VALIDATION OF LOCAL THERMAL EQUILIBRIUM IN UNSATURATED POROUS MEDIA WITH SIMULTANEOUS FLOW AND FREEZING

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ABSTRACT
Simultaneous flow and freezing, coupled with heat transfer, in unsaturated porous media is modeled using a unit cell to investigate the conditions under which thermal equilibrium in a local averaging volume (LAV) is applicable. The analysis gives parametric relations of the temperature differences between all the phases in LAV. It is shown that the validation of local thermal equilibrium largely depends on the gradients of $\text{Pe}_r$ and $\Theta_l$. Results from a numerical simulation of infiltration into frozen soils using the local volume averaging formulation are compared with the parametric analysis and found, in general, satisfying the criteria established in this study. However, increasing the surface infiltration rate or increasing soil permeability results in the breakdown of local thermal equilibrium.

Introduction

The concept of local thermal equilibrium has been widely used in modeling transport phenomena in porous media, especially used in the local volume averaging theory [1]. This concept states that in a local averaging volume (LAV) (a representative elementary volume containing all the phases and components in a porous medium) the average temperature in each phase is equal to the average temperature over the LAV. This assumption is justified for many theoretical and practical problems in which no phase change occurs in LAV. In some drying processes where phase change phenomena do occur such as evaporation, local thermal
equilibrium is still valid provided that rate of phase change is relatively small and convection and latent heat do not significantly contribute to the overall local thermal balance [2]. This is often the case where mass transfer in the process involved is primarily governed by diffusion [3]. Mathematically, local thermal equilibrium usually implies the following conditions [1],

\[(\Delta T)_\ell \ll (\Delta T)_L\]  \hspace{1cm} (1)

where the subscript \(\ell\) is the characteristic length scale for the LAV, and \(L\) is the length scale of the physical system studied.

There are many cases, especially in natural processes, where phase change in unsaturated porous media is strongly coupled with flow of one of the fluids undergoing phase change. Examples include snowmelt infiltration in frozen soils, an important process in a seasonal hydrological cycle [4]. In this case, supercooled water coexists with ice. Depending on the local percolation rate, subsequent melting or regelation causes strong fusion energy to be absorbed or released within LAV, which may well result in a breakdown of local thermal equilibrium depicted by inequality (1). In this paper, analyses are presented on the conditions under which the local thermal equilibrium assumption may or may not be applicable to such cases.

**Analysis for a Unit Cell**

Consider a porous medium that consists of supercooled liquid water, ice, gas mixture and solid matrix. A local averaging volume \(V\) for such a system is defined as a volume associated with a point in space (denoted by a position vector \(r\) in Fig. 1a) and containing all the phases in porous media. A quantity \(y\) is said to be 'spatially averaged' when it is defined as

\[
\bar{y}(r) = \frac{1}{V(r)} \int_{V(r)} y dV.
\]  \hspace{1cm} (2)

A quantity in an arbitrary phase \(j\) is said to be 'intrinsic phase averaged' when it is defined as

\[
\bar{y}_j = \frac{1}{V_j} \int_{V_j} y_j dV
\]  \hspace{1cm} (3)

where \(V_j\) is the volume of the \(j\) phase in \(V\). Local thermal equilibrium for a LAV having \(n\) phases requires

\[
T_{j_1} = T_{j_2} = \cdots = T_{j_n} = T.
\]  \hspace{1cm} (4)

We further idealize the LAV by constructing a unit cell such that the main coordinate axis is parallel to the direction of liquid flow and dominant temperature gradient, as shown in Fig. 1b. This assumption is made to simplify the analysis at a microscopical level and yet
FIG. 1 (a) Definition of a local averaging volume (LAV) and (b) an idealized unit cell showing one-dimensional, transient liquid flow, freezing/melting on the solid particle surface.

be able to link the results to a macroscopically one-dimensional, time-dependent transport process that an unsaturated, partially frozen, porous medium undergoes. The main physical phenomena involved in this process include liquid flow, melting or freezing, and thermal diffusion. Four phases coexist in the unit cell; solid particles, ice, liquid water and gaseous mixture (air and vapor). The volume fraction of each phase is defined as

\[ \epsilon_i = \frac{\delta_i}{\ell}, \quad \epsilon_l = \frac{\delta_l}{\ell}, \quad \epsilon_s = \frac{\delta_s}{\ell}, \quad \epsilon_g = 1 - \epsilon_i - \epsilon_l - \epsilon_s. \]  

