Heat and Mass Transfer of Freezing Water-Soil System

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To describe multiphase water (water vapor, ice, water liquid) distribution in freezing soil, mass and heat transfer equations using the methods of processes of irreversible thermodynamics are presented.

In this paper we derive equations describing fluxes (heat and mass) and transfer potential distributions (temperature and moisture content) for a freezing soil system. Within a given set of physical and mathematical restrictions the derived equations will account for transient conditions, multiphase systems, phase changes, and multieextensive property transfers. The development of these transfer equations involves defining the system and stating the physical conditions, developing conservation equations, developing flux equations subject to the proper use of the principles of thermodynamics of irreversible processes (linearized Onsager flux equations), and combining conservation and flux equations to yield the conservation equation.

**SYSTEM**

Figure 1 shows thermodynamically open actual freezing soil system $S_f$. Mass ($J_m$ is total mass flux) and heat ($J_q$ is heat flux) can flow into and out of the total system $S_f$ or any of the subsystems $S_C$ (freezing unsaturated system), $S_B$ (nonfreezing unsaturated system), and $S_A$ (nonfreezing saturated system). Subsystem $S_C$ is bounded by the soil surface and the frost front, $S_B$ by the frost front and the water table, and $S_A$ by the water table and an impervious layer.

To derive differential equations determining mass and heat transfer, this actual system (Figure 1) is simplified to an ideal (see the following list of physical and mathematical assumptions defining this ideality) general freezing soil system as shown in Figure 2. In Figure 2 the introduced wall-of-soil concept neglects the effect of gravity, and thus the derivation of equations is restricted to two-dimensional (horizontal) flow for moist soils. For drier soils for which gravity effects are indeed negligible the three-dimensional flow generality is preserved.

The proposed ideal system will have the following characteristics, which are in common use for nonfreezing water-soil systems as found in standard texts on subsurface hydrology.

1. Various changes in soil matrix, such as those due to swelling, frost heave, and expansion of water volume on ice lens formation in soil, are neglected.
2. Electrical and osmotic potentials are neglected (especially those caused by various ions and their concentration changes).
3. The gas phase in soil has uniform pressure throughout the system.
4. Fluid flow is laminar; hysteresis, viscous, and inertia effects are neglected.
5. Each fluid (gas, vapor, liquid) flow is connected through the system and is continuous.
6. Soils of high clay content (finer texture) and soils of high gravel content (coarser texture) are excluded; that is, we restrict ourselves to soil textures for which Darcy's law is commonly assumed to be valid.
7. The temperature at which freezing begins is assumed to be 0°C.
8. Heat transfer by convection (liquid, vapor) is neglected.
9. The soil within the given system is assumed to be a mathematically homogeneous and isotropic body.

Figure 3 summarizes parameters describing the volume of the idealized system at some arbitrary time $\tau$. This volume is separated into phases and species $i$. (Note that the designation of the mass species $i$ index is $i = 1, \cdots, 4$, whereas $i = 5$ represents heat.) The following
phases are present: gas, liquid, ice solid, and soil solid. The gas phase has two species, air ($i = 4$) and water vapor ($i = 1$). The remaining phases have only one species: water liquid, including bonded water ($i = 2$), ice ($i = 3$), and soil ($i = 0$). (Water liquid is defined as the sum of gravitational, capillary, and hygroscopic moisture.) If $m_i$ for $i = 1, \ldots, 4$ is the mass of species $i$, $u_i = m_i/m_o$ is the mass-based moisture content or specific mass content of species, and $\omega_i = m_i/V$ is the volume-based moisture content or bulk density of species, then the parameters may be named over species $i$ from 1 to 3. For species $i = 4$, $u_4$ is the specific mass content of dry air, and $\omega_4$ is the bulk density of dry air. The parameter $\omega_0$ is the dry bulk density of soil, and $V$ is the volume of the system. As is shown in Figure 2, the chosen freezing soil system is open; i.e., the flow of heat and mass through its boundaries, as well as phase changes (e.g., ice formation), takes place within these boundaries. The mass flow will consist of vapor and liquid flow. The heat and mass flow is caused by driving forces (or transfer forces) $\nabla \phi_i$, which are the gradients of the extensive property transfer potential $\phi_i$. The following transfer potentials describing the given system are used in this work: temperature potential $t$, where $t = ^\circ C$, for heat transfer; vapor concentration potential $x_i$, where $x_i = x_i(t)$ for moist soils or $x_i(u_4, t)$ for drier soils, for vapor mass transfer by diffusion; and capillary potential $\psi$, where $\psi = \psi(u_2, t)$, for liquid mass transfer by capillary absorption. (Moist soil in this work is defined as soil containing moisture in excess of hygroscopic moisture; i.e., drier soil is a limiting case of moist soil.) Additionally, it is assumed that heat and mass transfer is influenced by driving forces (see the flux equations to follow) caused by various coupling mechanisms.

