Spatial Distribution of Heat of Wetting in Porous Media

Lyle Prunty, professor
North Dakota State University
Department of Soil Science
Room 147 Walster Hall
Fargo, ND 58105
lprunty@ndsuext.nodak.edu

Written for presentation at the
2002 ASAE Annual International Meeting / CIGR XVth World Congress
Sponsored by ASAE and CIGR
Hyatt Regency Chicago
Chicago, Illinois, USA
July 28-July 31, 2002

Abstract. Heat generated when dry soil and water are mixed is known as heat of wetting. Models for coupled heat and water transport in unsaturated soil are part of global warming models and are used to predict moisture regimes of nuclear waste repositories. Since heat of wetting is part of the theory, a detailed examination of its implications is appropriate. The objective of this work is to examine the place of heat of wetting in the coupled equations of soil heat and water transport, to propose a modification of the usual way heat of wetting is introduced into the equations, and to examine the implications of the old and new equations with respect to spatial distribution of the effect. The differential heat of wetting term, $W$, is traditionally introduced into the energy conservation equation via the product of $W$ and the rate of change of water content. The proposed modification includes $W$ in the convection term of the energy equation. Calculation of the source term of the energy equation is used to illustrate the implications of the traditional and new forms of the energy equation with respect to the spatial distribution of heat generated during an isothermal redistribution of soil moisture. Results illustrate that if heat of wetting is to be included in a model at all, the new approach is to be preferred.

Keywords. thermal transport, coupled flow, temperature, models, soil water transport
Introduction
Heat generated when dry soil is mixed with water is known as heat of wetting. A calorimeter can be used to measure this heat. Examples of values for heat of wetting (Grim, 1953) are kaolinite = 6, illite = 17, smectite = 40 to 90 J g⁻¹.

Coupled soil water and heat flows are important considerations in design of nuclear waste storage facilities and electrical power cables. Global atmospheric models require input of land surface heat and water vapor fluxes, which have been calculated using computer models of the heat and water coupled soil fluxes (Milly and Eagleson, 1982). Some of these computer models have included heat of wetting while some have not. Those including the term, usually in a manner very similar to that formulated by deVries (1958), have been Milly and Eagleson (1980, 1982) and Nassar and Horton (1997). Those excluding the effect include a model by Salzmann et al. (2000), Wilson et al. (1994), and Fayer (2000) in model UNSAT-H version 3.0. Descriptions of some models do not make it clear if it is included or not.

The stated justification for omitting the heat of wetting effect is usually that it is relatively small compared to other effects. On the other hand, we have found that temperatures may increase to 8 °C when water is added to ordinary soil, as we describe later. Coupled heat and water transport in soils is an important topic in hydrology and soil physics. A new theoretical development to explain observations of water vapor movement in field experiments has recently been published (Parlange et al., 1998) and claims to overcome some shortcomings of the deVries (1958) approach, which has provided the primary theoretical basis heretofore.

Our objective is to calculate the spatial distribution of heat evolved from soil as a result of isothermal water redistribution under two forms of the energy equation. One form is that given by deVries (1958). The second form is a modification of the first, which accounts for convection of soil water potential and internal energy terms. The effect of condensation or evaporation is calculated separately.

Theory
The energy conservation approach used in “Simultaneous Transfer of Heat and Moisture in Porous Media” (deVries, 1958) is expressed in detail by equation (2.24) of Milly and Eagleson (1980) in the form

\[ C \frac{\partial T}{\partial t} + [L_o + c_p(T - T_o)] \theta_a \frac{\partial \theta}{\partial t} + [c_i \rho_i(T - T_o) - \rho_i W - c_p \rho_v(T - T_o) - L_o \rho_v] \frac{\partial \theta}{\partial t} = \nabla \cdot [\lambda \nabla T + \rho_i L D_{\psi \psi} \nabla \psi - c_i(T - T_o) q_m] \]

with the notation as listed in “Nomenclature” at the end.

For a long, slim column at constant \( T = T_o \) the equation simplifies considerably to

\[ L_o \theta_a \frac{\partial \rho_v}{\partial t} - [\rho_i W + L_o \rho_v] \frac{\partial \theta}{\partial t} = \nabla \cdot [\rho_i L_o D_{\psi \psi} \nabla \psi] + S_d = -L_o \nabla \cdot q_v + S_d \]

where \( S_d \) is a heat source term. The subscript \( d \) indicates association with the deVries model. This is the heat input rate needed to maintain the constant temperature, \( T_o \). Also, \( q_v \) is vapor flux (kg m⁻² s⁻¹).