(5)

Applying energy conservation and mass conservation laws to the liquid phase, we have\(^1\)

\[ \rho_l c_l \frac{\partial T_i^*}{\partial t^*} + \frac{\partial}{\partial x^*} (\rho_l h_t T_i^*) + \rho_l h_t \frac{\partial \delta_l}{\partial x^*} = k_l \frac{\partial}{\partial x^*} \left( \delta_l \frac{\partial T_i^*}{\partial x^*} \right) \]  

(6)

\[ \frac{\partial (u \delta_l)}{\partial x^*} = \frac{\partial \delta_l}{\partial t^*}. \]  

(7)

In developing the above energy equation, we assume that the temperature is averaged in direction perpendicular to the liquid flow, and the heat transfer (essentially by conduction) from the liquid to the ice is relatively small compared to the phase change and enthalpy flow terms. This assumption is generally justified because (1) local thermal equilibrium requirement is easily met under thermal diffusion-only conditions and (2) we are mainly interested in the case where phase change is significantly coupled with flow.

\(^1\)When a quantity appears in both dimensional and dimensionless forms, the one with an asterisk is dimensional.
With the dimensionless parameters defined in the nomenclature, the dimensionless forms of the above equations are (after some rearrangement)

\[
\frac{\partial T_i}{\partial t_i} + Pe_\epsilon T_i \frac{\partial \ln \epsilon_i}{\partial x} + T_i \frac{\partial Pe_\epsilon}{\partial x} + Pe_\epsilon \frac{\partial T_i}{\partial x} + \frac{1}{Ste} \frac{\partial T_i}{\partial t_i} = \frac{\partial^2 T_i}{\partial x^2} + \frac{\partial \ln \epsilon_i}{\partial x} \frac{\partial T_i}{\partial x}
\]

(8)

\[
\frac{\partial Pe_\epsilon}{\partial x} + Pe_\epsilon \frac{\partial \ln \epsilon_i}{\partial x} = \frac{\partial \ln \epsilon_i}{\partial t_i}.
\]

(9)

To linearize equations (8) and (9), the following approximations for \( y_j \) (\( j = 1, 2 \) and 3) obtained from Taylor’s series expansion with respect to \( \bar{y}_j \) are used

\[ y_1 y_2 \approx \bar{y}_2 y_1 + \bar{y}_1 \bar{y}_2, \quad y_1 y_2 y_3 \approx \bar{y}_3 y_1 + \bar{y}_1 \bar{y}_3 y_2 + \bar{y}_1 \bar{y}_2 y_3 \]

(10)

where

\[ \bar{y}_j = \int_0^1 y_j dx. \]

(11)

Note that according to the definition for the LAV shown in Fig. 1b, equation (11) is equivalent to equation (3).

Applying equation (10) to (8) and (9) and then integrating these two differential equations from \( x = 0 \) to \( x = 1 \), we have (note equation (11) is used)

\[
\frac{\partial T_i}{\partial t_i} + 3Pe_\epsilon T_0 (\Delta t \ln \epsilon_i) + T_0 \Delta t Pe_\epsilon + \frac{1}{Ste} \frac{\partial \ln \epsilon_i}{\partial t_i} \approx \Delta t \left( \frac{\partial T_i}{\partial x} \right) + (\Delta t \ln \epsilon_i)(\Delta t T_i)
\]

(12)

\[
\frac{\partial \ln \epsilon_i}{\partial t_i} \approx \Delta t Pe_\epsilon + Pe(\Delta t \ln \epsilon_i)
\]

(13)

where \( \Delta t y = y(x = 1, t) - y(x = 0, t) \) (\( y \) represents any variable in the above equation). In equation (12), \( Pe \Delta t T \) has been dropped because it is orders of magnitude smaller than other terms.