**Derivation of Transfer Equations**

**Conservation Equations**

If an extensive property balance is taken across an elemental volume (Figure 4) subject to all the restrictions forming an ideal freezing soil system, then one can write a general conservation equation for any extensive property [cf. Fitts, 1962] for the total system as

$$\frac{\partial (\omega G)}{\partial \tau} = -\nabla \cdot \mathbf{J}_\sigma + \phi_\sigma$$  \hspace{1cm} (1)
where $G$ is an extensive property per unit mass, $\phi_o$ is the internal source of this extensive property, and $\partial / \partial \tau$ is the time derivative at a fixed point relative to an external coordinate system. In separate species $i$ the conservation equation 1 becomes

$$\frac{\partial (\omega G_i)}{\partial \tau} = -\nabla \cdot J_i + \phi_o,$$  

If mass is considered as an extensive property, $G_i$ becomes

$$G_i = \omega_i / \omega$$  

or, if mass-based moisture content $u_i$ is used,

$$G_i = (\omega_i / \omega) u_i$$

the connection being that $\omega_i = \omega_i u_i$. By the use of conditions 3a and 3b the general extensive property conservation equation for species $i$ (2) may be written for the conservation of mass of species $i$ for the freezing soil system as

$$\frac{\partial (\omega_s u_i)}{\partial \tau} = -\nabla \cdot J_i + I_i, \quad i = 1, \ldots, 4$$

where $J_i$ is the local mass flux of species $i$ and $I_i$ is the specific strength of source (phase change). If we consider the total freezing soil system, the conservation of mass requires that the total specific strength of source vanish; i.e.,

$$\sum_{i=1}^{4} I_i = 0$$

Applying condition 5 to (4), we may write that the conservation of mass equation for the total system is

$$\frac{\partial (\omega_s u)}{\partial \tau} = -\nabla \cdot J_1 - \nabla \cdot J_2$$

where $u$ is total moisture content, $J_1$ is local vapor flux, and $J_2$ is local liquid flux. The above result is consistent with that proposed by Luikov [1966].

The corresponding conservation of energy equation becomes

$$c \omega_o \frac{\partial t}{\partial \tau} = -\nabla \cdot J_1 + \epsilon \lambda \omega_o \frac{\partial u}{\partial \tau}$$

where

- $c$, heat capacity of the system;
- $t$, temperature;
- $J_1$, heat flux;
- $\lambda$, latent heat of the phase change;
- $\epsilon$, species content factor, defined as the ratio of the moisture transfer to the phase change [Luikov, 1966].

Luikov has already indicated that an equation similar to (7) may be used for freezing ($t < 0^\circ C$, where $t_f = 0^\circ C$) as well as nonfreezing ($t > 0^\circ C$) water-soil systems. The heat capacity is a composite for the total system [Jumikis, 1966], and the latent heat $\lambda = \lambda_{12} = \lambda_m$ for $t > t_f$, or $\lambda = \lambda_{m2} = \lambda_{m2}$ for $t < t_f$. Similarly, species content factor $\epsilon = \epsilon_{12}$ for $t > t_f$ ($\epsilon_{12}$ is defined by Luikov from $I_1 = \epsilon_{12} \frac{\partial \omega_o u}{\partial \tau}$), or $\epsilon = \epsilon_m$ for $t < t_f$ ($\epsilon_m$ is defined by Luikov from $I_m = \epsilon_m \frac{\partial \omega_o u}{\partial \tau}$).

As is specified by Luikov [1966], $\epsilon$ is a constant; i.e., in the phase change term $\epsilon \lambda \omega_o \frac{\partial u}{\partial \tau}$ of (7), only $u = u(t)$. However, (7) can be generalized for the freezing system in question. Figure 5 shows a freezing system characterized by a moving freezing front. In this case, $L_f$ is the depth of frost penetration and is a continuous function of time during the transient
period, i.e., a time dependent condition brought on by altering a given boundary condition. The parameter \( \tau \) is the time when steady state flow returns (duration of transient state) and the frost front stops moving. The soil behind the frost front at any time contains ice, whereas the soil in front of the frost front contains no ice but mainly liquid water.

