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SOME APPROACHES TO MODELING PHASE CHANGE IN FREEZING SOILS

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ABSTRACT

Phase change effects associated with freezing soils dominate the thermal state of the soil regime. Furthermore, freezing of soil water influences the soil moisture regime by providing a moisture sink which tends to draw mobile soil moisture to freezing fronts. Consequently, it is critical to general purpose models that soil water phase change effects and the interrelated problem of estimating the moisture sink effects (i.e., conversion of liquid water to ice) be accurately modeled. The choice of such a model will not only influence the precision of simulated temperatures and water contents in a freezing soil, but also have a significant impact on computational efficiency. A review of several current models that assume unfrozen water content is functionally related to subfreezing temperatures indicate that within a freezing soil the soil water flow model and heat transport model parameters are restricted in spatial gradients according to the spatial gradient of modeled unfrozen water content. A freezing soil model based on the concept of isothermal phase change of soil water is proposed as an alternative approach.

INTRODUCTION

The possibility of numerically modeling the complex processes which occur in simultaneous heat and soil-moisture transport in a freezing soil has received much attention during the last decade. Early mathematical models for simulating the soil freezing process were proposed by Harlan (1973), and Guymon and Luthin (1974). More recent modeling efforts of coupled heat and soil-moisture transport in freezing soils include Sheppard et al. (1977), Jame (1978), Taylor and Luthin (1978), and Guymon et al. (1980). A comparison of these various modeling efforts indicates that the approaches used to simulate the soil freezing process differ. Guymon et al. use a so-called "isothermal" approach where the governing heat and moisture flow equations are solved independently and soil-water phase change is modeled within freezing soil by returning below freezing temperatures to the freezing point until the available soil water is frozen. The other referenced modeling efforts all assume that volumetric water content, θ, and temperature, T, are functionally related within a freezing region of soil

$$\theta = \theta(T), \quad T < 0°\text{C} \tag{1}$$

and numerically iterate between the coupled heat and moisture transport relations until values of θ and T are within a selected tolerance to the soil water freezing characteristic curve approximation; if temperatures are above freezing and the soil is ice free, then the functional relation of eqn. (1) is discontinued (Taylor and Luthin). Sheppard et al., however, used an alternative statement of eqn. (1) to eliminate the soil-moisture variable component by a volumetric water content to temperature gradient, and mathematically combined the coupled equations into a single relation based on temperature. This reduced formulation incorporated the so-called apparent heat capacity defined by

$$C_a = C_m + L_a\, \partial\theta/\partial T \tag{2}$$

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where C_a is the volumetric apparent heat capacity; C_m is the volumetric heat capacity of the soil-water–ice mixture; L_a is the volumetric latent heat of fusion of water; and the density of water, ρ_W, is assumed to be unity. Equation (2) was apparently originally presented in terms of volumetric ice content, but more commonly volumetric water content is used in eqn. (2) (Williams 1968 and Anderson et al. 1973).

Although Jame, and Taylor and Luthin numerically iterate and adjust solutions of the governing heat and moisture flow equations until eqn. (1) is satisfied, the underlying mathematical result is the solution of a single differential equation incorporating an appropriate apparent heat capacity term.

The Sheppard et al. mathematical model assumes negligible gravity effects in their vertical soil-water flow model, and relates soil-water pore pressure head to absolute temperature in order to combine both transport equations into an apparent heat capacity formulation including eqn. (2). Jame, and Taylor and Luthin, however, simulate coupled heat and moisture flow in a horizontal freezing soil column and use volumetric water content as the governing moisture transport variable.

In this paper, the two governing heat and soil-water flow mathematical models used in a horizontal freezing soil column problem will be combined into a single transport model similar to the vertical column model of Sheppard et al. Using the volumetric water content to temperature functional relationship assumption, the resulting combined transport model can be written in terms of either the moisture transport or heat transport variables (i.e. volumetric water content or temperature), with the apparent heat capacity term (or equivalent) included in the formulation. From the resulting combined model, it will be shown that severe limitations on the transport conduction parameters of thermal conductivity and soil-water diffusivity must be satisfied in order for the model to describe the soil-water freezing process.

The objective of this paper is twofold. The first objective is to evaluate the mathematical consistency of combining the assumptions in eqns. (1) and (2) with coupled heat and moisture transport models. A number of investigators assumes that soil-moisture transport in freezing soils can be modeled by an analogy to unsaturated soil-water flow theory where soil moisture driven by hydraulic gradients dominates, and the usual soil-water diffusivity can be modified by an ice-content correction or scaling factor in order to accommodate ice formation and its effect on soil-water flow. Additionally, the classical heat transport relation is assumed for heat flow within freezing soils, and heat transport due to convection by soil-water flow is assumed negligible in several models. Ice formation within freezing soils is modeled by an appropriate soil-moisture sink and heat source term based on the time rate of change of volumetric ice content within the freezing soil.

