Review: The mathematical representation of freezing and thawing processes in variably-saturated, non-deformable soils

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Abstract

Recently, there has been a revival in the development of models simulating coupled heat and water transport in cold regions. These models represent significant advances in our ability to simulate the sensitivity of permafrost environments to future climate change. However, there are considerable differences in model formulations arising from the diverse backgrounds of researchers and practitioners in this field. The variability in existing model formulations warrants a review and synthesis of the underlying theory to demonstrate the implicit assumptions and limitations of a particular approach. This contribution examines various forms of the Clapeyron equation, the relationship between the soil moisture curve and the soil freezing curve, and processes for developing soil freezing curves and hydraulic conductivity models for partially frozen soils. Where applicable, results from recent laboratory tests are presented to demonstrate the validity of existing theoretical formulations. Identified variations in model formulations form the basis for briefly comparing and contrasting existing models. Several unresolved questions are addressed to highlight the need for further research in this rapidly expanding field.

Keywords

Permafrost modeling, climate change, freezing soil, Clapeyron equation, soil freezing curve, hydraulic conductivity

Highlights

1) Models for simulating heat and water processes in freezing soils are summarized.
2) The sources of existing variations in the Clapeyron equation are explained.
3) Various formulations for the soil freezing curve are reviewed.
4) Best practices to develop a frozen soil hydraulic conductivity model are detailed.
5) Several unresolved questions are highlighted and addressed.

1. Introduction

Climate change-induced hydrological and ecological changes to arctic and subarctic regions have been well-documented [1-5]. These changes include: thawing permafrost, decreasing sea ice and glacier ice mass, and shifting biological indicators. Permafrost degradation could act as a positive feedback mechanism to climate change as thawing permafrost can release carbon and methane currently stored in northern soils [6-14]. Permafrost thaw can also affect hydrological regimes by increasing groundwater-surface water interactions and by mediating groundwater exchange between sub-permafrost and supra-permafrost aquifers [15-18]. Thus, understanding and characterizing permafrost thaw is an important component of the broader scientific investigation of the role of future climate change in altering high-latitude regions [19]. To address the concerns associated with permafrost thaw, recent contributions have employed coupled water and heat transport models to simulate hydraulic and thermal responses of idealized permafrost environments to a warming climate [e.g. [20-27]]. By accounting for transport of water, these contributions have expanded on other research that has assumed advective heat transport (and its impact on permafrost thaw rates) is insignificant [e.g. [28-30]]. Researchers developing or applying mathematical models to investigate the future state of subsurface hydrological processes in cold regions are faced with difficulties due to (1) a lack of a proper fundamental understanding of physical processes [31], (2) uncertainty regarding appropriate model parameterization to accurately simulate the dynamic freeze-thaw process, and (3) computational challenges arising from model complexity [23]. A thorough review of the underlying theory of freezing and thawing in unsaturated porous media should aid in addressing the first and second difficulty noted above and thereby assist model developers in this rapidly expanding field of research. A summary of previously published heat and water transport models for cold regions is presented prior to any detailed discussion regarding the underlying theory.

1.1. A history of mathematical models

The study of soil freezing and thawing has a fragmented history that is characterized by considerable inconsistencies in both nomenclature and underlying theories or methodologies. These incongruities stem in part from the diverse backgrounds (e.g. civil engineers, soil scientists, hydrologists, and hydrogeologists) of researchers and practitioners in this field. The quantitative study of freezing in soils has also been characterized by intermittent periods of research intensity and stagnation. For example, early studies describing the thermodynamics of freezing soils [32,33] were generally not expanded upon until two decades later when the quantitative study of frost heaving revived academic interest in this field [34-40].

The underlying theory presented in much of this seminal research [32-37] was soon incorporated into mathematical models of coupled water and energy transport in freezing soils. These models were developed in part to assist in the design of cold regions infrastructure as the oil and gas industry began to move increasingly north in the 1970's. Harlan [41] is typically credited for developing the first hydrodynamic-based model for simulating coupled water and heat transport in freezing porous media. This model was fundamentally based on a hydraulic analogy between Darcian fluid flow in unsaturated ice-free soils and fluid flow in partially frozen soils. This approach contrasted strongly with the capillary sink models employed by his contemporaries studying frost heave processes [42,43]. Guymon and Luthin [44] developed a similar model to Harlan's [41], by coupling a modified version of Richards' equation [45] to a one-dimensional conduction-advection heat transport equation. They also more clearly demonstrated how an equilibrium equation could be used to relate the pore water pressure and temperature in freezing or thawing soils. Jame [46] utilized a Crank-Nicholson scheme to solve modified forms of the equations presented by Harlan [41], and simulations from his model favorably compared to laboratory tests conducted on freezing unsaturated soil. Taylor and Luthin [47] created a mathematical model of coupled heat and moisture transfer in freezing soils that ignored the impacts of advective heat transport induced by moving groundwater. Their simulation results were in agreement with data obtained from the experimental freezing tests conducted by Jame and Norum [48] and Dirksen and Miller [39]. Hromadka et al. [49] presented a model in which the governing heat and soil-water transport equations were combined into either a single moisture or heat transport model via the derivative of the unfrozen water content-temperature relationship. This approach significantly improved computational efficiency.

This period of research intensity was followed by a relative quiescence until the late 1980's/early 1990's when further one-dimensional models of freezing soils began to emerge. Flerchinger and Saxton [50,51] developed the SHAW model for simulating simultaneous heat and water transport in freezing soils under tillage and crop residue effects; their model simulations were in agreement with measured soil temperature, frost depth and soil water data in Washington, USA. Johnsson and Lundin [52] applied the coupled soil water and heat transport model SOIL to study the influence of frost and snow on infiltration. Their simulations concurred with measured soil temperature and water content from a field site in northern Sweden. This model has since been further developed into the CoupModel, which also simulates frost heaving processes [53]. Newman [54] and Newman and Wilson [55] modified the geotechnical heat and mass transfer model SoilCover to include the effects of phase change and ice formation. Their model simulations successfully reproduce the temperature and moisture content data obtained from freezing tests conducted by Jame and Norum [56]. Guymon et al. [57] developed FROSTB to simulate heat and moisture flow and frost heave and thaw settlement. Shoop and Bigl [58] compared FROSTB simulations to their large-scale experimental investigations and found that FROSTB reasonably predicted frost penetration and heave, but over-predicted ice formation.

Zhao et al. [59] included the effects of phase changes in their one-dimensional water and energy transport model, and simulations were conducted to predict the thermal and hydraulic effects of infiltration in a partially saturated frozen ground. Hansson et al. [60] modified the existing HYDRUS-1D code to accommodate the hydraulic and thermal effects of freezing and thawing.

HYDRUS 1D simulations concurred with the freezing laboratory experiments conducted by Mizoguchi [61]. Zhang et al. [62] presented a frozen soil model that was capable of producing observed temperature and unfrozen water data collected from field sites in Minnesota and the Tibetan plateau. In these contributions, the accuracy and generality of the soil freezing calculations were improved, but the basic underlying theory was relatively unchanged from Harlan's work [41]. These one-dimensional models are only briefly described in the present contribution as most have already been reviewed and categorized by Li et al. [63].

More recently, questions regarding the impact of climate change on subsurface permafrost environments have emerged and created a demand for robust, multi-dimensional water and energy transport models. Ippisch [64] developed a rigorous three-dimensional groundwater flow and energy transport model to simulate coupled water, heat, gas, and solute transport in permafrost soils. Multi-phase transport was simulated using a two phase model to include both the water vapor and air phases. Ippisch [64] found that water vapor and solute transport did not significantly affect the subsurface thermal regime, but that advective heat transport was important near 0°C. Qualitative agreement was achieved between model simulations and measured unfrozen moisture content and temperature data obtained from an instrumented field site in the Svalbard archipelago, Norway. The Subsurface Transport Over Multiple Phases (STOMP) model [65,66] is a powerful, three-dimensional simulator of water, energy and solute transport in variably-saturated conditions and includes the dynamic freeze-thaw process. This two component (water and air) and three phase model was applied by Nichols et al. [67] to simulate a proposed benchmarking problem involving the freezing and thawing of a pipe.

McKenzie et al. [68] modified the existing groundwater flow and energy transport code SUTRA [69] to accommodate the thermal and hydrologic effects of freezing in fully saturated soils. The modified SUTRA code was applied to (1) replicate the analytical solution of Lunardini [70] for soil freezing in a three-layer system: thawed, frozen, and partially frozen, (2) reproduce measured subsurface temperatures from a peat bog in Minnesota, USA, and (3) solve two benchmark problems involving soil freezing. Li et al. [71] presented a finite element model for simulating three dimensional moisture and heat flow with phase change and freezing-induced soil deformation. Simulations of temperature profiles beneath a highway in the Qinghai-Tibetan Plateau agreed with measured field results. Bense et al. [25] developed a cold regions groundwater flow and heat transport model to simulate hydraulic and thermal processes in high-latitude aquifers. The governing coupled water and heat transport equations were solved by employing the finite element method with the FlexPDE software package. Bense et al. [20,25] applied this model to study climate change-induced hydraulic evolution of aquifers and the consequent increase in baseflow in idealized permafrost environments.

Liu and Yu [72] proposed a thermo-hydro-mechanical model to simulate the flow of heat and moisture and the associated soil mechanics in freezing soils. Results from their simulations concurred with data obtained from the classic freezing experiment by Mizoguchi [61] and measured temperature and moisture content data collected beneath a road in Ohio, USA.

Dall'Amico [73] and Dall'Amico et al. [74] presented a model to simulate freezing phenomena in variably-saturated soil. Model simulations compared favorably to temperature profiles generated from the Neumann solution for phase change without water flux [75] and experimental soil column freezing experiments conducted by Mizoguchi [61]. Tan et al. [76] developed a cold regions, coupled water and heat transport model which differed from many previous hydraulic models by accommodating the Soret effect (moisture redistribution due to temperature gradient) and segregation potential (the ratio of moisture redistribution to the temperature gradient) [77]. Their model simulations concurred with the laboratory experiments of Mizoguchi [61], and the model was subsequently applied to simulate the effects of design alternatives for the Galongla tunnel, Tibet.

Painter [78] developed the three-phase, non-isothermal model MarsFlo to simulate water and heat transport in frozen Martian environments [79]. This flexible and powerful code was validated by comparing model simulations to the soil freezing experiments documented by Mizoguchi [61] and Jame and Norum [56]. MarsFlo is one of the first models to consider both two components (gas and water) and three water phases (vapor, liquid water, and ice). The diffusive vapor transport formulation in MarsFlo was validated with an analytical solution. Painter [78] also demonstrated the application of MarsFlo to study the evolution of permafrost in Martian and terrestrial environments. Frampton et al. [24,26] later applied MarsFlo to simulate climate change impacts on subsurface thermal and hydraulic regimes in idealised permafrost environments.

