Sensitivity of Soil Coupled Heat and Mass Transfer Governing Equations to Hydraulic and Thermal Conductivities

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ABSTRACT

A pressure-based coupled heat and mass transfer model was used to simulate temperature and soil suction in a drying process within a clay soil column. Closed form functions were used for all parameters needed in the governing equations. Model predictions were compared with experimental data using the mean relative percentage deviation method. Thermocouples and mini-gypsum blocks were used to monitor the data collected hourly at different depths of the soil column. The model showed very high sensitivity to the proposed hydraulic conductivity function, while lower sensitivity was found for the proposed thermal conductivity function. This result highlights the importance of a proper hydraulic conductivity estimate while a rough estimate for thermal conductivity would have no significant adverse effect on the predicted values.

INTRODUCTION

The physics involved in the process of heat and mass transfer in agricultural soils has long been a subject of interest for researchers. The prediction of moisture and temperature profiles within unsaturated soil horizons under different boundary conditions is important for soil and water management. The mathematical analysis of the response of soil to atmospheric conditions tends to be complicated since the temperature and moisture dependence of the parameters involved in transport equations make these relationships highly nonlinear.

The pioneers in modeling coupled heat and mass transfer in porous media are Philip and de Vries (1957) and Luikov (1964). More recent formulations largely involve modifications of Philip and de Vries' and Luikov's approaches (Ten Berge, 1990; Thomas and King, 1992). Due to the complexity of the results, attempts have been made to analyze the coupling phenomenon and, if possible, to simplify the governing equations even to the point of decoupling. Studies have been conducted regarding sensitivity of the coupled governing equations to the phase conversion coefficient (Sidiropoulos and Tzimopoulos 1983) and to thermal effects on evaporation from soil (Milly 1984).

Two important parameters in the coupled heat and mass transfer governing equations are hydraulic conductivity and thermal conductivity. The object of this research is to show the sensitivity of the governing equations to variations in hydraulic and thermal conductivities.

Governing Equations

In a drying process, the coupled heat and mass transfer one-dimensional governing equations can be shown as (Thomas and King, 1992):

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$$C_{\psi\psi}\frac{\partial\psi}{\partial t}+C_{\psi T}\frac{\partial T}{\partial t}=\frac{\partial}{\partial z}\left(K_{\psi\psi}\frac{\partial\psi}{\partial z}\right)+\frac{\partial}{\partial z}\left(K_{\psi T}\frac{\partial T}{\partial z}\right)$$
(1)

$$C_{TT}\frac{\partial T}{\partial t}+C_{T\psi}\frac{\partial\psi}{\partial t}=\frac{\partial}{\partial z}\left(K_{TT}\frac{\partial T}{\partial z}\right)+\frac{\partial}{\partial z}\left(K_{T\psi}\frac{\partial\psi}{\partial z}\right)$$
(2)

where T is temperature (K), Ψ is matric suction or soil pressure (m) and t is time (s). Other parameters are defined as:

$$C_{\psi\psi}=C_{\theta}+C_{v}$$
(3)

$$C_{\psi T}=\frac{h}{\rho_{l}}(\eta-\theta_{l})\left(\frac{\partial\rho_{o}}{\partial T}-\frac{\rho_{o}\psi g}{R\,T^{2}}\right)$$
(4)

$$K_{\psi\psi}=K+K_{v}$$
(5)

$$K_{\psi T}=\frac{D_{vap}h}{\rho_{l}}\left(\frac{\partial\rho_{\_}}{\partial T}-\frac{g\psi\rho_{\_}}{RT^{2}}\right)$$
(6)

$$C_{TT}=\frac{C}{\rho_{l}}+LC_{\psi T}$$
(7)

$$C_{T\psi}=LC_{v}$$
(8)

$$K_{TT}=\frac{k}{\rho_{l}}+LK_{\psi T}$$
(9)

$$K_{T\psi}=LK_{v}$$
(10)

$$C_{\theta}=\partial\theta_{l}/\partial\psi$$
(11)

$$C_{v}=\frac{\rho_{\_}h}{\rho_{l}}\left[\frac{g(\eta-\theta_{l})}{RT}-C_{\theta}\right]$$
(12)

$$K_{v}=\frac{D_{vap}g\rho_{\_}h}{\rho_{l}RT}$$
(13)

where K and k are soil hydraulic (m/s) and thermal (W.m^{-1}.K^{-1}) conductivities, respectively. The remaining symbols are defined in the Notation following this article.