The second objective of this paper is to present an alternative modeling approach based on the previously mentioned isothermal concept. This second approach is based on the assumptions of an analogy to unsaturated soil-water flow theory and the classical heat transport relation (with convection), but somewhat relaxes the volumetric water content to temperature functional requirement. Soil water in excess of that predicted by the soil-water freezing characteristic curve is permitted, but further soil freezing is modeled isothermally until the soil-water content corresponds to the freezing characteristic curve.

SOIL-WATER PHASE CHANGE EFFECTS MODELED AS AN APPARENT HEAT CAPACITY

A horizontal freezing soil column will be discussed due to the extensive numerical model development and laboratory parameter estimations given in the literature (e.g. Jame 1978).

Soil water flow in freezing soils is generally assumed modeled by an analogy to unsaturated soil-water flow theory by

$$\frac{\partial}{\partial x}\left(D\,\frac{\partial \theta}{\partial x}\right) = \frac{\partial \theta}{\partial t} + \frac{\rho_I \partial \theta_I}{\rho_W \partial t} \tag{3}$$

where D is the appropriate freezing soil-water diffusivity. Equation (3) is based upon the assumption that soil water primarily moves as a liquid, driven by hydraulic gradients. Vapor movement and thermally driven moisture flow is assumed negligible (Fuchs 1978, for example).

Neglecting convected heat effects, heat flow in freezing soils is generally modeled by

$$\frac{\partial}{\partial x}\left(K_T\,\frac{\partial T}{\partial x}\right) = C_m\,\frac{\partial T}{\partial t} - L_a\,\frac{\rho_I}{\rho_W}\,\frac{\partial \theta_I}{\partial t} \tag{4}$$

where K_T is the thermal conductivity; θ_I is the volumetric ice content; L_a is the volumetric latent heat of fusion for liquid water; and ρ_I is the density of ice. A third major assumption in several current models is that water content and temperature are functionally related for below freezing temperatures (Sheppard et al., Taylor and Luthin, Jame)

$$\theta = \theta(T), \quad \theta \in R(T) \tag{5}$$

where $R(T)$ is the domain of functional definition for subfreezing temperatures.

From eqn. (5), the thermal gradient of water content is defined by (Jame, Sheppard et al.)

$$\hat{\theta} = \partial\theta/\partial T, \quad \theta \in R(T) \tag{6}$$

Therefore, eqns. (3), (4), (5) and (6) may be combined into one governing equation similar to the formulation of Sheppard et al.

$$\frac{\partial}{\partial x}\left[L_a D \frac{\partial \theta}{\partial x} + \frac{K_T}{\hat{\theta}} \frac{\partial \theta}{\partial x}\right] = \left[L_a + \frac{C_m}{\hat{\theta}}\right]\frac{\partial \theta}{\partial t}, \theta \in R(T) \tag{7}$$

or in simpler notation,

$$\left.\begin{aligned} &\frac{\partial}{\partial x}\left(\alpha_1 \frac{\partial \theta}{\partial x}\right) = \alpha_3 \frac{\partial \theta}{\partial t} \\ &\theta = \theta(T) \\ &\alpha_1 = L_a D + K_T/\hat{\theta} \\ &\alpha_3 = L_a + C_m/\hat{\theta} \end{aligned}\right\} \tag{8}$$

where α_3 is the corresponding apparent heat capacity term equivalent to eqn. (2) for volumetric water content used as the primary variable in eqn. (7). Thus, the $\theta = \theta(T)$ assumption leads to one equation incorporating an apparent heat capacity term (or equivalent) and ancillary relationships between parameters. Although from the above it is necessary to numerically solve only one equation, Jame (1978) and Taylor and Luthin (1978), for example, numerically solve each equation of state separately, and adjust solutions by an iteration procedure for an assumed $\theta = \theta(T)$.