ARCHY is a simulator of variably-saturated water, energy and solute transport developed by integrating two previous models: MAGHNUM [80] and TRAMP [81]. Rowland et al. [82] applied ARCHY to demonstrate the importance of advective heat transport in the formation of taliks below lakes in permafrost environments. Two emerging models that are currently being developed at Los Alamos National Laboratory (Artic Terrestrial Simulator, ATS [83] and PFLOTRAN [84]) perform simulations in powerful, parallel computational environments and will thereby enable researchers to investigate Artic processes at much higher spatiotemporal resolution.

Global and regional-scale land surface models have also recently incorporated soil freezing schemes, which have been directly or indirectly based on several of the models previously listed [85-88]. Such models are capable of simulating permafrost degradation at a coarse scale and assist in projecting future climate conditions [89]. However due to computing restrictions, the simulations of complex near-surface processes are generally sacrificed with increasing spatial scales.

1.2. Discrepancies between models: a basis for this review

The study of heat and water transport dynamics in permafrost regions is rapidly expanding due to the development of the increasingly complex models listed above. Unfortunately, early disagreements regarding the appropriate mathematical representation of freezing phenomenon still remain unresolved. Discrepancies between existing model mechanics become very apparent when these models are reviewed and compared. In this contribution, the theory of freezing and thawing processes in variably-saturated porous media and their effect on water transport are reviewed to highlight the underlying assumptions and limitations of particular formulations. Specifically, we discuss variations in the form of the Clapeyron equation (section 2), similarities between the soil water and soil freezing curves (section 3), variations in previously-published soil freezing curves (section 4), and diversities in methodologies for estimating the hydraulic conductivity of partially frozen soils (section 5). To our knowledge, this is the first synthesis of this body of research that spans several decades. Following the review of freezing and thawing theory, we briefly compare and contrast the models previously listed (Table 1) and offer suggestions for future research (section 6). In addition to review material, new and previously-published data are presented to demonstrate the accuracy of the current state of knowledge on the physics and thermodynamics of freezing and thawing phenomenon in porous media.

This contribution is focused on the theoretical development of models whose purpose is to simulate climate change-induced permafrost thaw and changing hydrogeologic and hydrologic regimes. Thus, this contribution will not contain a discussion on ice lensing and related soil deformation as these processes have been recently described in detail in several notable contributions [90-93]. Also, this contribution does not provide details regarding the formulation or parameterization of the governing heat transport equation in partially frozen soils. Readers interested in this formulation and parameterization are referred to classic contributions by Lunardini [70,94], Williams and Smith [95], and Farouki [96].

It should be noted that differences between model formulations often arise due to the various applications of these models. In general, model simulations can only provide answers to well-posed questions and thus all incorporate some degree of approximation. The appropriate level of model fidelity to physical processes is dependent on the simulation objectives. For example, models that are formulated to simulate the subsurface hydraulic and thermal response to surficial climate change may not need to accurately simulate the physics of ice lensing. We do not suggest that every heat and water transport simulator should incorporate all of the suggestions of the present contribution. Rather we provide details regarding various formulations and make suggestions regarding the ones which best represent physical processes. Interested model developers can then make informed decisions regarding which assumptions and simplifications to employ.

Table 1: Variations in the methodologies for models simulating water and heat transport in freezing soils

Numerical model reference[1]	Primary Focus of Model Development/ Application	Number of dimensions[2]	Clapeyron equation	Soil freezing curve	Soil diffusivity, permeability, or hydraulic conductivity[3]	Model verification/ validation
Harlan [41]	Moisture redistribution and infiltration in frozen soils	1	Modified Equation (3)	-[4]	-	--
Guymon and Luthin [44]	Coupled heat and moisture flow	1	Equation (3)	Gardner [147]	Gardner [147]	-
Jame [46]	Coupled heat and moisture flow (testing Harlan's approach)	1	Equation (2)	Piecewise linear	Piecewise linear + impedance	Experimental data and analytical solution
Taylor and Luthin [47]	Coupled heat and moisture flow with soil heaving	1	-	Piecewise linear and power function	Piecewise linear + impedance factor	Experimental data
Hromadka et al. [49]	Isothermal phase change model that combined heat and water transport equations.	1	-	Piecewise linear	Exponential function + impedance factor	--
Flerchinger and Saxton [51]	Coupled heat, moisture, and solute transport in agricultural settings	1	Modified Equation (7)	Brooks-Corey [151]	Modified Campbell [175]	Field data
Guymon et al. [57]	Prediction of frost heave and thaw settlement in pavements	1	-	Gardner [147]	Gardner [147] + impedance	Experimental and field data
Newman [54]	Unsaturated heat and water flux in a geotechnical model	1	Modified Equation (2)	Empirical form from Jame [46]	Fredlund et al. [153]	Experimental data
Ippisch [64]	Coupled water, heat, gas, and solute transport	3	Equation (2)	van Genuchten [154] or Brooks-Corey [151]	van Genuchten [154] or Brooks-Corey [151]	Field data
Hansson et al. [60]	Heat and moisture transport in sub-freezing temperatures with an application to study temperature beneath a road	1	Equation (3)	van Genuchten [154]	van Genuchten [154]+ impedance	Experimental data
White and Oostrom [65,66]	Simulator of coupled heat, mass, and solute transport	3	Modified Equation (2)	van Genuchten [154] or Brooks-Corey [151]	van Genuchyen [154] or Brooks-Corey [151]	Benchmark

Numerical model reference[1]	**Primary Focus of Model Development/ Application**	**Number of dimensions[2]**	**Clapeyron equation**	**Soil freezing curve**	**Soil diffusivity, permeability, or hydraulic conductivity[3]**	**Model verification/ validation**
Zhang et al. [62]	Development of soil parameterization scheme for cold regions	1	Equation (7)	Clapp and Hornberger [149]	Clapp and Hornberger [149]+ impedance	Field data
McKenzie et al. [68]	Ice formation in northern peatlands	3	-	Linear or exponential	Linear or independent impedance	Field data, analytical solution, benchmarks
Bense et al. [25]	Climate-induced evolution of permafrost aquifers	3	-	Undefined ‘smooth’ function	Empirical, equation	-
Liu and Yu [72]	Heat and water transfer in heaving soils	3	Equation (3)	van Genuchten [154] or Fredlund et al. [153]	van Genuchten [154] + impedance or Fredlund et al. [153]	Experimental data and field data
Painter et al. [78]	Two component, three phase transport in permafrost environments	3	Modified equation (2)	van Genuchten [154]	van Genuchten [154]	Experimental data and analytical solution
Dall’Amico et al. [74]	A robust model for heat and water flow in freezing unsaturated soils	3	Equation (7)	van Genuchten [154]	van Genuchten [154]+ impedance	Experimental data and analytical solution
Tan et al. [76]	Coupled heat and water flow + Soret effect/segregation potential	3	Equation (3)	van Genuchten [154]	Heaviside function	Experimental data and analytical solution
Sheshukov and Nieber [150]	Examination of various modes/stages of freezing in non-heaving soils + similarity solution	1	Equation (7)	Brooks-Corey [151]	Brooks-Corey [151] + impedance	Experimental data

[1]The contributions in the first column are organized by the publication date.

[2]This column represents the possible number of dimensions in the numerical model. Several recent contributions only performed simulations for two-dimensional cross-sections despite the three-dimensional capabilities of the model.

[3]In general, the hydraulic conductivity functions that were obtained from SWC’s following Mualem’s [161] or Burdine’s [162] approach are labeled in this column in accordance with the underling SWC formulation.

[4]In certain instances, the model information related to a particular column is missing, not clearly stated, or not applicable.

2. Variations of the Clapeyron equation

Cold regions water and heat transport models should be capable of simulating thermodynamic equilibrium conditions during phase change. The equilibrium relationship between the temperature and pressure in freezing soils is given by the Clapeyron equation, which is often termed the 'Clausius-Clapeyron equation', the 'freezing temperature equation', or the 'equilibrium equation'. Many disparate forms of this equation have been published. In most sources, these equations are presented with temperature expressed in degrees Kelvin; in the present contribution, temperature is expressed in Celsius.

The original form of the Clapeyron equation, which was derived from the thermodynamic concept of Gibbs free energy [97], can be generalized for multiple phases by first writing the Gibbs-Duhem relationship for each phase and then combining the resulting terms. This process is described in detail by Kay and Groenevelt [98] and Groenevelt and Kay [99]:

$$\frac{1}{\rho_w}\frac{dP_{wf}}{dT} - \frac{1}{\rho_i}\frac{dP_i}{dT} = \frac{H_f}{T + 273.15} \tag{1}$$

where T is the equilibrium freezing temperature [°C], H_f is the latent heat of fusion [L^2 t^{-2}], P_{wf} and P_i are the equilibrium gauge pressures in partially frozen soil for the liquid water and ice phases, respectively [M L^{-1} t^{-2}], and ρ_w and ρ_i are the water and ice densities, respectively [M L^{-3}]. Using basic thermodynamic principles, Loch [100] derived a slightly different form of the general Clapeyron equation for freezing soils by first integrating the Gibbs-Duhem expressions for each phase before combining the terms:

$$\frac{P_{wf}}{\rho_w} - \frac{P_i}{\rho_i} = \frac{H_f}{273.15}T \tag{2}$$

Many models have been primarily developed to simulate the migration of moisture or heat in partially frozen soil rather than freezing-induced deformation [e.g. [41,47,60]]. These models often do not account for the gauge pressure in the ice phase. Thus, the Clapeyron equation is given in a simpler format than equations (1) or (2) in accordance with earlier theoretical and experimental investigations of soil freezing. For example, Schofield [32] first demonstrated that the equilibrium freezing temperature is affected by matric potential due to the relationship between matric potential and free energy. The original equation proposed by Schofield [32] can be rewritten in a slightly revised form to represent a change in the equilibrium gauge pressure of water in freezing soil dP_{wf} due to a change in temperature dT .

$$\frac{dP_{wf}}{dT} = \frac{H_f\ \rho_w}{(T + 273.15)} \tag{3}$$

Equation (3) is predicated on the assumption that liquid water is coexisting with solid ice that is at constant pressure and density. Often, for the purpose of simplification, the T term in the denominator is removed. This simplification will have very little impact at temperatures close to 0°C.

$$\frac{dP_{wf}}{dT} \approx \frac{H_f \, \rho_w}{273.15} \tag{4}$$

Equations (3) and (4) indicate that the pore water pressure and the equilibrium freezing temperature are in a state of delicate balance. As temperature decreases and ice forms, liquid water content decreases, which decreases pressure and draws moisture toward the freezing front in a process known as cryosuction [101].