For calculating unsaturated soil hydraulic conductivity K, the following closed form function which is a combination of Brutsaert's (1967) and Blake's (1922) models and the well known van Genuchten's (1980) soil-water characteristic curve was used:

$$K=K_{s}\left[\frac{1}{\left(1+|\alpha\psi|^{n}\right)^{m}}\right]^{a}$$
(14)

For calculaning soil thermal conductivity

k, Johansen's (1975) model was used:

$$k=(k_{sat}-k_{dry})K_{e}+k_{dry}$$
(15)

where K_{e} is the Kersten normalized thermal conductivity that for fine textured soils is defined as (Farouki 1986):

$$K_{e}=log_{10}S+1.0,\qquad S>0.1$$
(16)

Johansen (1975) also presented the equations for saturated thermal conductivity k_{sat} and dry thermal conductivity k_{dry} of natural soils:

$$k_{sat}=k_{w}^{\eta_{w}}k_{q}^{\eta_{q}}k_{m}^{\eta_{m}}$$
(17)

$$k_{dry}=\frac{0.135\,\rho_{b}+64.7}{2720-0.947\,\rho_{b}}$$
(18)

where the soil sample particle density used in this study (2720 kg/m^{3}) is incorporated into equation (18).

In solving the governing equations, pressure and hydraulic conductivity were adjusted for temperature according to the following equations (Thomas and King, 1992):

$$\psi(\theta,T)=\frac{\sigma(T)}{\sigma(T_{r})}\psi_{ref}(\theta)$$
(19)

$$K(\theta,T)=\frac{\mu(T_{r})}{\mu(T)}K_{ref}(\theta)$$
(20)

Surface tension σ and dynamic viscosity μ are given as (Thomas and King, 1992):

$$\sigma(T)=0.117-0.00015T$$
(21)

$$\mu(T)=0.661\times(T-229)^{-1.56}$$
(22)

MATERIALS AND METHODS

A clear acrylic tube 200 mm in diameter, 160 mm in height, and 6.35 mm thick with a 6.35 mm thick solid base was used in three replicates. A solid base was used in order to direct moisture loss due to evaporation from the top surface. The sampled soil from Kernen research farm, north east of Saskatoon, Saskatchewan was classified as an Orthic Dark Brown Chernozem (Souster, 1979) with a clay texture (57% clay, 34% silt, 9% sand) according to the USDA soil classifica-

228

tion triangle. The organic matter of the soil was 4.83% determined by the dry combustion method. The soil was air dried, ground and sieved (< 4.5 mm) and brought to 31.8% ± 0.37 initial gravimetric water content. A bulk density of 1.15 Mg/m^3 that is similar to the range of bulk densities reported for the same location was chosen (Moazed, 1996). The relatively low bulk density of the clay soil was due to its high organic matter content. When preparing each soil layer for the specified bulk density in each container, a large diameter to depth ratio was chosen to ensure a uniform overall bulk density (Koolen, 1974). This was achieved by carefully packing 15 mm thick layers of a predetermined quantity of wetted soil using a manually driven hydraulic press.

To monitor soil moisture and temperature, mini-gypsum blocks (17 mm x 15 mm x 10 mm) and thermocouples were used in 15, 45, 75 and 135 mm depths. Data were collected hourly for a week using a Campbell 21X data-logger (Campbell Scientific, Inc., Logan, UT) and stored in a personal computer for further analysis (Figure 4).

Containers were kept in a 1.4 m^2 growth chamber located in the Phytotron facility of the University of Saskatchewan in which relative humidity and temperature, respectively, were set to 44% and 15 °C for sixteen hours and to 85% and 5 °C for eight hours. These approximate cyclic settings were chosen according to the local meteorological data representing the time of seeding which is usually in early May for a typical grain crop in Saskatoon area (Wittrock and Wheaton,1991; Environmental Canada, 1991).