To determine the ice content profile, considerations of mass transport may be used as outlined in Hromadka and Guymon (1980). Thus, eqn. (3) can be temporally and spatially discretized for numerical solution as follows:

$$\left\{\int_{\Omega_j} \theta_I \, dx\right\} \Big|_{\Delta t}^{2\Delta t} = \frac{\rho_W}{\rho_I} \int_{\Delta t}^{2\Delta t} \left\{D \frac{\partial \theta}{\partial x} \Big|_{\Gamma_j}\right\} dt - \frac{\rho_W}{\rho_I}\left\{\int_{\Omega_j} \theta \, dx\right\} \Big|_{\Delta t}^{2\Delta t} \tag{9}$$

where Δt is a numerical time step increment, Ω_j and Γ_j are spatial domains and boundaries respectively of soil column region, j. Appropriate basis or trial functions are substituted into eqn. (9) and indicated mathematical operations are carried out, yielding a matrix system very similar to that resulting from using the well-known finite-element method.

Some theoretical implications and problem limitations as posed by eqn. (7) can best be developed by examining a simulation of horizontal freezing in a soil column. Laboratory data obtained by Jame (1978) are used as a case study. Unsaturated soil-water diffusivity, $D(\theta)$, is assumed described as shown in Fig. 1, and water content is assumed to be a function

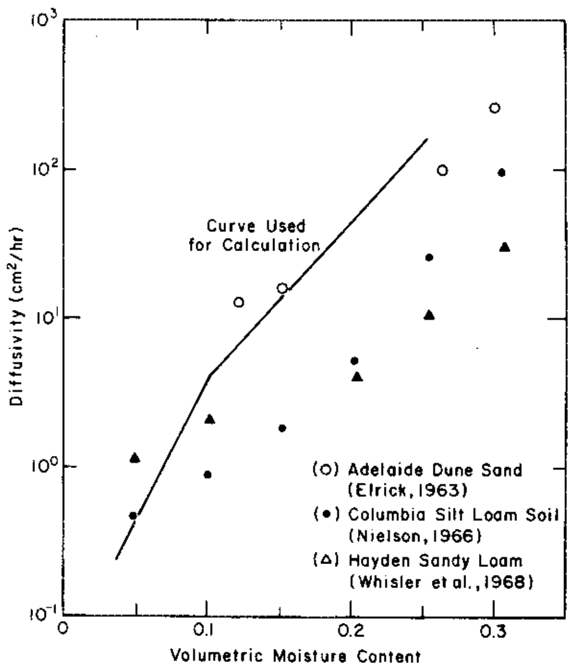

Fig. 1. Soil-water diffusivity versus unfrozen moisture content (Jame 1978).

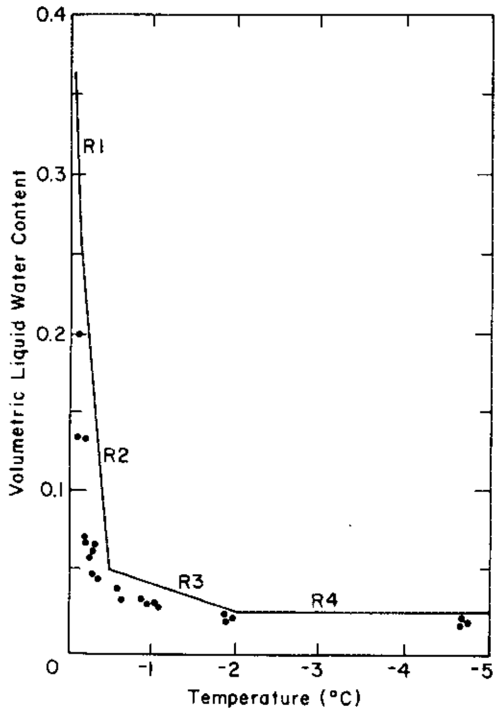

Fig. 2. Liquid water content versus temperature relationship showing experimental data and the approximate curve used in the computations (Jame 1978).

of temperature as shown in Fig. 2. These data are generally similar to data from frost susceptible soils. From Figs. 1 and 2, it can be shown that within region R_1 of the diffusivity curve, the magnitudes of $(C_m/\hat{\theta})$ and $(K_T/\hat{\theta})$ are less than one-half of one percent of the magnitudes of (L_a) and (DL_a), respectively. Accordingly, within region R_1 eqn. (7) may be numerically approximated for the given assumptions by

$$\left.\begin{aligned} &\frac{\partial}{\partial x}\left(D\,\frac{\partial\theta}{\partial x}\right) = \frac{\partial\theta}{\partial t} \\ &D = D(\theta,\theta_I) = D(\theta)/10^{10\theta_I} \\ &x \in R_1 \end{aligned}\right\} \tag{10}$$