Often the Clapeyron equation is expressed without differentials [102,103]. This form can be obtained from equation (3) by rearranging to isolate the pressure differential and integrating with respect to T and P_{wf}:

$$P_{wf} = H_f \rho_w \ln\left(\frac{T + 273.15}{273.15}\right) \tag{5}$$

It should be noted that equation (5) assumes that the water density is not temperature-dependent. This form is often further simplified by employing the first term in the Taylor expansion of the exponential function [34,62,63]:

$$\exp(x) \approx 1 + x \rightarrow x \approx \ln(1 + x) \tag{6}$$

If x is taken as T/273.15, equation (5) simplifies to the following:

$$P_{wf} \approx H_f \rho_w \frac{T}{273.15} \tag{7}$$

Equation (7) is equivalent to equation (5) to the first term in the Taylor expansion, which implies small variations about T=0°C. Equation (7) can be shown to be essentially identical to the form given in equation (4), but with pressure and temperature expressed without differentials. An algebraic manipulation will reveal that equations (3), (4), (5), and (7) are equivalent to or approximations of equation (1) when the pressure in the ice phase is constant. Similarly, equation (7) can be shown to be equivalent to equation (2) when the pressure in the ice phase is atmospheric (zero gauge pressure) or when the pressure in the water phase is measured relative to the pressure in the ice phase. Figure 1 shows the relationships between P_{wf} and T and indicates that the selection of the equilibrium equation has little effect at temperatures greater than -10°C.

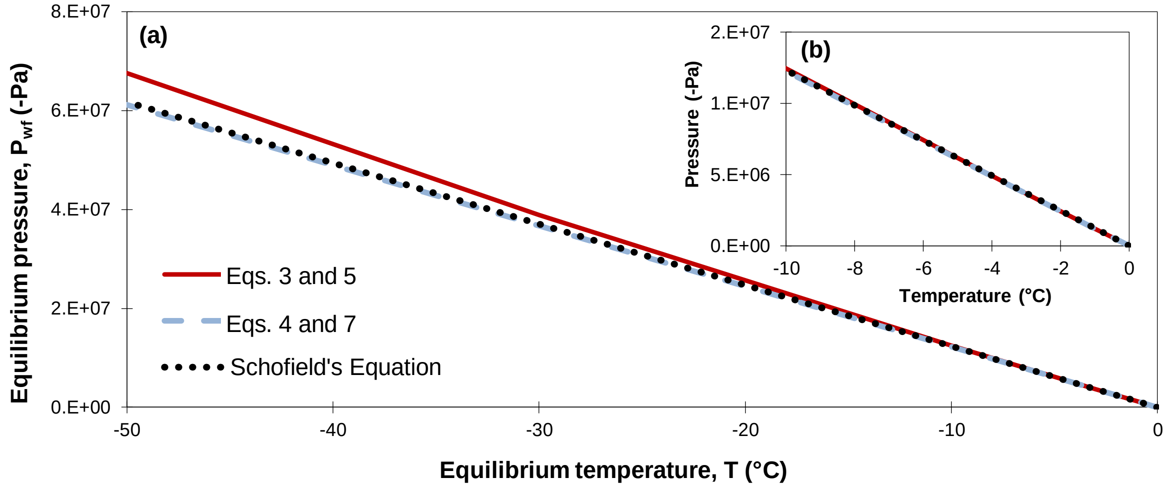

Fig. 1 (a) Comparison of the pressure-temperature equilibrium relationship for varying forms of the Clapeyron equation assuming T = 0°C at P_{wf} = 0 Pa. (b) Inset, amplified pressure-temperature relationship in range of temperature that is relevant for most applications (0 to -10°C). The various equations do not significantly deviate from each other in this range. Schofield's [32] equation was a simplified form of the Clapeyron equation expressed as pF = logT+4.1, where pF = log ($100P_{wf}\,\rho_w^{-1}\,g^{-1}$) and $10^{4.1} = 100H_f\,273.15^{-1}\,g^{-1}$.

Various other forms of the Clapeyron equation for freezing soils have been proposed that differ depending on the assumptions regarding the pressure in the ice phase. For example, Saetersdal [103] presented equations (8) and (9) as alternate forms of the Clapeyron equation:

$$\frac{dP_{wf}}{dT} = \frac{dP_i}{dT} = \frac{H_f}{(\rho_w^{-1} - \rho_i^{-1})(T + 273.15)} \tag{8}$$

$$\frac{dP_i}{dT} = \frac{H_f\,\rho_i}{(T + 273.15)} \tag{9}$$

According to Saetersdal [103], equation (8) is valid when a change in pressure in the ice phase is transferred to the liquid water phase and vice versa, and equation (9) is valid when the pore water pressure is constant, but the pressure in the ice phase varies. Other forms of the Clapeyron equation were presented by Kay and Groenevelt [98] and Groenevelt and Kay [99]. Dall'Amico [73] listed nine variations of the Clapeyron equation for freezing soils that have been employed by various model developers.

The Clapeyron equation can be manipulated to determine the freezing point depression due to pre-freezing negative pressures P_{w0} [M L^{-1} t^{-2}]. For example, equation (7) can be rearranged to the following form, which is valid at temperatures close to 0°C if the pressure in the ice phase is assumed to be constant, and thermodynamic equilibrium is achieved:

$$\Delta T = \frac{273.15\ P_{w0}}{H_f\ \rho_w} \tag{10}$$

where ΔT is the change in equilibrium temperature or the freezing point depression [°C] due to negative pressure. It should be noted that ΔT is equivalent in sign and magnitude to T, because at a water gauge pressure of zero, the freezing temperature is 0°C. Koopmans and Miller [38] suggested a more general freezing point depression equation, which was derived from an equation similar to (2), and which can be applied at any equilibrium point during freezing and which relaxes the null ice pressure assumption:

$$\Delta T = \left[\frac{P_{wf}}{\rho_w} - \frac{P_i}{\rho_i}\right] \times \frac{273.15}{H_f} \tag{11}$$

These Clapyeron-temperature depression formulations ignore freezing point depression due to solute concentration.

Freezing and thawing processes may not always occur at thermodynamic equilibrium, and at disequilibrium, the Clapeyron equation is invalid [73,105]. Disequilibrium phase change can occur at the onset of soil freezing because temperatures can decrease more rapidly than equilibrium ice formation. The possibility of disequilibrium states should not be neglected if the rate of temperature changes exceeds 0.1°C hr^{-1} in the range of 0 to -0.5°C. Numerical models that assume thermodynamic equilibrium based on the Clapeyron equation tend to overestimate cryosuction-induced water flow at the beginning of freezing because they overestimate the rate of ice formation based on the equilibrium assumption. Furthermore, disequilibrium pressure can occur during thawing and consequent infiltration, because ice content can decrease without a change in temperature. Accurately expressing these disequilibria with appropriate mathematical formula is important when considering freezing front phenomena or when simulating snowmelt infiltration and runoff during inhomogeneous ground thawing. The study and mathematical representation of disequilibrium phenomena is an emerging field of research.

3. Similarities between the soil water curve and the soil freezing curve

Most existing models for simulating water and heat transport in freezing soils predict the unfrozen water content in freezing soils based on an analogy between the soil freezing curve (SFC, the relationship between subzero temperatures and the unfrozen water content) and the soil water curve (SWC, the relationship between pore water suction and the moisture content). This relationship exists because liquid water is retained in the pore space during both desaturating processes (i.e. freezing or dessication) due to sorptive and capillary forces [106]. Beskow [107] initially proposed the concept that soil freezing is related to soil drying and that water flow to the freezing front in freezing soils is similar to water flow to the evaporative front in drying soils. Koopmans and Miller [38] demonstrated the analogy between the SFC and the SWC based on quantitative and qualitative parallels that exist between a drying, ice-free soil and a freezing, air-free soil. According to Koopmans and Miller [38], this analogy was valid for either soils where capillary forces govern (designated SS soil for solid-solid contact between particles), or soils where sorptive forces govern (designated SLS soils for solid-liquid-solid contact). In general, SS soils (e.g. sand or silt) are granular, coarse-grained soils characterized by rigid, capillary-like pores and (often) uniform grain size. Conversely, SLS soils (e.g. clays) are colloidal soils that are often platy-shaped, although rounded, corded and other grain orientations can also be found. The varying grain sizes and geometric orientations of these two soil classifications cause different forces (i.e. capillary or sorptive) to govern within the pore space and thereby affect the distribution of ice and unfrozen water during freezing or thawing.

The theoretical basis developed for relating the SWC and the SFC has been primarily founded on capillary theory. In a drying soil, the pressure discontinuity between air pressure and pore water pressure (i.e. the capillary pressure, P_a-P_w) at a curved air-water interface can be expressed using a form of the Young-Laplace equation [36,37]:

$$P_a - P_w = 2\frac{\sigma_{aw}}{r_{aw}} \tag{12}$$

where P_a is the air pressure [M L^{-1} t^{-2}], P_w is the pore water pressure [M L^{-1} t^{-2}], σ_{aw} is the specific energy of the air-water interface [M t^{-2}], and r_{aw} is the mean radius of the air-water interface curvature [L]. Similarly, Koopmans and Miller [38] theorized that a corresponding expression could be obtained for the ice-water interface in air-free, freezing soils. Unlike the original contribution, a distinction is made here between the pore water pressure in an ice-free soil P_w and the pore water pressure in a partially frozen soil P_{wf}:

$$P_i - P_{wf} = 2\frac{\sigma_{iw}}{r_{iw}} \tag{13}$$

where r_{iw} is the radius of the ice-water interface curvature [L], and σ_{iw} is the specific energy of the ice-water interface [M t^{-2}].

Equations (12) and (13) can be used to derive a new relationship that is valid if the radii of the two interfaces (i.e. ice-water and water-air) are the same:

$$P_a - P_w = \frac{\sigma_{aw}}{\sigma_{iw}}\left(P_i - P_{wf}\right) \tag{14}$$

Koopmans and Miller [38] used experimental SWC and SFC data to demonstrate that the ratio of the interface energies (σ_{aw}/σ_{iw}, equation 14) is approximately 2.20. In multicomponent flows, this scaling is denoted as a re-scaling of interfacial tensions [108]. Their results were consistent with the proposition that different phases of water could be at disparate pressures and still be in thermodynamic equilibrium due to the difference in the surface energies of the phase interfaces.

Koopmans and Miller [38] suggested that the pressure discontinuity relationship is simpler for SLS soils because sorptive forces govern rather than capillary forces, and the geometry of the liquid interface was assumed to be immaterially affected by the nature of the other pore constituent (ice or air):

$$P_a - P_w = P_i - P_{wf} \tag{15}$$

Based on this assumption, the pore water gauge pressure for drying, ice-free soil can be related to the pore water gauge pressure for freezing, air-free soil with the same liquid water saturation (same interface radii), assuming that the pressures in the ice and air phases are atmospheric [46]:

$$P_w = n \times P_{wf} \tag{16}$$

where n is 1.0 for SLS soils and 2.2 for SS soils. Because of the differences between equations (14) and (15), Koopmans and Miller [38] suggested that no fully-quantitative SFC-SWC relationship exists for soils that are not either fully SLS or fully SS. Additionally, their quantitative analogy was only valid for air-free freezing soils or ice-free drying soils. They also demonstrated that, similar to drying and wetting curves, freezing and thawing curves exhibit hysteresis. Black and Tice [109] determined that the quantitative relationship between the SWC and the SFC was only valid at similar bulk densities and, due to hysteresis, only drying curves could be related to freezing curves and only wetting curves could be related to thawing curves. When the conditions above were met, they found SFC parameters measured directly through experimentation were similar to those indirectly obtained from SWC parameters. This prompted them to suggest that SFC parameters obtained from freezing tests could be employed to infer SWC parameters.