Equations 1 and 2 were solved by an explicit finite difference method using a computer code written in FORTRAN 77 and proper closed form functions for the parameters involved (Keyhani, 1997). The imposing initial conditions at t = 0 are:

$\Psi = \Psi_o$ and $T = T_o$

It is assumed that the pressure and temperature are the same throughout the soil column. The boundary conditions at the surface at t = 0 are:

$T_1 = T_a = 15$ °C, $\Psi_1 = \Psi_a = -11130$ m (h = 0.44), for 16 hours,

$T_1 = T_a = 5$ °C, $\Psi_1 = \Psi_a = -2127$ m (h = 0.85), for 8 hours.

The boundary conditions at the bottom of the container (and around the wall), assuming no heat and mass transfer occurs, are:

$$\frac{\partial \psi}{\partial t} = 0 , \text{ and } \frac{\partial T}{\partial t} = 0$$

Sensitivity Analysis

To study the effect of overall hydraulic and thermal conductivity functions on the predicted values of temperature and water content obtained from the governing equations, after decreasing and increasing both functions by 20%, a mean relative percentage deviation (*MRPD*) procedure was adopted (Yang and Cenkowski, 1995). In this method, the sum of normalized absolute values of residuals is averaged over the number of observations (or measurements) multiplied by 100. The result is a number in percentage form representing the deviation of the theoretical and experimental approaches. The formula is:

$$MRPD = \frac{100}{N} \sum \frac{|y - y'|}{y} \qquad (23)$$

where *MRPD* is the mean relative percentage deviation, *y* is the measured value, *y'* is the estimated value and *N* is the number of observations. Excel 97 for Windows 98 was used for conducting the *MRPD* analysis.
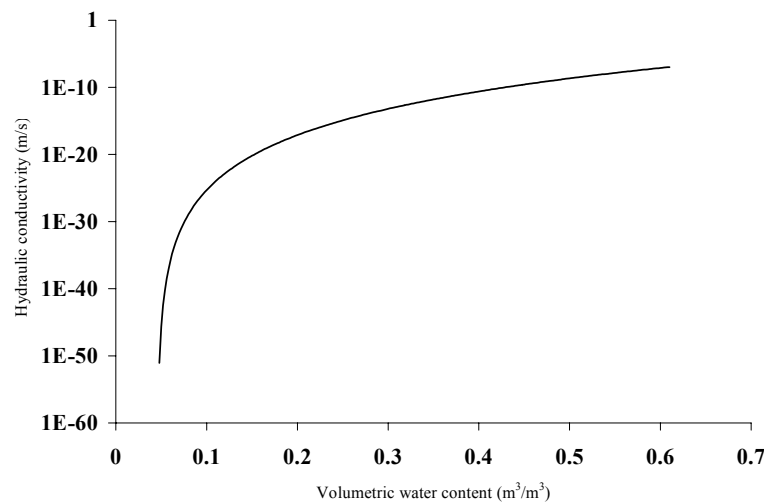
Figure 1. Variation of hydraulic conductivity with volumetric water content.

RESULTS AND DISCUSSION

Figures 1 and 2 show the graphs of the transport coefficients, hydraulic and thermal conductivities. Tables 1 and 2 show the results of changing hydraulic and thermal conductivities by ± 20%. Values presented for *MRPD* show the profound influence of the hydraulic conductivity function on predicted water contents (reflected in two-to three-fold *MRPD* values in Table 1).

These findings emphasize the importance of a proper estimation of hydraulic conductivity to minimize the overall deviation. The graph of the water content in Mg/Mg versus time for all replications and for different Ks' at 45 mm depth in the soil column is shown in Figure 3. To calculate the *MRPD*, the first 24 hour data were deleted due to the high

deviation involved for the time required for mini-gypsum blocks to reach a state of equilibrium with the soil medium.

On the other hand, a 20% change in thermal conductivity (decrease or increase) resulted in an almost 10% change in *MRPD* (Table 2). Since the accuracy required for predicting temperature is not usually high for agricultural purposes, a rough estimation of thermal conductivity may be sufficient.