Since

\[ n = \theta + \theta_a \]
where \( n \) is the total porosity, it follows, for a rigid soil matrix, that

\[
\frac{\partial \theta}{\partial t} = -\frac{\partial \theta_a}{\partial t} \tag{4}
\]

Using the above, we have

\[
L_o \left[ \frac{\partial}{\partial t} (\theta_a \rho_v) - \nabla \cdot (-q_v) \right] = \rho_l W \frac{\partial \theta}{\partial t} + S_d \tag{5}
\]

The left of this equation represents energy conversion during evaporation. The time derivative gives the rate of increase of vapor mass per unit volume and the gradient term subtracts the amount of that vapor mass increase attributable to vapor flow. The term with \( W \) on the right is the heat of wetting effect.

The energy equation (1) follows the formulation of deVries (1958) and Philip and deVries (1957). However, that formulation leaves out terms, usually considered small, which are necessary for a more precise analysis. Specifically, the gravitational potential energy is missing from the left side of (1) and there is no gradient of the differential heat of wetting flux plus the gravitational potential energy flux on the right.

Thus, we write

\[
gz \frac{\partial}{\partial t} (\rho_l \theta + \rho_v \theta_a) = \nabla \cdot [W q_l - g z q_m] + S_e \tag{6}
\]

where \( q_l \) is liquid water flux (kg m\(^{-2}\) s\(^{-1}\)) and \( S_e \) (\( e \) is for error) is as needed for the equality to hold.

The mass conservation equation, with no source term, is

\[
\frac{\partial}{\partial t} (\rho_l \theta + \rho_v \theta_a) = -\nabla \cdot q_m \tag{7}
\]

Thus, combining the mass conservation equation with the prior equation (6) yields

\[
0 = W \nabla \cdot q_l + q_l \nabla W - gz q_m + S_e \tag{8}
\]

Now, using \( q_l = q_m - q_v \) and employing (3) and (4) in (8) yields

\[
0 = -\rho_l W \left[ (1 - \frac{\rho_v}{\rho_l}) \frac{\partial \theta}{\partial t} + \frac{\theta_v}{\rho_l} \frac{\partial \rho_v}{\partial t} \right] - W \nabla \cdot q_v + q_l \nabla W - gz q_m + S_e \tag{9}
\]

Adding (5) and (9), employing (4) and rearranging leads to

\[
[L_o + W] \left[ \frac{\partial}{\partial t} (\theta_a \rho_v) - \nabla \cdot (-q_v) \right] = q_l \nabla W - gz q_m + S_e + S_d \tag{10}
\]
where the sum $S_e + S_d$ represents the true heat source term when all the additional terms are included in the heat conservation equation.

Now we can examine the various terms that contribute to the heat source, including their spatial distribution in the vertical column.

**Equations for Components of Evolved Heat**

**Heat of Wetting - $V$**

In (5) the term $\rho_l W \frac{\partial \theta}{\partial t}$ represents heat associated with moisture content change in the sense of deVries (1958), and we thus designate

$$V = -\rho_l W \frac{\partial \theta}{\partial t} \quad (11)$$

**Convected Gradient – $Q$**

In (10) the term $q_l \nabla W$ represents an energy rate of change at a point due to convection of liquid water with nonuniform $W$ (energy) content. Henceforth we use $Q$ for this quantity, so

$$Q = -q_l \nabla W \quad (12)$$

**Gravitational Dissipation – $G$**

In (10) the quantity $gq_m$ is similar in form to $Q$ above but is due to gradient of gravitational energy. Thus we use

$$G = gq_m \quad (13)$$

**Evaporation Energy – $E$**

The left side of (10) expresses the rate of energy conversion by evaporation. Although the left sides of (5) and (10) are different the $W$ term is very small compared to $L_0$ in the vertical column system we will examine, so $E$ is used to represent either the left side of (5) or (10). The definition used here is

$$E = (L_0 + W)[\frac{\partial}{\partial t}(\theta_a \rho_v) - \nabla(-q_v)] \quad (14)$$

**Overall**

With these definitions we see that (5) may be restated as

$$E_0 + V = S_d \quad (15)$$

and (10) may be restated as

$$E + Q + G = S_e + S_d \quad (16)$$
where $E_0$ in (15) designates that the $W$ term in (14) is omitted.