Figure 2a illustrates the ability of the Clapeyron equation (equation 5) to represent the relationship between negative pressures (suction pressure) and temperatures in freezing soils. The Clapeyron equation is valid with no modification, provided equilibrium is achieved and pressure is measured directly rather than estimated from an SWC. Figure 2b shows SWC and SFC data that were independently obtained from soils with the same bulk density using methods described in the caption. The Clapeyron equation (equation 5), with and without the n adjustment factor (equation 16), is also shown to illustrate the validity of using forms of the Clapeyron equation to relate SWC's and SFC's. As illustrated, the SWC-derived pressure and SFC-derived temperature may not perfectly match the theoretical relationships proposed by Koopmans and Miller [38]. For example, at temperatures close to 0°C, the kaolinite data (SLS soil) matches the Clapeyron equation with the adjustment factor n =2.2; however, in theory, this 2.2 adjustment factor should not apply for SLS soils. Additionally, both the sand (SS soil) and the kaolinite data appear to switch between the Clapeyron curve assuming a dominance of sorptive forces (n =1) versus the curve assuming a dominance of capillary forces (n =2.2) at temperatures around -5°C. This leads us to postulate a temperature-dependence for the n adjustment factor due to the fact that the governing retention force (capillary or sorptive) may switch with decreasing temperature and pressure [90,110, 111]. Thus, the classic SLS vs SS separation for the n adjustment factor [38] may be an inappropriate simplification. This temperature-dependence should be addressed in future research. The formation of ice reduces the effective porosity (i.e. porosity minus ice content) of freezing soils. For smaller effective porosities at low pressure and temperature, sorptive forces will likely govern (n = 1), and for larger effective porosities (close to 0°C), capillary forces may become significant (n = 2.2).

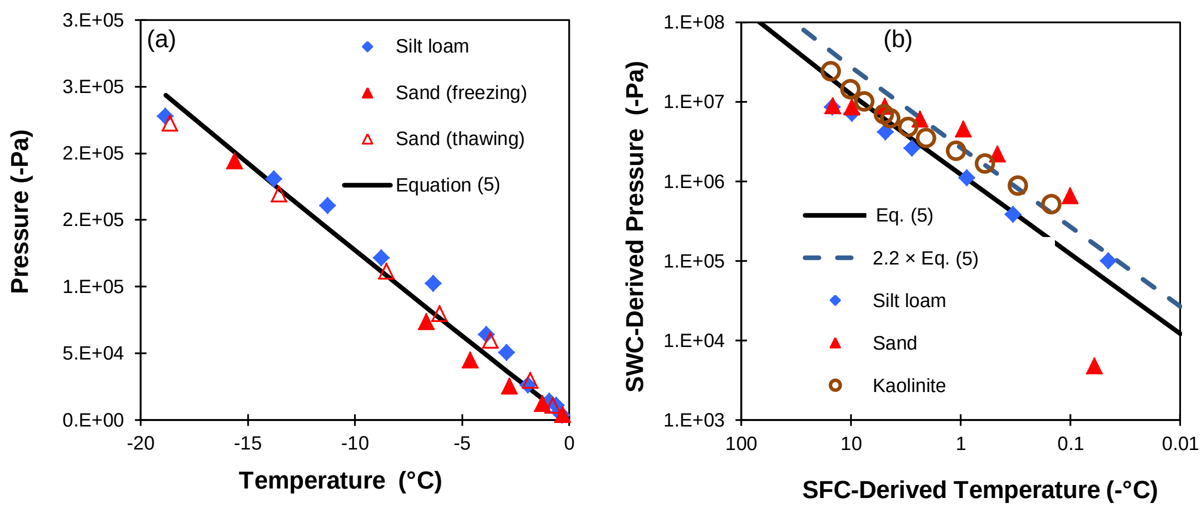

Fig. 2 (a) The negative pressure in freezing soils directly measured by a chilled-mirror potential sensor vs. measured temperature. The Clapeyron equation-predicted pressure (equation 5) for varying negative temperature is indicated by the solid line Adapted from [105]. For experimental details see [105]. **(b) Comparison of SWC and SFC at the same unfrozen water contents (unpublished data).** The measured SFC data were obtained from the pulsed nuclear magnetic resonance method. The measured SWC data were independently obtained from a combination of the hanging water method, the pressure plate method, and the dew point potensiometer. The theoretical Clapeyron relationships, with and without the equation (16) n factor, are shown by the dashed and solid lines, respectively.

Spaans and Baker [112] identified the following three limitations to the approach proposed by Koopmans and Miller [38]:

1. Freezing soils are often unsaturated, thus the air-free freezing restrictions are severely limiting.
2. Most soils in nature are neither fully SLS nor fully SS.
3. Determining the SWC becomes increasingly inaccurate and laborious as drying occurs; thus coupling of the SWC and the SFC is questionable at lower pressures.

They suggested that the last limitation noted above could be addressed by experimentally determining the water retention properties for soils from the SWC in the moist range and the SFC in the dry range. More recently, the chilled mirror technique has been adopted, which results in increased accuracy of an experimentally-derived SWC at lower soil water pressure [105].

Miller [40,43] attempted to address the first limitation identified above. For the case of unsaturated SS soils, he suggested that capillary forces are also affected by an air-ice interface. This interface yields a third pressure discontinuity equation (see equations 12 and 13):

$$P_i - P_a = 2\frac{\sigma_{ai}}{r_{ai}} \tag{17}$$

where r_{ai} is the radius of the air-ice interface curvature [L], and σ_{ai} is the specific energy of the air-ice interface [M t^{-2}]. This approach assumes that, like the water-air interface, the shape of the air-ice interface is adjusted to minimize interface energies. This assumption has been supported by observations of granulation in snow [40]. Miller [40,43] also demonstrated that the air-ice interface energy can be found from the addition of the energies for the air-water interface and the ice-water interface:

$$\sigma_{ai} = \sigma_{aw} + \sigma_{iw} \tag{18}$$

For the case of unsaturated SLS soils, the findings of Koopmans and Miller [38] regarding the ratio for air-water and ice-water interface energies can be applied in conjunction with equation (18) to yield:

$$\sigma_{ai} = \sigma_{aw} + \sigma_{iw} = \sigma_{aw} + \frac{1}{2.2}\sigma_{aw} = 1.45\sigma_{aw} \quad \text{or} \quad \sigma_{ai} = 3.2\sigma_{iw} \tag{19}$$

The interface energies σ_{aw}, σ_{iw}, and σ_{ai} have approximate values of 0.07 N m^{-1}, 0.03 N m^{-1}, and 0.10 N m^{-1} respectively at temperatures close to 0°C [43]. The coexistence of ice, air, water, and soil grains in freezing soils is depicted in Figure 3. Miller [40] proposed a function for the contact angle (ϕ, Figure 3) between the air-ice interface and the soil particle surface. According to Miller [42], ice pressure is only atmospheric when this contact angle is 68°. If the contact angle is less than this critical value, ice pressure is greater than air pressure, and if the contact angle is greater than this critical value, ice pressure is between air pressure and pore water pressure [46]. Because ice pressure caused by the air-ice interface energy should not be assumed to be zero if an air-ice interface exists [43], it is difficult to physically and quantitatively relate the SFC and the SWC quantitatively for unsaturated SS soils.

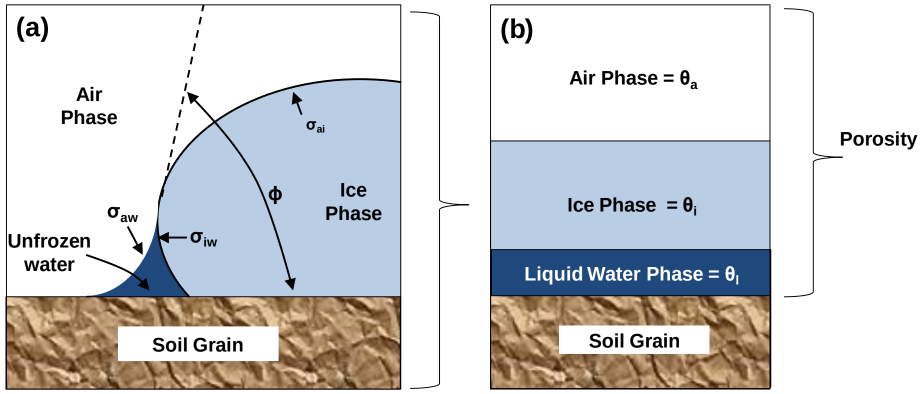

Fig. 3 Coexistence of water, air, ice, and soil grains in freezing soils. (a) The contact angle between the soil grains and the air-ice interface and the respective interface energies for the air-ice, water-ice, and air-water interfaces. (b) The volumetric contents for each phase in the pore space, where θ_a, θ_i, and θ_l represent the volumetric contents for the air, ice, and liquid water phase, respectively. Modified from [40].

A simplifying assumption that is often applied when relating a variably-saturated SFC to an SWC is that the unfrozen water content is independent of the initial total (frozen + unfrozen) water content. For example, Williams [34,35] experiments supported Fisher's [113] initial comments regarding the independence of unfrozen water content and initial total water content provided that the initial total water content is not less than the equilibrium unfrozen water content for a given temperature. Other researchers have also suggested through experimentation and/or thermodynamic theory that unfrozen water content is independent of initial total water content [e.g. 46,114].

More recently, researchers have developed or improved techniques for more accurately measuring unfrozen water content in freezing soils including: differential scanning calorimetry [115,116], time domain reflectometry (TDR) [117-122], nuclear magnetic resonance (NMR) [121,123-126] and ultrasonic techniques [127-129]. These technological advances have allowed researchers to further investigate the independence of unfrozen water on initial total water content. Tice et al. [123] measured unfrozen water content in freezing soils using pulsed NMR, and his results suggested that unfrozen water content increases with initial total water content. Similarly, Yong [130] and Suzuki [131] suggested that the unfrozen water content was higher at a given temperature for soils with higher initial total (frozen + unfrozen) water contents. However, Watanabe and Wake [121] and Akagawa et al. [126] have since demonstrated that experimental error can arise by not properly accounting for the signal from the ice phase when measuring the unfrozen water content by TDR or NMR methods. This experimental error can result in the erroneous conclusion that unfrozen water content increases significantly with increasing initial total water content. Also, equilibration time increases in fine soils or in soils with higher total water content. Because TDR and NMR measurements of unfrozen water contents assume equilibrium conditions, this increase in equilibrium time can yield additional experimental errors. Figure 4 shows the independence between initial total and unfrozen water contents for silt loam and sand when the ice signal correction factor is applied. As the temperature drops below the initial freezing temperature, the series with initially different moisture contents converge.