Summary and Conclusion

There are many parameters involved in the soil coupled heat and mass transfer governing equations among which hydraulic and thermal conductivities are of prime importance. Both hydraulic and thermal conductivities can be shown as closed form func-

Table 1. Mean relative percentage deviation for water content prediction with different hydraulic conductivties, K and no change in thermal conductivities, k.

Hydraulic Conductivity	$\dfrac{\sum |y_{wc} - y'_{wc}| / y_{wc}}{N} \times 100$				Average MRPD
(m/s)	15 mm	45 mm	75 mm	135 mm	(%)
0.8 *K*	7.47	5.32	10.9	0.385	6.02
K	8.07	0.884	2.45	0.339	2.94
1.2 *K*	8.54	8.10	8.74	0.268	8.55

y_{wc} = measured value; y'_{wc} = predicted value; N = number of observations; K = hydraulic conductivity

Table 2. Mean relative percentage deviation for temperature prediction with different thermal conductivties, k and no change in hydraulic conductivity, K.

Thermal *Conductivity*	$\dfrac{\Sigma\left|y_T - y'_T\right|/y_T}{N} \times 100$				Average MRPD
(W/m K)	15 mm	45 mm	75 mm	135 mm	(%)
0.8 *k*	1.18	0.810	0.448	0.316	0.689
k	1.21	0.893	0.551	0.370	0.756
1.2 *k*	1.24	0.967	0.653	0.474	0.834

y_T = measured value; y'_T = predicted value; N = number of observations; k = thermal conductivity

tions. The governing equations to predict the water content were sufficiently sensitive to a small change (± 20%) in hydraulic conductivity to lead to two-to three-folds *MRPD* values. On the other hand, the same range of changes of thermal conductivity led only to a 10% change in *MRPD* values. These results highlight the importance of a proper hydraulic conductivity estimate while a rough estimate of thermal conductivity would have no significant adverse effect on the predicted values. Full sensitivity analysis of the other parameters and the percentage of their contribution in predicting water content and temperature remains for future studies.

List of Notations

a fitting parameter in hydraulic conductivity function

C volumetric heat capacity (J.m^{-3}.K^{-1})

$$C_{TT} = \frac{C}{\rho_l} + LC_{\psi T}$$

$$C_{T\psi} = LC_v$$

$$C_v = \frac{\rho\, h}{\rho_l}\left[\frac{g(\eta - \theta_l)}{RT} - C_\theta\right]$$

C_θ specific water capacity, defined as $\dfrac{\partial \theta_l}{\partial \psi}$ (m^{-1})

$$C_{\psi T} = \frac{h}{\rho_l}\left(\eta - \theta_l\right)\left(\frac{\partial \rho_0}{\partial T} - \frac{\rho_0 \psi\, g}{RT^2}\right)$$
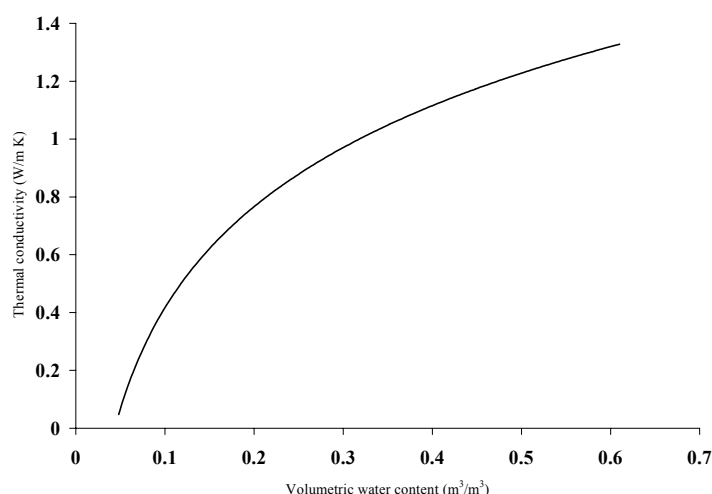

Figure 2. Variation of thermal conductivity with volumetric water content.