**Vertical Column Simulation**

Computer model, Simulation Program for Land-Surface Heat and Water Transport (SPLaSHWaTr, henceforth SPL herein) Version 2.4, is a matric head based numerical model for simulating the one-dimensional fluxes of moisture and heat in a vertical soil column (Milly, 1982). Properties of Plainfield sand suitable for use with the model are documented (Milly and Eagleson, 1982). Outputs from the model needed for our calculations were matric head ($h$ in cm), water content ($\theta$), liquid water flux ($q_l$) and vapor water flux ($q_v$). The model is based on a finite element scheme, so the column is divided into numerous elements. Nodes for the model are at the ends of the elements. The model output gives $h$ and $\theta$ values at the nodes and average flux values for the elements.

We used SPL to analyze a soil column 1 m = 100 cm long and filled with Plainfield sand with an initially uniform water content ($\theta$) at a matric potential of -50 cm. Boundary conditions were no water flow, vapor or liquid, at either end. In the vertical column, the water begins to redistribute immediately toward the equilibrium state of uniform hydraulic potential. The column dries at the top and becomes wetter at the bottom until the equilibrium state is achieved. Column temperature is fixed at reference temperature $T_0$.

For this process, $V$, $Q$, $G$, and $E$, which contribute to $S_d$ and $S_e$, can be evaluated. We calculated the spatial distribution of these quantities during redistribution.

The final (equilibrium) state of the column will be at uniform hydraulic potential, $\Psi = \psi + gz$. Consistent with this is a moisture content profile which decreases monotonically from its highest value at $z = 0$ (bottom of column) to its lowest value at $z = 100$ cm (top of column). This means, generally, that in the upper part of the column $\theta$ values will be lower than the initial values and in the lower part of the column they will be higher.

**Computational Details**

Milly and Eagleson (1980, p. 82 and 1982, p. 53) assign an exponential temperature dependence to matric potential. We express this in the form

$$h = H(\theta, T_0) e^{-a(T-T_0)}$$

(17)

where Milly and Eagleson (1982) assigned the value 0.0068 K$^{-1}$ to $a$. In the above equation $H(\theta, T_0)$ is the moisture characteristic function at temperature $T_0$. The expression for differential heat of wetting is

$$W = -(\psi + \Lambda) = -(\psi - T \frac{\partial \psi}{\partial T}) = -0.01g(h + Tah) = -0.01gh(1 + Ta)$$

(18)

where we have used $\psi$ (J kg$^{-1}$) = 0.01gh (cm) and at $T = 293$ K with the value of $a$ above we have $\Lambda = 0.1952h$. Thus, we used $W = -0.2932h$. (J kg$^{-1}$ when $h$ is in cm).

In the SPL model vapor flux is driven only by $Vh$ (see (5), in which $\psi$ has the same role as $h$). This results in nonzero vapor flux in a column with zero gradient of hydraulic potential [0.01g(h + z) if $h$ and z are in cm]. Since this is inconsistent with the equilibrium condition, it was necessary to correct the vapor
flux of SPL. This was done by adding to the vapor flux output by SPL the gravity driven component, which SPL ignores. This correction is of importance in the calculation of $E$ at the end nodes.

**Results and Discussion**

The SPL model was used to calculate moisture content profiles near the bottom (Fig. 1) and top (Fig. 2) of the column at various times ranging up to 12 h. Similarly, water flux was calculated near the bottom (Fig. 3) and top (Fig. 4) of the column at the same times. Outputs of moisture contents and fluxes from appropriate SPL runs were also used to calculate $V$, $Q$, $G$, and $E$ at 0.25 and 7.5 h near the column ends (Figs. 5-20).

