and *s* denote liquid, water, air, ice, and solid particles (in soils and rocks), respectively; C and L represent solid and liquid phases (in cement and concrete), respectively.

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