Following the similar steps, we can derive an energy equation and a continuity equation for the ice phase as follows

\[
\frac{\partial T_0}{\partial t_i} \approx \frac{a_i}{a_t} \left[ \Delta t \left( \frac{\partial T_i}{\partial x} \right) + (\Delta t \ln \epsilon_i) \Delta t T_i - \frac{a_t}{Ste \epsilon_i} \frac{\partial \ln \epsilon_i}{\partial t_i} \right]
\]

(14)

\[
\frac{\partial \ln \epsilon_i}{\partial t_i} \approx \frac{a_t}{a_i} \frac{\ln \epsilon_i}{\epsilon_i} \frac{\partial \epsilon_i}{\partial t_i},
\]

(15)

and for the solid phase, we only have the energy equation

\[
\frac{\partial T_s}{\partial t_i} \approx \frac{a_s}{a_i} \Delta t \left( \frac{\partial T_i}{\partial x} \right).
\]

(16)

For the sake of discussion, we define a rate of phase change as follows

\[
m = \frac{\partial \ln \epsilon_i}{\partial t_i}.
\]

(17)
A positive \( \dot{m} \) means melting while a negative \( \dot{m} \) indicates freezing.

After combining the continuity equation with the energy equation for each phase (except for the solid) with further algebraic manipulation, we finally arrive at the following expressions for the temperatures \( T_i, T_e \), and \( T_s \) (\( \sim \) reads 'is of the order of')

\[
\frac{\partial T_i}{\partial t} \sim -\left(3\overline{T_i} + \frac{1}{Ste}\right)P_{ef}(\Delta t \ln \varepsilon_i) - \left(\overline{T_i} + \frac{1}{Ste}\right)\Delta t P_e + \Delta t q_{ki} \quad (18)
\]

\[
\frac{\partial T_e}{\partial t} \sim -\left(\frac{c_i \overline{T_i}}{c_i \overline{T_e}}\right)\Delta t P_e + \frac{\overline{T_i}}{Ste}\Delta t \ln \varepsilon_i + \Delta t q_{ke} \quad (19)
\]

\[
\frac{\partial T_s}{\partial t} \sim \Delta t q_{ks} \quad (20)
\]

where \( \Delta t q_{ki} = \Delta t(\partial T_i/\partial x) + (\Delta t \ln \varepsilon_i)(\Delta t T_i), \) \( \Delta t q_{ke} = \Delta t(\partial T_e/\partial x) + (\Delta t \ln \varepsilon_i)(\Delta t T_i), \) \( \Delta t q_{ks} = \Delta t(\partial T_s/\partial x). \) These three terms represent the axial conduction heat flow in each phase. It should be reasonable to assume that these terms are of the same order; i.e., \( \Delta t q_{ki} \sim \Delta t q_{ke} \sim \Delta t q_{ks}. \) Note that if local thermal equilibrium breaks down, this assumption would not hold.

Subtracting equation (19) from (18), we arrive at an important relation for the temperature difference between the liquid and ice:

\[
\frac{\partial (T_i - \overline{T_i})}{\partial t} \sim -\left\{ \left[ \frac{1}{Ste} \left( \frac{c_i \overline{T_i}}{c_i \overline{T_e}} + 1 \right) + \overline{T_i} \right] \Delta t P_{ef} + \left[ \frac{1}{Ste} \left( \frac{c_i \overline{T_i}}{c_i \overline{T_e}} + 1 \right) + 3\overline{T_i} \right] \overline{T_i} \Delta t \ln \varepsilon_i \right\} . \quad (21)
\]