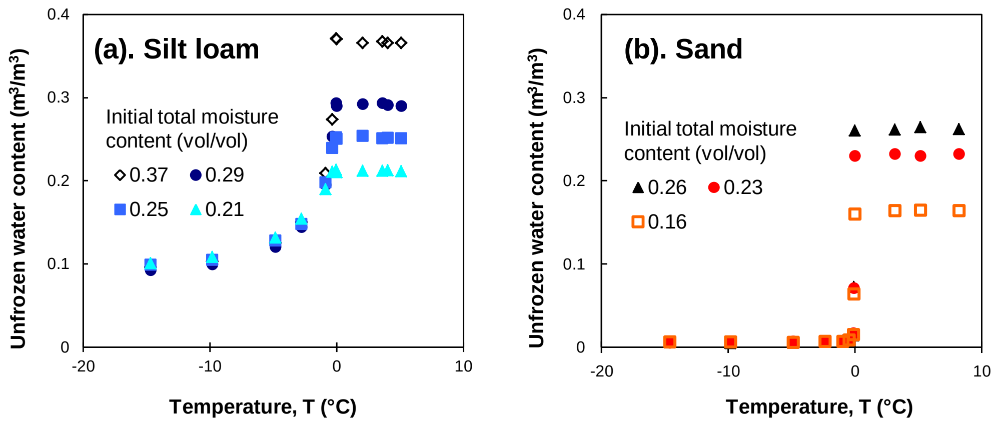

Fig. 4 Unfrozen water contents vs. temperature in unsaturated freezing silt loam (a) and sand (b) with different initial total water contents (indicated in the inset) measured by the pulsed nuclear magnetic resonance method with separate signals from ice and liquid water. Adapted from [121].

4. Previously developed soil freezing curves

4.1 SFC's not derived from SWC's

Mathematical models for simulating freezing or thawing in soils must incorporate some form of an SFC to relate the unfrozen moisture content to subzero temperatures. Numerous researchers have developed empirical SFC relationships that have been derived independently of any SWC data [e.g. [46,68,114,116,132,133]]. Where applicable, nomenclature has been adjusted in the present contribution to be consistent with conventional hydrology nomenclature (e.g. moisture content by % dry unit weight has been converted to volumetric moisture content). Based on the conservation of mass, the total water content θ_w (volume of water/total volume) is equivalent to the sum of the liquid water content (θ_l, Figure 3b) and the product of the ice content (θ_i, Figure 3b) and the ratio of ice density to water density:

$$\theta_w = \theta_l + \frac{\rho_i}{\rho_w}\theta_i \tag{20}$$

Sometimes, the density differences between ice and water are ignored, and the total water content is simply expressed as the sum of the ice and liquid water contents [68]:

$$\theta_w = \theta_l + \theta_i \tag{21}$$

If unfrozen water content is assumed to be independent of total water content, θ_l can be expressed as a function of temperature only. Anderson and Tice [114] and Anderson and Morgenstern [132] found that the relationship between the liquid water content and the temperature of freezing soils can be reasonably approximated with a power law:

$$\theta_l = \frac{\rho_s(1-\varepsilon)}{100\rho_w}\alpha(-T)^{\beta} \tag{22}$$

where ρ_s is the density of the soil solids [M·L^{-3}], ε is the porosity, and α and β are empirical fitting parameters. The SFC must be smooth and differentiable, because the apparent heat capacity term for freezing or thawing soils contains the derivative of the SFC [60,68]. The temperature derivative of equation (22) is:

$$\frac{\partial\theta_l}{\partial T} = -\frac{\rho_s(1-\varepsilon)}{100\rho_w}\alpha\beta(-T)^{\beta-1} \tag{23}$$

Values for α and β for many types of soil have been tabulated by Andersland and Ladanyi [134]. Anderson and Tice [114], Anderson and Morgenstern [132], and Blanchard and Frémond [135] demonstrated empirically that the α and β values can also be obtained from the specific surface area S [m^2 g^{-1}] for different types of soils:

$$\alpha = \exp\{0.5519\times\ln(S)+0.2168\} \tag{24}$$

$$\beta = -\exp\{-0.2640\times\ln(S)+0.3711\} \tag{25}$$

Thus, α and β can be shown to be dependent on basic soil types. For example, equation (24) indicates that α is typically higher for clays and other soil types with higher specific surface areas. Equations (22), (24), and (25) can be combined to express the unfrozen water content as a function only of temperature and specific surface area without the use of empirical fitting parameters α and β [46,54]. Tice et al. [136] demonstrated that empirical relationships could also be developed between the soil liquid limits and α and β. Thus, the SFC of a particular soil can be estimated from a few simple laboratory measurements. The proposed power relationship is several decades old; however, it is still commonly given in reference texts as a valid approach to estimating unfrozen water content in freezing soils [137,138].

Although it was empirically developed, the use of the power function for an SFC is also theoretically tenable. If it is assumed that the water film and soil surface act as flat parallel layers, the unfrozen water content can be expressed as follows [106,124,139-141]:

$$\theta_l = \kappa(-T)^{-1/3} \tag{26}$$

where κ is a parameter that includes the effect of specific surface area, water density, ice density, latent heat, and the Hamaker constant A [M L^2 s^{-2}]:

$$\kappa = S\rho_w\left(\frac{-273.15A}{6\pi\rho_i H_f}\right)^{1/3} \tag{27}$$

Comparing equation (26) to equation (22) indicates that a reasonable initial estimate for β could be -0.33, although β often differs from this value as a result of non-planar geometric orientations of the water film and soil surface or surface forces other than van der Waals [141]. Also equation (27) indicates that the κ parameter can be shown to be a function of specific surface, which concurs with the empirical relationships proposed by Anderson and Tice [114] and Anderson and Morgenstern [132]. It should be noted that equations (24) to (27) are formulated on the assumption that sorptive (surface) forces govern rather than capillary forces. Thus, these formulations are more valid for SLS soils or at lower temperatures when water is held to the soil (SS or SLS) particle surface by sorptive rather than capillary forces.

Jame [46] and McKenzie et al. [68] suggested that a simple piecewise linear function could approximate the SFC for saturated soils. This SFC is reproduced in a slightly modified form with the total water content replacing the porosity term in the original formulation to accommodate initially unsaturated conditions:

$$\begin{aligned} &\theta_l = mT + \theta_w \quad \text{if } T > T_{res} \\ &\theta_l = \theta_{res} \quad \text{if } T < T_{res} \end{aligned} \tag{28}$$

where m is the slope of the freezing function [T^{-1}], θ_{res} is the residual unfrozen water content, and T_{res} is the temperature at which the unfrozen water content is reduced to θ_{res}. A reasonable range of freezing temperature is 0 to -2°C [95]. Others have employed non-linear piecewise-freezing curves. For example, Kozlowski [116] achieved a good fit to measured unfrozen water in a clay soil by employing the following exponential piecewise SFC:

$$\begin{aligned} &\theta_l = \theta_w \quad \text{if } T > T_f \\ &\theta_l = \theta_{res} + (\theta_w - \theta_{res})\exp\left[\delta\left(\frac{\mathrm{T}_f - T}{T - T_{res}}\right)^{\chi}\right] \quad \text{if } T_f > T > T_{res} \\ &\theta_l = \theta_{res} \quad \text{if } T \le T_{res} \end{aligned} \tag{29}$$

where δ and χ are fitting parameters for this expression.

McKenzie et al. [68] and Ge et al. [22] suggested that an SFC could be obtained from a continuous exponential function. Herein, this SFC is modified slightly with the porosity replacing the total water content to allow for initially unsaturated conditions:

$$\theta_l = \theta_{res} + (\theta_w - \theta_{res})\exp\left(-\left(\frac{T}{w}\right)^2\right) \quad (30)$$

where w is a fitting parameter. The piecewise linear and exponential SFC's can also be shown to have smooth derivatives with respect to T on the interval of freezing [68]. Kozlowski and Nartowska [133] presented the following modified form of the exponential SFC proposed by Anderson and Tice [142]:

$$\theta_l = \exp\left(a + b\ln S + cS^d \ln(|T|)\right) \quad (31)$$

where a, b, c and d are empirical fitting parameters. Curves based on the power, piecewise linear, exponential, and Kozlowski's [116] SFC's are shown in Figure 5. The SFC given by Kozlowski and Nartowska [133] is not presented as this form can be shown to reduce to the power relationship (equation 22). The root-mean-square-error (RMSE) values in Figure 5 indicate that, for these experimental data, the Kozlowski [116] SFC matched the observed unfrozen water-temperature relationship far better than the power, piecewise-linear, or exponential SFC's.

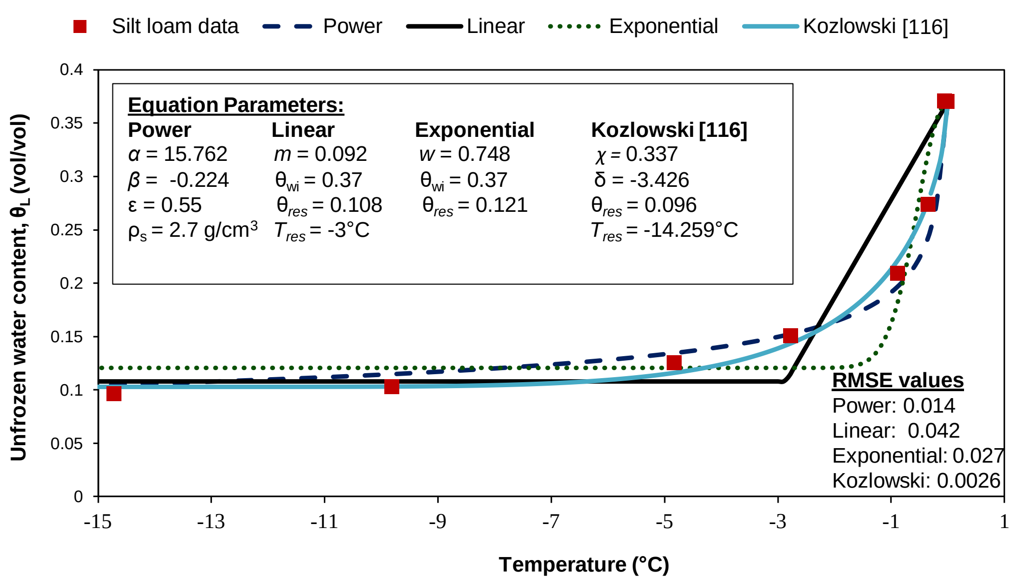

Fig 5. The power, piecewise linear, exponential and Kozlowski [116] SFC's fitted to the silt loam freezing data shown in Figure 4a by minimizing the RMSE. The equation parameters and the associated RMSE values are indicated.