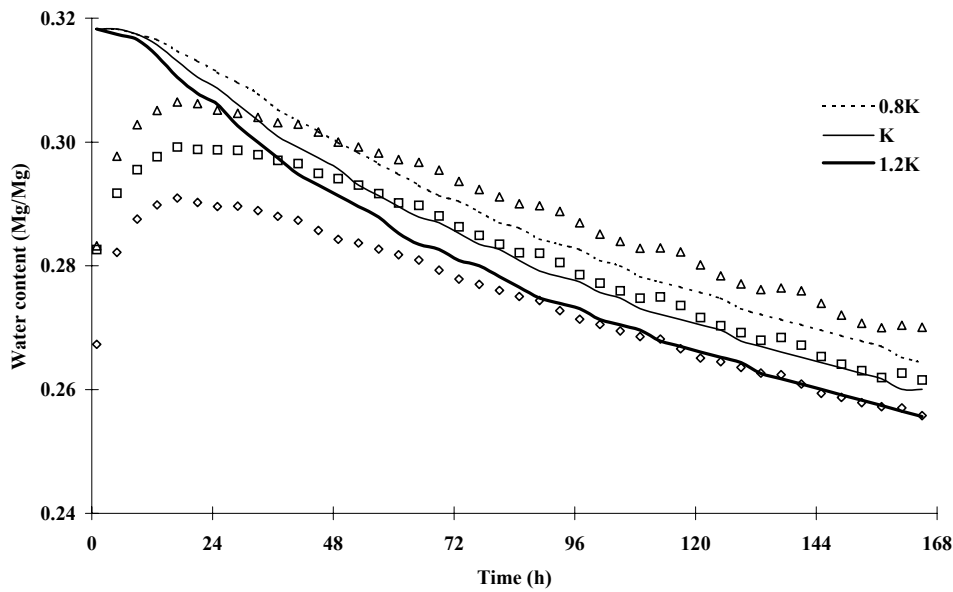**Figure 3**. Variation of measured and predicted water content with time. K:hydraulic conductivity (m/s).

$C_{\psi\psi} = C_\theta + C_v$

D_{vap} diffusion coefficient (m²/s)

g gravitational acceleration (m/s²)
h relative humidity
k soil thermal conductivity $(\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1})$
k_{dry} soil thermal conductivity in a dry state $(\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1})$
k_m thermal conductivity of soil minerals $(\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1})$
k_q thermal conductivity of quartz $(\text{W.m}^{-1}.\text{K}^{-1})$
k_{sat} soil thermal conductivity in a saturated state $(\text{W.m}^{-1}.\text{K}^{-1})$
k_w thermal conductivity of water $(\text{W m}^{-1}.\text{K}^{-1})$
K hydraulic conductivity (m/s)
K_e Kersten normalized thermal conductivity
K_{ref} hydraulic conductivity at reference temperature (m/s)
K_s saturated hydraulic conductivity (m/s)

$$K_{TT} = \frac{k}{\rho_l} + LK_{\psi T}$$

$$K_{T\psi} = LK_v$$

$$K_v = \frac{D_{vap}\, g \rho_{\_}\, h}{\rho_l RT}$$

$$K_{\psi T} = \frac{D_{vap} h}{\rho_l}\left(\frac{\partial \rho_{\_}}{\partial T} - \frac{g\psi \rho_{\_}}{RT^2}\right)$$