**Effects of \( \varepsilon_i \) and \( P_{ef} \) Gradients in the LAV**

In equation (18) \( \Delta t \ln \varepsilon_i \) and \( \Delta t P_{ef} \) represent the average gradients of \( \varepsilon_i \) and \( P_{ef} \) within the LAV. It is shown that the rate of liquid temperature is proportional to these two gradients (disregarding the sign). The \( \varepsilon_i \) and \( P_{ef} \) gradients reflect the rate of phase change under the flow condition \( \dot{m} \) (equation 17): therefore, any increase or decrease in \( \dot{m} \) significantly affects the change of \( T_i \). For example, the increase in the negative gradients of both \( \varepsilon_i \) and \( P_{ef} \) (i.e., freezing) results in a faster temperature increase rate for the liquid phase. In the meantime, it causes a faster decreasing rate for the ice temperature (see equation 19). In addition to the gradients, the rate of change for the ice temperature is also affected by the ratio \( \overline{T_i}/\overline{T_e} \) for given \( Ste \). The solid matrix temperature is primarily governed by thermal diffusion. By comparing equations (18), (19) and (20), it is clear that the time scales for temperature response from three different phases are different. This difference in time scales depends primarily, for the same Stephen number and material, on the strength of phase change heat source or sink, because the thermal diffusion contributions in liquid, ice and solid phases are generally of the same order.
It should be noted that when freezing occurs, i.e., \( m \) being negative, it is not necessary that the gradient of \( \epsilon_i \) has the same sign as that of \( \text{Pe} \). The same is true for melting situations. To discuss the contributions of individual gradients to the temperature change in a more practical manner, we will transform equation (21) from the microscopic level (\( \ell \) scale) to a macroscopic level (\( L \) scale) in the following section. Considering that the phase change between the ice and liquid causes the major temperature deviation in the LAV and the thermal conductivity of ice is four times of liquid water, we only present the result in term of \( \overline{T}_i - \overline{T}_L \).

### A Criterion for the Condition of Local Thermal Equilibrium

In equation (21), variables and parameters are defined using the length scale of \( \ell \). If we define transformation relations between the \( \ell \) and \( L \) scales such that \( \Delta \ell = \alpha \Delta L \), \( u_L = u_{\ell L}/\epsilon_i \), \( \text{Pe}_\ell = \text{Pe}(a_{\text{eff}}\ell)/(\alpha L) \), \( t_L = t_L(\ell L^3)/(a_{\text{eff}}\ell^2) \) and select the reference temperature difference \( \Delta T_{\text{ref}} = \Delta T^* \), we have

\[
\frac{\partial (\overline{T}_i - \overline{T}_\ell)}{\partial t_L} = \frac{\partial}{\partial t_L} \left( \frac{\overline{T}^* - \overline{T}_i}{\Delta T^*} \right) \sim \beta \left[ (\Gamma + \overline{T}_i)(-\Delta \text{Pe}) + (\Gamma + 3\overline{T}_i)\text{Pe}(\Delta \ln \epsilon_i) \right]
\]

(22)

where \( \beta = \alpha L/(\epsilon \ell) \).

Integrating equation (22) with respect to \( t_L \) (also considering \( \alpha \sim \epsilon \ell / L \), and \( \beta \sim 1 \)) yields

\[
\overline{T}_i - \overline{T}_\ell \sim \int_0^{t_L} \left[ (\Gamma + \overline{T}_i)(-\Delta \text{Pe}) + (\Gamma + 3\overline{T}_i)\text{Pe}(\Delta \ln \epsilon_i) \right] dt_L
\]

(23)

or

\[
\overline{T}_i - \overline{T}_\ell \sim [(\Gamma + \overline{T}_i)(-\Delta \text{Pe}) + (\Gamma + 3\overline{T}_i)\text{Pe}(\Delta \ln \epsilon_i)]_{\text{ave}} t_L
\]

(24)

where \( \Gamma = (1/\text{Ste})[c_i\epsilon_i/(c_i\epsilon_i) + 1] \).

In order for local thermal equilibrium being applicable, \( \overline{T}_i - \overline{T}_\ell \) has to be much less than unity; i.e., inequality (1) is to be satisfied. If we further modify (arbitrarily) inequality (1) as equivalent to

\[
|\Delta \ell T| < 0.1|\Delta T|, \text{ or } |\overline{T}_i - \overline{T}_\ell| < 0.1
\]

(25)

then the following relation establishes a bound within which local thermal equilibrium is generally satisfied

\[
\pm 0.1 = [(\Gamma + \overline{T}_i)\Delta \text{Pe} + (\Gamma + 3\overline{T}_i)\text{Pe}\Delta \ln \epsilon_i]_{\text{ave}} \text{Fo}
\]

(26)

where Fo is the Fourier number, \( a_{\text{eff}}\ell^2/L^2 \).