There are relatively few experimental studies that have measured SFC's for various soils types compared to the number of studies that have measured SWC's. This lack of research partly arises from persisting questions associated with the physical measurement of the freezing process. For example, Smerdon and Mendoza [143] observed hysteretic behavior in the thermal properties and TDR-measured unfrozen water content in peat using concurrent *in situ* and laboratory measurements. They suggested that the degree of hysteresis was dependent on liquid water content. He and Dyck [145] examined dialectric mixing models for measuring SFC and also observed significant hysteresis, which they attributed to supercooling and osmotic freezing point depression phenomena. Hysteretic phenomenon has also been reported by Parkin et al. [44] from recent field observations at sites in Ontario, Canada. They found that the best SFC fitting parameters changed by a factor of 0.09 between the freezing and thawing cycle, but this change did not concur with the predictions of previous research, which led them to suggest that the hysteresis may be 'more apparent than mechanistically real'. Parkin et al. [44] also observed that *in situ* measurements of SFC were difficult to obtain due to the lack of monotonically increasing or decreasing temperature cycles in natural environments. Thus, like the modelers, researchers measuring freezing processes in porous media are faced with several unresolved difficulties.

4.2 Previous SFC's derived from SWC's

The primary independent variable of the SWC is pressure, and the primary independent variable of the SFC is temperature. Thus, the Clapeyron equation can be utilized to convert between an SWC and SFC. In theory, at least for saturated soils, the pore water pressure associated with a negative temperature (P_{wf}) can first be found with a form of the Clapeyron equation and then related to an associated pore water pressure for a drying soil P_w according to equation (16). This P_w can be used to obtain the unfrozen water saturation from an appropriate SWC. In this sequential manner, an SFC can be developed from a previously existing SWC. For example, Flerchinger et al. [146] measured liquid water content in freezing soils using TDR and demonstrated that the parameters for SWC's obtained from pressure plate analyses were very close to SWC parameters deduced from SFC's directly obtained during freezing tests.

Several SWC-derived SFC's are given by Dall'Amico [73]. For example, Shoop and Bigl [58] applied a modified form of Gardner's [147] SWC to obtain the SFC for unfrozen water content in freezing or thawing soils. Luo et al. [148] utilized a common SFC derived from the Clapp and Hornberger [149] relationship. This was modified by Zhang et al. [62] to account for the effect of ice on the soil specific surface:

$$\theta_l = \varepsilon \left(\frac{\rho H_f \, T}{273.15 P_a} \right)^{-1/b} \left(1 + C_k \theta_i\right)^2 \tag{32}$$

where P_a is the air-entry pore water pressure [M L^{-1} t^{-2}], b is the empirical Clapp-Hornberger parameter, and C_k accounts for the effect of ice formation on matric potential (C_k~8) [62].

Sheshukov and Nieber [150] combined a simplified form of the Clapeyron relationship (equation 7) with the Brooks-Corey [151] SWC to obtain a relationship similar to the following:

$$\theta_l = \theta_{res} + \left(\varepsilon - \theta_{res}\right)\left(\frac{\rho_w H_f T}{P_a\, 273.15}\right)^{-1/b} \tag{33}$$

where b is the Brooks-Corey model exponent. Equation (33) is quite similar in form to the power relationship based on sorptive forces proposed in equations (22) and (26), although the Brooks-Corey model can accommodate capillary or sorptive forces as the b exponent will not necessarily match that of equation (26). At lower temperatures, when sorptive forces govern, equation (33) will, in theory, approach that of equation (26). Azmatch et al. [152] demonstrated that the form of the Clapeyron equation given in equation (5) can be effectively combined with the SWC proposed by Fredlund et al. [153] to obtain an accurate SFC. They also found that when soil freezing temperatures were converted to capillary pressures, the pressure vs. liquid saturation curves from the SFC and SWC were very close. The overlapping of the SWC and SFC occurred without any adjustment factor, such as the one proposed in equation (16), which was indicative of the presence of clays (i.e. SLS soils where n = 1.0).

Dall'Amico [73] demonstrated how the van Genuchten [154] SWC can be combined with a form of the Clapeyron equation to estimate liquid and ice saturations during freezing in unsaturated soils. He first obtained a depressed freezing temperature ΔT for unsaturated soil due to pre-freezing pressures (suction) according to equation (10). This new equilibrium temperature was used to obtain a relationship for further decreases in pressure due to subsequent freezing:

$$P_{wf} = P_{w0} + \frac{\rho_w H_f}{273.15}\left(T - \Delta T\right) \times H\left(T - \Delta T\right) \tag{34}$$

where H is the Heaviside function, P_{w0} is the pre-freezing pressure and P_{wf} is the new pressure induced by freezing [M L^{-1} t^{-2}]. Dall'Amico [73] theorized that the total water content θ_w could be obtained independently of the temperature according to the van Genuchten [154] SWC with P_{w0} as the input. He then proposed that the water could be partitioned into liquid water and ice saturations according to equations (35) and (36):

$$\theta_l = \theta_{res} + \left(\varepsilon - \theta_{res}\right)\left\{1 + \left[-a\,P_{w0} - a\frac{\rho_w H_f}{273.15}\left(T - \Delta T\right) \times H\left(T - \Delta T\right)\right]^n\right\}^{-m} \tag{35}$$

$$\theta_i = \frac{\rho_w}{\rho_i}\left(\theta_w - \theta_l\right) \tag{36}$$

where *a*, *n*, and *m* are the van Genuchten fitting parameters, and *ε* is porosity.

Watanabe et al. [103] demonstrated that an SFC could be formulated by combining equation (5) with the van Genuchten-type equation proposed by Durner [155] to accommodate heterogeneous pore structure:

$$\frac{\theta_l - \theta_{res}}{\left(\varepsilon - \theta_{res}\right)} = \left\{\left(1 - w_2\right)\left[1 + a_1\,\rho_w H_f\,\ln\left(\frac{T + 273.15}{273.15}\right)^{n_1}\right]^{-m_1} + w_2\left[1 + a_2\,\rho_w H_f\,\ln\left(\frac{T + 273.15}{273.15}\right)^{n_2}\right]^{-m_2}\right\} \tag{37}$$

where a_1, a_2, w_2, n_1, n_2, m_1, and m_2 are the Durner [155] fitting parameters.

Figure 6 depicts a general approach for determining unfrozen moisture content with the following steps: (1) the total water content can be obtained based on pre-freezing pressure from an SWC; (2) the freezing point depression due to initial (negative) pressure can be calculated (e.g. equation 10); (3) no freezing occurs until the soil temperature drops below the new depressed freezing temperature; (4) at temperatures below the depressed freezing temperature, ice formation begins and some unfrozen water remains in the pore space in accordance with the SFC; (5) at a given temperature below the depressed freezing point, the unfrozen water content can be taken directly from the adjusted SFC curve (e.g. equation 35). The ice content is equal to the total water content minus the unfrozen water content times the ratio of the water and ice densities (equation 36).

It should be noted that combining existing SWC's with a form of the Clapeyron equation to determine an SFC often renders the differentiating of the SFC and its subsequent incorporation into the apparent heat capacity term more difficult [60,68]. Given the small time steps required for unsaturated freezing simulations, the relative complexity of these SFC derivatives may currently limit their use in multi-dimensional or spatially extensive mathematical models.

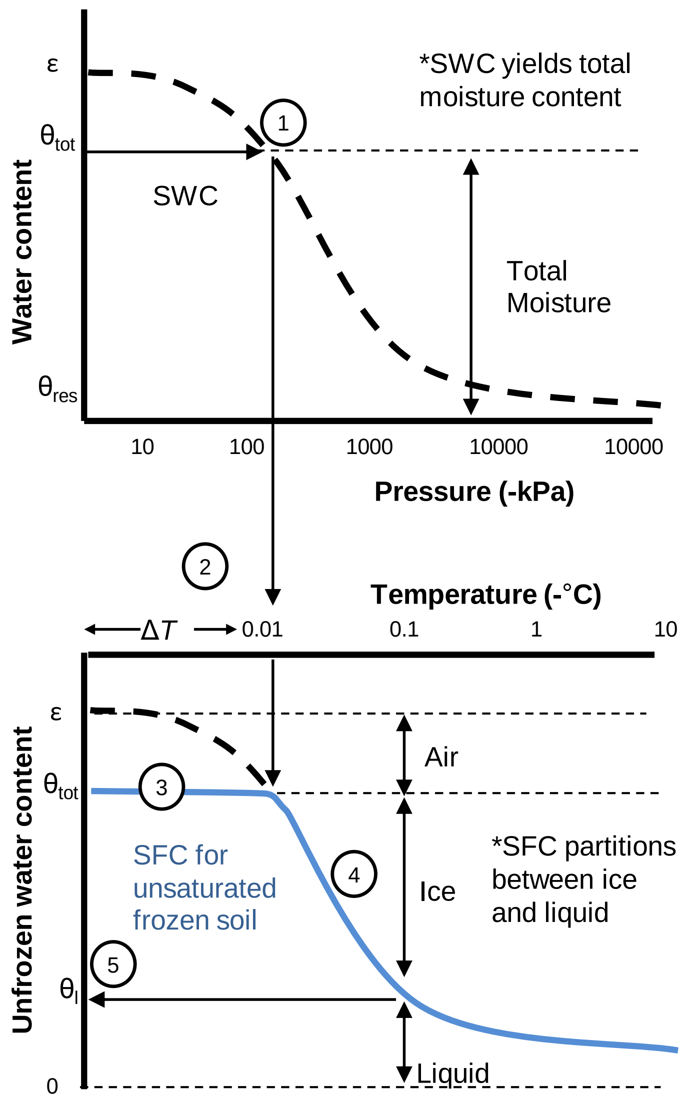

Fig. 6 The process for determining the unfrozen water content in variably saturated freezing or thawing soil. The steps in this figure are described in the text.

5. Hydraulic conductivity of partially frozen soils

Hydraulic conductivity in freezing soil (K_f) is reduced as ice accumulates in the pore space because the flow rate is dependent on the flow path cross-sectional area and pore geometry [156]. This phenomenon is typically simulated using one of three approaches: (1) a semi-theoretical approach based on capillary and sorptive theory, (2) a simple empirical formula expressing K_f as a function of temperature and independent of an SWC, and (3) a formula that estimates K_f from an SWC-derived hydraulic conductivity function of ice-free, drying soil.

Watanabe and Flury [157] developed an example of a type (1) freezing soil hydraulic conductivity models through the application of capillary and surface absorption theory. In this approach, the soil is treated as a bundle of cylindrical capilliaries, and the ice formation is assumed to occur in the center of the capilliaries. In a related approach, Lebeau and Konrad [110,158] developed a semi-theoretical hydraulic conductivity model for partially-frozen air-free porous media. In their model, water flow and hydraulic conductivity depend on both capillary and thin film flow processes (due to London-van der Waals and ionic electrostatic forces). These semi-theoretical hydraulic conductivity models have been shown to perform well when compared to field and laboratory data [110,157]; however, they are typically too complex to be incorporated into numerical models due to competing demands between model realism and computing capabilities.