$K_{\psi\psi} = K + K_v$

L latent heat of vaporization of water (J/Mg)
m fitting parameter in a soil-water characteristic function
n fitting parameter in a soil-water characteristic function
N number of observations
R universal gas constant $(\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1})$
S degree of saturation
t time (s)
T temperature (K)
$T_\circ$ initial soil temperature (K)
T_l soil surface temperature (K)
T_a environment temperature (K)
T_r reference temperature (K)
y measured value of a variable
y' estimated value of a variable
z vertical dimension (m)
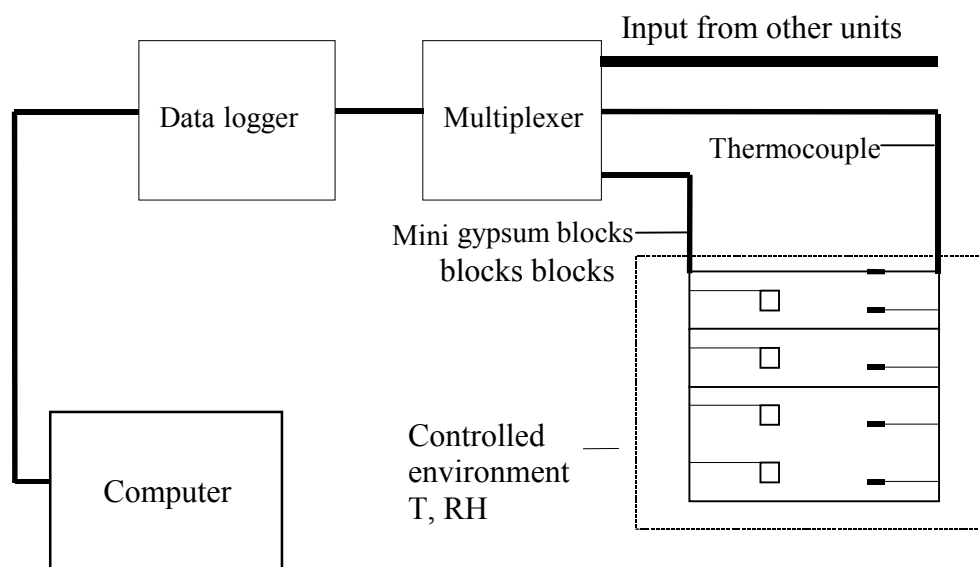α fitting parameter in a soil-water characteristic function

232

Figure 4. The schematic diagram of the experimental setup.
T and RH represent temperature and relative humidity, respectively.

η total porosity of soil (m^3/m^3)

η_a air porosity of soil (m^3/m^3)

η_m volume fraction of soil minerals (m^3/m^3)

η_o volume fraction of soil organic matter (m^3/m^3)

η_q volume fraction of quartz (m^3/m^3)

η_w volume fraction of water (m^3/m^3)

μ dynamic viscosity $(N \cdot s \cdot m^{-2})$

θ total volumetric water content (m^3/m^3)

θ_l volumetric water content in the liquid phase (m^3/m^3)

$\rho_\circ$ saturated vapor density (Mg/m^3)

ρ_b soil dry bulk density (Mg/m^3)

ρ_l liquid density (Mg/m^3)

σ surface tension (J/m)

ψ soil pressure or matric suction (m)

$\psi_\circ$ initial soil pressure or suction (m)

ψ_l soil surface pressure or suction (m)

ψ_a environment pressure (m)

ψ_{ref} soil suction at reference temperature (m)

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233

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حساسیت معادلات رفتاری انتقال حرارت و جرم مزدوج در خاک به ضرایب هدایت هیدرولیکی و حرارتی

ع. کیهانی و د. ولفسون

چکیده

یک مدل ریاضی انتقال حرارت و جرم مزدوج بر پایه فشار جهت شبیه‌سازی دما و مکش خاک در یک فرآیند خشک شدن در یک ستون خاک رسی مورد استفاده قرار گرفت. توابعی از نوع بسته جهت کلیه پارامترهای مورد نیاز در معادلات رفتاری به کار برده شدند. جواب‌های به دست آمده از مدل با داده‌های حاصل از آزمایش‌ها با استفاده از روش درصد انحراف میانگین نسبی مقایسه شدند. داده‌ها با استفاده از ترموکوپل‌ها و بلوک‌های گچی کوچک هر یک ساعت یک بار از اعماق مختلف ستون خاک جمع‌آوری شدند. مدل حساسیت بسیار بالایی را نسبت به تابع هدایت هیدرولیکی به کار گرفته شده از خود نشان داد در حالی که نسبت به تابع هدایت حرارتی حساسیت بسیار کمتر بود. نتایج به دست آمده

اهمیت ضریب هدایت هیدرولیکی را کاملاً مشخص می‌سازد. حال آنکه یک تخمـین نـه چنـدان دقیـق از ضریب هدایت حرارتی تاثیر منفی آنچنانی بر مقادیر حاصل از مدل نمی گذارد.