Fig. 2 shows the relationship between \( \Delta \text{Pe} \) and \( \text{Pe}\Delta \ln \epsilon_i \) and the specified upper and lower bounds, based on the above equation, within which the condition (25) is satisfied. The
FIG. 2 Upper and lower bounds within which the condition of $|\bar{T}_l - \bar{T}_s| < 0.1$ is satisfied: $\text{Fo}=0.0167$, Ste=0.101 for two different $\epsilon_l/\epsilon_i$.

example shown in Fig. 2 is for a water-ice system with $\epsilon_l/\epsilon_i = 10$, $\Delta T^* = 8K$, Fo=0.0167 and Ste=0.101, which is typical for a snow melt infiltration into a frozen soil [5]. The Fourier number of 0.0167 corresponds to 10 hours for a typical clay-loam soil with its characteristic depth of 1 m (see also Table 1). This time scale is long enough to cover both a rapid transient period and a relatively smooth change period. Similar graphs can be generated for other systems for which simultaneous phase change, flow and thermal diffusion take place. It can also be seen that as $\epsilon_l/\epsilon_i$ increases, the range of validation for local thermal equilibrium becomes narrower. This is generally expected for thawing processes. From an initially equilibrium state, an increase in the $\epsilon_l/\epsilon_i$ ratio implies an increase in the melting rate which tends to increase the temperature difference between the liquid and solid, given the same $\Delta \text{Pe}$ and $\text{Pe} \Delta (\ln \epsilon_l)$. For freezing, the large $\epsilon_l/\epsilon_i$ ratio usually occurs when ice crystals start to grow in the liquid adjacent to or on the surface of soil particles. It is known that the liquid is supercooled during an ice crystallization process [6]. This supercooling requirement easily makes local thermal equilibrium condition more restricted.

Validation from Numerical Results

The above discussion is all based on the unit cell, designated in Fig. 1, featuring one-dimensional flow and heat transfer for each phase at a microscopic level. Through dimensional analyses, a transformation from the microscopic scale to the macroscopic scale is made. Naturally, the next question would be how good the criterion established from such a model is as compared to the complete numerical simulation using the local volume averaging
Table 1 Physical Values Used in Numerical Simulation.

<table>
<thead>
<tr>
<th>$T_0^*$</th>
<th>°C</th>
<th>0.8</th>
<th>$T_0^*$</th>
<th>°C</th>
<th>0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>(et + et)/ε</td>
<td>0.35</td>
<td>1.0</td>
<td>Pe</td>
<td>k</td>
<td>0.15</td>
</tr>
<tr>
<td>ε</td>
<td>0.49</td>
<td>1.409</td>
<td>$\rho_0^*$</td>
<td>kg/m^3</td>
<td>4.63·10^{-7}</td>
</tr>
<tr>
<td>$a_{eff}$</td>
<td>0.574</td>
<td>10^{-14}</td>
<td>$a_{eff}$</td>
<td>m^2/s</td>
<td>1.0</td>
</tr>
<tr>
<td>K</td>
<td>W/m-K</td>
<td>10^{-14}</td>
<td>L</td>
<td>m</td>
<td></td>
</tr>
</tbody>
</table>

Technique—a macroscopic approach. Such a numerical model has been reported [5] for the investigation of simultaneous heat and mass transfer, percolation and freezing and thawing phenomena using snow melt infiltration at the soil-snow interface as a boundary condition. A complete formulation of the local volume averaged differential equations (energy, momentum, continuity and gas diffusion equations) was solved numerically. We pick up a typical case study for an initially frozen soil that is subject to a step temperature change and constant surface infiltration rate at the top of the soil. Some main physical data for this case are shown in Table 1, and the readers are referred to [5] for the details of formulation. We calculate the gradients of the volume averaged Pe and et from the numerical results, using finite differences and considering the following relations

$$\Delta Pe \approx \frac{\partial Pe}{\partial z} \Delta z, \Delta T \approx \frac{\partial T}{\partial z} \Delta z, \Delta \ln et \approx \frac{\partial \ln et}{\partial z} \Delta z,$$

where $\Delta z$ is the grid size. Thus the right hand side of equation (23) can be calculated.