where $D(\theta,\theta_I)$ is assumed defined by an adjustment to unsaturated diffusivity as described by Taylor and Luthin. Because data on hydraulic conductivity of frozen soil are not generally available, an estimate of frozen soil hydraulic conductivity is usually assumed for most models. The approach used by Taylor and Luthin which is based upon unfrozen soil water diffusivity is arbitrarily selected for study purposes. For region R_4 (Fig. 1), eqn. (7) may be examined in the limit to be

$$\lim_{\hat{\theta}\to 0}\left\{\frac{\partial}{\partial x}\left[\left(\frac{K_T}{\hat{\theta}} + DL_a\right)\frac{\partial\theta}{\partial x}\right] = \left(\frac{C_m}{\hat{\theta}} + L_a\right)\frac{\partial\theta}{\partial t}\right\}$$

$$= \left\{\frac{\partial}{\partial x}\left(K_T\,\frac{\partial T}{\partial x}\right) = C_m\,\frac{\partial T}{\partial t}\right\},\quad x \in R_4 \tag{11}$$

where the thermal parameters are functions of soil, water and ice fractions. Within regions R_2 and R_3, the magnitudes of (DL_a) and $(K_T/\hat{\theta})$ generally are such that neither term can be eliminated from the formulation.

For significant diffusivity values, difficulties may arise in attempting to model a zero moisture flux boundary condition while maintaining a freezing thermal gradient; that is, for $\theta = \theta(T)$,

$$\left.\begin{aligned} &D\,\frac{\partial\theta}{\partial x} = (D\hat{\theta})\frac{\partial T}{\partial x} = 0 \\ &K_T\frac{\partial T}{\partial x} \neq 0 \end{aligned}\right. \tag{12}$$

would be the boundary condition. Accordingly, diffusivity must be set to zero at the column boundary.

Another difficulty is possible accumulation of soil moisture above the water content value predicted by the characteristic curve, $\theta(T)$. For the horizontal freezing column problem (Jame, for example) where zero moisture flux occurs at the column boundaries at $x = (0, L)$, the $\theta = \theta(T)$ assumption necessarily implies that the thermal and moisture gradients are positive, for the freezing front advancing from $x = 0$. Also, a closed system freezing column problem can only have a depletion of unfrozen soil moisture, since an increase of moisture implies an increase of temperature by the $\theta(T)$ assumptions and eqns. (3) and (4). Hence, the governing relations within regions of freezing soil become

$$\left.\begin{aligned} &\frac{\partial}{\partial x}\left[\left(\frac{K_T}{\hat{\theta}} + DL_a\right)\frac{\partial\theta}{\partial x}\right] = \left(\frac{C_m}{\hat{\theta}} + L_a\right)\frac{\partial\theta}{\partial t},\quad 0<x<L \\ &\partial\theta/\partial t \leqslant 0,\quad t \geqslant 0 \\ &\theta = \theta(T) \end{aligned}\right\} \tag{13}$$

For $\partial\theta/\partial t = 0$,

$$-\frac{\partial}{\partial x}\left(K_{\mathrm{T}}\frac{\partial T}{\partial x}\right) = L_{\mathrm{a}}\frac{\partial}{\partial x}\left(D\frac{\partial\theta}{\partial x}\right) \tag{14}$$

which results in a specific formulation for thermal conductivity in a steady-state moisture content region for the models considered

$$\left.\begin{aligned} K_{\mathrm{T}} &= \frac{A_0}{(\partial T/\partial x)} - DL_{\mathrm{a}}\frac{\partial\theta}{\partial T} \\ \theta &= \theta(T) \\ \partial\theta/\partial t &= 0 \end{aligned}\right\} \tag{15}$$

For some region, $\hat{R}$, of the soil column where $\hat{\theta}$ is set to the constant value $\hat{\theta}_0$, A_0 can be evaluated such that eqn. (18) becomes

$$K_{\mathrm{T}} = \frac{(K_{\mathrm{T}}' + L_{\mathrm{a}}\hat{\theta}_0 D')\left(\dfrac{\partial T}{\partial x}\right)'}{\left(\dfrac{\partial T}{\partial x}\right)} - L_{\mathrm{a}}\hat{\theta}_0 D;\ x \in \hat{R} \tag{16}$$

where primes indicate known values. An approximate spatial gradient relationship is given by

$$\left.\begin{aligned} &\frac{\partial}{\partial x}\hat{K}_{\mathrm{T}} \approx -L_{\mathrm{a}}\hat{\theta}_0\frac{\partial D}{\partial x};\quad x \in \hat{R} \\ &\theta = \theta(T) \\ &\partial\theta/\partial t \approx 0 \\ &(\partial T/\partial x)'/(\partial T/\partial x) \approx 1 \end{aligned}\right\} \tag{17}$$

where $\hat{K}_{\mathrm{T}}$ denotes that thermal conductivity function which satisfies the steady-state moisture content relationship of eqn. (16).