Plots of $V$ (Fig. 5-8) show that this effect would cause heat flow out of the column near the bottom (Fig. 5 and 7) and into the column near the top (Fig. 6 and 8). At 0.25 h the bottom (Fig. 5) and top (Fig. 6) plots are very nearly reversed mirror images. At 7.5 h there is substantial departure from this symmetry, shown, for instance, by the -880 versus +730 µW m$^{-3}$ rates at 0 cm (Fig. 7) and 100 cm (Fig. 8).
Values of $Q$ (Fig. 9-12) indicate heat entering the column near both the bottom (Fig. 9 and 11) and top (Fig. 10 and 12). Thus the bottom and top graphs of $Q$ are mirror images, but not reversed. Again, at 7.5 h the symmetry is less than at 0.25 h, as verified by Fig. 11 (bottom) with a peak value of about 22 $\mu$W m$^{-3}$ versus 16 $\mu$W m$^{-3}$ for Fig. 12 (top). While $Q$ is at most 2% as great as $V$ at any point, $Q$ increases from 0.25 to 7.5 h, while $V$ decreases.
Gravitational energy dissipation, $G$, is always negative (Fig. 13-16). In contrast to all the other terms, the $G$ effect approaches zero at both ends and is at a uniform value of maximum difference from zero away from the ends. Again, the mirror image property of the 0.25 h plots (Fig. 13 and 14) is more exact than for the 7.5 h plots (Fig. 15 and 16). Away from the ends the value of $G$ is constant. It will, of course, decrease eventually as time proceeds.
The spatial distribution of evaporation energy conversion, $E$ (Fig. 17-20), is relatively about the same as for $V$ but $E$ is about three times greater in magnitude. These plots indicate, reasonably, that condensation takes place as water content increases (Fig. 17 and 19) and evaporation takes place as liquid water content decreases (Fig. 18 and 20).
Values of \( V, Q, G, \) and \( E \) calculated here are all too small to be of practical importance, we expect. Combined values of \( V + E \) approach only 20,000 \( \mu \text{W m}^{-3} = 0.02 \text{ W m}^{-3} \) maximum magnitude, and that level only in a small region. For some real soils, however, the heat of wetting effect can be fairly pronounced. For instance, we have conducted a simple experiment of adding 10 g of water to 15 g Fargo silty clay (oven dried and passing a 1mm sieve) and recorded temperature increases of 7 to 8 \( ^\circ \text{C} \) (Fig. 21). Since the total effect can be this large, we are inclined to view the discrepancy between the spatial distribution of \( V \), representing the traditional de Vries (1958) model, and the spatial distribution of \( Q + G \) as also of some significance.

![Figure 21. Temperatures in Fargo silty clay after placing water on top. Layer 1 is deepest (~3 cm) and has the gentlest temperature rise (>1200 s to peak). Layer 4 is nearest the soil surface and has the sharpest temperature rise (<100 s to peak).](image)

Besides considering the spatial aspects of the heat source terms, we have found it of interest to consider the initial and equilibrium states of the vertical column and the corresponding energy states. Here we consider the column to be one meter square in cross section, thus having a total volume of one cubic meter. Water mass in the block is 41.03 kg. We calculated the distribution of this water at equilibrium and were then able to calculate differences in gravitational and water potential energy between the initial (uniform \( \theta \)) and final (equilibrium) conditions.

At equilibrium the \( \theta \) and \( h \) values at \( z = 0 \) are 0.1416 and –19.39 cm, respectively. At \( z = 100 \) cm \( \theta \) and \( h \) are 0.0218 and –119.39 cm, respectively. The original \( \theta (0.04103) \) and \( h (-50.0 \text{ cm}) \) occur in the equilibrium column at \( z = 31.6 \) cm. The center of mass of the equilibrium water is at \( z = 35.58 \) cm.

The original center of mass was at 50.00 cm and the change in gravitational potential energy is found by \( \Delta U_g = mg \Delta z \) where \( m \) is the mass of water and \( g \) is acceleration of gravity. We find \( \Delta U_g = (41.03)(9.8)(35.58-50.00)/100 = -57.98 \text{ J} \). In the preceding, the difference was final energy less initial energy.

The difference in soil water matric potential energy may also be calculated. Consider

\[
d\Delta U_\psi = \psi dm
\]  

(19)
which says that a differential change in soil water matric potential energy (not including gravitational potential) is the product of $\psi$ (reversible work required to add an infinitesimal amount of water to soil at constant temperature) and $dm$ (differential mass of water added). This translates to

$$\Delta U_\psi = \sum \psi \Delta m = \sum 0.01g \bar{h} \rho V \Delta \theta$$  \hspace{1cm} (20)

where $V$ is the volume of soil at $\bar{h}$ (mean matric potential – cm) while moisture content changes by $\Delta \theta$. We used SPL to calculate at 1cm node spacing for the equilibrium state and found after adding up all the 1cm layers $\Delta U_\psi = +26.6$ J. Thus, gravity did 57.98 J of work to pull the water down to the equilibrium position but 26.6 J of that was needed to accomplish the redistribution of water and resides as potential matric energy of the soil water, discounting gravity effects.