To generalize (7), we must consider the phase change term with respect to possible temperature conditions \( t \leq t_f \). (The case \( t = t_f = 0 \degree C \), not covered in this work, represents the temperature at the frost front. At this temperature of the system, \( e \) and \( u \) remain constant, but \( L_f \) varies with time; hence \( L_f \) would have to be incorporated into the phase change term for the complex system involving a freezing zone behind the frost front, a moving frost front, and a nonfrozen zone in front of the frost front.)

The case \( t < t_f \) represents temperatures behind the frost front. For freezing partially frozen soil, \( u_s \) depends on \( t \); i.e., we assume that there is a unique relation \( u_s = u_s(t) \) as shown in Figure 6a for a given water-soil system. On the other hand, \( e \) for freezing soil can be related to moisture content by

\[
\varepsilon_{23} = \frac{u_3}{u_2 + u_3} \tag{8}
\]

Considering (8) and the assumption that \( u_s \) is a unique function of \( t \), i.e., \( u = u(t) \), we may say that \( \varepsilon \) depends on \( t \) and also that \( \varepsilon \) may be considered a unique function of \( t \), i.e., \( \varepsilon = \varepsilon(t) \), for the given soil system as shown in Figure 6b. Yet during the transient state change of the system the temperature of this system changes with respect to time, so that \( t = t(\tau) \). Thus \( \varepsilon \) depends on time; i.e., \( \varepsilon = \varepsilon(\tau) \) during the transient condition. The phase change term given in (7) can be expanded as

\[
\lambda_v \frac{\partial (\varepsilon u)}{\partial \tau} = \lambda_w \left( \frac{\partial u}{\partial \tau} + \frac{\partial \varepsilon}{\partial \tau} \right) \tag{9}
\]

The general conservation of energy equation therefore may be written as

\[
\lambda_w \frac{\partial t}{\partial \tau} = -\nabla \cdot J_s + \lambda_w \left( \frac{\partial u}{\partial \tau} + \frac{\partial \varepsilon}{\partial \tau} \right) \tag{10}
\]

**Flux Equations**

If the flux equations are derived by using the principles of the processes of irreversible thermodynamics [Fitts, 1962; DeGroot and Mazur, 1962], we may have (11) and (12). The Onsager ‘linear’ system of flux equations is given by

\[
J_i = \sum_i L_{ij} \nabla \phi_j \quad i, j = 1, \ldots, 5 \tag{11}
\]

where \( L_{ij} = L_{ji} \) (Onsager reciprocity relations satisfied) is the phenomenological or transfer coefficient, \( J_i \) is the local extensive property flux, \( \phi_j \) is the extensive property transfer potential, and \( \nabla \phi_j \) is the corresponding transfer force. The Onsager ‘nonlinear’ system of flux equations (the ‘linear’ system expanded into Taylor’s series) is given by

\[
J_i = \sum_i L_{ij} \nabla \phi_j + \frac{1}{2} \sum_i \sum_k L_{ijk} \nabla \phi_j \nabla \phi_k + \cdots \tag{12}
\]

where \( L_{ij} = L_{ji} \) and \( L_{ijk} = L_{ikj} = L_{jki} \) (Onsager reciprocity relation preserved). In either case it can be shown that water distribution in the unfrozen porous media is a limiting case in which the flux equation will reduce Darcy’s law:

\[
J = L \nabla \phi \tag{13}
\]

The Onsager nonlinear system of flux equations (12) is very complex, and its use might be justified for a freezing clay-water system [cf. Lielmezs and Kennedy, 1971]. However, in this work we have excluded clay-water systems, and so it may be assumed that the Onsager linear flux equations (11) are of sufficient generality to describe flux rates in the transfer equation for the freezing water-soil system (Figure 2).
To derive the Onsager linear system of flux equations from the principles of the processes of irreversible thermodynamics (for a general outline of the derivation see Fitts [1962] and DeGroot and Mazur [1962]), we state that the following transfer forces, based on the transfer potentials listed earlier [cf. Jumikis, 1966, Dirksen, 1964, and Philip, 1957], are the only transfer forces acting on this system (Figure 2): the heat transfer force $\nabla t$, the vapor transfer force $\nabla x_1$, and the liquid transfer force $\nabla \psi$. To obtain completed derived flux equations, the mass transfer forces are expressed in terms of the parameters of which the original transfer potentials are a function, i.e.,

$$\nabla x_1 \rightarrow \nabla u_2, \nabla t$$ (14)

for vapor and

$$\nabla \psi \rightarrow \nabla u_2, \nabla t$$ (15)

for liquid transfer (for justification of (14) and (15) see Philip [1957]).