For the sake of model simplicity, several researchers have proposed simple empirical hydraulic conductivity models for freezing soils that are functions only of the soil temperature (type 2). An example of these is the simple power relationship proposed by Nixon [159]:

$$K_f = K_0 / (-T)^{\delta} \tag{38}$$

where K_f is the hydraulic conductivity in freezing soils [L t^{-1}], K_0 is the hydraulic conductivity at -1°C [L t^{-1}], T is temperature in °C, and δ is the slope of the K_f-T relationship in a log-log plot. Another temperature-based hydraulic conductivity function that has been developed independently of any SWC is the power relationship proposed by Horiguchi and Miller [160]:

$$K_f = C \times T^D \tag{39}$$

where C and D are constant fitting parameters. Jame [46] and McKenzie et al. [68] suggested that, like the SFC, the hydraulic conductivity function for freezing soils could be simply approximated by employing a piecewise linear function:

$$\begin{aligned} K_f &= K_{sat}\left\{\left(\frac{K_{rel}-1}{(B_T)}\right)T+1\right\} \quad if\ T > B_T \\ K_f &= K_{rel} \times K_{sat} \quad if\ T < B_T \end{aligned} \tag{40}$$

where K_{sat} is the saturated unfrozen conductivity [L t^{-1}], K_{rel} is the minimum relative conductivity or the ratio of the minimum K_f to K_{sat} (e.g. 10^{-6}), and B_T is the temperature at which this minimum conductivity is first obtained. Temperature-based hydraulic conductivity functions typically yield stable calculations when they are employed in numerical models. However, it is generally difficult to obtain literature related to their parameterization and accuracy for different types of soils, and consequently, they are rarely implemented in recent numerical models.

Due to the limitations of the two approaches listed above, most models employ a hydraulic conductivity function for partially frozen soils that is developed from a SWC-derived hydraulic conductivity function for drying soils (type 3). This approach follows the classic formulations by Mualem [161] or Burdine [162], who developed models to predict unsaturated hydraulic conductivity from the knowledge of both the saturated hydraulic conductivity and the SWC. In this approach, the unfrozen hydraulic conductivity is expressed as a function of the unfrozen moisture content based on the derived SWC-hydraulic conductivity relationship [161,162]. The SFC can then employed to produce a model that expresses the hydraulic conductivity of partially frozen soil as a function of the temperature. For example, Tarnawski and Wagner [163] proposed that a Brooks and Cory [151] style conductivity function could be utilized to predict the hydraulic conductivity in freezing soil:

$$K_f = K_{sat}\left(\frac{\theta_l}{\varepsilon}\right)^{2b+3} \tag{41}$$

where b is an empirical parameter based on the soil particle size distribution. Similarly, Black [164] proposed that the hydraulic conductivity functions for unsaturated soil derived from the SWC models of Gardner [147], Brooks and Corey [151], and van Genuchten [154] could be employed to obtain relative conductivity functions for freezing soils.

All of these SWC-derived, unfrozen moisture content-conductivity relationships will not be reviewed in detail as their development and application is generally well understood. The main advantage of implementing a type (3) hydraulic conductivity model is that the model is well-defined and parameterized once the SWC and saturated conductivity values are known. The SWC or SFC are much easier to physically determine in a laboratory than the conductivity-pressure or conductivity-temperature relationship. The primary uncertainty that persists for relating relative hydraulic conductivity functions for drying soil and freezing soils is whether an additional hydraulic impedance term is required to account for the formation of ice and existence of the slip-free ice-water interface.

The question of whether to include an impedance factor originally arose from the study of Harlan's work [41]. Harlan [41] first proposed that the hydraulic conductivity of freezing soils would be the same as that of drying soils at the same liquid moisture saturation. This approach assumes similar film-water geometry in both instances. Harlan's [41] simulated water flow near the freezing front was over-predicted, which suggested that his approach also over-predicted hydraulic conductivity. To simulate this perceived reduction in hydraulic conductivity while still employing previously parameterized hydraulic conductivity functions for drying soils, several authors [e.g. [46,56,165]] proposed that a phenomenological impedance factor could be employed to further reduce the hydraulic conductivity of soils due to the presence pore ice. This impedance factor is often given in the following form [166]:

$$K_f = K_u \times 10\wedge(-EQ) \tag{42}$$

where K_u is the hydraulic conductivity [L t^{-1}] in unfrozen soils at the same negative pressure or liquid moisture content, 10^(-EQ) is the empirical impedance factor, Q is the mass ratio of ice ice to total water $(\rho_i\,\theta_i)/(\rho_w\,\theta_w)$, and E is the empirical constant that accounts for the reduction in permeability due to the formation of ice. In this approach, the K_u value is first found by entering the unfrozen water content into a hydraulic conductivity function for drying soil (e.g. van genuchten, Brooks-Corey, or Gardner). The K_f value is then obtained by further reducing this K_u value with the empirical impedance term. Taylor and Luthin [47] proposed the following expression for calculating the hydraulic conductivity of frozen soils, in which the impedance factor is given in a slightly different form:

$$K_f = K_u / 10\wedge(10\theta_i) \tag{43}$$

Mao et al. [167] proposed that the hydraulic conductivity of freezing porous media could be related to the hydraulic conductivity of unfrozen porous media through the application of a third impedance factor form:

$$K_f = K_u \times (1-\theta_i)^3 \tag{44}$$

Kahimba et al. [168] proposed a more physically-based function for simulating the reduction in hydraulic conductivity. They suggested that the hydraulic conductivity of partially frozen soil could be determined from a Brooks and Corey [151] relationship that was modified to account for the reduction in effective porosity due to the formation of pore ice. This approach is a slight modification on the original impedance concept:

$$K_f = K_{sat}\left(\frac{\rho_w g(\varepsilon-\theta_i)}{-P_{wf}}\right)^{3+\frac{2}{b}}\left(\frac{\theta_w-\theta_i}{\varepsilon-\theta_i}\right)^{3+\frac{2}{b}} \tag{45}$$

The empirical impedance factor has been adopted by numerous researchers [47,57,58,60, 62,72,74].

There are four objections to implementing an impedance factor in the hydraulic conductivity function. (1) Newman and Wilson [55] criticized the use of an empirical impedance factor because it is an arbitrary fitting parameter that is not physically-based. They suggested that since drying and freezing soils both lose liquid water from larger pore spaces first, the suction-conductivity relationship developed for drying, unsaturated soil should still apply for freezing, unsaturated soil. (2) In general, it is difficult to utilize an impedance factor to match the decrease in hydraulic conductivity due to the formation of ice at both high and low unfrozen moisture contents. For example, Watanabe [102] determined that including an impedance factor in the hydraulic conductivity term resulted in unreasonably low frozen zone permeability. Zhao et al. [169] showed that the apparent impedance factor (e.g. E in equation 42) was not a constant but was rather dependent on matric potential, which in turn depends on temperature. (3) The impedance factor can render the hydraulic conductivity function non-differentiable at temperatures close to 0°C. Prior to freezing, the impedance factor has no influence, but at the onset of freezing, the impedance factor changes the slope of the conductivity vs. moisture content curve and produces a discontinuity. This discontinuity can yield unstable calculations. (4) The empirical impedance factor must be determined inversely from experimental data [169,170] and this limits its applicability for other conditions. This process also creates inherent conflict when assessing model accuracy by comparing simulations to experimental data.

Due to the criticisms associated with the impedance factor, numerous researchers have adopted alternative techniques to represent the reduction in conductivity due to ice formation. For example, Newman and Wilson [55] suggested that classic unsaturated hydraulic conductivity models should be able to reproduce the relationship between unfrozen moisture content and conductivity without the use of an impedance factor provided that the SFC is accurate. They implemented the hydraulic conductivity model of Fredlund et al. [153], which is an integrated form of the SWC. By adopting this approach, Newman [54] obtained good agreement between simulated and measured ice saturations. Similarly, Painter [78] demonstrated that the SWC proposed by van Genuchten [154] could be combined with the hydraulic conductivity model of Mualem [161] to predict the hydraulic conductivity of partially frozen porous media without the use of an impedance factor.

Azmatch et al. [152] also demonstrated that the unsaturated conductivity model of Fredlund et al. [153] could be employed to accurately reproduce the hydraulic conductivity of frozen soil. Their approach differed from many others as they directly utilized an experimentally-derived SFC (rather than first deriving the SFC from the SWC) in conjunction the Fredlund et al. model [153] to estimate the hydraulic conductivity of partially frozen soil. Similarly, Watanabe et al. [171] demonstrated that the SFC could be directly or indirectly obtained to determine the hydraulic conductivity model for partially frozen soil. They measured both the SWC and SFC from laboratory freezing experiments conducted on a column of silty-loam and found that the closed-form Durner-Mualem [172] conductivity model obtained from either the SWC or the SFC concurred with experimental observations. This approach of directly measuring the SFC rather than indirectly inferring it from the SWC circumvents the need to relate the SWC and SFC via the *n*-adjustment factor (equation 16), the value of which is not well-established for soils that are neither fully SLS nor fully SS. Another advantage of this approach is that equilibrium conditions are not assumed. A disadvantage of directly utilizing the SFC is that SFC parameters have not been determined for most soil types to the extent that SWC parameters have.

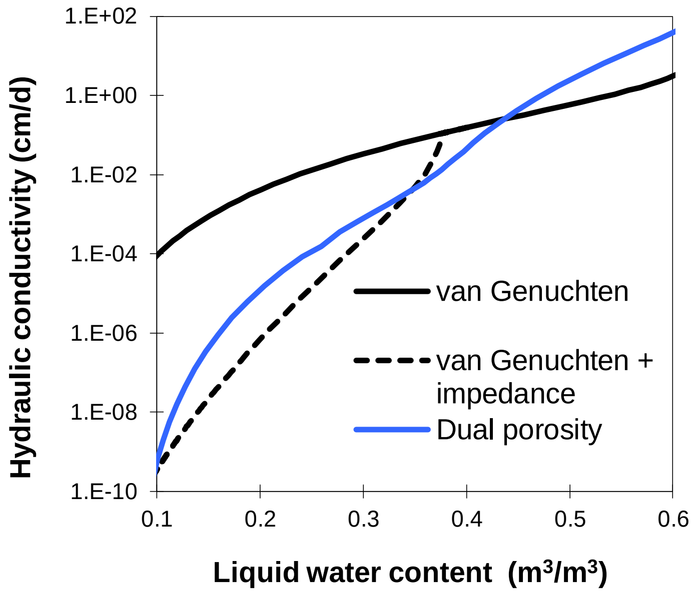

Fig 7. Estimated decrease in hydraulic conductivity as a function of the liquid water content according to the van Genuchten permeability equation (with and without the use of the impedance factor) and a dual porosity model. The impedance factor was obtained from an *E* value of 4 (equation 42). The van Genuchten parameters employed were: a= 0.0101 cm^{-1} and n = 1.35 for the van Genuchten cases with and without the impedance factor. The Durner-Mualem model [172] was utilised for the dual porosity curve with the a_1, n_1, a_2, n_2 parameters equal to 0.0133 cm^{-1}, 2.33, 0.0003 cm^{-1}, and 1.85, respectively. For more details, see Watanabe et al. [171].