For the dynamic case, in a freezing soil, eqn. (13) can be rewritten as

$$\left.\begin{aligned} &\frac{\partial}{\partial x}\left[\left(\frac{K_{\mathrm{T}}}{\hat{\theta}} + L_{\mathrm{a}}D\right)\frac{\partial\theta}{\partial x}\right] = \left(\frac{C_{\mathrm{m}}}{\hat{\theta}} + L_{\mathrm{a}}\right)\frac{\partial\theta}{\partial t} \\ &\frac{\partial\theta}{\partial t} < 0,\quad 0 < x < L \end{aligned}\right\} \tag{18}$$

where for unidirectional freezing in a soil-column (freezing front advancing from $x = 0$) the various gradients are generally given by

$$\left.\begin{aligned} &\partial\theta/\partial t \leqslant 0 \\ &\partial\theta/\partial x > 0 \\ &\partial^2\theta/\partial x^2 \leqslant 0 \\ &\partial K_{\mathrm{T}}/\partial x \leqslant 0 \\ &\partial D/\partial x \geqslant 0 \end{aligned}\right\} \tag{19}$$

From eqns. (18) and (19)

$$\frac{\partial}{\partial x}\left[\left(\frac{-K_{\mathrm{T}}}{\hat{\theta}}\right)\frac{\partial\theta}{\partial x}\right] \geqslant \frac{\partial}{\partial x}\left[(L_{\mathrm{a}}D)\frac{\partial\theta}{\partial x}\right] \tag{20}$$

which when expanded gives (for below freezing temperatures)

$$\frac{\partial}{\partial x}(DL_{\mathrm{a}}) \leqslant -\frac{\partial}{\partial x}\left(\frac{K_{\mathrm{T}}}{\hat{\theta}}\right) - \left(\frac{K_{\mathrm{T}}}{\hat{\theta}} + L_{\mathrm{a}}D\right)\frac{\partial^2\theta}{\partial x^2}\bigg/\frac{\partial\theta}{\partial x} \tag{21}$$

In order to avoid moisture accumulation at a constant temperature and preserve the $\theta(T)$ assumption, eqn. (21) must be satisfied for every water content profile. Thus, for the given model assumptions, the transport parameters are limited in spatial gradients according to the spatial gradient of water content. Especially important are the initial conditions of the problem which also bound the parameter spatial gradients as given in eqn. (21).

For example purposes, consider a strictly freezing horizontal soil-column problem with initial conditions given below (Fig. 3):

$$\left.\begin{aligned} &\theta = \theta(T)\ \text{(Fig. 2)} \\ &\theta(x=0,\ t \geqslant 0) = \theta_{\mathrm{b}} \\ &\theta(x=L,\ t=0) = \theta_0;\ \theta_{\mathrm{b}} < \theta_0 < \eta \\ &\theta(x, t=0) = (\theta_0 - \theta_{\mathrm{b}})x/L + \theta_{\mathrm{b}} \\ &\frac{\partial\theta}{\partial x}(x=L,\ t>0) = 0 \\ &\frac{\rho_{\mathrm{I}}}{\rho_{\mathrm{W}}}\theta_{\mathrm{I}} + \theta = \theta_0;\ t=0,\ 0<x<L \\ &\hat{\theta} > 0,\ 0<x<L \\ &T(x) < 0\ ^{\circ}\mathrm{C},\ 0 \leqslant x \leqslant L \end{aligned}\right\} \tag{22}$$

where η is the porosity. Thermal conductivity is assumed given by the DeVries (1966) equation

$$K_{\mathrm{T}} = K_{\mathrm{W}}\theta + K_{\mathrm{I}}\theta_{\mathrm{I}} + K_{\mathrm{S}}\theta_{\mathrm{S}} \tag{23}$$

where $(K_{\mathrm{W}}, K_{\mathrm{I}}, K_{\mathrm{S}})$ are the thermal conductivities of

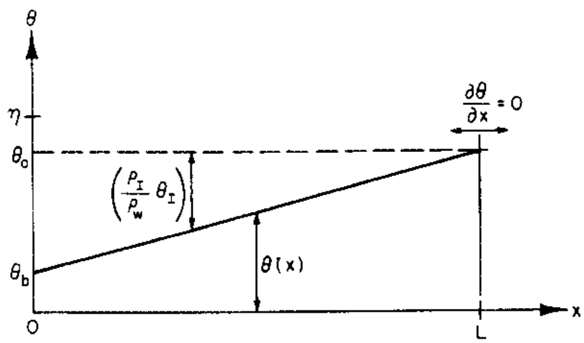

Fig. 3. Geometry for example initial condition problem.