If we follow the well-known procedure of derivation using the methods of irreversible thermodynamics [Fitts, 1962; DeGroot and Mazur, 1962], the overall mass flux equation for the freezing water-soil system, gravitational effects being neglected, is found to be

$$-(J_1 + J_2) = L'M'\nabla u_2 + L'M'\nabla t$$ (16)

where $L'$ is the resultant phenomenological coefficient after transformation of transfer forces is completed and mass fluxes are combined.

Equation 16 can be written in terms of soil moisture diffusivity $D_m$ as

$$-(J_1 + J_2) = \omega_0 D_m \nabla u_2 + \omega_0 D_m \delta \nabla t$$ (17)

Equation 17 represents modified Darcy’s law and compares with Luikov’s [1966] work, in which $\delta$ is the gradient coefficient. On the other hand, the heat flux equation in the expanded form may be written as

$$-J_5 = L_5'\nabla t$$ (18)

If we assume that the moisture content term in (18) is negligible, (18) reduces to

$$-J_5 = L_5'\nabla t = k\nabla t$$ (19)

where $k$ is the coefficient of the thermal conductivity of the system.

The transfer coefficients are obtained by comparing the limiting case of the flux equations (17 and 18) to existing simple flux equations (Darcy’s law and Fourier’s equation). For instance, Onsager mass transfer coefficients relate to soil moisture diffusivity, as has already been shown, i.e., $D_m = L_{ax}/w_m$, or, again, the Onsager heat transfer coefficient $L_\alpha$ relates to thermal conductivity $L_\alpha = k$. (The phenomenological coefficients relate to parameters such as soil moisture diffusivity, and these parameters in turn relate to experimentally measurable quantities such as capillary conductivity for $D_m$.)

The actual values of the Onsager coefficients, including cross coefficients, are determined by experiments; however, theoretical derivation may be possible, as is indirectly indicated by Stephan and Lucas [1971].

**Transfer Equations**

**Derivation of transfer equations.** The derived flux equations (17 and 19) (equation 19 is a simplified version of equation 18) are substituted into the corresponding conservation equations (6 and 10) to yield, first, the mass transfer equation,

$$\partial u / \partial t = \nabla (D_m \nabla u_2 + D_m \delta \nabla t)$$ (20)

and, second, the heat transfer equation,

$$\omega_0 \partial t / \partial t = \nabla (k\nabla t) + \lambda \omega_0 (\epsilon \partial u / \partial t + u \partial t / \partial t)$$ (21)

where $u$ is the moisture content and $D_m$, $D_m$, $\delta$, and $k$ are considered to be transfer parameters. These transfer parameters under specified conditions (if they are independent of position and time) may become transfer coefficients, i.e., may have constant values.

**Solution of transfer equations.** Proposed equations 20 and 21 are nonlinear; that is, the transfer coefficients are given as parameters describing the physical properties of the freezing water-soil system. This nonlinearity of (20) and (21) can be removed if conditions are simplified, i.e., if we divide the freezing water-soil system into zones of constant-valued transfer parameters (transfer coefficients).

We propose two specific freezing water-soil system models, the fixed freezing front and the moving freezing front. (We do not consider the nonfreezing water-soil system, which has already been discussed by Luikov [1966].) The
fixed freezing front (Figure 7) is simpler than the moving freezing front. The initial state of the fixed freezing front is defined as \( t = t_i = 0^\circ C = \text{const.} \) Consequently, one of the boundary conditions is altered instantaneously to \( t(0, \tau) < 0^\circ C \), and thus the transient state condition is set up at once. This system, which can be thermodynamically open or closed, reaches a steady state condition at some time \( \tau_e \). Solution of (20) and (21) becomes subject to these simplifying boundary conditions with the additional simplifying condition that, since across the freezing front (moving or fixed) transfer coefficients vary greatly [Jumikis, 1966; Dirksen, 1964; Kersten, 1949; Luikov, 1966], zoning the system with respect to constant values of transfer coefficients (parameters) is mandatory.

The moving freezing front (Figure 5) is a more general version of the fixed freezing front and is in effect commonly found in nature. The solutions of (20) and (21) are more difficult for this front; the suggested simplifying condition would be the zoning of the system in terms of the values of transfer coefficients.

As is indicated, when (20) and (21) are solved, they will determine the moisture and temperature distribution for a specified set of boundary conditions, that is, for specific freezing water-soil systems. Knowing this and obtaining the values of transfer coefficients, we can calculate the corresponding mass and heat fluxes for the given set of restricting conditions.

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REFERENCES


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