In the region near the bottom of the column water is flowing down at a slower rate because the matric potential gradient opposes and partially cancels out the gravitational potential gradient. As a particle of water moves downward in this region, at constant temperature, the quantity $(0.01gh + \Lambda + 0.01gz)$ can potentially increase. Consider this quantity when $\Lambda = 0.1952h$, as we illustrated earlier. In this case $(0.01gh + \Lambda + 0.01gz) = (0.2932h + 0.098z)$ and thus $-V(0.01gh + \Lambda + 0.01gz) = -0.2932 \bar{h} - 0.098$. This is the gradient of potential plus internal energy in the direction of flow. The numerical value of this quantity can be greater than zero for the vertical column we have considered since if $\bar{h} < -0.098/0.2932 = -0.334$ the above quantity is greater than zero and as equilibrium is approached $\bar{h}$ approaches $-1.0$. Thus, near the bottom of the column we find $\theta$ increasing and at the same time heat must enter the soil at that point to achieve energy balance, disregarding evaporation effects ($E$). An equivalent way of stating this is that $Q + G$ is positive near the lower end of the column. On the contrary, the results for $V$ suggest that in any region where moisture content is increasing at constant temperature the heat flow related to heat of wetting effects will always be out of the soil, as in Fig. 5 and 7, where $V$ is negative at the lower end. Thus we see that $Q + G$ and the $V$ sometimes result in opposite signs for the heat evolved and associated with the heat of wetting concept.

**Conclusion**

**Acknowledgements**

Joel Bell assisted in preparing the manuscript and figures and conducted the laboratory work collecting the data of Figure 21.

**References**


**Nomenclature**

\( C \) - volumetric heat capacity of soil \( J \, m^{-3} \, K^{-1} \)

\( c_l \) - specific heat capacity of liquid water \( J \, kg^{-1} \, K^{-1} \)

\( c_p \) - constant pressure specific heat capacity of water vapor \( J \, kg^{-1} \, K^{-1} \)

\( D_{ov} \) - diffusivity of water vapor \( m^{-1} \)

\( E \) – energy conversion rate from evaporation \( W \, m^{-3} \)

\( E_0 \) – same as \( E \) with \( W=0 \) \( W \, m^{-3} \)

\( g \) – acceleration of gravity \( m \, s^{-2} \)

\( G \) – energy conversion rate from gravitational energy gradient \( W \, m^{-3} \)

\( h \) – matric head of the SPL computer model \( cm \) [note that \( \psi=0.01gh \)]

\( L_0 \) - latent heat of vaporization at \( T_0 \) \( J \, kg^{-3} \, K^{-1} \)
$L$ - latent heat of vaporization at $T$  $J \cdot kg^{-3} \cdot K^{-1}$

$n$ – volume fraction pore space

$q_m$ - mass water flux  $kg \cdot m^{-2} \cdot s^{-1}$

$q_v$ - mass vapor flux  $kg \cdot m^{-2} \cdot s^{-1}$

$Q$ – energy conversion rate related to $W$ gradient

$S_d$ – heat source  $W \cdot m^{-3}$

$S_e$ – heat source  $W \cdot m^{-3}$

$t$ – time  $s$

$T$ - temperature  $K$

$T_0$ – reference temperature  $K$

$V$ – energy conversion associated with changing moisture content

$W$ - differential heat of wetting  $J \cdot kg^{-1}$

$z$ – vertical coordinate  $cm$ or $m$

$\Lambda$ - specific energy of adsorption  $J \cdot kg^{-1}$

$\theta$ - volume fraction liquid water

$\theta_a$ - volume fraction air

$\rho_l$ - liquid density (assumed constant)  $kg \cdot m^{-3}$

$\rho_v$ - vapor density  $kg \cdot m^{-3}$

$\lambda_v$ - thermal conductivity  $W \cdot m^{-1} \cdot K^{-1}$

$\psi$ - matric potential  $J \cdot kg^{-1}$

$\Psi$ - hydraulic potential  $J \cdot kg^{-1}$

$\nabla$ - gradient or divergence operator