water, ice and soil. Other pertinent parameter estimations are obtained from the laboratory data shown in Figs. (1) and (2). The unsaturated diffusivity shown in Fig. (1) is estimated by

$$D(\theta, \theta_I = 0) = 0.278e^{25.58\theta}, \quad 0.11 \leqslant \theta \leqslant 0.26 \quad (24)$$

Taylor and Luthin propose an ice accumulation correction factor, I, for freezing soils, such that

$$\left.\begin{aligned} D(\theta,\theta_I) &= D(\theta)/I \\ I &= 10^{10\theta_I} \end{aligned}\right\} \quad (25)$$

Thus, for below freezing temperatures

$$D(\theta,\theta_I) = 0.278e^{(25.58\theta-23.03\theta_I)}, \; 0.11 \leqslant \theta \leqslant 0.26 \quad (26)$$

The spatial gradient of diffusivity for below freezing temperatures is given by the chain rule

$$\frac{\partial D(\theta,\theta_I)}{\partial x} = \frac{\partial D}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial D}{\partial \theta_I}\frac{\partial \theta_I}{\partial x} \quad (27)$$

From eqn. (23)

$$\frac{\partial K_T}{\partial x} = K_W \frac{\partial \theta}{\partial x} + K_I \frac{\partial \theta_I}{\partial x} \quad (28)$$

From Fig. 2,

$$\theta(T) = 0.325 + 0.55T; \quad 0.11 \leqslant \theta \leqslant 0.26 \quad (29)$$

thus,

$$\hat{\theta} = \frac{\partial \theta}{\partial T} = 0.55 \equiv \hat{\theta}_0, \quad 0.11 \leqslant \theta \leqslant 0.26 \quad (30)$$

For the initial conditions of eqn. (22) and $0.11 \leqslant \theta \leqslant 0.26$,

$$\left.\begin{aligned} \frac{\partial \theta_I}{\partial x} &= -\frac{\rho_W}{\rho_I}\frac{\partial \theta}{\partial x} = -1.1\frac{\partial \theta}{\partial x} \\ \frac{\partial K_T}{\partial x} &= (K_W - 1.1K_I)\frac{\partial \theta}{\partial x} < 0 \\ \frac{\partial D(\theta,\theta_I)}{\partial x} &= 50.91\,D\frac{\partial \theta}{\partial x} \end{aligned}\right\} \quad (31)$$

For the initial conditions of eqn. (22), the statement of eqn. (7) is rewritten in terms of temperature as

$$\frac{\partial}{\partial x}\left[\left(L_a D\hat{\theta} + K_T\right)\frac{\partial T}{\partial x}\right] = [L_a\hat{\theta} + C_m]\frac{\partial T}{\partial t} \quad (32)$$

and from eqn. (2),

$$[L_a\hat{\theta} + C_m]\frac{\partial T}{\partial t} = C_a\frac{\partial T}{\partial t} \quad (33)$$

Equation 32 is expanded as

$$(L_a D\hat{\theta} + K_T)\frac{\partial^2 T}{\partial x^2} + \left[\frac{\partial}{\partial x}(L_a D\hat{\theta} + K_T)\right]\frac{\partial T}{\partial x} = C_a\frac{\partial T}{\partial t} \quad (34)$$

For $\hat{\theta}$ equal to the constant $\hat{\theta}_0$ per eqn. (30), the initial condition modeled temperature profile is linear and

$$\left.\begin{aligned} \frac{\partial}{\partial x}(L_a D\hat{\theta}_0 + K_T) &= \frac{C_a\dfrac{\partial T}{\partial t}}{\dfrac{\partial T}{\partial x}} \\ \partial T/\partial x &> 0 \end{aligned}\right\} \quad (35)$$

but from eqn. (4), the initial condition of the test problems implies

$$\frac{\partial K_T}{\partial x}\frac{\partial T}{\partial x} = C_m\frac{\partial T}{\partial t} - L_a\frac{\rho_I}{\rho_W}\frac{\partial \theta_I}{\partial t} \quad (36)$$

Thus,

$$\left.\begin{aligned} 0 &> C_m\frac{\partial T}{\partial t} - L_a\frac{\rho_I}{\rho_W}\frac{\partial \theta_I}{\partial t} \\ \frac{\partial K_T}{\partial x} &< 0 \end{aligned}\right\} \quad (37)$$