Watanabe and Wake [173] suggested that the hydraulic conductivity derived from classic SWC models, such as the Brooks-Corey [151] and van Genuchten [154] models, are incapable of accurately predicting the hydraulic conductivity at very cold temperatures because they were developed for moderate suction. For example, the residual water content in the van Genuchten equation [154] can result in unrealistically high hydraulic conductivities in frozen regions. Additionally, the pressure change near 0°C significantly affects water migration during freezing; this pressure change can be more accurately expressed in a dual porosity model. Hence, modified versions of the van Genuchten equation [154] that account for soil heterogeneities can be utilized to predict hydraulic conductivity in partially frozen soils [e.g. [155,172, 174]]. These modified dual porosity SWC's and relative hydraulic conductivity functions are more flexible and accurate at low unfrozen moisture contents. Following this approach, Watanabe et al. [171] demonstrated that the dual-porosity SWC of Durner [155, 172] could be utilized to accurately represent the SFC and hydraulic conductivity of a column of partially frozen silt loam. Figure 7 demonstrates the hydraulic effect (i.e. the reduction in conductivity) of including the impedance factor or employing a dual porosity model. As Figures 7 indicates, the impedance factor forces the relative permeability function to be non-differentiable at the onset of freezing, and it may cause unrealistic pressure and unstable model calculations. The dual porosity curve in Figure 7 is fully differentiable, but it still produces the general effect of the impedance factor at low unfrozen water contents. Furthermore, as shown in Figure 8, the Durner [155] SWC-derived SFC (dual porosity) has been shown to be able to replicate measured pressures in freezing soils much better than the van Genuchten-derived SFC (Figure 8b). Errors in water pressure can translate to unreasonably high conductivities and water migration (Figure 8c), thereby necessitating the use of an impedance factor. Thus, recent research suggests that Harlan's [41] over-estimation of hydraulic conductivity arose primarily from employing an inaccurate SFC and conductivity function rather than an improper understanding of the hydraulic impedance of pore ice. However, this notion remains a matter of ongoing research and debate.

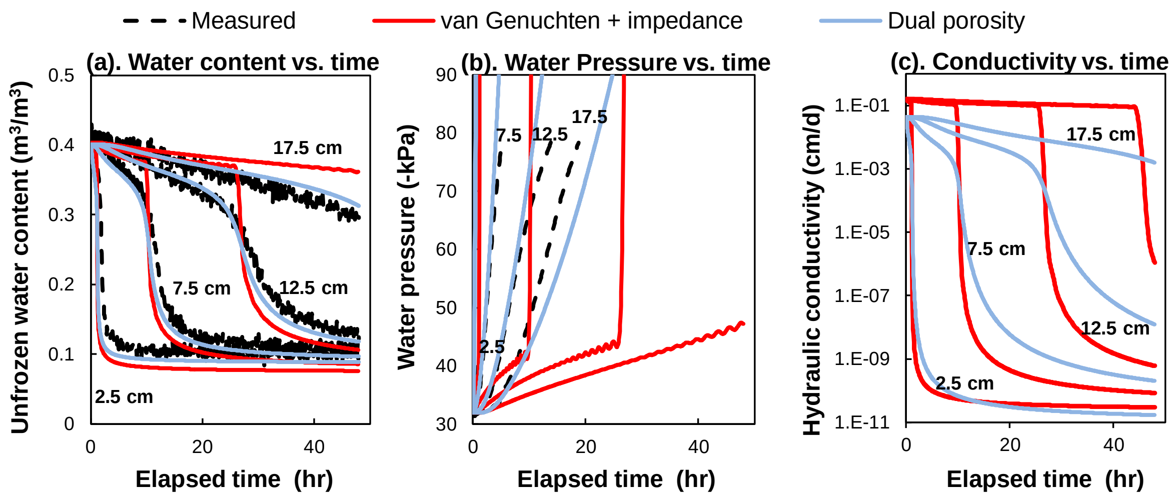

Fig 8. Results from a freezing soil (loam) experiment conducted and detailed by Watanabe et al. [102] **for unsaturated freezing soils: (a) simulated and measured unfrozen water content vs. time, (b) simulated and measured water pressure vs. time , and (c) simulated hydraulic conductivity vs. time.** Modified from Watanabe et al. [102]. The dual porosity SWC of Durner [155] and hydraulic conductivity model of Priesack and Durner [172] were employed. Simulations were performed in HYDRUS with freezing alterations. See [171] for further modeling details.

6. Conclusions

A number of unresolved differences persist for simulating coupled thermal and hydraulic processes in freezing or thawing soils. These theoretical differences have resulted in a variety of methodologies in existing mathematical models, which are summarized in Table 1. Outstanding questions related to these disparate methodologies and the underlying theory discussed in this contribution are highlighted below. Not all of these questions are answered definitively. Where applicable, the need for additional research is highlighted.

1. **Which form of the Clapeyron equation is most appropriate?**

Many of the models listed in Table 1 employ simplified version of the Clapeyron equation, such as equations (3), (4), (5), or (7). One of the primary assumptions invoked when employing these simplified versions of the Clapeyron equation is that the pore water pressure is measured relative to the pressure in the ice phase, which is often implicitly assumed to be atmospheric [73,74]. Accurately simulating the pressure in the ice phase becomes important when freezing-induced mechanical deformations are considered in the model environment [90-92]. Miller [43] criticized the hydraulic model of soil freezing developed by Harlan [41] and others who ignored the pressure in the ice phase and stated: 'Perhaps with judicious tinkering, the hydraulic model can be modified to yield some useful estimates of heaving behavior but not because it is physically realistic'. Therefore, assuming atmospheric pressure in the ice phase certainly limits the ability of the model to simulate frost heave phenomena [73,91]. It is, however, reasonable to implement a simplified Clapeyron equation to simulate coupled heat and water processes in freezing soils, provided that the model scope does not include mechanical deformation. Thus, the appropriate Clapeyron equation is dependent on the model scope. It should also be noted that the Clapeyron relationship is only valid during equilibrium; thus it is inappropriate to apply this equation at disequilibrium, such as during early-stage freezing. Incorporating more complex forms of the Clapeyron equation into several of the existing model methodologies to accommodate heaving processes and accounting for disequilibrium freezing are potential areas of significant research and development.

2. **Is the unfrozen moisture content independent of the initial total moisture content?**

Many have demonstrated through experimentation and/or thermodynamic theory that the unfrozen water content is independent of the initial total water content [34,46,112-114,176,177], while others have suggested a dependence [123,130,131]. Recent research [121,126] has demonstrated that errors were made in these previous studies [123,131] because the ice phase signal was not properly accounted for in the TDR or NMR measurements of unfrozen water content. Thus except in certain cases, such as in saline soils or very high porosity soils, the unfrozen moisture content has been shown to be independent of the initial total moisture content. These observations greatly facilitate the development of SFC's for unsaturated soils.

3. **Should the pressure discontinuity adjustment based on the ratio of the interfacial energies be included when relating the SFC and the SWC?**

As indicated in equations (14) and (16), Koopmans and Miller [38] suggested that the pore water pressure in freezing, saturated soils can be related to the pore water pressure in drying, unsaturated soils. The *n* adjustment factor suggested by Koopmans and Miller [38] is 2.2 for saturated capillary-dominated SS soils and 1.0 for saturated sorption-dominated SLS soils. However, very few researchers have accounted for this when relating the SWC to the SFC. For example, Sheshukov and Nieber [150] acknowledged the existence of this *n* factor, but then ignored it for the sake of simplicity. Ignoring the *n* factor can yield a reasonable SFC if the SWC parameters are adjusted accordingly; however, for the sake of consistency between the SFC and the SWC it is preferable to employ the *n* adjustment factor. Many of the models that have been developed could align much more closely with the capillary theory advanced by Miller [43] by including the adjustment factor based on the ratio of the interfacial energies for capillary-dominated soils. Future research is required to investigate the temperature-dependence of this factor for different types of soils and identify temperatures or unfrozen moisture contents at which sorptive forces may govern even in SS soils.

4. Is the application of an impedance factor necessary?

Despite the fact that several researchers have strongly suggested that this impedance factor is arbitrary, unscientific, and unnecessary [e.g. [54,157]], recent numerical models still continue to utilize an impedance factor when simulating freezing-induced reduction in permeability [e.g. [72,150]]. In general, the impedance factor may be practically useful when employing simple (inaccurate) SWC's, but its application is highly skeptical from a mathematical or physical perspective. Previous research has demonstrated that it is preferable to employ a more accurate SWC and relative conductivity function such as a dual porosity model, as these have been shown to produce reasonable results without the use of an impedance factor.

In summary, a multidisciplinary effort by agronomists, engineers, and hydrogeologists has resulted in a number of mathematical models each employing distinct, and sometimes poorly justified algorithms. To date, there is no generally-accepted unified theory for simulating freezing and thawing processes in unsaturated porous media. Further theoretical work and laboratory and field testing are required to test the validity of existing approaches for simulating the physics and thermodynamics of unsaturated freezing and to establish a framework to identify when existing simplifications or methodologies are invalid. Because the unfrozen water content is known to affect thermal, hydraulic, and stress properties of soils, cryogenic soils will continue to be studied by researchers with diverse backgrounds and interests. However, as more flexible and robust models continue to be developed, an interdisciplinary approach is preferred to reduce the tendency of one discipline to rediscover and solve problems already encountered in other disciplines. We hope that the questions highlighted above may incite model developers from varying backgrounds to progress towards a unified approach in order to resolve these issues and provide valuable information regarding the response of high-latitude or high-altitude soils to future climate change.

We also recommend that models investigating heat transport processes in high-latitude soils accommodate advective heat transport, as this has been shown to accelerate permafrost degradation in certain hydrogeological environments [21,22,178]. Most of the models summarized in the present contribution include advective heat transport, but recent studies of the thermal evolution of permafrost soils still frequently assume conduction is the only significant heat transport mechanism in high-latitude regions [19,28,29,179,180]. Admittedly, numerical models designed to examine large-scale climate change processes in high-latitude soils are often faced with competing demands between model complexity and realism and model computing capabilities. However, with the emergence of increasingly capable computing environments [83,64], model complexity can also be increased. Increasing model capabilities should also enable researchers to incorporate several of the recommendations listed in the preceding paragraphs to enhance model fidelity to physical processes. These recommendations include: (1) employing SFC's derived from well-established SWC's via the Clapeyron equation coupled to capillary theory and (2) utilizing accurate SWC-derived hydraulic conductivity functions that circumvent the need for an arbitrary empirical impedance factor. Accurately simulating the migration of moisture in high-latitude soils will produce corresponding accurate simulations of advective heat transport, and consequently more realistic simulations of the timing, pattern, and magnitude of permafrost thaw. Many of the models listed in this contribution have already incorporated the recommendations above, but future research must be conducted to investigate the parameterization of these models for large-scale permafrost thaw simulations.

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