Fig. 3 shows the calculated $A \Delta Pe$, $Pe \Delta T$ and $BPe \Delta \ln et$ as a function of Fo with $A = \Gamma + \tilde{T}_t$ and $B = \Gamma + 3\tilde{T}_t$. The profiles shown in Fig. 3 are for $z = 0.02$ and 0.04, the first two nodal points adjacent to the soil surface ($z = 0$) where infiltration occurs and phase change is the strongest. It can be seen that the term $Pe \Delta T$ is negligibly small as compared with other terms in equation (22), which justifies the assumption used to arrive at equation (21). For $Pe_0 = 0.15$, the increase in $K$ from $10^{-14}$ to $10^{-13}$ m^2 has little effect on the gradients of $Pe$ and $\ln et$ (Fig. 3a and b). However, for the high Peclet number ($Pe_0 = 0.5$) and high permeability ($K = 10^{-13}$ m^2), these two gradients increase dramatically (Fig. 3c).

It is therefore understood that in the latter case, local thermal equilibrium may not be a valid assumption. Shown in Fig. 4a and b, the calculated $|T_i - T_s|$ is less than 0.1 while in Fig. 4c for the high surface infiltration rate and strong near-surface phase change, $|T_i - T_s|$ is up to 0.4 (the point A) at Fo = 0.0167. If we find the corresponding $\Delta Pe$ and $Pe \Delta \ln et$ (the points C and B, respectively), we can show them on Fig. 2 where this state is outside the bounds within which $|T_i - T_s|$ is less than 0.1. This comparison proves that the criteria established in equations (24) and (26) are reasonable, and the associated assumptions are
justified. It can then be concluded that for high Peclet numbers and high permeabilities the numerical solutions based on the local volume averaging technique are less accurate and may be unstable.

FIG. 3 Quantities $A \Delta \overline{P}_e$, $B \overline{P}_e \Delta \overline{T}$ and $\overline{P}_e \Delta \ln \eta$ at $z = 0.02$ and 0.04, calculated from the numerical simulation, as a function of Fo for three different $Pe_0$ and $K$.

FIG. 4 Quantities $\overline{T}_l - \overline{T}_i$, $\Delta \overline{P}_e$ and $\overline{P}_e \Delta \ln \eta$ at $z = 0.02$ and 0.04, calculated from the numerical simulation, as a function of Fo for three different $Pe_0$ and $K$. 
Acknowledgement

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Nomenclature

\begin{align*}
\alpha & \quad \text{thermal diffusivity, } k/(\rho c) \\
c & \quad \text{heat capacity} \\
F & \quad \text{Fourier number, } at^*/L^2 \\
h & \quad \text{enthalpy of fusion, } J \, \text{kg}^{-1} \\
k & \quad \text{thermal conductivity, } \text{W m}^{-1}\text{K}^{-1} \\
K & \quad \text{permeability, m}^2 \\
\ell & \quad \text{length scale of the local averaging volume, m} \\
L & \quad \text{physical length of porous media, m} \\
\dot{m} & \quad \text{rate of freezing or melting} \\
Pe & \quad \text{Peclet number, } uL/a_{\text{eff}} \\
q & \quad \text{conduction heat flux} \\
St & \quad \text{Stephen number, } c_i\Delta T_{\text{ref}}^*/h \dot{m} \\
t & \quad \text{time, } at^*/\ell^2 \\
T & \quad \text{temperature, } T^*/\Delta T_{\text{ref}} \\
u & \quad \text{velocity, m/s} \\
x & \quad \text{coordinate axis, } x^*/\ell \\
y & \quad \text{arbitrary variable} \\
z & \quad \text{soil depth, } z^*/L \\
\text{Greek Symbols} \\
\alpha, \beta & \quad \text{transform factors, } \beta = \nu/(\epsilon \ell) \\
\Delta & \quad \text{difference} \\
\epsilon_j & \quad \text{volume fraction of } j \text{ phase} \\
\epsilon & \quad \text{porosity} \\
\rho & \quad \text{density} \\
\text{Subscripts} \\
i & \quad \text{ice} \\
l & \quad \text{liquid} \\
\ell & \quad \text{based on the scale } \ell \\
L & \quad \text{based on the scale } L \\
o & \quad \text{at } z = 0 \\
s & \quad \text{solid} \\
sc & \quad \text{supercooling} \\
\text{Superscripts} \\
s & \quad \text{dimensional} \\
- & \quad \text{average}
\end{align*}

References


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