Since convected heat is assumed negligible in this example, it can be assumed that initially

$$\partial T/\partial t \leqslant 0 \tag{38}$$

but

$$\frac{\partial T}{\partial t} = \frac{\partial T}{\partial \theta}\frac{\partial \theta}{\partial t}, \quad T < 0°\mathrm{C} \tag{39}$$

Thus, for the initial condition of the test problem

$$\partial\theta/\partial t \leqslant 0 \tag{40}$$

Therefore, from eqns. (18), (35), (38) and (40)

$$\frac{\partial DL_a}{\partial x} \leqslant -\frac{\partial}{\partial x}\frac{K_T}{\hat{\theta}_0} \tag{41}$$

is a necessary condition to preserve the $\theta(T)$ assumption for the freezing soil test problem. From eqn. (34), the restrictions of eqn. (41) also apply in a freezing soil where temperature (or moisture) gradients are linear. The conditions of eqn. (41) can also be determined from eqn. (7) by a development similar to the above.

For thermal parameters assumed given by

$$\left.\begin{aligned} K_W &= 4.8 \text{ cal/h cm °C} \\ K_I &= 19 \text{ cal/h cm °C} \\ L_a &= 80 \text{ cal/cm}^3 \end{aligned}\right\} \tag{42}$$

eqn. (41) can be evaluated for the initial conditions of the test problem as

$$\left.\begin{aligned} \frac{\partial DL_a}{\partial x} &= 4072.8\, D\frac{\partial \theta}{\partial x} \text{ cal/h cm}^2 \\ \frac{\partial}{\partial x}\left(\frac{K_T}{\hat{\theta}}\right) &= -29.3\frac{\partial\theta}{\partial x} \text{ cal/h cm}^2 \end{aligned}\right\} \tag{43}$$

but $\partial\theta/\partial x > 0$ by Fig. 3. Thus, from the initial condition of the test problem and eqns. (41) and (43), a necessary requirement for preserving the $\theta(T)$ assumption is

$$\left.\begin{aligned} &D(\theta,\theta_I) \leqslant 0.0072 \text{ cm}^2\text{/m} \\ &0 < x < L \end{aligned}\right\} \tag{44}$$

The conditions of eqn. (44) cannot generally be satisfied for the considered domain $0.11 < \theta < 0.26$.

For modeling purposes, it is assumed that eqn. (41) must be satisfied for any moisture content profile. The results of eqn. (41) can also be derived from eqn. (21) by considerations of linear water content profiles. A major implication of eqn. (41) is that for the $\theta(T)$ assumption to remain valid, the soil freezing front must essentially continually advance into the soil column. The requirement of eqn. (20) implies that the net heat efflux must never be exceeded by the net influx of latent heat (influx due to moisture transport). Since the assumed initial condition ice and water content profile are arbitrary for the problem of Fig. 3, the $\theta(T)$ assumption and resulting apparent heat capacity term formulation indicates that the models that incorporate these are restricted to a limited class of soil freezing problems.

SOIL-WATER PHASE CHANGE EFFECTS MODELED AS AN ISOTHERMAL PROCESS

Guymon et al. (1980) propose a model of simultaneous flux of heat and moisture in freezing and thawing soils that assumes latent heat effects can be modeled as an isothermal process. The concepts employed in this model are discussed below.

Consider the heat budget ΔQ required to alter a unit volume soil-water–ice mixture by a temperature change of $\mathrm{d}T$ in a time interval of $\mathrm{d}t$,

$$\Delta Q = C_m\,\mathrm{d}T - L_a\frac{\rho_I}{\rho_W}\frac{\partial\theta_I}{\partial t}\,\mathrm{d}t \tag{45}$$

Equation (45) can be rewritten as

$$\Delta Q = C_m\frac{\partial T}{\partial t}\,\mathrm{d}t - L_a\frac{\rho_I}{\rho_W}\frac{\partial\theta_I}{\partial t}\,\mathrm{d}t \tag{46}$$

where temperature is a differentiable function of time.

Application of eqn. (46) to problems where the water content of the soil can also be assumed to be a differentiable function of temperature permits the rewriting

$$\Delta Q = \left(C_m + L_a\frac{\partial\theta}{\partial T}\right)\frac{\partial T}{\partial t}\,\mathrm{d}t \tag{47}$$

which establishes the apparent heat capacity formulation of eqn. (2), where applicable.

Assuming that the convected moisture enters the soil system at approximately the temperature of the freezing point depression, a small drop in temperature ΔT (in time Δt) of the soil-ice–water mixture is modeled by a heat budget of

$$\Delta Q = L_a [\theta' - \theta(T_0)] - L_a \frac{\partial \theta}{\partial T} \Delta T - C_m \Delta T \quad (48)$$

where θ' is the volumetric moisture content at the beginning of the process; $\theta(T_0)$ is the volumetric water content described by the thermal soil-water characteristic curve for temperature T_0, T_0 is the initial temperature of the system, ΔT is the temperature drop (assumed negative), and ΔQ is the heat lost from the system during time step Δt.

From eqn. (48), three macroscopic thermodynamic cases are accommodated in the lumped isothermal model for a strictly freezing process

$$L_a [\theta' - \theta(T_0)] = \Delta Q \quad (49)$$

$$L_a [\theta' - \theta(T_0)] > \Delta Q \quad (50)$$

$$L_a [\theta' - \theta(T_0)] < \Delta Q \quad (51)$$

Equation (49) is associated with isothermal freezing in a static thermal and moisture regime. Relation (50) also indicates isothermal freezing (i.e. no temperature variation) but additionally indicates possible moisture accumulation. Equation (51) occurs with a temperature change of the system ΔT (during time step Δt) determined from eqn. (48)

$$\Delta T = \frac{L_a[\theta' - \theta(T_0)] - \Delta Q}{L_a \dfrac{\partial \theta}{\partial T} + C_m} \quad (52)$$

The ice accumulation term is calculated by

$$\frac{\rho_I}{\rho_W} \frac{\partial \theta_I}{\partial t} \mathrm{d}t = \begin{cases} \dfrac{\Delta Q}{L_a}, & \text{if } \Delta Q \leqslant L_a [\theta' - \theta(T_0)] \\ [\theta' - \theta(T_0)] - \dfrac{\partial \theta}{\partial T} \Delta T, & \\ \quad \text{if } \Delta Q > L_a[\theta' - \theta(T_0)] & \end{cases} \quad (53)$$

Assume $\theta(T)$ approximated by a set of linear functions defined on a discretized thermal domain per Fig. 2. Then for an appropriate temperature subdomain for $T_a \leqslant T \leqslant T_b$

$$\theta(T) = \beta_0 + \beta_1 T \quad (54)$$

where β_0, β_1 are constant soil parameters, and

$$\partial\theta(T)/\partial T = \beta_1 \quad (55)$$

Thus, for a small change in temperature ΔT (ΔT negative), eqn. (48) and eqn. (55) are modeled by

$$\Delta Q = \{L_a[\theta' - \theta(T_0)] - L_a \beta_1 \Delta T\} - C_m \Delta T \quad (56)$$

where the term in brackets represents an isothermal freezing process.

The terms within the braces of eqn. (56) may be approximated numerically by decoupling the ice formation terms from the general heat transfer equation and allocating the subsequent heat evolution to a latent heat budget. As the ice content increases, the thermal and moisture parameters are adjusted. Ice formation is interpreted as a moisture sink in the moisture transfer relation. Only when the necessary heat evolution has occurred, is a soil mixture's temperature allowed to recede below the freezing point depression, hence modeling the isothermal phase change process.

DISCUSSION

Although there are no apparent theoretical problems in applying the apparent heat capacity concept to numerical models that deal only with the thermal regime of freezing soils, there may be problems when using this concept to numerically model simultaneous thermal and moisture states of freezing soils. This is particularly true in regions where the thermal (or moisture content) spatial gradients are approximately linear, resulting in invalidation of the water content to temperature functional relationship as shown herein. In the literature, numerical models employing this approach require small time-steps (on the order of centimeters). Using currently proposed numerical modeling approaches shows that assumptions imbedded in these models lead to inconsistencies when these models use the apparent heat capacity approach in its present form. Either an apparent heat capacity formulation based upon open freezing situations where moisture is mobile will have to be prepared or alternative means of accounting for latent heat effects are required.

An alternative modeling approach is proposed which is based on an isothermal soil-water freezing submodel. Such an approach leads to a self-consistent model. From a practical standpoint, time-step sizes can be relatively large, of the order of hours, and spatial discretization can also be relatively large, of the order of 0.5 meters. Models that have been developed and employed are able to accurately simulate thermal and moisture states of freezing soils over long time spans, of the order of years. The ability to use large discretization and achieve stable, accurate results over a long simulation period will become increasingly important as more complex problems are attempted which require two or three spatial dimensions. It is emphasized that the proposed isothermal approach is a lumped thermodynamic assumption used for predictive modeling. No claim is made that such a modeling assumption describes the microscopic thermodynamic behavior of water freezing or thawing in a soil.

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